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Fabio Bagarello
Roberto Passante
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Non-Hermitian Hamiltonians in Quantum Physics

Selected Contributions from the 15th International Conference on Non-Hermitian Hamiltonians in Quantum Physics, Palermo, Italy, 18–23 May 2015

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Preface

This volume collects the selected contributions presented at or inspired by the *15th International Workshop on Pseuso-Hermitian Hamiltonians in Quantum Physics* (PHHQP15), held in Palermo, Italy, from May 18 to 23, 2015. This workshop was the 15th in the series of international meetings that was started in 2003. These meetings were mainly attended by mathematicians and physicists interested in the study of non-Hermitian operators and Hamiltonians, and in their physical applications. About 80 mathematicians and physicists attended the 2015 Workshop in Palermo.

Even though mathematicians have deeply studied several aspects of the spectral theory of operators since long time, the realization that non-Hermitian Hamiltonians with PT symmetry may have a real spectrum has produced a growing interest in theoretical physicists for this subject. From the mathematical side this renewed perspective concerning operators with real spectrum has put on the stage new methods aimed to find conditions for a non-self-adjoint operator to have a real spectrum or it has led to revisiting (and, often, generalizing) older concepts (similarity, affinity, metric operators, etc.) as tools for studying this problem. From a physical point of view the main outcome of this unconventional approach to quantum mechanics has been the exploration of several new and interesting models.

Started as a pure mathematical problem, the subject of non-Hermitian Hamiltonians with PT (parity-time) symmetry has rapidly grown in the past years. It has also attracted much interest for its possible applications in physics, since when it was shown that non-Hermitian Hamiltonians with PT symmetry can have a real spectrum.

Nowadays, in fact, PT-symmetric non-Hermitian Hamiltonians have found application in several areas of physics, for example in quantum optics, condensed matter physics, non-equilibrium statistical physics, and quantum field theory, from both the theoretical and experimental points of view. Typical important systems that can be described by non-Hermitian Hamiltonians endowed with PT symmetry are open systems with balanced gain–loss terms, where gain–loss mechanisms break the Hermiticity while preserving the PT symmetry. Realistic examples are given by

optical waveguides and periodic lattices with balanced absorption or amplification. Other relevant aspects that have received great attention in recent times are, among the others, PT-symmetry breaking phase transitions and formation of exceptional points and spectral singularities.

The papers in this volume will cover several aspects of PT-symmetric non-Hermitian Hamiltonians, investigating both mathematical and physical aspects of the research topics mentioned above.

Palermo, Italy

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We thank these Institutions for making possible this meeting. We also thank speakers, contributors, chairpersons, and participants.

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Our special thanks go to the local organizing committee, Giorgia Bellomonte, Francesco Gargano, Margherita Lattuca, Salvatore Spagnolo, Salvatore Triolo, and Francesco Tschinke, for the great job they did.

Palermo, Italy

Fabio Bagarello
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Contents

Real Discrete Spectrum of Complex PT-Symmetric Scattering Potentials

Zafar Ahmed, Joseph Amal Nathan, Dhruv Sharma and Dona Ghosh

Abstract We investigate the parametric evolution of the real discrete spectrum of several complex PT symmetric scattering potentials of the type $V(x) = -V_1 F_e(x) + iV_2 F_o(x)$, $V_1 > 0$, $F_e(x) > 0$ by varying V_2 slowly. Here e, o stand for even and odd parity and $F_{e,o}(\pm\infty) = 0$. Unlike the case of Scarf II potential, we find a general absence of the recently explored accidental (real to real) crossings of eigenvalues in these scattering potentials. On the other hand, we find a general presence of coalescing of real pairs of eigenvalues at a finite number of exceptional points. After these points, real discrete eigenvalues become complex conjugate pairs. We attribute such coalescings of eigenvalues to the presence of a finite barrier (on the either side of $x = 0$) which has been linked to a recent study of stokes phenomenon in the complex PT-symmetric potentials.

The discovery [1] that the complex PT-symmetric Hamiltonians may have real discrete spectrum has given rise to PT-symmetric quantum mechanics. The coalescing of real discrete eigenvalues at a parametric point and their transition to complex conjugate eigenvalues just after has been known earlier as a phenomenon of spontaneous breaking of complex PT-symmetry. The exactly solvable complex PT-symmetric Scarf II scattering potential

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$$V_S(x) = -V_1\ \mathrm{sech}^2 x + i V_2\ \mathrm{sech}\ x\ \tanh x, \quad V_1, V_2 \in \mathscr{R}, V_1 > 0, \tag{1}$$

has been well known to display spontaneous breaking of PT-symmetry when [2] $|V_2| = V_{2c} = 1/4 + V_1$ ($2m = 1 = \hbar^2$). In the theory of exceptional points (EPs) of non-Hermitian potentials [3], the value(s) of $|V_2| = V_{2c}$ are called EPs where the real pairs of eigenvalues coalesce and just after they turn into complex conjugate pairs. Exactly at these values the corresponding eigenstates become linearly dependent and the Hamiltonian looses diagonalizability.

A recent study of the Stoke's phenomenon of complex PT-symmetric potentials claims [4] the occurrence of level-coalescing (they call it level-crossings) at infinite exceptional points in the potential $V(x) = ig(x^3 - x)$. In [4], this potential is called "PT-symmetric double well" with "two wells at $x = \pm 1/\sqrt{3}$". Such potentials as having this feature have been claimed to have infinite number level-coalescings. However, in more simple terms this $V(x)$ is such that its imaginary part has a finite barrier on the either side of $x = 0$ according as g is positive or negative. In this work, we show that evolution of several complex PT-symmetric scattering potentials whose imaginary part has a barrier on the either side of $x = 0$ have a finite number of level-coalescings at the critical values $|V_2| = V_{2c}$. It is important to recall that the complex PT-symmetric potentials $V(x) = x^2 + igx$, $V(x) = igx^3$, $V(x) = -V_1 \mathrm{sech}^2 x + i V_2 \tanh x$ [5] do not entail coalescing of levels and exceptional points. However, the interesting potential $V(x) = x^4 + igx$ [6] does have them.

Recently, it has been found that the potential (1) has a very interesting property wherein real discrete eigenvalues cross at special values V_{2*} of $|V_2|$. This phenomenon has been called accidental crossing [7] of real discrete eigenvalues in one-dimension. As in one dimension, the degeneracy (two (distinct) linearly independent eigenstates having coincident eigenvalue) cannot occur consequently the crossing levels have linearly dependent eigenstates. This gives rise to loss of diagonalizability of the Hamiltonian which in turn hampers the completeness of the spectrum of the potential.

Interestingly, the solvable regularized one-dimensional complex harmonic oscillator (RCHO) [8, 9] potential also had this feature of level-crossings however this came up more clearly in two recent presentations [10, 11].

In the parlance of exceptional points of non-Hermitian Hamiltonians the above-mentioned two types (real to real, real to complex) of crossings of levels may not be distinguished. However the real to real crossing of eigenvalue appears to be so rare, that so far only two potentials RCHO [8, 9] and Scarf II (1) have yielded it. Curiously, the former is only binding (infinite spectrum) potential that does not allow scattering whereas the latter allows both bound (finite spectrum) and scattering states.

So, with the motivation of studying level coalescings (and any possibility of level-crossings), we propose to find the parametric evolution of the finite number of eigenvalues for five models of complex PT-symmetric scattering potentials (see Fig. 1) employing various methods.

We shall be solving the one-dimensional time-independent Schrödinger equation

$$\frac{d^2\psi(x)}{dx^2} + \frac{2\mu}{\hbar^2}[E - V(x)]\psi(x) = 0 \tag{2}$$

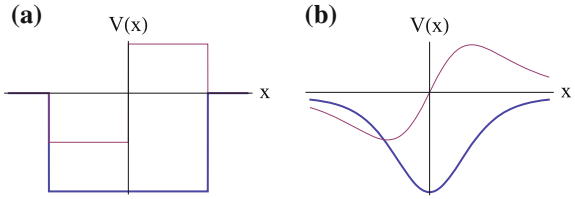

Fig. 1 Schematic depiction of the Complex PT-symmetric scattering potentials, real part (*thick line*), imaginary part (*thin line*). **a** Represents the rectangular well $V_R(x)$ (4) and **b** represents $V_S(x)$ (1), $V_G(x)$ (5), $V_F(x)$ (6), $V_H(x)$ (7) and $V_{WC}(x)$ (14)

for five models of one-dimensional complex PT-symmetric scattering potentials. These potentials (see Fig. 1) essentially vanish at $x = \pm\infty$ and their real part constitutes a well which support only a finite numbers of real discrete eigenvalues. Their imaginary parts are the corresponding anti-symmetric profile. These potential wells are piece-wise constant rectangular, Gaussian, $-(1 + x^4)^{-1}$, $-\text{sech}\, x$ and Wigner-Coulomb profiles.

We would like to outline our method of finding real discrete eigenvalues by numerical integration of the Schrödinger equation (2). Let us define $k = \sqrt{-2\mu E}/\hbar$. We take the general solution of (2) as $\psi(x < -L) = Ce^{kx}$, $\psi(-L < x < L) = Au(x) + Bv(x)$, $\psi(x > L) = De^{-kx}$. Here $u(x)$ and $v(x)$ are linearly independent solutions of (2), their initial values as $u(0) = 1, u'(0) = 0$ and $v(0) = 0, v'(0) = 1$ to start the integration to both left and right side up to $-L$ and $+L$, respectively. L is sufficiently large distance to be chosen. We match these piece-wise solutions and their first derivatives at $x = -L, 0, L$. Finally, we eliminate A, B, C, D in the resulting equations to obtain the eigenvalue formula

$$\frac{ku(L) + u'(L)}{kv(L) + v'(L)} = \frac{ku(-L) - u'(-L)}{kv(-L) - v'(-L)} \tag{3}$$

to find the eigenvalues.

We choose the distance L such that the final results (eigenvalues) have the desired accuracy. For all the calculations here we use $2\mu = 1 = \hbar^2$. Using (3), we fix a value of V_1 so that there are at least 6 real discrete eigenvalues for the real potential well ($V_2 = 0$) by varying $E = -V_1$ to $E = 0$. Next, V_2 is proposed to vary slowly till we get real pairs of eigenvalue curves which coalesce. We call these special values of V_2 as V_{2c} which are known as exceptional points (EPs) of non-Hermitian potential. Nonetheless, we are interested to see whether or not there will be crossings of real discrete eigenvalues from real to real when we vary V_2. The eigenvalues of complex PT-symmetric potentials (4, 5, 6, 7, 14) considered here in the sequel satisfy $E_n(-V_2) = E_n(V_2)$, we therefore evaluate $E_n(V_2)$ only for $V_2 > 0$.

First, to confirm our numerical method, we take up the well known rectangular complex PT-symmetric profile [12] of width $2a$.

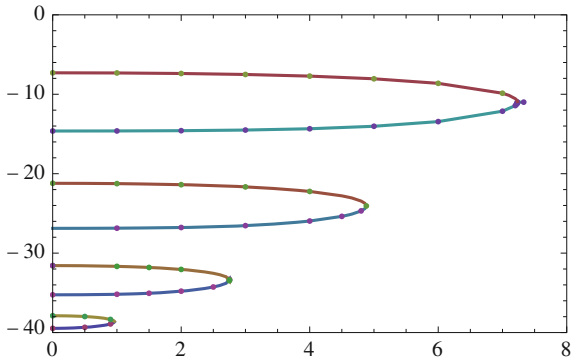

Fig. 2 The parametric evolution of real discrete spectrum, $E_n(V_2)$, for rectangular potential with $V_1 = 40$ and $a = 2$, notice that there are no level-crossings, but the eigenvalue pairs do coalesce at the exceptional points $|V_2| = 0.96, 2.75, 4.88, 7.33$. The *solid line* is due to numerical integration using (3) and the *dots* are due to the exact analytic method using (9)

$$V_R(x) = -V_1\Theta_1(x) - iV_2\Theta_2(x), \Theta_1(x) = \begin{cases} 1, & |x| \le a \\ 0, & |x| > a \end{cases}, \Theta_2(x) = \begin{cases} 0, & |x| \ge a \\ -1, & -a < x < 0 \\ 1, & 0 \le x < a \end{cases} \quad (4)$$

which is also solvable analytically (see (9)). The potential (4) being of finite support we take $L = a = 2$. In Fig. 1, the solid lines are due to numerical integration method using (3). No crossing (real to real) of eigenvalues is observed but eigenvalues coalesce at $|V_2| = V_{2c} = 0.96, 2.75, 4.88, 7.33$. Next, we find the evolution of eigenvalues of Gaussian model for $V_1 = 50$

$$V_G(x) = V_1 e^{-x^2} + iV_2 x e^{-x^2}, \quad V_1, V_2 \in \mathscr{R}, V_1 > 0. \quad (5)$$

By this method a distance of $L = 10$–12 has been found sufficient for the convergence of eigenvalues. In Fig. 3, the solid lines represent the result due to (3). The exceptional points for this potential (5) are $|V_2| = V_{2c} = 43.26, 55.55, 63.70$ and the crossing of levels is not found. In Fig. 4, the parametric evolution of the spectrum of

$$V_F(x) = \frac{-V_1}{1+x^4} + \frac{iV_2 x}{1+x^4}, \quad V_1, V_2 \in \mathscr{R}, V_1 > 0 \quad (6)$$

is presented. The pairs of eigenvalues are well separated from each other and the levels do not cross. They do coalesce at $|V_2| = V_{2c} = 19.39, 38, 87, 46.35$, we have fixed $V_1 = 50$. So, for $|V_2| < 19.39$ all the discrete eigenvalues are real and PT-symmetry is un-broken. After this critical value, the initial discrete eigenvalues start disappearing. Let us now consider sech-hyperbolic potential

$$V_H = -V_1 \text{sech}\, x + iV_2 \text{sech}\, x \tanh x, \quad V_1, V_2 \in \mathscr{R}, V_1 > 0 \quad (7)$$

whose real part is sech x unlike the Scarf II potential (1). See in Fig. 5, the eigenvalue pairs are well separated without crossing each other, they coalesce at $|V_2| = V_{2c} =$ 25.37, 31.15, 34.92, 37.35.

In the following, we find eigenvalues of (4) alternatively by the exact and analytic method which will also confirm the results in Fig. 2. We insert this potential in the Schrödinger equation (2). Assuming $2m = 1 = \hbar$, we define

$$p = a\sqrt{E + V_1 - iV_2}, \quad q = a\sqrt{E + V_1 + iV_2}, \quad r = ak, \quad k = \sqrt{-E}. \tag{8}$$

The solution of (1) for this potential can be written as $\psi(x < -a) = Fe^{kx}$, $\psi(-a < x < 0) = C \sin qx + D \cos qx$, $\psi(0 < x < a) = A \sin px + B \cos px$, $\psi(x > a) = Ge^{-kx}$. By matching these solutions and their first derivative at $x = -a, 0, a$, we eliminate A, B, C, D, F, G to get the eliminant as

$$2pqr \cos p \cos q + p(r^2 - q^2) \cos p \sin q + q(r^2 - p^2) \sin p \cos q - r(p^2 + q^2) \sin p \sin q = 0, \tag{9}$$

which serves as an analytic eigenvalue equation to be solved by varying E from $-V_1$ to 0. By fixing $V_1 = 20$, and $a = 2$, we obtain the parametric evolution of the spectrum of (4). These results are shown by dots in Fig. 2. See an excellent agreement between the two.

Below, we propose to find the eigenvalues of the Gaussian potential (5) potential alternatively by the diagonalization of $H = p^2/(2\mu) + V_G(x)$ in the harmonic oscillator (HO) basis. For HO basis $|n\rangle$, we know that $H_0 = -\frac{d^2}{dx^2} + x^2$, $H|n\rangle = (2n + 1)|n\rangle$, where $2\mu = 1 = \hbar^2$, $\hbar\omega = 2$. Using the well known $a, a^\dagger$ operators, we know that

$$\langle m|p^2|n\rangle = -\frac{\sqrt{(n-1)n}}{2}\,\delta_{m,n-2} + \frac{(2n+1)}{2}\,\delta_{m,n} - \frac{\sqrt{(n+1)(n+2)}}{2}\,\delta_{m,n+2}. \tag{10}$$

More interestingly the following required matrix elements can be found analytically with help of available but rare integrals [13]

$$\langle m|e^{-x^2}|n\rangle = \cos[(m-n)\pi/2]\frac{\Gamma[(m+n+1)/2]}{\sqrt{2\pi m!n!}}, \tag{11}$$

and

$$\langle m|xe^{-x^2}|n\rangle = \begin{cases} \frac{(m-n)}{2\sqrt{2}\sin[(m-n)\pi/2]}\frac{\Gamma[(m+n)/2]}{\sqrt{2\pi m!n!}}, & \text{if, } m+n = \text{odd} \\ 0, & \text{otherwise.} \end{cases} \tag{12}$$

Using (10, 11, 12), we write the matrix elements $h_{m,n} = \langle m|H|n\rangle$ to get the eigenvalues as

$$\det|h_{m,n} - E\,\delta_{m,n}| = 0. \tag{13}$$

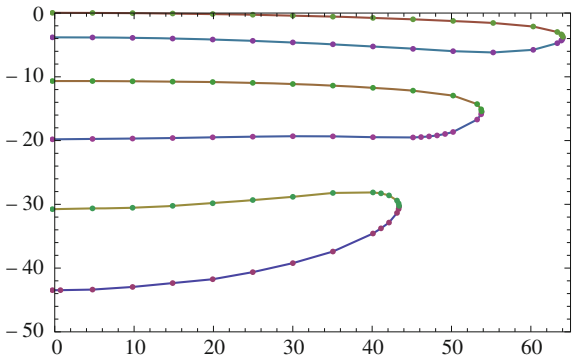

Fig. 3 The same as in Fig. 2, for $V_G(x)$ (5), when $V_1 = 50$. The *solid line* is due to (3) and *dots* are due to (13). The exceptional values are $|V_2| = 43.26, 55.55, 63.70$

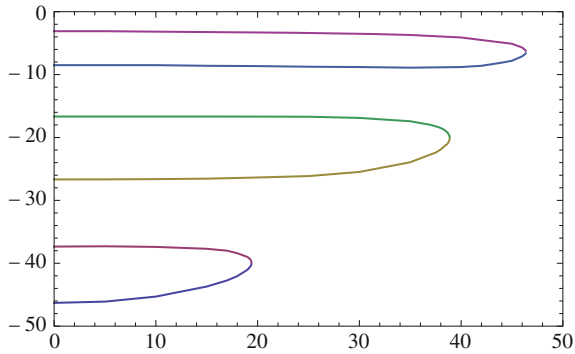

Fig. 4 The same as in Fig. 2, for $V_F(x)$ (6). These results are due to (3) and the exceptional point are $|V_2| = 19.39, 38, 87, 46.35$ and $V_1 = 50$

In Fig. 3, see the excellent agreement between solid lines (using (3) and dots (obtained by diagonalization using (13)).

Our last model to be discussed is the Wigner-Coulomb type complex PT-symmetric scattering potential expressed as

$$V_{WC}(x) = \frac{-V_1}{1+x^2} + \frac{iV_2 x}{1+x^2}, \quad V_1, V_2 \in \mathscr{R}, V_1 > 0. \tag{14}$$

The Schrödinger equation for this potential is known to be unamenable. A special case ($V_1 = V_2$) of this potential is $V_{WC}(x) = \frac{iV_2}{x-i}$ which is a complex regularized PT-symmetric potential and on the real line $x \in (-\infty, \infty)$ its discrete spectrum is null. This may well be understood by realizing that for any real value of E it gives rise to only one classical turning point (for bound states there should at least be two turning points). This special case also serves to a priori indicate that $V_{2c} < V_1$. The aforementioned special case of complex Coulomb potential has been treated [14, 15] on a special complex trajectory to find a real discrete spectrum.

In order to solve the eigenvalue equation $H\psi = E\psi$, where $H = [\frac{p^2}{2\mu} + V(x)]$. Here we use a special method [16, 17] wherein we find the roots of E by solving the determinantal equation

$$\det |\langle m|(1+x^2)H - Ex^2)|n\rangle - E\delta_{m,n}| = 0, \tag{15}$$

where $|n\rangle$ are the well known harmonic oscillator eigenstates. The motive behind choosing this method [16, 17] is two-fold. The matrix elements like $\langle m|(1+x^2)^{-1}|n\rangle$ cannot be found analytically. As the determinant becomes larger and larger, the analytic matrix elements are more desirable. Secondly, the imaginary part of this potential (1) like the Coulomb potential varies as $\sim 1/|x|$, asymptotically. This insufficiently rapid asymptotic fall off of the coulomb potential brings in the typical problems in the integration of the Schrödinger for asymptotic values. We again take $2\mu = 1 = \hbar^2$, $\hbar\omega = 2$ the eigenvalue equation (2) can be expressed as

$$\det |\mathscr{H}_{m,n}(E)| = 0$$
$$\mathscr{H}_{m,n} = \langle m|p^2|n\rangle + \langle m|x^2p^2|n\rangle - (E+V_1)\langle m|n\rangle + iV_2\langle m|x|n\rangle - E\langle m|x^2|n\rangle. \tag{16}$$

$$\langle m|x|n\rangle = \sqrt{\frac{n}{2}}\,\delta_{m,n-1} + \sqrt{\frac{(n+1)}{2}}\,\delta_{m,n+1} \tag{17}$$

$$\langle m|x^2|n\rangle = \frac{\sqrt{(n-1)n}}{2}\,\delta_{m,n-2} + \frac{(2n+1)}{2}\,\delta_{m,n} + \frac{\sqrt{(n+1)(n+2)}}{2}\,\delta_{m,n+2} \tag{18}$$

$$\begin{aligned}\langle m|x^2p^2|n\rangle = &-\sqrt{(n-3)(n-2)(n-1)n}\,\delta_{m,n-4}/4 + \sqrt{n(n-1)}\,\delta_{m,n-2}\\ &+ (2n^2+2n-1)\,\delta_{m,n} - \sqrt{(n+1)(n+2)}\,\delta_{m,n+2}/4\\ &- \sqrt{(n+1)(n+2)(n+3)(n+4)}\,\delta_{m,n+2}/4\\ &- \sqrt{(n+1)(n+2)(n+3)(n+4)}\,\delta_{m,n+4}/4.\end{aligned} \tag{19}$$

Curiously, the parametric evolution of eigenvalues obtained for this potential is qualitatively different from the other ones: $V_R(x)$, $V_G(x)$, $V_F(x)$, $V_H(x)$ discussed above. See in Fig. 6, the initial eigenvalue curves are longer which go on becoming shorter for higher eigenvalues. Once again there are no crossings of eigenvalues, but eigenvalues coalesce at $|V_2| = 19.73, 10.87, 5.53, 2.75$ (Fig. 5).

Most importantly, for all the scattering potentials considered here, we find that the change of the depth parameter V_1 changes the number of discrete eigenvalues and the subsequent values of exceptional points where energy levels coalesce and just after they become complex conjugate pairs. Based on our calculations, we can claim that by changing V_1 we do not detect any real to real crossings of discrete eigenvalues as

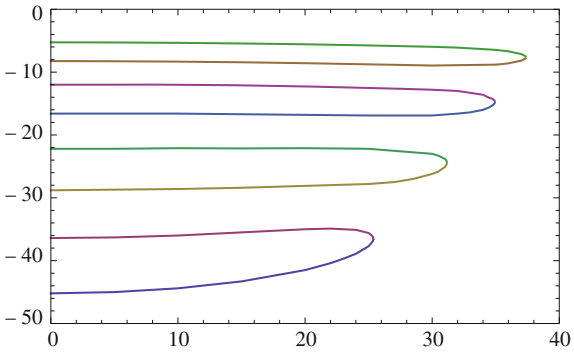

Fig. 5 The same as in Fig. 2, for $V_H(x)$ (7), $V_1 = 50$. The exceptional points are $|V_2| =$ 25.37, 31.15, 34.92, 37.35

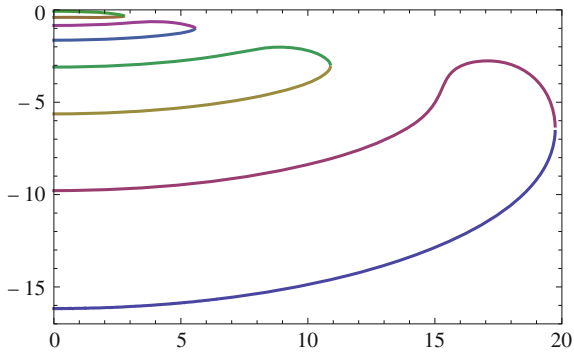

Fig. 6 The same as Fig. 2, for the Wigner-Coulomb potential (14), $V_1 = 20, a = 2$. The exceptional points are $|V_2| =$ 19.73, 10.87, 5.53, 2.74. These results are due to the special method [12, 13] of diagonalization (16)

it happens [7] in the case of complex PT-symmetric Scarf II scattering potential of the similar shape as in Fig. 1a, b.

To conclude, in this paper we have found parametric evolution of eigenvalues for five complex PT-symmetric scattering potentials employing different methods. Such works are instructive and desirable especially when complex PT-symmetry makes way in to textbooks of quantum mechanics. Unlike the Scarf II, these scattering potentials do not give rise to the real to real crossing of discrete eigenvalues. In this regard, the present work also attracts the attention on Scarf II (and also the RCHO) as two highly exceptional cases of accidental crossings of eigenvalues. The reason behind their specialty needs to be investigated. However, the PT-symmetric scattering potentials discussed here do display a general coalescing of eigenvalues at a finite number exceptional points, we attribute this phenomenon to the occurrence of a finite barrier either side of $x = 0$. This may be sufficient but not a necessary condition on a potential for the occurrence of level-coalescing. Further confirmations and investigations are welcome in this regard.

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Geometrical and Asymptotical Properties of Non-Selfadjoint Induction Equation with the Jump of the Velocity Field. Time Evolution and Spatial Structure of the Magnetic Field

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Abstract We study asymptotic solutions of the nonlinear system of MagnetoHydrodynamics. The solutions are assumed to jump rapidly near certain 2D-surface in 3D-space. We study the time behavior of the solution. In particular, we derive free boundary problem for the limit values of the magnetic field and the velocity field of the fluid. This problem governs also the evolution of the surface of the jump. We derive equations on the moving surface, describing the evolution of the field profile. In particular, we prove that the effect of the instantaneous growth of the magnetic field takes place only for degenerate asymptotic modes. This effect is deeply connected with non-Hermitian structure of the linearized induction operator.

1 Introduction

Equations of Magnetohydrodynamics (the MHD equations) describe the motion of the magnetic field in a conducting fluid. This nonlinear system of PDE's consists of the Navier-Stokes equations for the velocity field of the fluid and the Maxwell

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equations for the magnetic field. The equations are coupled by the term, describing the Lorenz force. The MHD equations describe, in particular, evolution of the magnetic fields of planets, stars and galaxies. Usually the viscosity and the resistance of the fluid are small enough and one can study the asymptotic solutions of the system with respect to the corresponding small parameter. This problem was studied in a lot of papers; note that in linear approximation the structure of the asymptotics is the subject of the famous dynamo theory (see, e.g. [1–12]). The main mathematical problem (which is still open) is to prove the existence of exponentially growing solutions.

The alternative effect was studied in [13, 14] (in linear approximation also). Namely, we described the instantaneous growth of the magnetic field, induced by the jump of the velocity field of the fluid. In another words, we studied the asymptotics of the solution for the Cauchy problem for linear induction equation with rapidly varying velocity field. We assumed that this field had a rapid jump in a small vicinity of the fixed 2D surface. We proved that the solution grows rapidly with respect to the corresponding small parameter, and has a delta-type singularity near the surface of the jump. This effect is a result of the non-Hermitian structure of the linearized induction operator—in certain sense the operator of the problem is close to the Jordan block.

Here we study the analogous problem for the complete nonlinear system. We describe the asymptotic structure of the solution with a rapid jump near 2D-surface. Now the surface is not fixed—it moves in time together with the solution. We obtain the special free boundary problem which governs the movement of the surface. We also study the possibility of the instantaneous growth of the magnetic field. It appears that the growth is possible only in the case of so called degenerate Alfwen modes; the latter appear if the main term of the magnetic field is tangent to the surface of the jump.

2 Statement of the Problem

2.1 The Cauchy Problem with the Jump of Initial Fields

We denote by $B(x,t)$ and $V(x,t)$ the magnetic and velocity fields in a conducting fluid (B, V are time-dependent vector fields in R^3). This pair of vector functions satisfy the following nonlinear MHD system

$$\frac{\partial B}{\partial t} + (V,\nabla)B - (B,\nabla)V = \varepsilon^2\mu\triangle B \tag{1}$$

$$\frac{\partial V}{\partial t} + (V,\nabla)V - (B,\nabla)B + \nabla P = \varepsilon^2\nu\triangle V \tag{2}$$

$$(\nabla, V) = 0, \quad (\nabla, B) = 0. \tag{3}$$

Here $P(x,t)$ is a scalar function, which can be expressed in terms of B and the pressure of the fluid, ν μ are positive numbers, characterizing hydrodynamic and magnet viscosities, $\varepsilon \to 0$ is a small parameter.

Let us consider for the system (1) initial data of the form

$$B|_{t=0} = B^0\left(\frac{\Phi_0(x)}{\varepsilon}, x, \varepsilon\right), \quad V|_{t=0} = V^0\left(\frac{\Phi_0(x)}{\varepsilon}, x, \varepsilon\right), \tag{4}$$

where $\Phi_0(x)$ is a smooth scalar function, divergence free vector fields $B^0(y,x,\varepsilon)$, $V^0(y,x,\varepsilon)$ depend smoothly on all arguments and tend to limits $B^{0,\pm}(x,\varepsilon)$, $V^{0,\pm}(x,\varepsilon)$ as $y \to \pm\infty$ faster then any power of y. We assume that the equation $\Phi_0(x) = 0$ defines a smooth compact surface $M_0 \subset R^3$ and $\Phi(x,t) < 0$ inside the domain, bounded by the surface. Without the loss of generality one can assume also that in the vicinity of the surface $|\Phi_0|$ equals the distance from M_0 in the normal direction; in particular, in this vicinity $|\nabla\Phi_0| = 1$.

Remark 1 Vector fields of this type define "smoothened" discontinuities—as $\varepsilon \to 0$ they tend to the discontinuous functions with the jump on the surface M_0. The corresponding weak limits have the form

$$\mathscr{B}^0 = B^{0,+}(x,0) + \theta_{M_0}(B^{0,-}(x,0) - B^{0,+}(x,0)),$$

$$\mathscr{V}^0 = V^{0,+}(x,0) + \theta_{M_0}(V^{0,-}(x,0) - V^{0,+}(x,0)),$$

where θ_{M_0} is the Heaviside function on M_0.

In the next sections we describe the asymptotic solutions to the Cauchy problem (1)–(4) under some additional assumptions concerning the initial fields. These assumptions define separate nonlinear modes.

2.2 Degenerate and Nondegenerate Alfwen Modes

The structure of the asymptotic solution to the Cauchy problem (1)–(4) depends essentially of the presence of the points of the initial surface, in which $B^0(y,x,0)$ is tangent to M_0. We will study two limit cases: in the first case there are no such points (nondegenerate modes) while in the second one B^0 is tangent to M_0 everywhere (degenerate mode). We do not study the problem of nonlinear interaction of modes; note that even in linear approximation this problem is highly nontrivial (for WKB-type solutions this problem was studied recently in [15]). Note that it is easy to prove that, according to the equations governing the motion of the surface, the points of tangency can not appear or disappear—the absence or presence of these points is a property of the initial data.

If there is no tangency, on can extract the single nondegenerate mode with the help of additional conditions on the initial fields; these conditions (which are well

known in the MHD theory) state that the fields $\frac{\partial V^0(y,x,0)}{\partial y}$ and $\frac{\partial B^0(y,x,0)}{\partial y}$ must coincide up to a sign. To be definite, we chose the sign "+"; so for nondegenerate mode we assume additionally that

$$\frac{\partial V^0(y,x,0)}{\partial y} = \frac{\partial B^0(y,x,0)}{\partial y}. \tag{5}$$

For the degenerate mode we assume that B is tangent to M:

$$(B^0(y,x,0), \nabla\Phi_0))|_{M_0} = 0. \tag{6}$$

Our goal is the description of the formal asymptotic solution as $\varepsilon \to 0$ of the Cauchy problem (1–4) under additional conditions (5) or (6).

3 Formulation of the Results. Nondegenerate Modes

Here we describe the structure of asymptotic solution corresponding to nondegenerate mode. The main term of asymptotics is defined by the free boundary problem for the limit fields as $y \to \pm\infty$ and by the equation on the moving surface, describing the profile of the rapidly varying field. Surprisingly, the latter equation appears to be linear.

3.1 Free Boundary Problem for Limit Fields

Let the conditions (5) are fulfilled; we denote by $u_0(y,x)$, $w_0(x)$ the main terms of the sum and the difference of the velocity field and the magnetic field in the initial instant of time:

$$u_0 = V^0(y,x,0) + B^0(y,x,0), \quad w_0 = V^0(y,x,0) - B^0(y,x,0).$$

Let $u_0^{\pm}$, $w_0^{\pm}$ be the limits of u_0, w_0 as $y \to \pm\infty$. Let us consider the following free boundary problem: for a finite time interval $t \in [0,T]$ we seek for a smooth compact surface $M_t \in R^3$ and for smooth vector fields $u^{\pm}(x,t)$, $w^{\pm}(x,t)$ and scalar functions $P_0^{\pm}(x,t)$, defined in the internal (D_t^-) and external (D_t^+) domains and satisfying for $x \in D_t^{\pm}$ the following equations

$$\frac{\partial u^{\pm}}{\partial t} + (w^{\pm}, \nabla)u^{\pm} + \nabla P_0^{\pm} = 0, \tag{7}$$

$$\frac{\partial w^{\pm}}{\partial t} + (u^{\pm}, \nabla)w^{\pm} + \nabla P_0^{\pm} = 0, \tag{8}$$

$$(\nabla, u^{\pm}) = (\nabla, w^{\pm}) = 0. \tag{9}$$

We put also the conditions on the surface

$$[w] = 0, \quad [P_0] = 0, \quad [u_n] = 0, \quad -\frac{\partial \Phi}{\partial t} = w_n, \quad x \in M_t \tag{10}$$

and the initial conditions

$$\Phi|_{t=0} = \Phi_0(x), \quad u^{\pm}|_{t=0} = u_0^{\pm}, \quad w^{\pm}|_{t=0} = w_0^{\pm}, \quad x \in D_0^{\pm}. \tag{11}$$

Here $\Phi(x, t)$ denote the distance (with the appropriate sign) from the surface M_t in the normal direction, $u_n = (u, \nabla\Phi)|_{M_t}$, $w_n = (w, \nabla\Phi)|_{M_t}$, symbol $[f]$ denotes the jump of the function f:

$$[f] = f^+|_{M_t} - f^-|_{M_t}.$$

Remark 2 The surface M_t is defined by the equation $\Phi(x, t) = 0$; the boundary condition $-\frac{\partial \Phi}{\partial t} = w_n$ means that the surface moves along the trajectories of the vector field w.

3.2 Linear Equations on the Moving Surface, Describing the Rapidly Varying Part of the Solution

Let Φ, $u^{\pm}$, $w^{\pm}$, $P_0^{\pm}$ be the smooth solution of the free boundary problem, formulated above. Let us consider 3D surface $\Omega \subset R^4$, defined by the equation $\Phi(x, t) = 0$ (trace of the moving surface M_t). Note that the field $\partial/\partial t$, generally speaking, is not tangent to this surface; we denote by ∂_t the projection of $\partial/\partial t$ to the tangent plane to Ω. We denote by $\hat{w}$ the projection of the field $w|_{M_t}$ to the tangent plane to M_t and let $\mathscr{B}$ be the second fundamental form operator (that is the operator in the tangent plane with the eigenvalues equal to the principle curvatures and eigenvectors equal to the principle directions). The rapidly varying part of the main term of asymptotic solution—vector field h on the surface M_t—satisfies the Cauchy problem

$$\mathscr{L}_{\partial_t} h + \alpha y \frac{\partial h}{\partial y} + \hat{\nabla}_{\hat{w}} h - w_n \mathscr{B} h = \frac{1}{2}(\mu + \nu)\frac{\partial^2 h}{\partial y^2}, \tag{12}$$

$$h|_{t=0} = \Pi(u_0 - u_0^-)|_{M_0}. \tag{13}$$

Here $\hat{\nabla}$ denotes the covariant derivative on the surface M_t, $\mathscr{L}$ denotes Lie derivative on Ω, Π is the projection to the tangent plane to M_t,

$$\alpha = \frac{\partial}{\partial \Phi}|_{M_t} \left(\frac{\partial \Phi}{\partial t} + (w, \nabla\Phi) \right).$$

Remark 3 Vector field h satisfies the Cauchy problem for the linear parabolic system—evidently, this system has a unique solution for any finite time interval.

Remark 4 Equation (12) is analogous to the advection-diffusion equations on the moving surface M_t. Advection is governed by the field $\hat{w}$, while diffusion is presented by the terms in the right hand site, containing viscosity. The system additionally contains the second fundamental form operator $\mathscr{B}$; the corresponding term describes the influence of the curvature of M_t on the growth or the decay of the field h. In particular, in the area of hyperbolic points the corresponding term induces the growth of the one component of the field and the decay of the another component, while in the area of elliptic points both components have the tendency to grow or to decrease simultaneously.

3.3 Asymptotic Solution of the Cauchy Problem

General structure of nondegenerate mode is described by the following theorem.

Theorem 1 *Let for $t \in [0, T]$ there exists a smooth solution Φ, $w^{\pm}$, $u^{\pm}$, $P_0^{\pm}$ to the free boundary problem (7)–(11) as well as the smooth solution of the corresponding linearized problem (see (36)–(40)) and the analogous problem with a smooth right hand side. Then there exist formal series*

$$B = \sum_{k=0}^{\infty} \varepsilon^k B_k\left(\frac{\Phi(x,t)}{\varepsilon}, x, t\right), \quad V = \sum_{k=0}^{\infty} \varepsilon^k V_k\left(\frac{\Phi(x,t)}{\varepsilon}, x, t\right),$$
$$P = \sum_{k=0}^{\infty} \varepsilon^k P_k\left(\frac{\Phi(x,t)}{\varepsilon}, x, t\right), \qquad (14)$$

satisfying the Cauchy problem (1)–(4) with the initial fields, satisfying (5). Moreover,

$$\lim_{y\to\pm\infty} V_0 = \frac{1}{2}(u^{\pm} + w^{\pm}), \quad \lim_{y\to\pm\infty} B_0 = \frac{1}{2}(u^{\pm} - w^{\pm}),$$

the function P_0 does not depend on the rapid variable y and coincides with $P_0^{\pm}$ in $D_t^{\pm}$. On the surface M_t the tangent $\hat{V}$, $\hat{B}$ and normal V_n, B_n components of the fields V_0, B_0 have the form

$$V_n(x,t) = \frac{1}{2}(u_n + w_n), \quad B_n(x,t) = \frac{1}{2}(u_n - w_n), \qquad (15)$$

$$\hat{V}(y,x,t) = \frac{1}{2}(h(y + c(x,t)) + u^{-}(x,t) + \hat{w}(x,t)), \qquad (16)$$

$$\hat{B}(y,x,t) = \frac{1}{2}(h(y + c(x,t)) + u^{-}(x,t) - \hat{w}(x,t)). \tag{17}$$

Here $c(x,t)$ is a smooth function, satisfying the equation, obtained in Sect. 5 (see. (34)).

Remark 5 Initial conditions for the function c depend on the vectors $\frac{\partial}{\partial\varepsilon}|_{\varepsilon=0}B^0$, $\frac{\partial}{\partial\varepsilon}|_{\varepsilon=0}V^0$. So the asymptotic solution is "asymptotically unstable"—small $(O(\varepsilon))$ variation of initial conditions leads to the big $(O(1))$ variation of the asymptotics. However, the limit fields $B_0^{\pm}$, $V_0^{\pm}$ and the profile $h(y)$ do not change as a result of such a variation—$O(\varepsilon)$—variation of the initial conditions lead to the $O(\varepsilon)$—shift of the surface of the jump.

4 Formulation of the Results. Degenerate Mode

Here we describe the structure of asymptotic solution, corresponding to the degenerate mode. Just as in the nondegenerate case, the main term of asymptotic solution is defined from the free boundary problem and from the system of equations on the moving surface. However, the latter equations now are essentially more complicated—they form a nonlinear system for two vector fields and one scalar function. The main property of this system—the possibility of the instantaneous growth of the magnetic field.

4.1 Free Boundary Problem for the Limit Fields

Let the conditions (6) be fulfilled; let us consider the following free boundary problem. On the finite time interval $t \in [0,T]$ we seek for smooth compact surface $M_t \in R^3$, vector fields $B_0^{\pm}(x,t)$, $V_0^{\pm}(x,t)$ and scalar functions $P_0^{\pm}(x,t)$, defined in the internal (D_t^-) and external (D_t^+) domains with respect to M_t and satisfying for $x \in D_t^{\pm}$ the following equations

$$\frac{\partial V_0^{\pm}}{\partial t} + (V_0^{\pm},\nabla)V_0^{\pm} - (B_0^{\pm},\nabla)B_0^{\pm} + \nabla P_0^{\pm} = 0, \tag{18}$$

$$\frac{\partial B_0^{\pm}}{\partial t} + (V_0^{\pm},\nabla)B_0^{\pm} - (B_0^{\pm},\nabla)V_0^{\pm} = 0, \qquad (\nabla, V_0^{\pm}) = (\nabla, B_0^{\pm}) = 0, \tag{19}$$

boundary conditions

$$B_n = 0, \quad [P_0] = 0, \quad [V_n] = 0, \quad -\frac{\partial \Phi}{\partial t} = V_n, \quad x \in M_t \tag{20}$$

and initial conditions

$$\Phi|_{t=0} = \Phi_0(x), \quad V_0^{\pm}|_{t=0} = V^{0,\pm}, \quad B_0^{\pm}|_{t=0} = B^{0,\pm}, \quad x \in D_0^{\pm}. \tag{21}$$

Here $\Phi(x,t)$ equals the distance (with the appropriate sign) from the surface M_t in the normal direction, $V_n = (V_0, \nabla\Phi)|_{M_t}$, $B_n = (B_0, \nabla\Phi)|_{M_t}$, the symbol $[f]$ denotes the jump of f:

$$[f] = f^+|_{M_t} - f^-|_{M_t}.$$

Remark 6 Surface M_t is defined by the equation $\Phi(x,t) = 0$; the boundary condition $-\frac{\partial\Phi}{\partial t} = V_n$ means that the surface moves along the trajectories if the field V_0.

4.2 Equations on the Moving Surface, Describing the Rapidly Varying Fields

Let Φ, $V_0^{\pm}$, $B_0^{\pm}$, $P_0^{\pm}$ be the smooth solution of the free boundary problem, formulated in the previous section. The rapidly varying part of the solution—two vector fields v, b on the surface M_t—satisfy the Cauchy problem

$$\mathscr{L}_{\partial_t} v + \hat{\nabla}_v v + \kappa y \frac{\partial v}{\partial y} - 2V_n \mathscr{B} v - \hat{\nabla}_b b + \hat{\nabla}\mathscr{P} = a\frac{\partial b}{\partial y} + \nu\frac{\partial^2 v}{\partial y^2}, \tag{22}$$

$$\mathscr{L}_{\partial_t} b + \{v, b\} + \kappa y \frac{\partial b}{\partial y} = a\frac{\partial v}{\partial y} + \mu\frac{\partial^2 b}{\partial y^2}, \tag{23}$$

$$(\hat{\nabla}, v) = 0, \quad (\hat{\nabla}, b) + \frac{\partial a}{\partial y} = 0, \tag{24}$$

$$v|_{t=0} = \Pi(V^0|_{M_0}), \quad b|_{t=0} = \Pi(B^0|_{M_0}). \tag{25}$$

Here $\mathscr{P} = (P_0 + \frac{1}{2}V_n^2)|_{M_t}$, a is a smooth scalar function, $\kappa = \frac{\partial}{\partial\Phi}|_M \left(\frac{\partial\Phi}{\partial t} + (V_0, \nabla\Phi)\right)$.

Remark 7 Equations (22) are close to the Prandtl equations for the boundary layer and their generalizations, describing vortex structures in the fluid (see [16–18]).

Remark 8 Function a can be excluded from the system—it can be expressed from the last equation:

$$a(y,x,t) = a^-(x,t) + \int_{-\infty}^{y} (\hat{\nabla}, b)dy.$$

The limit function $a^-(x,t)$ can be computed from the linearized free boundary problem; at the initial instant of time this function has the form $\left(\frac{\partial}{\partial\varepsilon}|_{\varepsilon=0}(B^{0,-}, \nabla\Phi_0\right)$. So the $O(\varepsilon)$-variation of the initial field implies the variation of the function a and

the vector fields v, b—the main term of asymptotic solution. Moreover, using the form of (22) it is easy to see, that even if at the initial instant of time the magnetic field is small ($B^0 = O(\varepsilon)$), during arbitrary small time $t > 0$ the field grows to the value $O(1)$. The same effect (instantaneous growth of the magnetic field, caused be the jump of the velocity field)—was described in the paper [13] in linear approximation. Note that, analogous to the linear situation, the magnetic field in this case is localized in the small vicinity of M_t (evidently, $B_0^{\pm} = 0$ if $B^0 = O(\varepsilon)$).

4.3 Asymptotic Solution of the Cauchy Problem

The structure of the degenerate mode is described by the following theorem.

Theorem 2 *Let for $t \in [0, T]$ there exists smooth solution Φ, $V_0^{\pm}$, $B_0^{\pm}$, $P_0^{\pm}$ for the free boundary problem (18)–(21), as well as the smooth solution for the linearized problem with the smooth right hand side. Let the system (22)–(25) admits smooth solution h, v, a. Then there exist power series*

$$B = \sum_{k=0}^{\infty} \varepsilon^k B_k \left(\frac{\Phi(x,t)}{\varepsilon}, x, t \right), \quad V = \sum_{k=0}^{\infty} \varepsilon^k V_k \left(\frac{\Phi(x,t)}{\varepsilon}, x, t \right),$$

$$P = \sum_{k=0}^{\infty} \varepsilon^k P_k \left(\frac{\Phi(x,t)}{\varepsilon}, x, t \right), \qquad (26)$$

satisfying the Cauchy problem (1)–(4) with the initial fields, satisfying (6). Moreover,

$$\lim_{y \to \pm\infty} V_0 = V_0^{\pm}, \quad \lim_{y \to \pm\infty} B_0 = B_0^{\pm},$$

the function P_0 does not depend on y and coincides in the domains $D_t^{\pm}$ with $P_0^{\pm}$. On the surface M_t the tangent $\hat{V}$, $\hat{B}$ and the normal V_n, B_n components of the fields V_0, B_0 have the form

$$V_n(x,t) = (V_0^{+}, \nabla\Phi)|_{M_t}, \quad B_n(x,t) = 0, \qquad (27)$$

$$\hat{V}(y,x,t) = v(y + d(x,t)), \quad \hat{B}(y,x,t) = b(y + d(x,t)). \qquad (28)$$

Here $d(x,t)$ is the smooth function, which can be expressed in terms of the limit fields $V_1^{\pm}$, $B_1^{\pm}$.

5 Construction of the Asymptotic Solution

Here we give the proof of the Theorem 1; the proof of the Theorem 2 is analogous.

5.1 Division in the Asymptotic Modes

We seek for the formal asymptotic solution of the Cauchy problem (1)–(4) (i.e. for the the formal series, satisfying the corresponding equations and initial conditions) in the form (14); we assume that $\Phi(x,t)$, $B_k(y,x,t)$, $V_k(y,x,t)$, $P_k(y,x,t)$ are smooth functions of all arguments, and $B_k \to B_k^{\pm}(x,t)$, $V_k \to V_k^{\pm}(x,t)$, $P_k \to P_k^{\pm}(x,t)$ as $y \to \pm\infty$ faster than any power of y. We denote by M_t the surface, defined by the equation $\Phi(x,t) = 0$; we assume that this surface is smooth and compact, $\Phi < 0$ inside M_t and in certain vicinity of this surface $|\Phi(x,t)|$ coincides with the distance from the point x to M_t in the normal direction (we can always provide this property with the help of re-expansions in (14)). Moreover, we assume that $|\nabla\Phi| \geq C > 0$ in R^3. Further we will usually omit the index t in the notation of the surface.

Let us substitute the series (14) to the equations (1) and consider the summands in the both sides of equality, containing equal powers of ε. The summands, containing ε^{-1}, lead to the equation

$$\left(\frac{\partial\Phi}{\partial t} + (V_0, \nabla\Phi)\right)\frac{\partial B_0}{\partial y} - (B_0, \nabla\Phi)\frac{\partial V_0}{\partial y} = 0, \tag{29}$$

$$\left(\frac{\partial\Phi}{\partial t} + (V_0, \nabla\Phi)\right)\frac{\partial V_0}{\partial y} - (B_0, \nabla\Phi)\frac{\partial B_0}{\partial y} + \nabla\Phi\frac{\partial P_0}{\partial y} = 0.$$

$$\frac{\partial}{\partial y}(B_0, \nabla\Phi) = 0, \quad \frac{\partial}{\partial y}(V_0, \nabla\Phi) = 0.$$

Note that the left hand sides of these equalities decay rapidly as $|y| \to \infty$, hence, due to the well-known estimate [19]

$$F(x,y) = F(x,y)|_{x\in M, y=\Phi/\varepsilon} + \Phi\left(\frac{\partial}{\partial\Phi}F(x,y)\right)|_{x\in M, y=\Phi/\varepsilon} + \dots$$

$$= F(x,y)|_{x\in M, y=\Phi/\varepsilon} + \varepsilon y\left(\frac{\partial}{\partial\Phi}F(x,y)\right)|_{x\in M, y=\Phi/\varepsilon} + \dots = F(x,y)|_{x\in M, y=\Phi/\varepsilon} + O(\varepsilon)$$

these summands can be mod $O(\varepsilon)$ restricted to the surface M. Note that this equality is obtained with the help of Taylor expansion with respect to the distance from M; in further approximations with respect to ε we will take into account all the summands of this expansion.

Multiplying (29) by the vector $\nabla\Phi$, we obtain

$$\frac{\partial P_0}{\partial y}|_M = 0.$$

We will have to prolong functions, rapidly decaying in y, from M to the vicinity of this surface. We will use the following rule: the functions and the fields will be prolonged in such a way, that they will not depend on Φ (i.e. will satisfy equations $\nabla_{\nabla\Phi} F = 0$). In particular, as $\frac{\partial P_0}{\partial y}|_M = 0$, we will assume that this derivative vanishes everywhere.

Note that, if (29) has nontrivial solutions, the determinant of 2×2 matrix

$$\begin{matrix} \left(\frac{\partial\Phi}{\partial t} + (V_0, \nabla\Phi)\right)|_M & (B_0, \nabla\Phi)|_M \\ (B_0, \nabla\Phi)|_M & \left(\frac{\partial\Phi}{\partial t} + (V_0, \nabla\Phi)\right)|_M \end{matrix}$$

vanishes; this implies one of the two following conditions.

1. The rang of this matrix is equal to unity; in this case we have on M

$$\frac{\partial B_0}{\partial y} = \pm\frac{\partial V_0}{\partial y}, \quad \frac{\partial\Phi}{\partial t} + (V_0, \nabla\Phi) = \pm(B_0, \nabla\Phi).$$

2. The rang is equal to zero; in this case

$$\frac{\partial\Phi}{\partial t} + (V_0, \nabla\Phi)|_M = 0, \quad (B_0, \nabla\Phi)|_M = 0,$$

and we have no conditions on the vectors $\frac{\partial B_0}{\partial y}$, $\frac{\partial V_0}{\partial y}$.

These two cases correspond to nondegenerate and degenerate modes; consider the first case. We chose the mode, corresponding to the "+" sign; in another words, we assume that the initial fields satisfy (5). So (1) are fulfilled up to mod$O(1)$, if

$$\frac{\partial P_0}{\partial y} = 0, \quad \frac{\partial}{\partial y}(V_0 - B_0) = 0,$$

$$\frac{\partial}{\partial y}(V_0, \nabla\Phi) = 0, \quad \frac{\partial}{\partial y}(B_0, \nabla\Phi) = 0,$$

$$\left(\frac{\partial\Phi}{\partial t} + (V_0 - B_0, \nabla\Phi)\right)|_M = 0.$$

5.2 Free Boundary Problem for the Limit Fields

Now let us equate summands, containing ε^0, in both sides of (1). Consider first these equations in the domains $D_\pm$, i.e. in the points which do not belong to M. At these points $y \to \infty$, so in the corresponding equalities one can $\mathrm{mod}\, O(\varepsilon^\infty)$ pass to the limit $y \to \pm\infty$; thus we have

$$\frac{\partial V_0^\pm}{\partial t} + (V_0^\pm, \nabla V_0^\pm) - (B_0^\pm, \nabla) B_0^\pm + \nabla P_0 = 0,$$

$$\frac{\partial B_0^\pm}{\partial t} + (V_0^\pm, \nabla) B_0^\pm - (B_0^\pm, \nabla V_0^\pm) = 0,$$

$$(\nabla, V_0^\pm) = (\nabla, B_0^\pm) = 0.$$

Let us denote $u = V_0 + B_0, w = V_0 - B_0$; in the previous section we showed, that w does not depend on y. Consider the sum and the difference of the equations for $V_0^\pm$ an $B_0^\pm$; evidently we obtain (7). As P_0, w do not depend on y, at the points of M $P_0^+ = P_0^-$, $w^+ = w^-$; moreover, the function $(V_0 + B_0, \nabla\Phi)$ also does not depend on y, hence $u_n^+ = u_n^-$, where $u_n^\pm$ denote the limits of the normal components of the vector u in the points of M. Thus the fields $u^\pm$, w and the functions P_0, Φ satisfy (10) (we remind, that the equation for the function Φ was obtained earlier). Evidently, initial conditions (11) are also fulfilled. Further we will assume that Φ, w, $u^\pm$, P_0 is a smooth solution of (7)–(11).

5.3 Equations on the Moving Surface

Let us return to the equations, appearing from the summands, multiplied by ε^0. Due to the equations of the previous section, the left hand sides of these equations vanish as $y \to \pm\infty$, hence they can be restricted $\mathrm{mod}\, O(\varepsilon)$ to the surface M. We have

$$\begin{aligned}
&\frac{\partial V_0}{\partial t} + (V_0, \nabla) V_0 + (B_0, \nabla\Phi)\left(\frac{\partial V_1}{\partial y} - \frac{\partial B_1}{\partial y}\right) \\
&\quad - (B_1, \nabla\Phi)\frac{\partial B_0}{\partial y} + (V_1, \nabla\Phi)\frac{\partial V_0}{\partial y} - (B_0, \nabla) B_0 + \nabla P_0 + \nabla\Phi \frac{\partial P_1}{\partial y} \\
&\quad + y\frac{\partial}{\partial\Phi}\left((\Phi_t + (V_0, \nabla\Phi))\frac{\partial V_0}{\partial y}\right) - y\frac{\partial}{\partial\Phi}\left((B_0, \nabla\Phi)\frac{\partial B_0}{\partial y}\right) - \nu\frac{\partial^2 V_0}{\partial y^2} = 0, \\
&\frac{\partial B_0}{\partial t} + (B_0, \nabla\Phi)\left(\frac{\partial B_1}{\partial y} - \frac{\partial V_1}{\partial y}\right) + \{V_0, B_0\} + (V_1, \nabla\Phi)\frac{\partial B_0}{\partial y} - (B_1, \nabla\Phi)\frac{\partial V_0}{\partial y} \\
&\quad + y\frac{\partial}{\partial\Phi}\left((\Phi_t + (V_0, \nabla\Phi))\frac{\partial B_0}{\partial y}\right) - y\frac{\partial}{\partial\Phi}\left((B_0, \nabla\Phi)\frac{\partial V_0}{\partial y}\right) - \mu\frac{\partial^2 B_0}{\partial y^2} = 0,
\end{aligned}$$

$$\frac{\partial}{\partial y}(V_1, \nabla\Phi) + (\nabla, V_0) = 0,$$

$$\frac{\partial}{\partial y}(B_1, \nabla\Phi) + (\nabla, B_0) = 0.$$

Here we took into account the summands of order $O(1)$, neglected in the previous approximation (second summands of the Taylor expansion with respect to the distance form M).

Let us rewrite the equations in the following form:

$$(B_0, \nabla\Phi)\left(\frac{\partial B_1}{\partial y} - \frac{\partial V_1}{\partial y}\right) + (V_1, \nabla\Phi)\frac{\partial B_0}{\partial y} - (B_1, \nabla\Phi)\frac{\partial V_0}{\partial y} = F,$$

$$(B_0, \nabla\Phi)\left(\frac{\partial V_1}{\partial y} - \frac{\partial B_1}{\partial y}\right) + (V_1, \nabla\Phi)\frac{\partial V_0}{\partial y} - (B_1, \nabla\Phi)\frac{\partial B_0}{\partial y} + \nabla\Phi\frac{\partial P_1}{\partial y} = G,$$

$$\frac{\partial}{\partial y}(V_1, \nabla\Phi) = g \quad \frac{\partial}{\partial y}(B_1, \nabla\Phi) = f, \quad f - g = 0 \tag{30}$$

(the last equality follows from the equation $(\nabla, w) = 0$ in R^3).

Let us project the second vector equation to the tangent plane to M and then let us consider the sum and the difference of the obtained vector equations. Taking into account that $\frac{\partial V_0}{\partial y} = \frac{\partial B_0}{\partial y}$ as well as (29), we obtain

$$2(B_0, \nabla\Phi)\frac{\partial w_1}{\partial y} = \Pi(G) - F, \tag{31}$$

$$2(w_1, \nabla\Phi)\frac{\partial V_0}{\partial y} = \Pi(G) + F, \tag{32}$$

where $w_1 = V_1 - B_1$ and Π is the projector to the tangent plane. Projecting the same equation to the normal direction to M, we obtain

$$\frac{\partial P_1}{\partial y} = (G, \nabla\Phi). \tag{33}$$

Proposition 1 *Equation* (32) *can be reduced to the form*

$$\mathscr{L}_{\partial_t} H + (\alpha y + \beta)\frac{\partial H}{\partial y} + \hat{\nabla}_{\hat{w}} H - w_n \mathscr{B} H = \frac{1}{2}(\mu + \nu)\frac{\partial^2 H}{\partial y^2}, \tag{34}$$

where $H = \Pi(u - u^-)|_M$, $\alpha = \frac{\partial}{\partial \Phi}|_M \left(\frac{\partial \Phi}{\partial t} + (w, \nabla\Phi)\right)$, $\beta = (w_1, \nabla\Phi)$.

Proof First we prove that the vector F is tangent to M; let us compute its normal component. Taking into account the equality $(\nabla\Phi, \partial V_0/\partial y) = 0$, after direct computations we obtain

$$-(F, \nabla\Phi) = \left(\frac{\partial}{\partial t} + (w, \nabla)\right)(B_0, \nabla\Phi) - (B_0, \nabla)\left(\frac{\partial \Phi}{\partial t} + (w, \nabla\Phi)\right).$$

Note that the first summand is independent of y; taking into account the equality $(\Phi_t + (w, \nabla\Phi))|_M = 0$, one can rewrite the second summand in the form

$$-(B_0, \nabla\Phi)\frac{\partial}{\partial \Phi}|_M \left(\frac{\partial \Phi}{\partial t} + (w, \nabla\Phi)\right).$$

This function is also independent of y. Note that the vector F vanishes as $|y| \to \infty$, hence $(F, \nabla\Phi) = 0$.

Thus (32) can be rewritten in the form

$$2(w_1, \nabla\Phi)\frac{\partial V_0}{\partial y} = \Pi(G + F)$$

Using the explicit expressions for F and G, we have

$$\Pi\left(\frac{\partial u}{\partial t} + (w, \nabla)u + \nabla P_0 + y\alpha\frac{\partial u}{\partial y} - \frac{\mu + \nu}{2}\frac{\partial^2 u}{\partial y^2}\right) + \beta\frac{\partial u}{\partial y} = 0.$$

Let us subtract from this equation the equality

$$\Pi\left(\frac{\partial u^-}{\partial t} + (w, \nabla)u^- + \nabla P_0^-\right)|_M = 0.$$

Note that P_0 does not depend on y and the vector $\partial u/\partial y$ is tangent to M. Using these facts, we obtain

$$\Pi\left(\frac{\partial \hat{H}}{\partial t} + (w, \nabla)\hat{H}\right) + (\alpha y + \beta)\frac{\partial H}{\partial y} = \frac{\mu + \nu}{2}\frac{\partial^2 H}{\partial y^2},$$

where $\hat{H} = u - u^-$, $H = \hat{H}|_M$ (note, that, according to (10), this vector is tangent to M). Further computation of the projection is quite analogous to the calculation, presented in [20]. Namely: we expand the vector $\partial/\partial t$ to the tangent and normal components to the 3D surface $\cup_t M_t \subset R^4$. Cumbersome computations lead to the formulae

$$\Pi\left(\frac{\partial \hat{H}}{\partial t}+(w,\nabla)\hat{H}\right)=\Pi\left(\{\frac{\partial}{\partial t},\hat{H}\}+(\hat{w},\nabla)\hat{H}+w_n\frac{\partial \hat{H}}{\partial \Phi}\right)$$

$$=\{\partial_t,H\}+\hat{\nabla}_{\hat{w}}H+\Pi\left(\left(\frac{\partial \Phi}{\partial t}+w_n\right)\frac{\partial \hat{H}}{\partial \Phi}-\frac{\partial \Phi}{\partial t}(\hat{H},\nabla)\frac{\partial}{\partial \Phi}\right)$$

$$=\mathscr{L}_{\partial_t}H+\hat{\nabla}_{\hat{w}}H-w_n\mathscr{B}H.$$

Equation (34) contains the coefficient β, depending on the first correction w_1; so the equations for the main part of the asymptotics appear to be linked with the equations, appearing in the next approximations. However, the form of the function h appears to be independent on the correction w_1—the latter function influences only the shift of the argument y, i.e. the small (of order ε) shift of the surface M_t. Formally: the following assertion can be verified directly.

Proposition 2 *Equation (34) is invariant with respect to the transformation*

$$H(y,x,t)\to H(y+c(x,t),x,t),\quad \beta\to\beta+\partial_t(c)+(\hat{w},\nabla)c.$$

Corollary 1 *Let $h(y,x,t)$ be the solution of the Cauchy problem (12), while the scalar function $c(x,t)$ on the surface M_t satisfies the equation*

$$\partial_t(c)+(\hat{w},\nabla)c+\beta(x,t)=0,\quad c(0)=0. \tag{35}$$

Then the vector field $H(y,x,t)=h(y+c,x,t)$ satisfies (30) and $H|_{t=0}=(u_0-u_0^-)|_{M_0}$.

5.4 Construction of the Main Part of the Asymptotic Solution and Description of the Further Terms

The free boundary problem determines the functions $B_0^{\pm}$, $V_0^{\pm}$, Φ, w, P_0 and $(u,\nabla\Phi)$. In order to construct the main term of the asymptotics one has to prolong the vector field h to the entire space and to compute the phase shift $c(x,t)$. Note that $h\to 0$ as $y\to-\infty$ and $h\to(u^+-u^-)|_M$ as $y\to-\infty$; so the vector field h can be represented in the form

$$h=\eta(y)(u^+-u^-)|_M+h_0(y,x,t),\quad \eta(y)=\frac{1}{2}(1+\tanh y),\quad h_0\to 0\ \ as\ \ y\to\pm\infty.$$

Let us define the field $U(y,x,t)$ in the entire space as follows

$$U(y,x,t)=\eta(y)(u^+(x,t)-u^-(x,t))+u_0(y,x,t),$$

where the decaying function u_0 is the standard prolongation of h_0 (($\nabla_{\nabla\Phi} u_0 = 0$, $u_0|_M = h_0$)). Now the vector field u is defined in the entire space up to the shift of the argument y ($u(y, x, t) = U(y + c, x, t)$). In order to determine this shift, we consider the $O(\varepsilon^1)$-approximation. Considering the corresponding equations in the domains $D_\pm$ and passing to the limits $y \to \pm\infty$, we obtain

$$\frac{\partial V_1^\pm}{\partial t} + (V_1^\pm, \nabla)V_0^\pm + (V_0^\pm, \nabla)V_1^\pm - (B_0^\pm, \nabla)B_1^\pm - (B_1^\pm, \nabla)B_0^\pm + \nabla P_1^\pm = 0,$$

$$\frac{\partial B_1^\pm}{\partial t} + (V_1^\pm, \nabla)B_0^\pm + (V_0^\pm, \nabla)B_1^\pm - (B_0^\pm, \nabla)V_1^\pm - (B_1^\pm, \nabla)V_0^\pm = 0,$$

$$(\nabla, V_1^\pm) = (\nabla, B_1^\pm) = 0.$$

The sum and the difference of these equations have the form

$$\frac{\partial w_1^\pm}{\partial t} + (u^\pm, \nabla)w_1^\pm + (u_1^\pm, \nabla)w + \nabla P_1^\pm = 0, \tag{36}$$

$$\frac{\partial u_1^\pm}{\partial t} + (w^\pm, \nabla)u_1^\pm + (w, \nabla)u_1^\pm + \nabla P_1^\pm = 0, \tag{37}$$

$$(\nabla, u_1^\pm) = (\nabla, w_1^\pm) = 0, \tag{38}$$

where $u_1 = V_1 + B_1$. Boundary conditions on the surface M_t come from (30, 33): integrating them with respect to y, we obtain

$$[w_1^n] = 0, \quad [w_1] = -\frac{1}{(B_0, \nabla\Phi)} \int_{-\infty}^{\infty} F dy, \quad [u_1^n] = \int_{-\infty}^{\infty} (f + g) dy,$$

$$[P_1] = \int_{-\infty}^{\infty} (G, \nabla\Phi) dy. \tag{39}$$

Evidently, the initial conditions have the form

$$u_1^\pm|_{t=0} = (V_1^0 + B_1^0)^\pm, \quad w_1^\pm|_{t=0} = (V_1^0 - B_1^0)^\pm, \quad V_1^0 = \frac{\partial V^0}{\partial \varepsilon}|_{\varepsilon=0}, \quad B_1^0 \frac{\partial B^0}{\partial \varepsilon}|_{\varepsilon=0}. \tag{40}$$

Remark 9 Boundary conditions (39) do not depend on the phase shift $c(x, t)$.

Let $w_1^\pm, u_1^\pm, P_1^\pm$ be the smooth solution of the problem (36)–(40); substituting the function $\beta = (w_1, \nabla\Phi)|_M$ (which is independent of y) to (35) and solving this equation, we obtain the phase shift $c(x, t)$. Now the main term of asymptotic solution is described completely.

The corrections can computed analogously; in order to describe the k-th summand of the asymptotic series, one has to take into account three approximations—$O(\varepsilon^{k-1})$, $O(\varepsilon^k)$ and $O(\varepsilon^{k+1})$.

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PT Symmetric Classical and Quantum Cosmology

Alexander A. Andrianov, Chen Lan and Oleg O. Novikov

Abstract The classical cosmology of flat space can be realized in a phenomenological scalar field model for dark energy: a two-field model of quintessence and phantom fields. When the model is supplied by a proper field mixing term it becomes analytically solvable for exponential potentials. The motivation is given for replacing a phantom field by a normal pseudoscalar field with complex but PT-symmetric potential (PTom). The comparison of two approaches in their prediction for the fate of our Universe is done in figures. The quantum cosmology of flat space is realized in the Arnowitt-Deser-Misner approach by means of the Wheeler-DeWitt equations. Taking into account the isotropy and homogeneity of space the ADM approach is reduced to only quantized component of space-time metric—Friedmann-Robertson-Walker factor. The quantum models supplied with appropriate mixing kinetic terms turn out to be also integrable for exponential potentials and the exact analytical solutions are obtained for wave functionals of quantum PT symmetric cosmology. Lessons and perspectives for developing PT symmetric Classical and Quantum Cosmology are discussed.

1 Outline

The main purpose of this work is to elucidate alternative ways for phenomenological description of dark energy in the universe with scalar fields both in classical and in quantum cosmology. Last decades were very rich in getting more precise values of cosmological parameters, especially, after the data collecting by the Satellite Observatory PLANCK [1, 2]. We start with brief survey of basic features of modern cosmology.

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By now the cosmology state-of-art can be summarized as follows:

- Nowadays our Universe is essentially space-flat: large-scale homogeneous and isotropic.
- Its fine structure—galaxies, stars and Cosmic Microwave Background, represents small fluctuations which could be theoretically explained as perturbations on a flat background.
- Universe evolution after Big Bang and inflation [3] was in average space-flat as it is supported by BAO and CMB data obtained by COBE, WMAP, PLANCK (see an updated review in [1]).
- However the space-averaged energy density ε and pressure p governing the Universe evolution are somewhat unusual: dark energy dominates over dark and visible matter and it obeys the equation of state $p = w\varepsilon$ (in the linear approximation) for which the observations prove $w \sim -1$ [2]. The question is what is its essence: *cosmological constant with* $w = -1$ *or dark energy medium with* $w < -1$ [4]? The modern observations have not yet excluded the latter option [2] (see Sect. 2).
- The future of our Universe strongly depends on the dark energy equation of state if w is a dynamic time-dependent variable. It may have a dramatic end with singular behavior of energy density and/or pressure (Big Crunch, Big Rip... [5–7]). In the vicinity of singularities the classical gravitational theory is not anymore adequate and must be extended to a quantum version accepting the quasiclassical approximation far from turning points.

The content and purpose of this work can be briefly formulated in the following items:

- The classical cosmology of flat space based on equation of state $w = p/\varepsilon \simeq -1$ can be realized in a phenomenological scalar field model for dark energy (Sect. 3): a two-field hybrid model [8] of quintessence field ($w > -1$) with normal kinetic energy and a phantom one ($w < -1$) with negative kinetic energy. The new type of hybrid models (Sect. 4) is supplied by a field mixing term which makes it separable and analytically solvable [9] for exponential potentials [10–22].
- However the phantom matter is troublesome, its energy is not bounded below and its classical cosmology may end up in the Big Rip. In this work we advocate for another type of scalar matter: a pseudoscalar one with PT symmetric complex potentials (Sect. 3) as a cure for above mentioned problems [23, 24]. PT symmetry means a discrete symmetry under simultaneous space-parity reflection and time-reversal transformations (the latter one realized in the Wigner sense).
- Therefore the motivation of this work is threefold: to replace a linearly unstable phantom mechanics by the linearly stable PT symmetric mechanics [23, 24] which simulates a phantom-like solution at the classical level (for introducing PT symmetry see [25–28]); to bound a "classical" trajectory (a saddle point solution) in the PT symmetric sector of a hybrid model with the help of negative classical potential unbounded below; to fix the separation constant in the integrable hybrid model in its quantum realization and thereby to remove (quasi)energy degeneracy. In this paper we derive the consistent quantum hybrid model (Sect. 4) which

includes two separable dynamics: one is a quintessence model and another one is a PT symmetric mechanics with complex exponential (Liouville) potential (in passing, we notice that real exponential potentials for scalar backgrounds in cosmology are inspired by the string theory [18]). Therefore a phantom field part is replaced by a pseudoscalar field with normal kinetic term and complex but PT-symmetric potential ("PTom"). The comparison of two approaches to (classical) hybrid models is done in Sect. 5 and their predictions for the fate of our Universe are illustrated in figures.

- The quantum cosmology of flat space is realized in the Arnowitt-Deser-Misner (ADM) approach by means of the Wheeler-DeWitt (WdW) equations [5]. Taking into account the isotropy and homogeneity of space the ADM approach is reduced so that the only quantized component of space-time metric, the Friedmann-Robertson-Walker (FRW) factor, is associated to time reparametrization (the mini-superspace model [5]).
- The new type of quantum hybrid models (Sect. 6) supplied by appropriate mixing kinetic terms turn out to be integrable for exponential potentials [9] and the exact analytical solutions are obtained for wave functionals of quantum PT symmetric hybrid cosmology. The consistency conditions are obtained from boundness of wave functions at large values of fields. They fix uniquely the separation constant and the dependence of energy spectrum on parameters of a hybrid model.
- Lessons and perspectives for developing PT symmetric Classical and Quantum Cosmology are discussed in Conclusions.

2 Geometry of Flat Space Evolution

Flat-space Universe evolution (in *cosmic time* τ) is described by a diagonal metric tensor

$$ds^2 = d\tau^2 - a^2(\tau)d\mathbf{x}^2. \tag{1}$$

The *Hubble variable* $h \equiv \dot{a}/a$ characterizes the Universe expansion and satisfies the Friedmann equation

$$h^2 = \frac{\kappa^2}{3}\varepsilon, \quad \kappa^2 = 8\pi G = M_{Pl}^{-2} \tag{2}$$

where ε is the space averaged energy density of massive matter, radiation and dominantly of **dark energy** populating the Universe.

Flat space is induced by a diagonal energy-momentum tensor

$$\left(T_{\mu\nu}\right) = \begin{pmatrix} \epsilon & 0 & 0 & 0 \\ 0 & p & 0 & 0 \\ 0 & 0 & p & 0 \\ 0 & 0 & 0 & p \end{pmatrix} \tag{3}$$

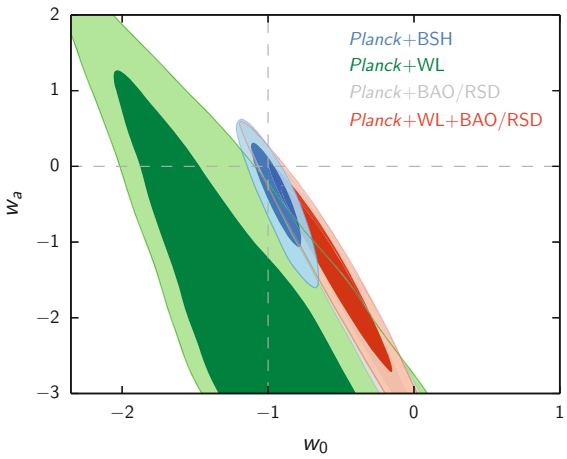

Fig. 1 Experimental fit (PLANCK [2]) of $w = w_0 + w_a(1-a) + \mathcal{O}((1-a)^2)$ against time ($a = a(\tau)$): dynamic equation of state. $a < 1$ corresponds to the past decreasing in time and $a > 1$ for the future

with an isotropic and homogeneous pressure $p = w\varepsilon$ (equation of state of the Universe). The pressure is also determined by the Hubble variable

$$p = -\frac{3}{\kappa^2}\Big(\frac{2}{3}\dot{h} + h^2\Big). \tag{4}$$

If the Hubble variable is constant then $w = -1$. If $w < -1$ a matter is "phantom"-like (with negative kinetic energy, see below). In the equation of state $w = w_0 + w_a(1-a) + \mathcal{O}((1-a)^2)$ is normalized so that $a < 1$ corresponds to the past and $a = 1$ at present. If $w_0 + w_a < -1$ but $w_0 < 0$, $w_a < 0$ then at present or in the future the interplay is possible between dominance of a "normal" dark energy with $w > -1$ and a phantom one with $w < -1$!? For this to take place one needs a two field composition—*quintom* (Fig. 1).

3 Cosmology of Scalar Matter

The gravitational action for individual components of scalar field dark energy can be taken as

$$S = \int d^4x\sqrt{-g}\Big(-\frac{1}{2\kappa^2}R \pm \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - V(\phi)\Big), \tag{5}$$

where the signs are "+" for normal matter and "−" for phantom matter.

By variation of the metric in scalar field action one derives the energy density and the pressure,

$$\varepsilon = \pm\frac{1}{2}(\dot{\phi})^2 + V(\phi), \quad p = \pm\frac{1}{2}(\dot{\phi})^2 - V(\phi) \tag{6}$$

for both ones we have normalized the potential $V \geq 0$. Evidently in the equation of state, $w > -1$ or < -1 depending on the kinetic energy sign. Thus in order to fit an experimentally acceptable dynamic equation of state we can combine the two scalar fields in the *quintom* model including a quintessence field with normal kinetic term and a phantom one with negative kinetic energy,

$$S = \int d^4x \sqrt{-g}\Big(-\frac{1}{2\kappa^2}R + \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}\partial_\mu\tilde{\phi}\partial^\mu\tilde{\phi} - V(\phi) - \tilde{V}(\tilde{\phi})\Big). \tag{7}$$

However the phantom matter is troublesome, its energy is not bounded below, its presence breaks various energy conditions and its classical cosmology ends up in the Big Rip.

Are there alternatives which could bring stability of evolution? *PT symmetric pseudoscalar interactions with complex potentials* may help!

Take the pseudoscalar field action with a potential $V(i\tilde{\phi})$ (with real analytical function $V(x)$) instead of a $V(\tilde{\phi})$ and a normal kinetic energy,

$$S = (Vol.)\int dt\, e^{3\rho}\Big(\frac{1}{2}(\dot{\tilde{\phi}})^2 - V(i\tilde{\phi})\Big), \tag{8}$$

for the metric (1). It is PT symmetric for ϕ pseudoscalar under parity reflection $\mathscr{P}\phi_t = -\phi_t$ and Wigner's time reflection as complex conjugation $i \to -i$, i.e. $\mathscr{P}\mathscr{T}i\phi_t = i\phi_{-t}$.

From this action equation of motion for ϕ reads,

$$\ddot{\phi} + 3\rho'\dot{\phi} + iV'(i\phi) = 0 \tag{9}$$

Among various complex solutions there is a particular purely imaginary one $\phi = -i\xi$ so that

$$-\ddot{\xi} - 3\rho'\dot{\xi} + V'(\xi) = 0 \tag{10}$$

that is expected for a phantom field ξ. Its choice is *unique* to provide the real energy and pressure and correspondingly it leads $w < -1$. The PT symmetric model behaves different at a quantum level and have different stability properties compared to the usual phantom field. The perturbations around the classical solutions should be considered along the real axis,

$$\phi = -i\xi_{class} + \delta\phi \tag{11}$$

As a result the effective Hamiltonian becomes positively defined [23, 24]. To separate the fields with PT symmetry from usual phantoms we coin a new name—*PTom*.

4 Model with Quintessence and PT Fields

In order to fit the recent observations of large scale universe we need a composition of two scalar fields: quintessence and PTom ones. Hence let us consider the following model with two scalar fields minimally coupled to the gravity [9]:

$$S = \int d^4x \sqrt{-g}\Big(-\frac{1}{2\kappa^2}R + \frac{1}{2}M_{\phi\phi}\partial_\mu\phi\partial^\mu\phi + \frac{1}{2}M_{\tilde\phi\tilde\phi}\partial_\mu\tilde\phi\partial^\mu\tilde\phi + iM_{\phi\tilde\phi}\partial_\mu\phi\partial^\mu\tilde\phi - Ve^{\lambda\phi} + \tilde V e^{i\tilde\lambda\tilde\phi}\Big), \tag{12}$$

where all parameters are real to preserve the following symmetry,

$$t \mapsto -t, \quad i \mapsto -i, \quad \phi \mapsto \phi, \quad \tilde\phi \mapsto -\tilde\phi. \tag{13}$$

The mixing term in kinetic energy is introduced to guarantee the separability of equations of motion for scalar fields (analytic integrability). For the same purpose we select out exponential potentials. Then this model turns out to be integrable [9] (see below).

The full set of independent variables in gravity is related to the entire metric $g_{\mu\nu}$ which could be decomposed into the pure space-like part g_{ab}; $a, b = 1, 2, 3$ and the remaining variables $g_{00} \equiv N$; $g_{0a} \equiv N_a$. The latter ones can be taken as Lagrange multipliers and therefore create constraints (Arnowitt-Deser-Misner approach). After J.A.Wheeler we name the 6-dimensional space of functions g_{ab} as a *superspace*. It has the signature $(-1, 1, 1, 1, 1, 1)$.

If the space and matter are dominantly homogeneous and isotropic, one can select out the Friedman-Robertson-Walker minisuperspace for the only spatially uniform variable $a(t) \equiv \exp\rho(t)$,

$$ds^2 = N^2(t)\,dt^2 - e^{2\rho(t)}\,d\mathbf{x}^2, \qquad \phi = \phi(t), \quad \tilde\phi = \tilde\phi(t). \tag{14}$$

with $N(t)$ being a *lapse* variable. It provides the time-reparametrization invariance which is a remnant of GR invariance against coordinate diffeomorphisms. The action for such a minisuperspace takes the form

$$S = \int dt\, e^{3\rho}\Big(-\frac{3}{\kappa^2}\frac{\dot\rho^2}{N} + M_{\phi\phi}\frac{\dot\phi^2}{2N} + M_{\tilde\phi\tilde\phi}\frac{\dot{\tilde\phi}^2}{2N} + iM_{\phi\tilde\phi}\frac{\dot\phi\dot{\tilde\phi}}{N} - NVe^{\lambda\phi} + N\tilde V e^{i\tilde\lambda\tilde\phi}\Big). \tag{15}$$

Then the Euler-Lagrange equation obtained by variation of N is a Friedmann equation,

$$h^2 = \frac{\dot\rho^2}{N^2} = \frac{\kappa^2}{3}\left[M_{\phi\phi}\frac{\dot\phi^2}{2N^2} + M_{\tilde\phi\tilde\phi}\frac{\dot{\tilde\phi}^2}{2N^2} + iM_{\phi\tilde\phi}\frac{\dot\phi\dot{\tilde\phi}}{N^2} + Ve^{\lambda\phi} - \tilde V e^{i\tilde\lambda\tilde\phi}\right] \tag{16}$$

Because to be physically meaningful the metrics should be real h^2 should be real and positive. This can be only achieved if ϕ is real and $\tilde\phi = -i\xi$ is purely imaginary. This also guarantees that the Lagrangian and the pressure are real on classical solutions.

It is convenient to search for the classical solutions in the Hamiltonian formulation. The canonical momenta are

$$p_\rho = -\frac{6}{\kappa^2}e^{3\rho}\frac{\dot\rho}{N}, \qquad p_\phi = \frac{e^{3\rho}}{N}\left(M_{\phi\phi}\dot\phi + iM_{\phi\tilde\phi}\dot{\tilde\phi}\right),$$
$$p_{\tilde\phi} = \frac{e^{3\rho}}{N}\left(iM_{\phi\tilde\phi}\dot\phi + M_{\tilde\phi\tilde\phi}\dot{\tilde\phi}\right), \qquad p_N = 0. \tag{17}$$

As always in the gravitational theory, the Hamiltonian becomes a pure constraint (equivalent to (16)) with a Lagrangian multiplier N,

$$H = Ne^{-3\rho}\left[-\frac{\kappa^2}{12}p_\rho^2 + \frac{M_{\tilde\phi\tilde\phi}}{2\mathscr{D}}p_\phi^2 + \frac{M_{\phi\phi}}{2\mathscr{D}}p_{\tilde\phi}^2 - \frac{iM_{\phi\tilde\phi}}{\mathscr{D}}p_\phi p_{\tilde\phi}\right.$$
$$\left. + Ve^{6\rho+\lambda\phi} - \tilde V e^{6\rho+i\tilde\lambda\tilde\phi}\right]. \tag{18}$$

where $\mathscr{D} = M_{\phi\phi}M_{\tilde\phi\tilde\phi} + M^2_{\phi\tilde\phi}$.

To eliminate the dependence of the exponent term on the different degrees one should to perform the generalized canonical transformation:

$$\chi = \lambda\phi + 6\rho, \quad \pi = \frac{1}{\lambda}p_\phi, \quad \tilde\chi = \tilde\lambda\tilde\phi - 6i\rho, \quad \tilde\pi = \frac{1}{\tilde\lambda}p_{\tilde\phi}, \tag{19}$$

$$\omega = p_\rho - \frac{6}{\lambda}p_\phi + \frac{6i}{\tilde\lambda}p_{\tilde\phi}, \tag{20}$$

with π, $\tilde\pi$ and ω being new canonical momenta for χ, $\tilde\chi$ and ρ correspondingly. Then the Hamiltonian takes the form

$$H = Ne^{-3\rho}\left[-\frac{\kappa^2}{12}\omega^2 - \kappa^2\omega\pi + i\kappa^2\omega\tilde\pi + \frac{1}{2}D\pi^2 + \frac{1}{2}\tilde D\tilde\pi^2\right.$$
$$\left. -i\left(\lambda\tilde\lambda\frac{M_{\phi\tilde\phi}}{\mathscr{D}} - 6\kappa^2\right)\pi\tilde\pi + Ve^{\chi} - \tilde V e^{i\tilde\chi}\right]. \tag{21}$$

where we introduced,

$$D = \lambda^2\frac{M_{\tilde\phi\tilde\phi}}{\mathscr{D}} - 6\kappa^2, \quad \tilde D = \tilde\lambda^2\frac{M_{\phi\phi}}{\mathscr{D}} + 6\kappa^2. \tag{22}$$

Note that the new canonical momentum ω is conserved on the constraint surface, i. e.

$$\{\omega, H\} = -3H \approx 0. \tag{23}$$

For arbitrary choice of constants this model is not exactly solvable in the case of several fields. Let us assume a special form of the kinetic term matrix satisfying the condition:

$$\lambda\tilde{\lambda}\frac{M_{\phi\tilde{\phi}}}{\mathscr{D}} = 6\kappa^2, \tag{24}$$

so that the kinetic energy of the fields becomes diagonalized. As will be shown below this permits the separation of variables in the classical as well as in the quantum case.

5 Classical Solutions

Classical solutions can be easily found by solving Hamiltonian equations of motion. Let us choose the gauge

$$N = e^{3\rho}.$$

The equations of motion on the constraint surface $H = 0$ can be written in the form,

$$\begin{aligned}
&\dot{\chi} = \{\chi, H\} \simeq -\kappa^2\omega + D\pi, && \dot{\pi} = \{\pi, H\} \simeq -Ve^{\chi}, \\
&\dot{\tilde{\chi}} = \{\tilde{\chi}, H\} \simeq i\kappa^2\omega + \tilde{D}\tilde{\pi}, && \dot{\tilde{\pi}} = \{\tilde{\pi}, H\} \simeq i\tilde{V}e^{i\tilde{\chi}}, \\
&\dot{\rho} = \{\rho, H\} \simeq -\frac{\kappa^2}{6}\omega - \kappa^2\pi + i\kappa^2\tilde{\pi}, && \dot{\omega} = \{\chi_a, H\} \simeq 0.
\end{aligned} \tag{25}$$

The general solution for this system supplemented with the constraint is:

$$\begin{aligned}
\rho = \rho_0 + \kappa^4\omega t\Big(\frac{1}{\tilde{D}} - \frac{1}{D} - \frac{1}{6\kappa^2}\Big) + \frac{\kappa^2}{D}\ln\cosh^2(Pt - Q) \\
- \frac{\kappa^2}{\tilde{D}}\ln\cosh^2(\tilde{P}t - \tilde{Q}),
\end{aligned} \tag{26}$$

$$e^{\chi} = \frac{2P^2}{DV}\frac{1}{\cosh^2(Pt - Q)}, \qquad e^{i\tilde{\chi}} \equiv e^{\xi} = \frac{2\tilde{P}^2}{\tilde{D}\tilde{V}}\frac{1}{\cosh^2(\tilde{P}t - \tilde{Q})}, \tag{27}$$

$$\pi = -\frac{2P}{D}\tanh(Pt - Q) + \frac{\kappa^2}{D}\omega, \quad i\tilde{\pi} = -\frac{2\tilde{P}}{\tilde{D}}\tanh(\tilde{P}t - \tilde{Q}) + \frac{\kappa^2}{\tilde{D}}\omega, \tag{28}$$

$$P^2 = \frac{\kappa^2\omega^2}{24}(6\kappa^2 + D/2 + CD), \qquad \tilde{P}^2 = \frac{\kappa^2\omega^2}{24}(6\kappa^2 - \tilde{D}/2 + C\tilde{D}), \tag{29}$$

where C, Q and $\tilde{Q}$ are arbitrary constants.

Note that for χ to be purely real and $\tilde{\chi}$ being purely imaginary requires

$$\frac{P^2}{DV} > 0, \quad \frac{\tilde{P}^2}{\tilde{D}\tilde{V}} > 0, \tag{30}$$

and this condition constraints the classically allowed values of C. For $D, \tilde{D}, V > 0$ it yields $P^2 > 0, \tilde{P}^2 > 0$.

At large positive t the metric factor ρ behaves as a linear function. If its coefficient is positive,

$$\rho \sim \text{const} + \alpha_+ t, \quad \alpha_\pm = \pm\kappa^4\Big(\frac{1}{\tilde{D}} - \frac{1}{D} - \frac{1}{6\kappa^2}\Big)\omega + \frac{2\kappa^2}{D}P - \frac{2\kappa^2}{\tilde{D}}\tilde{P} \tag{31}$$

If $\alpha_+ > 0$ this means the unlimited expansion of the universe. However the cosmic time (1),

$$\tau = \int^t dt' N = \int^t dt' e^{3\rho} \sim \text{const} \cdot e^{\alpha_+ t} \tag{32}$$

also tends to infinity. Thus this singularity happens to be unreachable. On the other hand if $\alpha_+ < 0$ the limit of $t \to +\infty$ corresponds to the infinite contraction of the universe at finite cosmic time—the Big Crunch. Similar arguments can be given for the early history of the universe in the model. Then $\alpha_- < 0$ corresponds to the Big Bang singularity while $\alpha_- > 0$ to the contraction for infinite time in the past.

Alternatively we could consider hermitian phantom field,

$$\begin{aligned} S = \int d^4x \sqrt{-g}\Big(&-\frac{1}{2\kappa^2}R + \frac{1}{2}M_{\phi\phi}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}M_{\xi\xi}\partial_\mu\xi\partial^\mu\xi \\ &+ M_{\phi\xi}\partial_\mu\phi\partial^\mu\xi - Ve^{\lambda\phi} - \tilde{V}e^{\tilde{\lambda}\xi}\Big), \end{aligned} \tag{33}$$

which is classically equivalent to the PTom model considered above up to the different sign of the potential to ensure the stability under slow perturbations. Again the condition (24) allows to separate the variables and obtain exact solution. However now the condition (30) yields,

$$\tilde{P}^2 = -\tilde{P}_\Phi^2 < 0 \tag{34}$$

which leads to a qualitatively different behaviour of the solutions [9],

$$\begin{aligned} \rho =& \rho_0 + \kappa^4\omega t\Big(\frac{1}{\tilde{D}} - \frac{1}{D} - \frac{1}{6\kappa^2}\Big) + \frac{\kappa^2}{D}\ln\cosh^2(Pt - Q) \\ &- \frac{\kappa^2}{\tilde{D}}\ln\cos^2(\tilde{P}_\Phi t - \tilde{Q}_\Phi), \end{aligned} \tag{35}$$

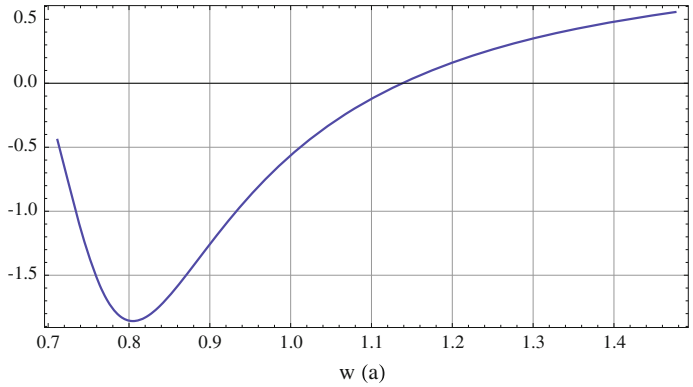

Fig. 2 The equation of state w as a function of a metric factor a for PTom model. The phantom-like dark energy era is *transient*, i.e. holds only during a finite time

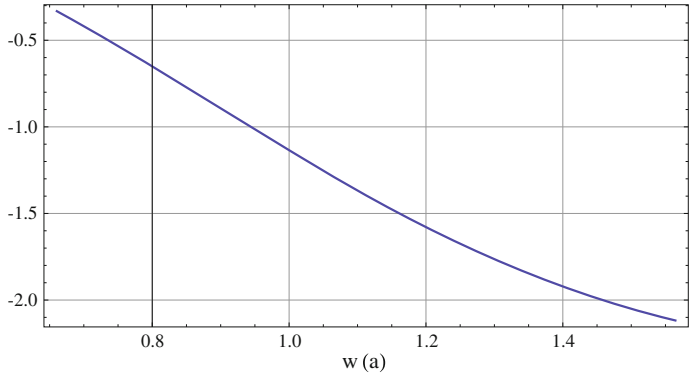

Fig. 3 The equation of state w as a function of a metric factor a for the phantom model. The phantom era continues till it ends in the Big Rip

For phenomenologically appropriate value of $\tilde{D} > 2\kappa^2$ (which means that the characteristic scale of the phantom field is below the Planck scale) the cosmological evolution results in Big Rip. Using (2), (4) we can obtain the equation of state $w = p/\varepsilon$ as a function of $a = \exp \rho$. Typical behaviour is depicted on the figures.

Figures 2 and 3 are normalized tentatively to the PLANCK data reconstruction near $a \leq 1$ [2].

6 Quantum Cosmology: Wheleer-DeWitt Equation

The WdW equation for the minisuperspace under consideration is obtained by canonical quantization for the Hamilton function (18):

$$Ne^{-3\rho}\Big[\hbar^2\frac{\kappa^2}{12}\,\partial_\rho^2-\frac{\hbar^2}{2}\frac{M_{\tilde\phi\tilde\phi}}{\mathscr{D}}\partial_\phi^2+i\hbar^2\frac{M_{\phi\tilde\phi}}{\mathscr{D}}\partial_\phi\partial_{\tilde\phi}$$
$$-\frac{\hbar^2}{2}\frac{M_{\phi\phi}}{\mathscr{D}}\partial_{\tilde\phi}^2+Ve^{6\rho+\lambda\phi}-\tilde V e^{6\rho+i\tilde\lambda\tilde\phi}\Big]\Psi(\rho,\phi,\tilde\phi)=0. \tag{36}$$

The factor $Ne^{-3\rho}$ will not play the role in finding the solutions and thus it will be taken equal one by an appropriate choice of gauge.

Canonical transformation (19)–(20) in the quantum case becomes simply the coordinate transformation and the corresponding transformation of the partial derivatives after which the equation takes the form

$$\Big[\hbar^2\frac{\kappa^2}{12}\,\partial_\rho^2+\hbar^2\kappa^2\partial_\rho\partial_\phi-i\hbar^2\kappa^2\partial_\rho\partial_{\tilde\phi}-\frac{\hbar^2}{2}D\partial_\chi^2-\frac{\hbar^2}{2}\tilde D\partial_{\tilde\chi}^2$$
$$-i\hbar^2\Big(\lambda\tilde\lambda\frac{M_{\phi\tilde\phi}}{\mathscr{D}}-6\kappa^2\Big)\partial_\chi\partial_{\tilde\chi}+Ve^{\chi}-\tilde V e^{i\tilde\chi}\Big]\Psi(\rho,\chi,\chi)=0. \tag{37}$$

where we used the definitions (22).

Because now there is no ρ in the potential, it is convenient to perform the Fourier transform,

$$\Psi(\rho,\chi,\tilde\chi)=\int d\omega\, e^{i\omega\rho/\hbar}\Psi(\omega,\chi,\tilde\chi),$$
$$\Big[-\frac{\kappa^2}{12}\omega^2+i\hbar\kappa^2\omega\partial_\chi+\hbar\kappa^2\omega\partial_{\tilde\chi}-\frac{\hbar^2}{2}D\partial_\chi^2-\frac{\hbar^2}{2}\tilde D\partial_{\tilde\chi}^2$$
$$-i\hbar^2\Big(\lambda\tilde\lambda\frac{M_{\phi\tilde\phi}}{\mathscr{D}}-6\kappa^2\Big)\partial_\chi\partial_{\tilde\chi}+Ve^{\chi}-\tilde V e^{i\tilde\chi}\Big]\Psi(\omega,\chi,\tilde\chi)=0. \tag{38}$$

In the case of the special form of the kinetic term matrix

$$\lambda\tilde\lambda\frac{M_{\phi\tilde\phi}}{\mathscr{D}}=6\kappa^2, \tag{39}$$

the mixed term is canceled and partial solutions can be obtained by separation of variables,

$$\Psi(\omega,\chi,\tilde\chi)=\Psi_\chi(\omega,\chi)\Psi_{\tilde\chi}(\omega,\tilde\chi), \tag{40}$$

6.1 Hermitian Quintessence Sector

Let us first consider the equation for the hermitian field,

$$\Big[-\frac{\kappa^2}{12}\omega^2\Big(\frac12+C\Big)+i\hbar\kappa^2\omega\,\partial_\chi-\hbar^2\frac{D}{2}\,\partial_\chi^2+Ve^{\chi}\Big]\Psi_\chi(\omega,\chi)=0, \tag{41}$$

After the variable change

$$\Psi_\chi = \exp\left[\frac{i}{\hbar}\frac{\kappa^2\omega}{D}\chi\right]f, \qquad z = \frac{2}{\hbar}\sqrt{\frac{2V}{D}}e^{\chi/2} \tag{42}$$

we obtain the modified Bessel equation

$$\begin{aligned} &[z^2\partial_z^2 + z\partial_z + \nu^2 - z^2]f(\omega, z) = 0, \\ &\nu = \frac{4P}{\hbar D}, \qquad P^2 = \frac{\kappa^2\omega^2}{24}(6\kappa^2 + D/2 + CD), \end{aligned} \tag{43}$$

with P expressed similarly to the classical solution (29).

The selection of the solution may be done based on the condition of square integrability by ρ from $-\infty$ to $+\infty$ to ensure the π_ρ operator hermiticity and the self-consistency of the Dirac or BRST/BFV (Becchi–Rouet–Stora–Tyutin/Batalin–Fradkin–Vilkovisky) quantization scheme [29]. Because this condition has to be satisfied for any value of $\{\phi\}$ it yields the decreasing of the solution at large values of χ. Such solution exists only for $P^2 > 0$ in the form,

$$\Psi_\chi(\omega, \chi) = \exp\left[\frac{i}{\hbar}\frac{\kappa^2\omega}{D}\chi\right]K_{i\nu}\left(\frac{2}{\hbar}\sqrt{\frac{2V}{D}}e^{\chi/2}\right), \tag{44}$$

where $K_{i\nu}(z)$ is the modified Bessel function of the second kind (Macdonald function). The solution decreases at $\chi \to +\infty$,

$$\Psi_\chi(\omega, \chi) \sim \frac{\pi^{1/2}\sqrt{\hbar}}{2}\left(\frac{V}{2D}\right)^{1/4} e^{-\chi/4}\exp\left[-\frac{2}{\hbar}\sqrt{\frac{2V}{D}}e^{\chi/2}\right]\exp\left[\frac{i}{\hbar}\frac{\kappa^2\omega}{D}\chi\right]. \tag{45}$$

and oscillates at $\chi \to -\infty$,

$$\begin{aligned} &\Psi_\chi(\omega, \chi) \sim -\sqrt{\frac{\pi}{\nu\sinh\nu\pi}}\exp\left[\frac{i}{\hbar}\frac{\kappa^2\omega}{D}\chi\right]\left[\sin\left(\frac{\nu\chi}{2} - \delta\right) + O(e^\chi)\right], \\ &\delta = \nu\ln\frac{1}{\hbar}\sqrt{\frac{2V}{D}} + \arg[\Gamma(1 + i\nu)]. \end{aligned} \tag{46}$$

Of course to ensure good behaviour at the Big Bang and the existence of the quasiclassical spacetime one should consider wavepackets. However due to the Hamiltonian constraint the question can not be discussed without specifying the functional space of the PT symmetric sector first.

6.2 Pseudohermitian PT Symmetric Sector

Let us now consider the equation corresponding to the part of the solution depending on PTom field,

$$\left[-\frac{\kappa^2}{12}\omega^2\left(\frac{1}{2}-C\right)+\hbar\kappa^2\omega\,\partial_{\tilde{\chi}}-\hbar^2\frac{\tilde{D}}{2}\,\partial^2_{\tilde{\chi}}-\tilde{V}e^{i\tilde{\chi}}\right]\Psi_{\tilde{\chi}}(\omega,\tilde{\chi})=0, \tag{47}$$

To get rid of the linear term we have to perform the following non-unitary transformation,

$$\Psi_{\tilde{\chi}}=\exp\left[\frac{1}{\hbar}\frac{\kappa^2\omega}{\tilde{D}}\tilde{\chi}\right]\tilde{f}(\tilde{\chi}) \tag{48}$$

$$\left(-\partial^2_{\tilde{\chi}}-\frac{2\tilde{V}}{\hbar^2\tilde{D}}e^{i\tilde{\chi}}\right)\tilde{f}(\tilde{\chi})=-\frac{4\tilde{P}^2}{\hbar^2\tilde{D}^2}\tilde{f}(\tilde{\chi}). \tag{49}$$

Choosing new variable,

$$\tilde{z}=2i\sqrt{\frac{2\tilde{V}}{\hbar^2\tilde{D}}}e^{i\tilde{\chi}/2} \tag{50}$$

we get the Bessel equation,

$$\left(\tilde{z}^2\partial^2_{\tilde{z}}+\tilde{z}\partial_{\tilde{z}}+\tilde{z}^2+E\right)f(\tilde{z})=0,\quad E=\frac{16\tilde{P}^2}{\hbar^2\tilde{D}^2} \tag{51}$$

The independent solutions read,

$$\Psi^{\pm}_E=\exp\left[\frac{1}{\hbar}\frac{\kappa^2\omega}{\tilde{D}}\tilde{\chi}\right]J_{\pm i\sqrt{E}}\left(2i\sqrt{\frac{2\tilde{V}}{\hbar^2\tilde{D}}}e^{i\tilde{\chi}/2}\right). \tag{52}$$

We notice that a similar equation was analyzed in [30] but for negative real E and respectively for purely real order of Bessel functions. However the Curtright's choice is in disagreement with linear stability of the model (15).

Using the series representation of the Bessel function [31, 8.402] we can rewrite the solutions as,

$$\Psi^{\pm}_E=\exp\left[\frac{1}{\hbar}\frac{\kappa^2\omega}{\tilde{D}}\tilde{\chi}\mp\frac{\sqrt{E}}{2}\tilde{\chi}\right]\pm\sqrt{E}\Phi_{\pm E}(\tilde{\chi}), \tag{53}$$

where

$$\Phi_{\pm\sqrt{E}}(\tilde{\chi}) = \frac{1}{2^{\pm i\sqrt{E}}} \sum_{n=0}^{+\infty} \frac{1}{n!\Gamma(\pm i\sqrt{E}+n+1)} \left(\frac{2\tilde{V}}{\hbar^2\tilde{D}}\right)^n e^{in\tilde{\chi}}, \tag{54}$$

The sum is convergent everywhere and thus $\Phi_{\pm E}(\tilde{\chi})$ is a periodic function. The only undesirable behaviour comes from the exponential factor. However it becomes constant in the special case $\sqrt{E} = \frac{2}{\hbar}\frac{\kappa^2\omega}{\tilde{D}}$ which fixes $C = \frac{1}{2}$. This constraint is in concordance with the linear stability.

As result we obtain the following solutions of the Wheeler-DeWitt equation with sufficiently regular behaviour on the real axes of χ and $\tilde{\chi}$,

$$\Psi = \int_{-\infty}^{+\infty} d\omega\, A(\omega) e^{i\omega\rho/\hbar} \exp\left[\frac{i}{\hbar}\frac{\kappa^2\omega}{D}\chi\right] K_{i\nu}\left(\frac{2}{\hbar}\sqrt{\frac{2V}{D}}e^{\chi/2}\right)\Phi_{\sqrt{E}}(\tilde{\chi}) \tag{55}$$

$$\nu = \frac{2\kappa\omega}{\hbar D}\sqrt{\kappa^2 + \frac{D}{6}}, \qquad \sqrt{E} = \frac{2}{\hbar}\frac{\kappa^2\omega}{\tilde{D}} \tag{56}$$

The construction of the biorthogonal basis suitable for building physical state space using these solutions as well as the full quasiclassical analysis is postponed for the future analysis.

7 Conclusions

In this work we analyzed the implementation of dark energy in evolutionary universe based on a pseudoscalar field model with complex but PT-symmetric potential (PTom) [23, 24].

- In contrast to the phantom scalar scenario the PTom dark energy is supplied with linear stability even for rapid perturbations. The stability criterion differs from the one for the phantom field stable under slow perturbations and allows to avoid the catastrophic evolution resulting in Big Rip. In that analysis the possible influence of the gravitational perturbations has not been taken into account yet.
- We found that both classical and quantum (restricted to minisuperspace) models with appropriate mixing kinetic terms turn out to be integrable for exponential potentials. In such a case the exact analytical solutions are obtained for classical trajectories and for wave functionals of quantum PT symmetric cosmology. Classical trajectories demonstrate the aforementioned difference in ultimate fate of the universe.
- The requirement of sufficiently regular behaviour of the solutions of PT symmetric Wheeler-DeWitt equations with exponential potentials imposes extra constraint on the spectral parameter space leaving it one-dimensional. This is unexpected

from the classical point of view and may signal a nontrivial quasiclassical limit. Perspectives for developing PT symmetric Quantum Cosmology are dependent on a correct mathematical definition of resolution of identity for dual Riesz spaces generated by these solutions. With the physical state space known it will be possible to construct observables and study the evolution of wavepackets. It represents the program for future research.

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Operator (Quasi-)Similarity, Quasi-Hermitian Operators and All that

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Abstract Motivated by the recent developments of pseudo-Hermitian quantum mechanics, we analyze the structure generated by unbounded metric operators in a Hilbert space. To that effect, we consider the notions of similarity and quasi-similarity between operators and explore to what extent they preserve spectral properties. Then we study quasi-Hermitian operators, bounded or not, that is, operators that are quasi-similar to their adjoint and we discuss their application in pseudo-Hermitian quantum mechanics. Finally, we extend the analysis to operators in a partial inner product space (PIP-space), in particular the scale of Hilbert space s generated by a single unbounded metric operator.

1 Introduction

More than fifty years ago, Dieudonné [14] defined quasi-Hermitian operators as those bounded operators A which satisfy a relation of the form

$$GA = A^*G, \tag{1}$$

where G is a *metric operator*, i.e., a strictly positive self-adjoint operator. The same relation makes sense, however, for unbounded operators A also, under suitable conditions. In any case, the operator G then defines a new metric (hence the name) and a new Hilbert space, with inner product $\langle G\cdot|\cdot\rangle$ (called physical in some applications), in which A is symmetric and may possess a self-adjoint extension. In particular, the

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Dieudonné relation (1) implies that the operator A is similar to its adjoint A^*, in some sense, so that the notion of similarity plays a central rôle in the theory.

In most of the literature, the metric operator G is assumed to be bounded, with bounded inverse. However, the example of the Hamiltonian of the imaginary cubic oscillator, $H = p^2 + ix^3$, shows that bounded metric operators with unbounded inverse do necessarily occur [22]. In that case, the notion of similarity must be replaced by that of *quasi-similarity*. In fact, the notions of similarity and quasi-similarity between operators on Banach spaces have a long history, notably in the context of spectral operators, in the sense of Dunford [15, Sect. XV.6]. A spectral operator of scalar type is an operator that can be written as $A = \int_{\mathbb{C}} \lambda \, \mathrm{d}E(\lambda)$, where $E(\cdot)$ is a bounded (but not necessarily self-adjoint) resolution of the identity.[1] Every such operator is similar to a normal operator [15, Sect. XV.6, Theorem 4]. Spectral operators of scalar type with real spectrum and, *a fortiori*, self-adjoint operators, are quasi-Hermitian. Thus we are led to generalize the notion of similarity of operators, in particular in the unbounded case. We will also need an alternative definition of quasi-Hermitian operators, better adapted to the presence of unbounded metric operators.

On the physical side, the motivation for such an analysis stems from recent developments in the so-called Pseudo-Hermitian quantum mechanics. This is an unconventional approach to quantum mechanics, based on the use of a non-self-adjoint Hamiltonian, that can be transformed into a self-adjoint one by changing the ambient Hilbert space, via a metric operator, as explained above.[2] These Hamiltonians are in general assumed to be $\mathscr{P}\mathscr{T}$-symmetric, that is, invariant under the joint action of space reflection ($\mathscr{P}$) and complex conjugation ($\mathscr{T}$). Typical examples are the $\mathscr{P}\mathscr{T}$-symmetric, but non-self-adjoint, Hamiltonians $H = p^2 + ix^3$ and $H = p^2 - x^4$. Surprisingly, both of them have a purely discrete spectrum, real and positive. In fact, they are quasi-Hermitian. An early analysis of $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians may be found in the review papers of Bender [9] and Mostafazadeh [19]. Since then, a large body of literature has been devoted to this topic. An overview of the recent works, including the various physical applications, is presented in [10, 11]. The recent conference PHHQP15 (Palermo, May 2015) offers a vivid panorama of the present status of the theory. A large number of contributions to the latter may be found in the present volume.

Coming back to the present paper, we note that unbounded metric operators have been introduced in several recent works [6–8, 20] and an effort was made to put the whole machinery on a sound mathematical basis. In particular, we have explored in [2, 3, 5] the properties of unbounded metric operators, in particular, their incidence on similarity and on spectral data. We will quickly survey those papers here, omitting all proofs.

To conclude, let us fix our notations. The framework in a separable Hilbert space $\mathscr{H}$, with inner product $\langle \cdot | \cdot \rangle$, linear in the first entry. Then, for any operator A in $\mathscr{H}$, we denote its domain by $D(A)$ and its range by $R(A)$.

[1] Non-self-adjoint resolutions of the identity have recently be studied by Inoue and Trapani [17].

[2] Self-adjoint operators are usually called *Hermitian* by physicists.

2 Metric Operators

We start with the central object of the study, namely, *metric operators*.

Definition 1 By a metric operator in a Hilbert space $\mathscr{H}$, we mean a strictly positive self-adjoint operator G, that is, $G > 0$ or $\langle G\xi|\xi\rangle \geqslant 0$ for every $\xi \in D(G)$ and $\langle G\xi|\xi\rangle = 0$ if and only if $\xi = 0$.

Of course, G is densely defined and invertible, but need not be bounded; its inverse G^{-1} is also a metric operator, bounded or not. We note that, given a metric operator G, both $G^{\pm 1/2}$ and, more generally, $G^{\alpha}(\alpha \in \mathbb{R})$, are metric operators. As we noticed in the introduction, in most of the literature on Pseudo-Hermitian quantum mechanics, the metric operators are assumed to be bounded with bounded inverse, although there are exceptions. In the sequel, however, we will consider the general case where G and G^{-1} may be both unbounded.

2.1 The General Case

Given a metric operator G, consider the domain $D(G^{1/2})$ and equip it with the following norm

$$\|\xi\|_{R_G}^2 = \left\|(I+G)^{1/2}\xi\right\|^2, \ \xi \in D(G^{1/2}), \tag{2}$$

where I denotes the identity operator. Since this norm is equivalent to the graph norm,

$$\|\xi\|_{\mathrm{gr}}^2 := \|\xi\|^2 + \left\|G^{1/2}\xi\right\|^2, \tag{3}$$

this yields a Hilbert space, denoted $\mathscr{H}(R_G)$, dense in $\mathscr{H}$. Next, we equip that space with the norm $\|\xi\|_G^2 := \left\|G^{1/2}\xi\right\|^2$ and denote by $\mathscr{H}(G)$ the completion of $\mathscr{H}(R_G)$ in that norm and corresponding inner product $\langle\cdot|\cdot\rangle_G := \langle G^{1/2}\cdot|G^{1/2}\cdot\rangle$. Hence, we have $\mathscr{H}(R_G) = \mathscr{H} \cap \mathscr{H}(G)$, with the so-called projective norm [1, Sect. I.2.1], which here is simply the graph norm (3). Then we define $R_G := I + G$, which justifies the notation $\mathscr{H}(R_G)$, by comparison of (2) with the norm $\|\cdot\|_G^2$ of $\mathscr{H}(G)$.

Now we perform the construction described in [1, Sect. 5.5], and largely inspired by interpolation theory [12]. First we notice that the conjugate dual $\mathscr{H}(R_G)^{\times}$ of $\mathscr{H}(R_G)$ is $\mathscr{H}(R_G^{-1})$, the completion of $\mathscr{H}$ with respect to the norm defined by R_G^{-1}, and one gets the triplet

$$\mathscr{H}(R_G) \ \subset \ \mathscr{H} \ \subset \ \mathscr{H}(R_G^{-1}). \tag{4}$$

Proceeding in the same way with the inverse operator G^{-1}, we obtain another Hilbert space, $\mathscr{H}(G^{-1})$, and another triplet

$$\mathscr{H}(R_{G^{-1}}) \ \subset \ \mathscr{H} \ \subset \ \mathscr{H}(R_{G^{-1}}^{-1}). \tag{5}$$

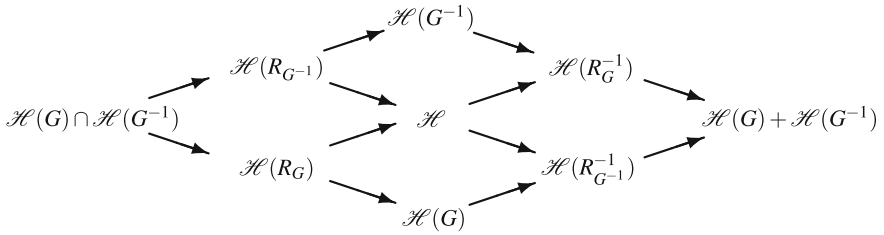

Fig. 1 The lattice of Hilbert spaces generated by a metric operator

Then, taking conjugate duals, it is easy to see that one has

$$\mathscr{H}(R_G)^\times = \mathscr{H}(R_G^{-1}) = \mathscr{H} + \mathscr{H}(G^{-1}), \tag{6}$$

$$\mathscr{H}(R_{G^{-1}})^\times = \mathscr{H}(R_{G^{-1}}^{-1}) = \mathscr{H} + \mathscr{H}(G). \tag{7}$$

In these relations, the r.h.s. is meant to carry the inductive norm (and topology) [1, Sect. I.2.1], so that both sides are in fact unitary equivalent, hence identified.

By the definition of the spaces $\mathscr{H}(R_{G^{\pm 1}})$ and the relations (6)–(7), it is clear that all the seven spaces involved constitute a lattice with respect to the lattice operations

$$\mathscr{H}_1 \wedge \mathscr{H}_2 := \mathscr{H}_1 \cap \mathscr{H}_2, \tag{8}$$

$$\mathscr{H}_1 \vee \mathscr{H}_2 := \mathscr{H}_1 + \mathscr{H}_2. \tag{9}$$

Completing that lattice by the extreme spaces $\mathscr{H}(R_G) \cap \mathscr{H}(R_{G^{-1}}) = \mathscr{H}(G) \cap \mathscr{H}(G^{-1})$ and $\mathscr{H}(R_G^{-1}) + \mathscr{H}(R_{G^{-1}}^{-1}) = \mathscr{H}(G) + \mathscr{H}(G^{-1})$ (these equalities follow from interpolation), we obtain the diagram shown on Fig. 1, which completes the corresponding one from [2]. Here also every embedding, denoted by an arrow, is continuous and has dense range.

Next, on the space $\mathscr{H}(R_G)$, equipped with the norm $\|\cdot\|_G^2$, the operator $G^{1/2}$ is isometric onto $\mathscr{H}$, hence it extends to a unitary operator from $\mathscr{H}(G)$ onto $\mathscr{H}$. Analogously, $G^{-1/2}$ is a unitary operator from $\mathscr{H}(G^{-1})$ onto $\mathscr{H}$. In the same way, the operator $R_G^{1/2}$ is unitary from $\mathscr{H}(R_G)$ onto $\mathscr{H}$, and from $\mathscr{H}$ onto $\mathscr{H}(R_G^{-1})$.[3]

Typical examples would be weighted L^2 spaces in which G and G^{-1} are multiplication operators in $\mathscr{H} = L^2(\mathbb{R}, \mathrm{d}x)$, both unbounded, so that the three middle spaces are mutually noncomparable. For instance, one could take $G = x^2$, so that $R_G = 1 + x^2$, or $G = e^{ax}$, $G^{-1} = e^{-ax}$. The corresponding lattices are given in [5].

An interesting variant of the last example is the LHS of analytic functions described in [1, Sect. 4.6.3], in which the order parameter is the opening angle of a sector, instead of the rate of growth at infinity. This LHS simplifies considerably the formulation of scattering theory, in the form presented by van Winter, as explained in [1, Sect. 7.2]. Let us give some details.

[3]The space $\mathscr{H}(R_G^{-1})$ is (three times) erroneously denoted $\mathscr{H}(R_{G^{-1}})$ in [2, p. 4]; see Corrigendum.

Define $G(a,b)$ $(-\pi < a < b < \pi)$ as the space of all functions $f(z)$, $z = re^{i\varphi}$, which are analytic in the open sector $S_{a,b} := \{z = re^{i\varphi},\ a < \varphi < b\}$, and such that the integral $\int_0^\infty |f(re^{i\varphi})|^2\, dr < \infty$ is uniformly bounded in $\varphi \in (a,b)$. It turns out that the family $\{G(a,b),\ -\frac{\pi}{2} \leqslant a < b \leqslant \frac{\pi}{2}\}$ may be identified, via a Mellin transform, with a part of a LHS of weighted L^2 spaces. First, for $-\frac{\pi}{2} \leqslant a \leqslant \frac{\pi}{2}$, define the Hilbert space

$$L^2(a) := \left\{ f : \int_{-\infty}^{+\infty} e^{ax}\, |f(x)|^2\ \mathrm{d}x < \infty \right\} = L^2(r_a),\ \text{with}\, r_a(t) = e^{-ax}. \qquad (10)$$

Then consider the lattice generated by the family $L^2(a)$, $L^2(0) = L^2$ and $L^2(-a)$, following the construction described previously. The infimum is $L^2(a) \wedge L^2(b) = L^2(a) \cap L^2(b) = L^2(a \wedge b)$ and the supremum $L^2(a) \vee L^2(b) = L^2(a) + L^2(b) = L^2(a \vee b)$, with $r_{a\wedge b}(x) = \min(r_a(x), r_b(x))$ and $r_{a\vee b}(x) = \max(r_a(x), r_b(x))$. As usual, these norms are equivalent to the projective, resp. inductive, norms. For instance, the following two norms are equivalent

$$\|f\|^2_{L^2(r_{a\wedge -a})} = \int_{-\infty}^{+\infty} e^{a|x|} |f(x)|^2\ \mathrm{d}x \asymp \int_{-\infty}^{+\infty} (e^{ax} + e^{-ax}) |f(x)|^2\ \mathrm{d}x.$$

Next, the discrete lattice of nine spaces may be converted into a continuous one by interpolation. This yields $\{L^2(a), -\frac{\pi}{2} \leqslant a \leqslant \frac{\pi}{2}\}$. Thus we obtain a LHS, with extreme spaces $V^\# = L^2\left(-\frac{\pi}{2}\right) \cap L^2\left(\frac{\pi}{2}\right)$, $V = L^2\left(-\frac{\pi}{2}\right) + L^2\left(\frac{\pi}{2}\right)$, which are themselves Hilbert space s. In addition, all spaces are obtained at the first generation, i.e., they are all of the form $L^2(c \wedge d)$ or $L^2(c \vee d)$.

In the case $0 < a < b$, one gets the picture shown in Fig. 2. Duality corresponds to symmetry with respect to the center (i.e., L^2): $a \wedge b \iff -b \vee -a$.

2.2 *Bounded Versus Unbounded Metric Operators*

Now, if G is *bounded,* the triplet (4) collapses, in the sense that all three spaces coincide as vector spaces, with equivalent norms (thus we identify them). Similarly, one gets $\mathscr{H}(R_{G^{-1}}) = \mathscr{H}(G^{-1})$ and $\mathscr{H}(R^{-1}_{G^{-1}}) = \mathscr{H}(G)$. So we are left with the triplet

$$\mathscr{H}(G^{-1}) \ \subset\ \mathscr{H}\ \subset\ \mathscr{H}(G). \qquad (11)$$

Then $G^{1/2}$ is a unitary operator from $\mathscr{H}(G)$ onto $\mathscr{H}$ and from $\mathscr{H}$ onto $\mathscr{H}(G^{-1})$, whereas $G^{-1/2}$ is a unitary operator $\mathscr{H}(G^{-1})$ onto $\mathscr{H}$ and from $\mathscr{H}$ onto $\mathscr{H}(G)$.

If G^{-1} is also bounded, then the spaces $\mathscr{H}(G^{-1})$ and $\mathscr{H}(G)$ coincide with $\mathscr{H}$ as vector spaces and their norms are equivalent to (but different from) the norm of $\mathscr{H}$.

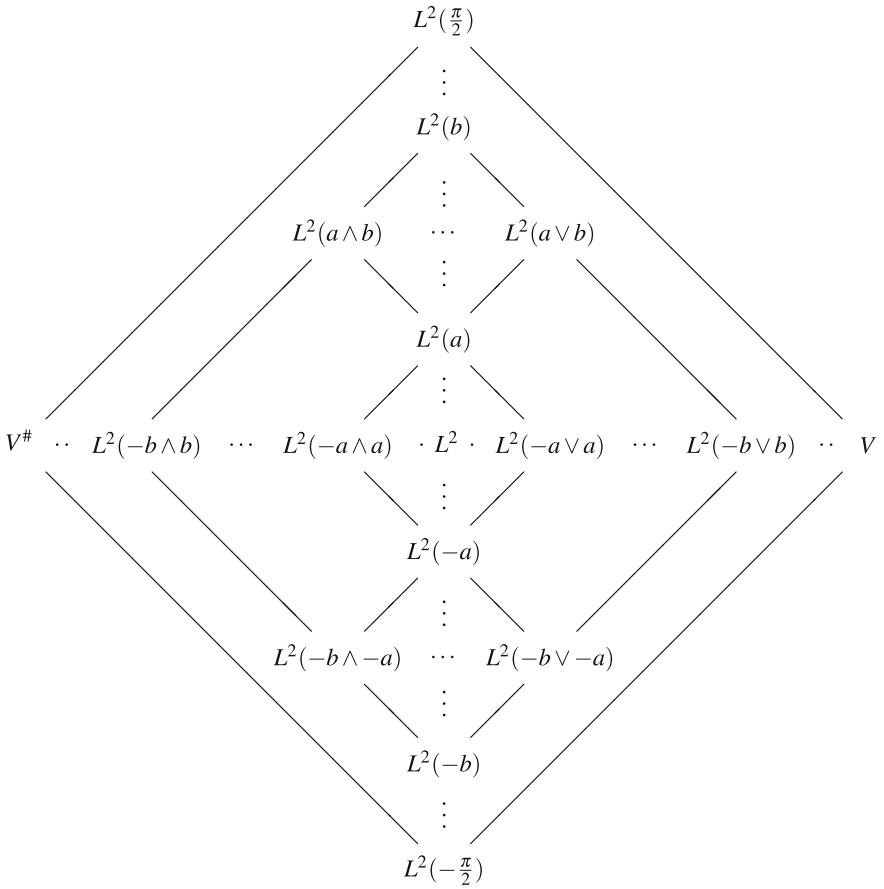

Fig. 2 The van Winter LHS (from [1])

Let now G be *unbounded*, with $G > 1$.[4] Then the norm $\|\cdot\|_G$ is equivalent to the norm $\|\cdot\|_{R_G}$ on $D(G^{1/2})$, so that $\mathscr{H}(G) = \mathscr{H}(R_G)$ as vector spaces and thus also $\mathscr{H}(G^{-1}) = \mathscr{H}(R_G^{-1})$. On the other hand, G^{-1} is bounded. Hence we get the triplet

$$\mathscr{H}(G) \ \subset \ \mathscr{H} \ \subset \ \mathscr{H}(G^{-1}). \tag{12}$$

In the general case, we have $R_G = I + G > 1$ and it is also a metric operator. Thus we have now

$$\mathscr{H}(R_G) \ \subset \ \mathscr{H} \ \subset \ \mathscr{H}(R_G^{-1}). \tag{13}$$

[4]Since G is self-adjoint, the expression $G > 1$ makes sense as a shortcut for $\langle G\xi\,|\xi\rangle > \|\xi\|^2\,, \forall\,\xi \in D(G)$.

In both cases one recognizes that the triplet (12), resp. (12), is the central part of the discrete scale of Hilbert spaces built on the powers of $G^{1/2}$, resp. $R_G^{1/2}$. This means, in the first case, $V_{\mathscr{G}} := \{\mathscr{H}_n, n \in \mathbb{Z}\}$, where $\mathscr{H}_n = D(G^{n/2})$, $n \in \mathbb{N}$, with a norm equivalent to the graph norm, and $\mathscr{H}_{-n} = \mathscr{H}_n^{\times}$:

$$\ldots \subset \mathscr{H}_2 \subset \mathscr{H}_1 \subset \mathscr{H} \subset \mathscr{H}_{-1} \subset \mathscr{H}_{-2} \subset \ldots \tag{14}$$

Thus $\mathscr{H}_1 = \mathscr{H}(G)$ and $\mathscr{H}_{-1} = \mathscr{H}(G^{-1})$. In the second case, one simply replaces $G^{1/2}$ by $R_G^{1/2}$ and performs the same construction.

In fact, one can go one more step. Namely, following [1, Sect. 5.1.2], we can use quadratic interpolation theory [12] and build a continuous scale of Hilbert spaces $\mathscr{H}_\alpha$, $0 \leqslant \alpha \leqslant 1$, between $\mathscr{H}_1$ and $\mathscr{H}$, where $\mathscr{H}_\alpha = D(G^{\alpha/2})$, with the graph norm $\|\xi\|_\alpha^2 = \|\xi\|^2 + \|G^{\alpha/2}\xi\|^2$ or, equivalently, the norm $\left\|(I+G)^{\alpha/2}\xi\right\|^2$. Indeed every G^α, $\alpha \geqslant 0$, is an unbounded metric operator. Next we define $\mathscr{H}_{-\alpha} = \mathscr{H}_\alpha^{\times}$ and iterate the construction to the full continuous scale $V_{\mathscr{G}} := \{\mathscr{H}_\alpha, \alpha \in \mathbb{R}\}$.

3 Similar and Quasi-similar Operators

In this section we collect some basic definitions and facts about similarity of linear operators in Hilbert spaces and discuss a generalization of this notion called quasi-similarity. Throughout most of the section, G will denote a *bounded* metric operator.

3.1 Similarity

In order to state precisely what we mean by similarity, we first define intertwining operators [2].

Definition 2 Let $\mathscr{H}$, $\mathscr{K}$ be Hilbert spaces, $D(A)$ and $D(B)$ dense subspaces of $\mathscr{H}$ and $\mathscr{K}$, respectively, $A : D(A) \to \mathscr{H}$, $B : D(B) \to \mathscr{K}$ two linear operators. A bounded operator $T : \mathscr{H} \to \mathscr{K}$ is called a *bounded intertwining operator* for A and B if

(io_1) $T : D(A) \to D(B)$;
(io_2) $BT\xi = TA\xi$, $\forall\, \xi \in D(A)$.

Remark 1 If T is a bounded intertwining operator for A and B, then $T^* : \mathscr{K} \to \mathscr{H}$ is a bounded intertwining operator for B^* and A^*.

Definition 3 Let A, B be two linear operators in the Hilbert spaces $\mathscr{H}$ and $\mathscr{K}$, respectively. Then, we say that A and B are *similar*, and write $A \sim B$, if there exists a bounded intertwining operator T for A and B with bounded inverse $T^{-1} : \mathscr{K} \to \mathscr{H}$, which is intertwining for B and A.

Actually, this notion of similarity is equivalent to the standard one. Indeed, we will see in Proposition 5 that $A \sim A^*$ with a bounded metric operator G, with bounded inverse, if and only if $A_{sa} := G^{1/2} A G^{-1/2}$ is self-adjoint. The same result is given in [18, Proposition 1].

If $A \sim B$ and $T : \mathscr{H} \to \mathscr{K}$ is unitary, A and B are *unitarily equivalent*, in which case we write $A \overset{u}{\sim} B$. We notice that $\sim$ and $\overset{u}{\sim}$ are equivalence relations. Also, in both cases, one has $T D(A) = D(B)$.

Similarity of A and B is symmetric, preserves both the closedness of the operators and their spectra. But, in general, it does not preserve self-adjointness.

As we will see in Proposition 1 below, similarity preserves also the resolvent set $\rho(\cdot)$ of operators and the parts in which the spectrum is traditionally decomposed: the point spectrum $\sigma_p(\cdot)$, the continuous spectrum $\sigma_c(\cdot)$ and the residual spectrum $\sigma_r(\cdot)$. Note we follow the definition of [15], according to which the three sets $\sigma_p(A), \sigma_c(A), \sigma_r(A)$ are disjoint and $\sigma(A) = \sigma_p(A) \cup \sigma_c(A) \cup \sigma_r(A)$.

We proceed now to show the stability of the different parts of the spectrum under the similarity relation $\sim$, as announced above [2, Propositions 3.7 and 3.9].

Proposition 1 *Let A, B be closed operators such that $A \sim B$ with the bounded intertwining operator T. Then,*

(i) $\rho(A) = \rho(B)$.
(ii) $\sigma_p(A) = \sigma_p(B)$. *Moreover if $\xi \in D(A)$ is an eigenvector of A corresponding to the eigenvalue λ, then $T\xi$ is an eigenvector of B corresponding to the same eigenvalue. Conversely, if $\eta \in D(B)$ is an eigenvector of B corresponding to the eigenvalue λ, then $T^{-1}\eta$ is an eigenvector of A corresponding to the same eigenvalue. Moreover, the multiplicity $m_A(\lambda)$ of λ as eigenvalue of A is the same as its multiplicity $m_B(\lambda)$ as eigenvalue of B.*
(iii) $\sigma_c(A) = \sigma_c(B)$.
(iv) $\sigma_r(A) = \sigma_r(B)$.

Now it has been argued forcefully by Krejčiřík et al. [18] that, in the case of non-self-adjoint operators, the spectrum yields a rather poor information and should be replaced by the pseudospectrum [13, Chap. 9], defined as follows. Given $\varepsilon > 0$, the pseudospectrum of an operator A is the set

$$\sigma_\varepsilon(A) := \sigma(A) \cup \{z \in \mathbb{C} : \left\|(A - zI)^{-1}\right\| > \varepsilon^{-1}\}. \tag{15}$$

The pseudospectrum $\sigma_\varepsilon(A)$ contains the spectrum $\sigma(A)$, but may be much larger, in particular for badly behaved operators. It is called *trivial* if there exists a fixed constant $C > 0$ such that, for all $\varepsilon > 0$,

$$\sigma_\varepsilon(A) \subset \{z \in \mathbb{C} : \mathrm{dist}(z, \sigma(A)) < C\varepsilon\}, \tag{16}$$

that is, $\sigma_\varepsilon(A)$ is contained in a tubular neighborhood of $\sigma(A)$. It is known that the pseudospectra of self-adjoint and normal operators are trivial. More interestingly, if

$A \sim A^*$, that is, A satisfies Dieudonné's relation (1) with G bounded and boundedly invertible, then the pseudospectrum of A is trivial [18].

Another useful characterization of the pseudospectrum is the following. If $\varepsilon > 0$ and $z \notin \sigma(A)$, then $z \in \sigma_\varepsilon(A)$ if and only if there exists $\xi \in D(A)$ such that

$$\|(A - zI)\xi\| < \varepsilon \|\xi\| .$$

It is easily seen that, if $A \sim B$ with the bounded intertwining operator T then, putting $\tau := \|T\| \cdot \|T^{-1}\|$, one has

$$\sigma_{\varepsilon\tau^{-1}}(B) \subseteq \sigma_\varepsilon(A) \subseteq \sigma_{\varepsilon\tau}(B). \tag{17}$$

Another yet characterization of the pseudospectrum of A is in terms of the *numerical range* $\Theta(A) := \{\langle A\xi|\xi\rangle, \xi \in D(A), \|\xi\| = 1\}$. Then, according to [18, Eq. (4)], if $\mathbb{C} \setminus \overline{\Theta(A)}$ is connected and has a non-empty intersection with $\rho(A)$, one has

$$\{z \in \mathbb{C} : \mathrm{dist}(z, \sigma(A) < \varepsilon\} \subseteq \sigma_\varepsilon(A) \subseteq \left\{z \in \mathbb{C} : \mathrm{dist}(z, \overline{\Theta(A)} < \varepsilon\right\}. \tag{18}$$

3.2 Quasi-similarity

The notion of similarity discussed in the previous section is often too strong, thus we seek a weaker one. A natural step is to drop the boundedness of T^{-1}.

Definition 4 We say that A is *quasi-similar* to B, and write $A \dashv B$, if there exists a bounded intertwining operator T for A and B which is invertible, with inverse T^{-1} densely defined (but not necessarily bounded).

Note that, even if T^{-1} is bounded, A and B need not be similar, unless T^{-1} is also an intertwining operator. Indeed, T^{-1} does not necessarily map $D(B)$ into $D(A)$, unless of course if $TD(A) = D(B)$. If $A \dashv B$, with the bounded intertwining operator T, then $B^* \dashv A^*$ with the bounded intertwining operator T^*.

As already remarked in [3], there is a considerable confusion in the literature concerning the notion of quasi-similarity. In particular, this notion has been introduced by Sz.-Nagy and Foiaş [23, Chap. 2, Sect. 3], under the name of *quasi-affinity*.

Next, we ask to what extent quasi-similarity affects the properties of spectra, that is, we look for the analogue of Proposition 1.

Proposition 2 *Let A, B be closed and densely defined, and assume $A \dashv B$ with the bounded intertwining operator T. Then:*

(i) $\sigma_p(A) \subseteq \sigma_p(B)$ *and, for every* $\lambda \in \sigma_p(A)$, *one has* $m_A(\lambda) \leqslant m_B(\lambda)$.
(ii) $\sigma_r(B) \subseteq \sigma_r(A)$.

(iii) *If $T\,D(A) = D(B)$, then $\sigma_p(B) = \sigma_p(A)$.*
(iv) *If T^{-1} is bounded and $T\,D(A)$ is a core for B, then $\sigma_p(B) \subseteq \sigma(A)$.*
(v) *If T^{-1} is everywhere defined and bounded, then $\rho(A) \setminus \sigma_p(B) \subseteq \rho(B)$ and $\rho(B) \setminus \sigma_r(A) \subseteq \rho(A)$.*
(vi) *Assume that T^{-1} is everywhere defined and bounded and $T\,D(A)$ is a core for B; then*

$$\sigma_p(A) \subseteq \sigma_p(B) \subseteq \sigma(B) \subseteq \sigma(A).$$

This situation is important for applications, since it gives some information on $\sigma(B)$ once $\sigma(A)$ is known. For instance, if A has a pure point spectrum, then B is isospectral to A. Also, if A self-adjoint and $A \dashv B$ via an intertwining operator T with bounded inverse T^{-1}, then B has real spectrum.

3.2.1 A Bounded Example

As an example, consider, in the Hilbert space $L^2(\mathbb{R})$, the operator Q of multiplication by x, defined on the dense domain $D(Q) = \left\{ f \in L^2(\mathbb{R}) : \int_{\mathbb{R}} x^2 |f(x)|^2 \,\mathrm{d}x < \infty \right\}$. Given $\varphi \in L^2(\mathbb{R})$, with $\|\varphi\| = 1$, let $P_\varphi := \varphi \otimes \overline{\varphi} = |\varphi\rangle\langle\varphi|$ denote the projection operator onto the one-dimensional subspace generated by φ and A_φ the operator with domain $D(A_\varphi) = D(Q^2)$ defined by

$$A_\varphi f = \langle (I + Q^2) f | \varphi \rangle (I + Q^2)^{-1} \varphi, \quad f \in D(A_\varphi).$$

Then, it is easily seen that $P_\varphi \dashv A_\varphi$ with the bounded intertwining operator $T := (I + Q^2)^{-1}$. Clearly P_φ is everywhere defined and bounded, but the operator A_φ is closable if, and only if, $\varphi \in D(Q^2)$. When this condition is satisfied, A_φ is bounded and everywhere defined. Then the two operators have a pure point spectrum and we have $\sigma(A_\varphi) = \sigma_p(A_\varphi) = \sigma(P_\varphi) = \sigma_p(P_\varphi) = \{0, 1\}$.

In this case we can compute explicitly the pseudospectra. Let $\alpha, \beta \in \mathbb{C}$. Then

$$\|(\alpha I + \beta P_\varphi)\psi\|^2 = |\alpha|^2 \|\psi\|^2 + (2\,\mathrm{Re}(\alpha\overline{\beta}) + |\beta|^2) |\langle \psi | \varphi \rangle|^2.$$

If $\|\psi\| = 1$, the supremum of this expression is $\max\{|\alpha|^2, |\alpha + \beta|^2\}$. Hence

$$\|\alpha I + \beta P_\varphi\| = \max\{|\alpha|, |\alpha + \beta|\}. \tag{19}$$

If $z \in \mathbb{C} \setminus \{0, 1\}$ we have

$$(P_\varphi - zI)^{-1} = \frac{1}{z(1-z)} P_\varphi - \frac{1}{z} I. \tag{20}$$

Thus

$$\|(P_\varphi - zI)^{-1}\| = \max\left\{ \frac{1}{|z|}, \frac{1}{|1-z|} \right\}.$$

Then using the definition (15), we get

$$\sigma_\varepsilon(P_\varphi) = \{z \in \mathbb{C} : |z| < \varepsilon\} \cup \{z \in \mathbb{C} : |z-1| < \varepsilon\}, \tag{21}$$

that is, the pseudospectrum of P_φ is contained in the union of two (possibly overlapping) disks around 0 and 1. Hence it is trivial, as expected. In addition, we easily see that $\Theta(A)$ is the segment [0,1], so that the relation (18) is satisfied.

As for A_φ, rewriting it as $u_\varphi \otimes \overline{v_\varphi}$, where $u_\varphi = (I+Q^2)^{-1}\varphi$, $v_\varphi = (I+Q^2)\varphi$, we see that it is neither self-adjoint, nor normal and $\|A_\varphi\| = \|u_\varphi\|\,\|v_\varphi\|$. Next $\sigma(A_\varphi) = \sigma_p(A_\varphi) = \{0, 1\}$ and one has

$$(A_\varphi - \lambda)^{-1} = -\frac{I}{\lambda} + \frac{A_\varphi}{\lambda(1-\lambda)}$$

(the spectral representation (20) is not available here, since A_φ is not normal!). On the other hand, the numerical range of A_φ is

$$\Theta(A_\varphi) = \{\langle v_\varphi|\xi\rangle\langle\xi|u_\varphi\rangle,\ \|\xi\| = 1\},$$

so that $|\Theta(A_\varphi)| \leqslant \|u_\varphi\|\,\|v_\varphi\| = \|A_\varphi\|$. Therefore, $\sigma_\varepsilon(A_\varphi)$ contains the union of two (possibly overlapping) disks around 0 and 1 and it is contained in an ε-neighborhood of the disk of radius $\|A_\varphi\|$, hence it is trivial too.

3.2.2 An Unbounded Example

As another example, consider the following closed operators in $L^2(\mathbb{R})$

$$\begin{aligned}(Af)(x) &= f'(x) - \frac{2x}{1+x^2} f(x),\\ (Bf)(x) &= f'(x),\end{aligned}$$

defined on $D(A) = D(B) = W^{1,2}(\mathbb{R})$. Then $A \dashv B$ with the intertwining operator $T = (I+Q^2)^{-1}$, bounded with unbounded inverse. An explicit calculation shows that $\sigma(A) = \sigma(B) = \sigma_c(B) = i\,\mathbb{R}$, whereas $\sigma_p(A) = \emptyset$, $\sigma_r(A) = \sigma_p(A^*) = i\,\mathbb{R}$ and $\sigma_c(A) = \emptyset$. Thus, here quasi-similarity does not preserve the different parts of the spectra, although it preserves the spectra as a whole.[5]

Concerning the pseudospectra, take first the operator of derivation B. Taking a Fourier transform, we get for $\widehat{B}$ a multiplication operator $(\widehat{B} - \lambda I)\widehat{f}(p) = (ip - \lambda)\widehat{f}(p)$. Therefore

$$\|(\widehat{B} - \lambda I)^{-1}\| = \max_{p\in\mathbb{R}} |ip - \lambda|^{-1}.$$

[5]This corrects a gap in a result given in [2, 5].

Take $\lambda = \varepsilon + iy$, ε small, $y \in \mathbb{R}$. Then

$$\left\|(\widehat{B} - \lambda I)^{-1}\right\| = \max_{p\in\mathbb{R}} |i(p-y) - \varepsilon|^{-1} = \max_{p\in\mathbb{R}} [\varepsilon^2 + (p-y)^2]^{-1/2} = \varepsilon^{-1}.$$

Thus $\sigma_\varepsilon(B)$ is a strip $\{z \in \mathbb{C} : |\mathrm{Re}\, z| \leqslant \varepsilon\}$, centered on the spectrum $\sigma(B) = i\mathbb{R}$, and it is obviously trivial.

For the operator A, however, we cannot conclude, although we conjecture that it is also a vertical strip around the imaginary axis.

3.2.3 Generalizations

The discussion concerning the projection operator P_φ of Sect. 3.2.1 can be easily generalized.

Let H be self-adjoint or normal, with pure point spectrum $\sigma(H) = \sigma_p(H) = \{x_j,\, j \in \mathbb{N}\}$ and corresponding spectral projections P_j:

$$\sum_j P_j = I, \quad P_j P_k = \delta_{jk} P_j, \quad H = \sum_j x_j P_j.$$

Then, for $\lambda \notin \{x_j,\, j \in \mathbb{N}\} = \sigma(H)$,

$$(H - \lambda I)^{-1}\psi = \sum_j \frac{1}{x_j - \lambda} P_j \psi$$

and

$$\|(H - \lambda I)^{-1}\| = \sup_{j\in\mathbb{N}} \frac{1}{|x_j - \lambda|}.$$

Hence

$$\sigma_\varepsilon(H) = \bigcup_{j\in\mathbb{N}} \{\lambda \in \mathbb{C} :\ |x_j - \lambda| < \varepsilon\}.$$

Thus the quasispectrum of H contains the union of (possibly overlapping) disks around the eigenvalues x_j, $j \in \mathbb{N}$. Hence the quasispectrum of H is trivial, in the sense that, for ε small, $\sigma_\varepsilon(H)$ is an ε-neighborhood of $\sigma(H)$.

This can probably be generalized to a normal or self-adjoint operator with a continuous spectrum.

In general, however, the question to what extent quasi-similarity preserves the pseudospectra of operators is still open.

We can only state the following simple results. Let $A \dashv B$ with the bounded intertwining operator T. Let $\varepsilon > 0$ and $z \in \sigma_\varepsilon(A)$. Then there exists $\xi \in D(A)$ such that

$$\|(A - zI)\xi\| < \varepsilon \|\xi\|.$$

Put $\eta = T\xi$; then,

$$\|(B - zI)\eta\| = \|(B - zI)T\xi\| = \|T(A - zI)\xi\| \leqslant \|T\|\|(A - zI)\xi\| < \varepsilon\|T\|\|\xi\|.$$

Hence

$$\|(B - zI)\eta\| < \varepsilon\|T\|\|T^{-1}\eta\|.$$

Similarly one can show that if $z \in \sigma_\varepsilon(B)$, then there exists $\xi \in D(A)$ such that

$$\|T(A - zI)\xi\| < \varepsilon\|T\xi\| \leqslant \varepsilon\|T\|\|\xi\|.$$

Therefore, if $z \notin \sigma(A)$, it follows that $z \in \sigma_{\varepsilon\|T\|}(T(A - zI))$.

We remark that these considerations imply the inclusions (17), valid when $A \sim B$.

It turns out that the notion of quasi-similarity can be extended, without change, to the case where the intertwining operator is unbounded, provided one adds to Definition 2 the extra condition

(io$_0$) $D(TA) = D(A) \subset D(T)$.

The resulting situation, however, is quite pathological and we will not pursue this topic here.

4 Quasi-Hermitian Operators

Intuitively, a quasi-Hermitian operator A is an operator which is Hermitian when the space is endowed with a new inner product. We will make this precise in the sequel, generalizing the original definition of Dieudonné [14].

Definition 5 A closed operator A, with dense domain $D(A)$, is called *quasi-Hermitian* if there exists a metric operator G, with dense domain $D(G)$ such that $D(A) \subset D(G)$ and

$$\langle A\xi|G\eta\rangle = \langle G\xi|A\eta\rangle, \quad \xi, \eta \in D(A). \tag{22}$$

We say that A is *strictly quasi-Hermitian* if, in addition, $AD(A) \subset D(G)$ or, equivalently, $D(GA) = D(A)$.

In the last case, one has $A^*G\eta = GA\eta$, $\forall\, \eta \in D(A)$. This means that A is quasi-Hermitian in the sense of Dieudonné, that is, it satisfies the relation $A^*G = GA$ on the dense domain $D(A)$. Therefore, A is strictly quasi-Hermitian if, and only if, $A \dashv A^*$.

Take first G bounded and G^{-1} possibly unbounded. According to the analysis of Sect. 2.2, we are facing the triplet (11), namely,

$$\mathscr{H}(G^{-1}) \subset \mathscr{H} \subset \mathscr{H}(G),$$

where $\mathscr{H}(G)$ is a Hilbert space, the completion of $\mathscr{H}$ in the norm $\|\cdot\|_G$. Thus we have now two different Hilbert spaces and the question is how operator properties are transferred from $\mathscr{H}$ to $\mathscr{H}(G)$. Notice that we are recovering here the standard situation of pseudo-Hermitian quantum mechanics [9, 11].

4.1 Bounded Quasi-Hermitian Operators

Let A be a bounded operator in $\mathscr{H}$. If A is quasi-Hermitian, it follows that the metric operator G in (22) is bounded with bounded inverse. Indeed we have

Proposition 3 *Let A be bounded. The following statements are equivalent.*

(i) *A is quasi-Hermitian.*
(ii) *There exists a bounded metric operator G, with bounded inverse, such that GA $(= A^*G)$ is self-adjoint.*
(iii) *A is metrically similar to a self-adjoint operator K, i.e. $A = G^{-1/2}KG^{1/2}$, with K self-adjoint.*

As a consequence of this proposition, bounded quasi-Hermitian operators coincide with bounded spectral operators of scalar type and real spectrum, mentioned in Sect. 1 [16].

4.2 Unbounded Quasi-Hermitian Operators

Let again G be bounded, but now we take A unbounded and quasi-Hermitian, that is, exactly the situation expected for non-self-adjoint Hamiltonians.

First we investigate the self-adjointness of A as an operator in $\mathscr{H}(G)$.

Proposition 4 *Let G be bounded. If A is self-adjoint in $\mathscr{H}(G)$, then GA is symmetric in $\mathscr{H}$ and A is quasi-Hermitian. If G^{-1} is also bounded, then A is self-adjoint in $\mathscr{H}(G)$ if, and only if, GA is self-adjoint in $\mathscr{H}$.*

The real, and difficult, problem is the converse, namely, given the closed operator A, possibly unbounded, to find a metric operator G that makes A quasi-Hermitian and self-adjoint in $\mathscr{H}(G)$. We will not give recipes for answering the question (presumably they have to be found for each case separately), but we will reformulate it in various forms. The first result is rather strong.

Proposition 5 *Let A be closed and densely defined. Then the following statements are equivalent:*

(i) *There exists a bounded metric operator G, with bounded inverse, such that A is self-adjoint in $\mathscr{H}(G)$.*

(ii) *There exists a bounded metric operator G, with bounded inverse, such that $GA = A^*G$, i.e., $A \sim A^*$, with intertwining operator G.*
(iii) *There exists a bounded metric operator G, with bounded inverse, such that $G^{1/2}AG^{-1/2}$ is self-adjoint.*
(iv) *A is a spectral operator of scalar type with real spectrum.*

In particular, the equivalence of conditions (ii) and (iii) reproduces the standard notion of similarity mentioned after Definition 3.

Condition (i) of Proposition 5 suggests the following definition.

Definition 6 Let A be closed and densely defined. We say that A is *quasi-self-adjoint* if there exists a bounded metric operator G, such that A is self-adjoint in $\mathscr{H}(G)$.

In particular, if any of the conditions of Proposition 5 is satisfied, then A is quasi-self-adjoint. Notice that the definition of quasi-self-adjointness does *not* require that G^{-1} be bounded.

Proposition 5 characterizes quasi-self-adjointness in terms of similarity of A and A^*. Instead of requiring that A be similar to A^*, we may ask that they be only quasi-similar. The price to pay is that now G^{-1} is no longer bounded and, therefore, Proposition 5 is no longer true. Instead we have only

Proposition 6 *Let A be closed and densely defined. Consider the statements*

(i) *There exists a bounded metric operator G such that $GD(A) = D(A^*)$, $A^*G\xi = GA\xi$, for every $\xi \in D(A)$, in particular, $A \dashv A^*$, with intertwining operator G.*
(ii) *There exists a bounded metric operator G, such that $G^{1/2}AG^{-1/2}$ is self-adjoint.*
(iii) *There exists a bounded metric operator G such that A is self-adjoint in $\mathscr{H}(G)$, i.e., A is quasi-selfadjoint.*
(iv) *There exists a bounded metric operator G such that $GD(A) = D(G^{-1}A^*)$, $A^*G\xi = GA\xi$, for every $\xi \in D(A)$, in particular, $A \dashv A^*$, with intertwining operator G.*

Then, the following implications hold:

$$(i) \Rightarrow (ii) \Rightarrow (iii) \Rightarrow (iv).$$

If the range $R(A^*)$ of A^* is contained in $D(G^{-1})$, then the four conditions (i)–(iv) are equivalent.

4.3 Pseudo-Hermitian Hamiltonians

Analyzing pseudo-Hermitian Hamiltonians, Mostafazadeh [20] constructs a so-called physical Hilbert space, with help of a very strong assumption. Instead, we will assume that the Hamiltonian H is quasi-Hermitian in the sense of Definition 5

and possesses a (large) set of vectors, $\mathscr{D}_G^\omega(H)$, which are analytic in the norm $\|\cdot\|_G$ and are contained in $D(G)$ [21]. This means that every vector $\phi \in \mathscr{D}_G^\omega(H)$ satisfies the relation

$$\sum_{n=0}^{\infty} \frac{\|H^n\phi\|_G}{n!}\, t^n < \infty, \text{ for some } t \in \mathbb{R},$$

so that

$$\mathscr{D}_G^\omega(H) \subset D(H) \subset D(G) \subset D(G^{1/2}) \subset \mathscr{H}.$$

Then the construction proceeds as follows.

Endow $\mathscr{D}_G^\omega(H)$ with the norm $\|\cdot\|_G$ and take the completion $\mathscr{H}_G$, which is a closed subspace of $\mathscr{H}(G)$. An immediate calculation then yields

$$\langle \phi | H\psi \rangle_G = \langle H\phi | \psi \rangle_G, \ \forall\, \phi, \psi \in \mathscr{D}_G^\omega(H),$$

that is, H is a densely defined symmetric operator in $\mathscr{H}_G$. Since it has a dense set of analytic vectors, it is essentially self-adjoint, by Nelson's theorem [21], hence its closure $\overline{H}$ is a self-adjoint operator in $\mathscr{H}_G$. The pair $(\mathscr{H}_G, \overline{H})$ may then be interpreted as the physical quantum system.

Next $W_{\mathscr{D}} := G^{1/2} \restriction \mathscr{D}_G^\omega(H)$ is isometric from $\mathscr{D}_G^\omega(H)$ into $\mathscr{H}$, hence it extends to an isometry $W = \overline{W_{\mathscr{D}}} : \mathscr{H}_G \to \mathscr{H}$. The range of W is a closed subspace of $\mathscr{H}$, denoted $\mathscr{H}_{\text{phys}}$, and the operator W is unitary from $\mathscr{H}_G$ onto $\mathscr{H}_{\text{phys}}$. Therefore, the operator $h = W\,\overline{H}\,W^{-1}$ is self-adjoint in $\mathscr{H}_{\text{phys}}$. This operator h is interpreted as the genuine Hamiltonian of the system, acting in the physical Hilbert space $\mathscr{H}_{\text{phys}}$.

If $\mathscr{D}_G^\omega(H)$ is dense in $\mathscr{H}$, $W(\mathscr{D}_G^\omega(H))$ is also dense, $\mathscr{H}_G = \mathscr{H}(G)$, $\mathscr{H}_{\text{phys}} = \mathscr{H}$ and $W = G^{1/2}$ is unitary from $\mathscr{H}(G)$ onto $\mathscr{H}$.

Now, the author of [20] assumes that H has a basis of eigenvectors. Since every eigenvector is automatically analytic, the present construction construction generalizes that of [20]. This applies, for instance, to the example given there, namely, the $\mathscr{PT}$-symmetric operator $H = \frac{1}{2}(p - i\alpha)^2 + \frac{1}{2}\omega^2 x^2$ in $\mathscr{H} = L^2(\mathbb{R})$, for any $\alpha \in \mathbb{R}$, which has an orthonormal basis of eigenvectors.

5 Quasi-Hermitian Operators and Lattices of Hilbert Spaces

The construction given in (8), (9) can be generalized to a family of metric operators. Let $\mathscr{O}$ be a family of metric operators, containing I, and assume that

$$\mathscr{D} := \bigcap_{G \in \mathscr{O}} D(G^{1/2})$$

is a dense subspace of $\mathscr{H}$. To each operator $X \in \mathscr{O}$, associate the Hilbert space $\mathscr{H}(X)$ as before. On that family, consider the lattice operations

$$\mathscr{H}(X \wedge Y) := \mathscr{H}(X) \cap \mathscr{H}(Y), \quad \mathscr{H}(X \vee Y) := \mathscr{H}(X) + \mathscr{H}(Y), \tag{23}$$

corresponding to the metric operators

$$X \wedge Y := X \dot{+} Y, \quad X \vee Y := (X^{-1} \dot{+} Y^{-1})^{-1},$$

where $X \dot{+} Y$ stands for the form sum of $X, Y \in \mathscr{O}$ [24].

Define the set $\mathscr{R} = \mathscr{R}(\mathscr{O}) := \{G^{\pm 1/2} : G \in \mathscr{O}\}$ and the corresponding domain $\mathscr{D}_{\mathscr{R}} := \bigcap_{X \in \mathscr{R}} D(X)$. Let now Σ denote the minimal set of self-adjoint operators containing $\mathscr{O}$, stable under inversion and form sums, with the property that $\mathscr{D}_{\mathscr{R}}$ is dense in every H_Z, $Z \in \Sigma$. Then, by [1, Theorem 5.5.6], $\mathscr{O}$ generates a lattice of Hilbert spaces $\mathscr{J} := \mathscr{J}_\Sigma = \{\mathscr{H}(X),\ X \in \Sigma\}$ and a *partial inner product space* (PIP-space) V_Σ with central Hilbert space $\mathscr{H} = \mathscr{H}(I)$ and total space $V = \sum_{G \in \Sigma} \mathscr{H}(G)$. The "smallest" space is $V^\# = \mathscr{D}_{\mathscr{R}}$. The compatibility and the partial inner product read, respectively, as

$$\xi \# \eta \iff \exists\, G \in \Sigma \text{ such that } \xi \in \mathscr{H}(G),\ \eta \in \mathscr{H}(G^{-1}),$$
$$\langle \xi | \eta \rangle_{\mathscr{J}} = \langle G^{1/2} \xi | G^{-1/2} \eta \rangle_{\mathscr{H}}.$$

We shall denote the partial inner product simply as $\langle \xi | \eta \rangle := \langle \xi | \eta \rangle_{\mathscr{J}}$, since it coincides with the inner product of $\mathscr{H}$ whenever $\xi, \eta \in \mathscr{H}$.

We denote by $\mathrm{Op}(V_\Sigma)$ the space of *operators* in V_Σ [1, Chap. 3]. Whenever $A \in \mathrm{Op}(V_\Sigma)$, we denote by $\mathrm{j(A)}$ the set of pairs $\{(X, Y) \in \Sigma \times \Sigma\}$ such that $A : \mathscr{H}(X) \to \mathscr{H}(Y)$, continuously (i.e. bounded). Given $(X, Y) \in \mathrm{j}(A)$, we denote by $A_{YX} : \mathscr{H}(X) \to \mathscr{H}(Y)$ the (X, Y)-representative of A, i.e., the restriction of A to $\mathscr{H}(X)$. Then A is identified with the collection of its representatives:

$$A \simeq \{A_{YX} : (X, Y) \in \mathrm{j}(A)\},$$

which is a (maximal) coherent family of bounded operators : if $\mathscr{H}(W) \subset \mathscr{H}(X)$, $\mathscr{H}(Y) \subset \mathscr{H}(Z)$, then $A_{ZW} = E_{ZY} A_{YX} E_{XW}$, where $E_{YX} : \mathscr{H}(X) \to \mathscr{H}(Y)$ is the representative of the identity operator (embedding) when $\mathscr{H}(X) \subset \mathscr{H}(Y)$. Every operator $A \in \mathrm{Op}(V_\Sigma)$ has an adjoint $A^\times$ defined by

$$\langle A^\times \eta | \xi \rangle = \langle \eta | A \xi \rangle, \text{ for } \xi \in \mathscr{H}(X), \eta \in \mathscr{H}(Y^{-1}).$$

In particular, $(X, X) \in \mathrm{j}(A)$ implies $(X^{-1}, X^{-1}) \in \mathrm{j}(A^\times)$ and $A^{\times\times} = A$, i.e., there are no extensions (this is what 'maximal' means above).

Finally, an operator A is called *symmetric* if $A = A^\times$. Therefore, if A is symmetric, $(X, X) \in \mathrm{j}(A)$ implies $(X^{-1}, X^{-1}) \in \mathrm{j}(A)$. Then, by interpolation, $(I, I) \in \mathrm{j}(A)$, that is, A has a bounded representative $A_{II} : \mathscr{H} \to \mathscr{H}$ [12].

5.1 *Similarity of* PIP*-Space Operators*

Let G be any metric operator. If $(G, G) \in \mathsf{j}(A)$, then $\mathsf{B} = G^{1/2} A_{GG} G^{-1/2}$ is bounded on $\mathscr{H}$ and $A_{GG} \dashv \mathsf{B}$.

Next, let $(G, G) \in \mathsf{j}(A)$, G bounded, with G^{-1} unbounded, so that $\mathscr{H}(G^{-1}) \subset \mathscr{H} \subset \mathscr{H}(G)$. Consider the restriction A of A_{GG} to $\mathscr{H}$ and assume that $D(\mathsf{A}) = \{\xi \in \mathscr{H} : A\xi \in \mathscr{H}\}$ is dense in $\mathscr{H}$, which is not automatic. Then $\mathsf{A} \dashv \mathsf{B}$ (both acting in $\mathscr{H}$). On the other hand, $\mathsf{B}\, G^{1/2}\eta = G^{1/2} A\, \eta,\ \forall\, \eta \in \mathscr{H}(G)$ and $G^{1/2} : \mathscr{H}(G) \to \mathscr{H}$ is a unitary operator. Therefore, A and B are unitarily equivalent (but acting in different Hilbert spaces).

Let now $(G, G) \in \mathsf{j}(A)$, G unbounded, with G^{-1} bounded, so that $\mathscr{H}(G) \subset \mathscr{H} \subset \mathscr{H}(G^{-1})$. Then $A : \mathscr{H}(G) \to \mathscr{H}(G)$ is a densely defined operator in $\mathscr{H}$. Then $A_{GG} \dashv\vdash B$; in addition $A_{GG} \overset{u}{\sim} B$ (in different Hilbert spaces), since $G^{\pm 1/2}$ are unitary between $\mathscr{H}$ and $\mathscr{H}(G)$.

5.2 *The Case of Symmetric* PIP*-Space Operators*

A recurring question in quantum mechanics is to show that a given symmetric (in the usual sense) operator A in a Hilbert space $\mathscr{H}$, typically the Hamiltonian, is self-adjoint. More generally, one may ask whether A is similar in a some sense to a self-adjoint operator. We might start from a quasi-Hermitian operator A on $\mathscr{H}$, e.g. a $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian. If A is a symmetric, densely defined, operator in the Hilbert space $\mathscr{H}$, it makes sense to ask for the existence of self-adjoint *extensions* of A, using, for instance, quadratic forms or von Neumann's theory of self-adjoint extensions.

However, there is another possibility. Namely, given a operator A in a space $\mathscr{K} \supset \mathscr{H}$, symmetric in some sense, it is natural to ask directly whether A has *restrictions* that are self-adjoint in $\mathscr{H}$. The answer is given essentially by the KLMN theorem.[6] This celebrated theorem (which has already a PIP-space flavor in its Hilbert space formulation) can be extended to a PIP-space [1, Theorems 3.3.27 and 3.3.28]. Thus we formulate the question in the context of a PIP-space, such as V_Σ defined above. Actually, there is no other possibility than the KLMN approach, since every operator $A \in \mathrm{Op}(V_\Sigma)$ satisfies the condition $A^{\times\times} = A$, there is no room for extensions.

Thus let $A = A^\times \in \mathrm{Op}(V_\Sigma)$ be a symmetric operator. If $(G, G) \in \mathsf{j}(A)$, we have seen above that A as a bounded restriction A_{II} to $\mathscr{H}$. Clearly the assumption $(G, G) \in \mathsf{j}(A)$ too strong for applications ! Assume instead that $(G^{-1}, G) \in \mathsf{j}(A)$, G bounded with unbounded inverse, so that $\mathscr{H}(G^{-1}) \subset \mathscr{H} \subset \mathscr{H}(G)$. Then one can apply the KLMN theorem, which reads now as

[6] KLMN stands for Kato, Lax, Lions, Milgram, Nelson.

Theorem 1 *Given a symmetric operator $A = A^\times$, assume there is a bounded metric operator G with an unbounded inverse, for which there exists a $\lambda \in \mathbb{R}$ such that $A - \lambda I$ has a boundedly invertible representative $(A - \lambda I)_{GG^{-1}} : \mathscr{H}(G^{-1}) \to \mathscr{H}(G)$. Then $A_{GG^{-1}}$ has a unique restriction to a self-adjoint operator A in the Hilbert space $\mathscr{H}$, with dense domain $D(\mathsf{A}) = \{\xi \in \mathscr{H} : A\xi \in \mathscr{H}\}$. In addition, $\lambda \in \rho(\mathsf{A})$.*

If there is no bounded G such that $(G^{-1}, G) \in \mathsf{j}(A)$, one can use the KLMN theorem in the Hilbert scale $V_{\mathscr{G}}$ built on the powers of $G^{-1/2}$ or $(R_G)^{-1/2}$.

Theorem 2 *Let $V_{\mathscr{G}} = \{\mathscr{H}_n, n \in \mathbb{Z}\}$ be the Hilbert scale built on the powers of the operator $G^{\pm 1/2}$ or $(R_G)^{-1/2}$, depending on the (un)boundedness of $G^{\pm 1}$ and let $A = A^\times$ be a symmetric operator in $V_{\mathscr{G}}$.*

(i) Assume there is a $\lambda \in \mathbb{R}$ such that $A - \lambda I$ has a boundedly invertible representative $(A - \lambda I)_{nm} : \mathscr{H}_m \to \mathscr{H}_n$, with $\mathscr{H}_m \subset \mathscr{H}_n$. Then A_{nm} has a unique restriction to a self-adjoint operator A in the Hilbert space $\mathscr{H}$, with dense domain $D(\mathsf{A}) = \{\xi \in \mathscr{H} : A\xi \in \mathscr{H}\}$. In addition, $\lambda \in \rho(\mathsf{A})$.

(ii) If the natural embedding $\mathscr{H}_m \to \mathscr{H}_n$ is compact, the operator A has a purely point spectrum of finite multiplicity, thus $\sigma(\mathsf{A}) = \sigma_p(\mathsf{A})$, $m_{\mathsf{A}}(\lambda_j) < \infty$ for every $\lambda_j \in \sigma_p(\mathsf{A})$ and $\sigma_c(\mathsf{A}) = \emptyset$.

However, there is no known (quasi-)similarity relation between $A_{GG^{-1}}$ or A and another operator!

6 Conclusion

In this Chapter, we have introduced a natural generalization of similarity between operators, better adapted to the unbounded case, and we have obtained some results on the preservation of spectral properties under this quasi-similarity. The best case is that of a bounded metric operator with unbounded inverse. This is precisely the situation that arises in some models of Pseudo-Hermitian quantum mechanics, with a $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian [22]. Thus it is imperative to clarify the underlying mathematical structure.

We have seen that the consideration of unbounded metric operators leads naturally to the formalism of PIP-spaces, more precisely, a lattice or a scale of Hilbert spaces. This means that PIP-space techniques are available and should be studied systematically in concrete examples. Indeed it turns out that exploiting the connection between metric operators and PIP-spaces does in certain cases improve the quasi-similarity of operators. More precisely, given a symmetric operator $A = A^\times$ in a PIP-space with central Hilbert space $\mathscr{H}$, one can apply the KLMN theorem, which may yield a self-adjoint restriction of A in $\mathscr{H}$. Then additional quasi-similarity relations follow.

Of course, many open problems subsist. In view of the applications, notably in pseudo-Hermitian QM, the most crucial ones concern the behavior of spectral properties under some generalized similarity with an unbounded metric operator. In the same vein, there are few results about the spectral properties of self-adjoint

operators derived in a PIP-space context from a symmetric operator via the KLMN theorem. Then, of course, one should investigate the connection between these two types of problems. In particular, one needs to investigate in more details the spectral properties of symmetric operators in a PIP-space, and in a LHS in the first place. Some preliminary results in that direction may be found in [4]. Another topic that deserves a deeper scrutiny is the notion of pseudospectra and its behavior under (quasi-) similarity.

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Generalized Jaynes-Cummings Model with a Pseudo-Hermitian: A Path Integral Approach

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Abstract We use the coherent state path integral and a angular model for the spin to solve the generalized Jaynes-Cummings model with a pseudo-hermitian Hamiltonian and nonlinear Kerr cavity. The propagators are given explicitly as perturbation series. These are summed up exactly. The energy spectrum and the bi-orthonormal basis of states are deduced.

1 Introduction

In recent years the study of some non-hermitian Hamiltonian with real spectrum have given rise to a growing interest in the literature. Bender and Boettcher were the first who have suggested replacing the condition of self-adjointness by the weaker condition of PT symmetry, leads sometimes to real eigenvalues of the non-Hermitian Hamiltonian [1–3].

However pairs of complex conjugate eigenvalues appear when the PT (parity-time) symmetry is broken spontaneously. This is also illustrated nicely with the help of a nonhermitian but PT invariant potential with quasi-exactly solvable eigenvalues [4]. By using an additional C (conjugation operator) symmetry [5], an inner product whose associated norm is positive definite could be constructed. As a result the Hamiltonian and its eigenstates can be extended to complex domain so that the associated eigenvalues are real and underlying dynamics is unitary.

In an another approach Mostafazadeh [6–8] has shown that the reality of spectrum of nonhermitian Hamiltonian is due to so called pseudo-hermiticity properties of the Hamiltonian.

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A Hamiltonian is called η pseudo-hermitian if it satisfies the relation

$$A^{\dagger} = \eta A \eta^{-1}, \tag{1}$$

where η is a linear hermitian operator.

Furthermore this operator gives an equivalent Hermitian theory by means of a similarity transformation. However if quantum mechanics is formulated in terms of functional (path) integrals, the metric operator makes only an implicit appearance and Green functions are calculated as functional integrals in the normal way. This approach was mainly initiated in [9].

Recent investigations of the non-hermitian hamiltonian for a modulated Jaynes-Cummings model with PT symmetry have been made by Bagarello et al. [10], the authors show that, for an appropriate choice of the modulation parameters, the state amplitudes in a generic n-excitation subspace obey the same equations of motion that can be obtained from a static non-Hermitian Jaynes-Cummings Hamiltonian with PT symmetry, that is with an imaginary coupling constant, also they generalize the well-known diagonalization of the Jaynes-Cummings Hamiltonian to the non-Hermitian case in terms of pseudo-bosons and pseudo-fermions. Saaidi et al. [11] showed that the interaction of an electromagnetic field of circular polarization with an atom can create a non-Hermitian Hamiltonian (see Eq. (24) of [11]), and Mandal [12], find that the energy eigenvalues for this system are real even though the interaction is not PT (parity-time) symmetry. We note that this problem [12] has been recently studied using spin coherent state path integral [13, 14].

In this paper, using the coherent state path integral and angular representation for the spin, we solve the generalized Jaynes-Cummings model with pseudo hermitian Hamiltonian and nonlinear Kerr cavity, governed by the Hamiltonian [15].

$$H = H_0 + H_1, \tag{2}$$

with

$$H_0 = \left[\omega_c + \frac{1}{2}\left(\beta_1 + \beta_2\right)\right] a^{\dagger} a + \chi a^{\dagger 2} a^2 \tag{3}$$

and

$$H_1 = \frac{1}{2}\left[\omega_a + \left(\beta_1 - \beta_2\right) a^{\dagger} a\right] \sigma_z + \lambda \left[a^{\dagger m} a^l \sigma_+ - a^{\dagger l} a^m \sigma_-\right]. \tag{4}$$

Here λ is the field-atom coupling constant, ω_c is the field frequency, ω_a is the transition frequency between the excited and ground states of the atom, β_1 et β_2 are parameters describing the intensity-dependents Stark effect, of two-levels that are due to the virtual transition between the two levels, σ_+, σ_-, σ_z are the usual Pauli matrices, with $\sigma_{\pm} = \frac{1}{2}\left(\sigma_x \pm i\sigma_y\right)$, χ is non-linear dispersive part of the third-order

of the Kerr effect, and $a^\dagger$, a are the creation and annihilation operators of the cavity field respectively, and defined as

$$a^\dagger = \frac{p + i\omega m x}{\sqrt{2m\omega\hbar}}, \qquad a = \frac{p - i\omega m x}{\sqrt{2m\omega\hbar}} \tag{5}$$

with

$$a\,|n\rangle = \sqrt{n}\,|n-1\rangle\,, \quad a^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{6}$$

where the notation $|n\rangle$ for number eigenvectors for the oscillator has been adopted.

Note that this Hamiltonian is not hermitian as,

$$H^\dagger \neq H \tag{7}$$

as $\sigma_\pm^\dagger = \sigma_\mp^\dagger$. Under parity transformation i.e. $[x \to -x;\ p \to -p]$, σ do not change sign as it is an axial vector but as it clear from the (5) that both the creation and annihilation operators change sign [12].

$$P\sigma P^{-1} = \sigma, \quad PaP^{-1} = -a, \quad Pa^\dagger P^{-1} = -a \tag{8}$$

Note the interaction term of the Hamiltonian in (4) changes sign under parity operation .

The time reversal operator for the system of spin half particles is $T = -i\sigma_y K$ where K is complex conjugation operator. We note the changes of following quantities under time reversal transformation as [12],

$$T\sigma T^{-1} = -\sigma, \ T\sigma_\pm T^{-1} = -\sigma_\mp \qquad TaT^{-1} = -a, \quad Ta^\dagger T^{-1} = -a \tag{9}$$

From (8) and (9) we can see that the Hamiltonian in (2) is not PT symmetric,

$$PTH\,(PT)^{-1} \neq H \tag{10}$$

However this Hamiltonian is σ_z-pseudo-hermitian

$$\sigma_z H \sigma_z^{-1} = H^\dagger \tag{11}$$

where we have used the relations $\sigma_z\sigma_\pm\sigma_z = -\sigma_\pm$.

In case of η pseudo-hermitian Hamiltonian the choice of the operator η is not unique [6, 7]. Therefore we look for whether our Hamiltonian is pseudo-hermitian with respect to any other operator. Indeed it is also pseudo-hermitian with respect to parity operator if l+m is odd as,

$$PHP^{-1} = H^\dagger \tag{12}$$

Finally we found a symmetry of our Hamiltonian. It is invariant under the symmetry generated by the combined operator, $P\sigma_z$ i.e.

$$\left[H, P\sigma_z\right] = 0. \tag{13}$$

Our motivation for considering this problem via the path integral formalism is the following. Firstly the propagator for the spin-field interaction is written by construction in the standard form $\sum_{\text{path}} \exp\left(iS\left(\text{path}\right)/\hbar\right)$, where S is the action that describes the system. The discrete variable related to spin is then inserted as a continuous path using coherent states. Within this approach the formulation that uses the concept of trajectory is more suitable for a discussion of the semiclassical case, which is based on the determination of the classical path [16, 17]. Secondly, the biorthonormal eigenvectors with the corresponding eigenvalues arise naturally in this formulation, and one can deduce the symmetry $P\sigma_z$ of the system considered, since the metric operator makes only an implicit appearance and Green functions are calculated as functional integrals in the normal way contrary to algebraic methods [12] one need to know in advance the symmetry of the system to solve it.

Our paper is organized as follows. In the next section we give some notation and the spin coherent state path integral for spin $\frac{1}{2}$ system for our further computations. In Sect. 3, after setting up a path integral formalism for the propagator, we perform the direct calculations over the angular variables. Accordingly, the integration over the bosonic variables is easy to carry out and the result is given as a perturbation series. These are summed up exactly and the explicit result of the propagator is directly computed and the bi-orthonormal basis of states is then deduced. Finally, in Sect. 4, we present our conclusions.

2 The Solutions via Path-Integral Formulation

There are several ways to represent the spin in the path integral formalism [18, 19] We use the simplest way [16], which consists in:

-replacing σ by unit vector $\mathbf{n}$ directed according to (θ, φ) (Fig. 1)

-associating a coherent state $|\Omega\rangle$

$$|\Omega\rangle = |\theta, \varphi\rangle = e^{-i\varphi S_z} e^{-i\theta S_y} |\uparrow\rangle . \tag{14}$$

obtained from two rotations of the angles θ and φ around z and y axes over the state $|\uparrow\rangle$, and whose scalar product and projector are respectively:

$$\langle\Omega|\,\Omega'\rangle = \cos\frac{\theta}{2}\cos\frac{\theta'}{2}e^{\frac{i}{2}(\varphi-\varphi')} + \sin\frac{\theta}{2}\sin\frac{\theta'}{2}e^{-\frac{i}{2}(\varphi-\varphi')}, \tag{15}$$

$$\frac{1}{2\pi}\int d\varphi d\cos(\theta)\,|\Omega\rangle\,\langle\Omega| = \mathbf{I}. \tag{16}$$

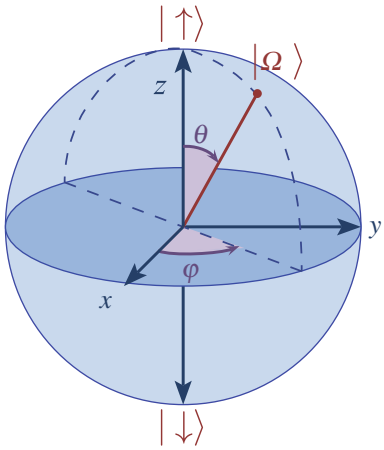

Fig. 1 Angles θ and φ of the unit vector corresponding to state $|\Omega\rangle$

As for the coherent states $|Z\rangle$ relative to bosons, the properties are known. These are:

-the eigenstate of the annihilation operator a ($\left[a, a^{\dagger}\right] = 1$)

$$a\,|Z\rangle = Z\,|Z\rangle\,, \tag{17}$$

-they can also be created from a vacuum state $|0\rangle$ by applying a unitary operator called displacement operator

$$|Z\rangle = e^{Za^{\dagger} - Z^{*}a}\,|0\rangle\,. \tag{18}$$

The scalar product and the projector operator are respectively in this case

$$\langle Z|\,Z'\rangle = \exp\left(Z^{*}Z' - \frac{1}{2}\left(|Z|^{2} + \left|Z'\right|^{2}\right)\right), \tag{19}$$

$$\int \frac{d^{2}Z}{\pi}\,|Z\rangle\,\langle Z| = 1. \tag{20}$$

Now we move to the description of the system via path integral.

For this we consider the quantum state $|Z, \theta, \varphi\rangle$ where Z and the polar angles (θ, φ) are the field and spin related variables.

The transition amplitude from the initial state $|Z_i, \theta_i, \varphi_i\rangle$ at $t_i = 0$ to the final state $\left|Z_f, \theta_f, \varphi_f\right\rangle$ at $t_f = T$ is defined with the matrix elements of the evolution operator:

$$K\,(f, i; T) = \langle Z_f, \theta_f, \varphi_f \mid \mathbf{T}_D \exp(-i \int_0^T H dt) \mid Z_i, \theta_i, \varphi_i\rangle, \tag{21}$$

where $\mathbf{T}_D$ is the Dyson chronological operator. Thus the propagator take the following form:

$$K(f,i;T) = \lim_{N\longrightarrow\infty} \int \prod_{n=1}^{N} \frac{d^2 Z_n}{\pi} \prod_{n=1}^{N+1} \langle Z_n | e^{-i\varepsilon H_0} | Z_{n-1} \rangle \times$$
$$\lim_{N\longrightarrow\infty} \int \prod_{n=1}^{N} \frac{d\cos(\theta_n) d\varphi_n}{2\pi} \prod_{n=1}^{N+1} \left[\langle \Omega_n \mid \Omega_{n-1} \rangle - i\varepsilon \langle \Omega_n | H_1 | \Omega_{n-1} \rangle \right], \quad (22)$$

where

$$Z_{N+1} = Z_f, \quad \Omega_{N+1} = \Omega_f \quad and \quad Z_0 = Z_i, \quad \Omega_0 = \Omega_i. \quad (23)$$

Then the propagator related to our problem (22) takes the form of a Feynman path integral:

$$K = \int \mathscr{D}(\text{path}) \exp(i\,\text{Action}), \quad (24)$$

which means in our case

$$K(f,i;T) = \lim_{N\longrightarrow\infty} \int \prod_{n=1}^{N} \frac{d^2 Z_n}{\pi} \int \prod_{n=1}^{N} \frac{d\cos(\theta_n) d\varphi_n}{2\pi}$$
$$\times \exp\left\{ \sum_{n=1}^{N+1} \left[-Z_n^* \Delta Z_n - i\varepsilon \left(\omega_c + \frac{1}{2}(\beta_1 + \beta_2) \right) Z_n^* Z_{n-1} - i\varepsilon \chi Z_n^{*2} Z_{n-1}^2 \right.\right.$$
$$\left.\left. - \frac{|Z_n|^2 + |Z_{n-1}|^2}{2} + \log < \Omega_n | \Omega_{n-1} \rangle - i\varepsilon \frac{\langle \Omega_n | H_1 | \Omega_{n-1} \rangle}{< \Omega_n | \Omega_{n-1} \rangle} \right] \right\}. \quad (25)$$

After having obtained the conventional form, it remains to integrate it, in order to extract the interesting physical properties. We proceed thus to the calculation of $K(f,i;T)$.

3 The Propagator Calculation

It is well-known that the time-continuous coherent-state path-integral approach breaks down for the spin path integral. Specifically when the Hamiltonian is quadratic in the generator of the algebra used to construct the coherent states, the path integral fails to reproduce the correct results obtained through an operator approach [20]. Detailed analysis of the origin of these difficulties makes it clear that the only way to avoid them is by working with the proper discrete-time formalism [21].

We note that (25) is written like the following discrete-time form

$$K\,(f,i;T)=\lim_{N\longrightarrow\infty}\int\prod_{n=1}^{N}\frac{d^2Z_n}{\pi}\prod_{n=1}^{N+1}\langle Z_n|\,e^{-i\varepsilon H_0}\,|Z_{n-1}\rangle\lim_{N\longrightarrow\infty}\int\prod_{n=1}^{N}\frac{d\cos(\theta_n)d\varphi_n}{2\pi}$$
$$\prod_{n=1}^{N+1}\left(\cos\tfrac{\theta_n}{2}e^{+\frac{i}{2}\varphi_n},\ \sin\tfrac{\theta_n}{2}e^{-\frac{i}{2}\varphi_n}\right)R(Z_n,t_n)\begin{pmatrix}\cos\frac{\theta_{n-1}}{2}e^{-\frac{i}{2}\varphi_{n-1}}\\ \sin\frac{\theta_{n-1}}{2}e^{+\frac{i}{2}\varphi_{n-1}}\end{pmatrix},\qquad(26)$$

where the unitary matrix (to first order in ε) $R(Z_n,t_n)$ is given by

$$R(Z_n,t_n)=\left[e^{-i\varepsilon\frac{1}{2}(\omega_a+(\beta_1-\beta_2)Z_n^*Z_n)\sigma_z}+i\varepsilon K(Z_n,t_n)\right],\qquad(27)$$

where

$$K(Z_n,t_n)=\begin{pmatrix}0 & +\lambda Z_n^{*m}Z_n^l\\ -\lambda Z_n^{*l}Z_n^m & 0\end{pmatrix}.\qquad(28)$$

Let us integrate over all angular variables θ_n and φ_n, then (26) becomes

$$K\,(f,i;T)=\lim_{N\longrightarrow\infty}\int\prod_{n=1}^{N}\frac{d^2Z_n}{\pi}\prod_{n=1}^{N+1}\langle Z_n|\,e^{-i\varepsilon H_0}\,|Z_{n-1}\rangle$$
$$\times\left(\cos\tfrac{\theta_f}{2}e^{\frac{i}{2}\varphi_f},\ \sin\tfrac{\theta_f}{2}e^{-\frac{i}{2}\varphi_f}\right)R(Z,T)\begin{pmatrix}\cos\frac{\theta_i}{2}e^{-\frac{i}{2}\varphi_i}\\ \sin\frac{\theta_i}{2}e^{\frac{i}{2}\varphi_i}\end{pmatrix}.\qquad(29)$$

With

$$R(Z,T)=\prod_{\leftarrow n=1}^{N}\left[(-1)^n\,R(Z_n,t_n)\right]=\begin{pmatrix}\mathscr{R}_{11}(Z,T) & \mathscr{R}_{12}(Z,T)\\ \mathscr{R}_{21}(Z,T) & \mathscr{R}_{22}(Z,T)\end{pmatrix}\qquad(30)$$

The arrow under the product symbol indicates the time ordering operation, and $\mathscr{R}_{ij}(Z,T)$ are the matrix elements of $R(Z,T)$.

We develop the product (of matrix 2×2) which appear in the expression (29) we can see that (30) takes the following form [13].

$$R(Z,T)=\lim_{N\longrightarrow\infty}\prod_{n=1}^{N}\left[(-1)^n\,R(Z_n,t_n)\right]$$
$$=(-1)^N\left[e^{-i\int_0^T ds\omega\sigma_z}+i\int_0^T ds_1e^{-i\int_{s_1}^T ds\omega\sigma_z}K(s_1)e^{-i\int_0^{s_1}ds\omega\sigma_z}\right.$$

$$+(i)^2\int_0^T ds_1\int_0^{s_1} ds_2 e^{-i\int_{s_1}^{T} ds\omega\sigma_z} K(s_1) e^{-i\int_{s_2}^{s_1} ds\omega\sigma_z} K(s_2) e^{-i\int_{0}^{s_2} ds\omega\sigma_z} +$$

$$\cdots + i^{N+1}\int_0^T ds_1\int_0^{s_1} ds_2\cdots\int_0^{s_N} ds_{N+1} e^{-i\int_{s_1}^{T} ds\omega\sigma_z} K(s_1) e^{-i\int_{s_2}^{s_1} ds\omega\sigma_z}$$

$$\times K(s_2)\cdots K(s_N) e^{-i\int_{s_{N+1}}^{s_N} ds\omega\sigma_z} K(s_{N+1})+\cdots\Bigg] \tag{31}$$

We have put:

$$\omega = \frac{1}{2}\left(\omega_a + (\beta_1-\beta_2) Z^* Z\right). \tag{32}$$

These matrix elements are respectively the following:

$$\mathscr{R}_{11}(Z,T) = \mathscr{R}^*_{22}(Z,T) = e^{-i\int_0^T ds\omega} + \sum_{n=1}^{\infty}\Bigg[(-i\lambda)^{2n}\int_0^T ds_1\int_0^{s_1} ds_2\cdots\int_0^{s_{2n-1}} ds_{2n}$$

$$\times e^{-i\int_{s_1}^{T} ds\omega} Z_1^{*m} Z_1^l e^{+i\int_{s_2}^{s_1} ds\omega}\cdots Z_{2n}^m Z_{2n}^{*l} e^{-i\int_0^{s_{2n}} ds\omega}\Bigg] \tag{33}$$

$$\mathscr{R}_{12}(Z,T) = -\mathscr{R}^*_{21}(Z,T) = -i\lambda\int_0^T ds_1 e^{-\frac{i}{2}\int_{s_1}^{T}\omega dt} Z^{*m} Z^l \mathscr{R}^*_{11}(Z,s_1) \tag{34}$$

which can be rearranged to expressed (29) in the form of a sum of four terms:

$$K(f,i;T) = \left(\cos\tfrac{\theta_f}{2} e^{\frac{i}{2}\varphi_f}\ \sin\tfrac{\theta_f}{2} e^{-\frac{i}{2}\varphi_f}\right)\begin{pmatrix} K_{11} & K_{12}\\ K_{21} & K_{22}\end{pmatrix}\begin{pmatrix}\cos\frac{\theta_i}{2} e^{-\frac{i}{2}\varphi_i}\\ \sin\frac{\theta_i}{2} e^{\frac{i}{2}\varphi_i}\end{pmatrix} \tag{35}$$

The first term of (35) for example will be written as:

$$K_{11}(f,i;T) = \cos\frac{\theta_f}{2}\cos\frac{\theta_i}{2} e^{\frac{i}{2}(\varphi_f-\varphi_i)}\Big\{K_0^+(Z_f,Z_1;T-s_1)$$

$$+\sum_{n=1}^{\infty}\Bigg[(-i\lambda)^{2n}\int_0^T ds_1\int_0^{s_1} ds_2\cdots\int_0^{s_{2n-1}} ds_{2n}$$

$$\times\int\frac{d^2Z_1}{\pi}\cdots\int\frac{d^2Z_{2n}}{\pi} K_0^+(Z_f,Z_1;T-s_1) Z_1^{*m} Z_1^l$$

$$\times K_0^-(Z_1,Z_2;s_1-s_2) Z_2^m Z_2^{*l}\cdots Z_{2n}^m Z_{2n}^{*l} K_0^+(Z_{2n},Z_i;s_{2n})\Bigg]\Big\}. \tag{36}$$

It has been expressed in function of new core

$$K_0^{\pm}\left(Z'', Z'; s''-s'\right) = \int \mathscr{D}Z^* \mathscr{D}Z \exp\left\{ i \int_{s'}^{s''} dt \left[\frac{i}{2}\left(Z^*\cdot Z - Z\cdot Z^*\right) - \chi Z^{*2} Z^2 \right.\right.$$
$$\left.\left. - \left(\omega_c + \frac{1}{2}\left(\beta_1+\beta_2\right) \pm \frac{1}{2}\left(\beta_1-\beta_2\right)\right) Z^* Z \pm \frac{1}{2}\omega_a \right] \right\}. \tag{37}$$

which we propose to calculate it.

It is natural first to trait the term $Z^{2*}Z^2$ appeared in (37) as a perturbation. For this we develop the exponential perturbation term.

$$\begin{aligned} & K_0^{\pm}\left(Z'', Z'; s''-s'\right) \\ &= \left\{ K_{00}^{\pm}\left(Z'', Z'; s''-s'\right) + \sum_{n=1}^{\infty} \left[(-i\chi)^n \int_0^T ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n \right.\right. \\ & \times \int \frac{d^2 Z_1}{\pi} \cdots \int \frac{d^2 Z_n}{\pi} K_{00}^{+}\left(Z'', Z_1; T-s_1\right) Z_1^{*2} Z_1^2 \\ & \left.\left. \times\ K_{00}^{\pm}\left(Z_1, Z_2; s_1-s_2\right) Z_2^{*2} Z_2^2 \times \cdots \times Z_n^{*2} Z_n^2 K_{00}^{\pm}\left(Z_n, Z'; s_n\right) \right] \right\}, \end{aligned} \tag{38}$$

with

$$K_{00}^{\pm}\left(Z'', Z'; s''-s'\right) = \sum_{k=1}^{\infty} \frac{\left(Z''^* Z'\right)^k}{k!} \exp\left(-\frac{\left|Z''\right|^2 + \left|Z'\right|^2}{2} \right)$$
$$\times \exp\left(-i \left[k \left[\omega_c + \frac{1}{2}\left(\beta_1+\beta_2\right) \pm \frac{1}{2}\left(\beta_1-\beta_2\right) \right] \pm \frac{1}{2}\omega_a \right] \left(s''-s'\right) \right). \tag{39}$$

We integrate over all variables Z_n in (38) using the formula

$$\int \frac{dZ^* dZ}{\pi} Z^{*m} Z^n e^{-Z^* Z} = \delta_{nm} \sqrt{m!}\sqrt{n!}. \tag{40}$$

It comes then

$$K_0^{\pm}\left(Z'', Z'; s''-s'\right) = K_{00}^{\pm}\left(Z'', Z'; s''-s'\right) e^{-i\chi(k+2)(k+1)\left(s''-s'\right)}. \tag{41}$$

We substitute (39) in (41) we get

$$K_0^{\pm}\left(Z'', Z'; s''-s'\right) =$$

$$= \sum_{k=0}^{\infty} \frac{\left(Z''^{*} Z'\right)^{k}}{k!} \exp\left(-\frac{\left|Z''\right|^{2} + \left|Z'\right|^{2}}{2}\right) \exp\left(-i\chi\,(k+2)\,(k+1)\,(s''-s')\right)$$
$$\exp -i\left[k\left[\omega_c + \frac{1}{2}(\beta_1+\beta_2) \pm \frac{1}{2}(\beta_1-\beta_2)\right] \pm \frac{1}{2}\omega_a\right](s''-s') \tag{42}$$

Then (36) becomes:

$$K_{11}(f,i;T) = \cos\frac{\theta_f}{2}\cos\frac{\theta_i}{2} e^{\frac{i}{2}(\varphi_f-\varphi_i)} \exp\left(-\frac{\left|Z_f\right|^{2} + \left|Z_i\right|^{2}}{2}\right) \sum_{k=0}^{\infty} \left\{ \frac{Z_f^{*k} Z_i^{k}}{k!} \right.$$
$$\times \exp\left(-i\left[\chi\left(k^2+3k+2\right) + k\left[\omega_c+\beta_1\right] + \frac{1}{2}\omega_a\right]T\right)$$
$$\left. \times \left[1 + \sum_{n=1}^{\infty}\left[-\varpi_{ml}^{2}\right]^{n} \int_0^T ds_1 e^{i\Delta_1 s_1} \cdots \int_0^{s_{2n-1}} e^{-i\Delta_1 s_{2n}} ds_n\right]\right\} \tag{43}$$

with

$$\varpi_{ml}^{2} = \lambda^{2} \frac{[(k+l)!]^{2}}{k!\,(k+l-m)!}. \tag{44}$$

and

$$\Delta_1 = \omega_a + k\,(\beta_1-\beta_2) + (m-l)\,[\omega_c+\beta_2] + \chi\,(2k+3)\,(m-l) - \chi\,(m-l)^{2} \tag{45}$$

This last expression (43) can be written in the more convenient form. In effect we put first

$$F(0,T) = \sum_{n=1}^{\infty}\left[\left(-\varpi^{2}\right)^{n} \int_0^T ds_1 e^{i\Delta_1 s_1} \int_0^{s_1} ds_2 e^{-i\Delta_1 s_2} \cdots \int_0^{s_{2n-1}} ds_{2n} e^{-i\Delta_1 s_{2n}}\right] \tag{46}$$

and we pass at its Laplace's transformation and applied it the convolution theorem

$$\widetilde{F}(0,p) = \int_0^{\infty} dT e^{-pT} F(0,T) = \frac{1}{p}\sum_{n=1}^{\infty}\left[\frac{-\varpi_{ml}^{22}}{p(p-i\Delta_1)}\right]^{n}. \tag{47}$$

The result is again series which is here simply equal at:

$$\widetilde{F}(p) = \frac{p-i\Delta_1}{p(p-i\Delta_1) - \varpi_{ml}^{2}} - \frac{1}{p}. \tag{48}$$

According to [11] we find that under the condition of reality

$$\left(\frac{\Delta_1}{2}\right)^2 - \varpi_{ml}^2 \geq 0 \tag{49}$$

Equation (43) take the following form

$$K_{11}(f,i;T) = \cos\frac{\theta_f}{2}\cos\frac{\theta_i}{2}e^{\frac{i}{2}(\varphi_f-\varphi_i)}\exp\left(-\frac{|Z_f|^2+|Z_i|^2}{2}\right)$$
$$\times\sum_{k=0}^{\infty}\frac{\left(Z_f^*Z_i\right)^k}{k!}\left(\cos\Omega_1 T - i\frac{\Delta_1}{2\Omega_1}\sin\Omega_1 T\right)e^{-i\eta_1 T}. \tag{50}$$

where

$$\eta_1 = \chi\left(k^2+3k+2\right)+k\left[\omega_c+\beta_1\right]+\frac{k}{2}\left(\beta_1-\beta_2\right)+\frac{1}{2}(m-l)\left[\omega_c+\beta_2\right]$$
$$+\frac{1}{2}\chi(2k+3)(m-l)-\frac{1}{2}\chi(m-l)^2, \tag{51}$$

and

$$\Omega_1 = \sqrt{\frac{\Delta_1^2}{4}-\varpi_{ml}^2}. \tag{52}$$

Note that $F(0,T)$ is written in the form e^{-iET} with E being real, hence these eigenvalues are real provided $\left(\frac{\Delta_1}{2}\right)^2 - \varpi_{ml}^2 \geq 0$

The calculation of all other matrix elements in (35) is achieved by following the same procedure outlined above. Hence we obtain:

$$K(f,i;T) = \exp\left(-\frac{|Z_f|^2+|Z_i|^2}{2}\right)\sum_{k=0}^{\infty}\left\{\frac{\left(Z_f^*Z_i\right)^k}{k!}\right.$$
$$\times\left[\cos\frac{\theta_f}{2}\cos\frac{\theta_i}{2}e^{\frac{i}{2}(\varphi_f-\varphi_i)}\left(\cos\Omega_1 T - i\frac{\Delta_1}{2\Omega_1}\sin\Omega_1 T\right)e^{-i\eta_1 T}\right.$$
$$+\sin\frac{\theta_f}{2}\sin\frac{\theta_i}{2}e^{-\frac{i}{2}(\varphi_f-\varphi_i)}\left(\cos\Omega_2 T + i\frac{\Delta_2}{2\Omega_2}\sin\Omega_2 T\right)e^{-i\eta_2 T}$$
$$-i\lambda\cos\frac{\theta_f}{2}\sin\frac{\theta_i}{2}e^{\frac{i}{2}(\varphi_f+\varphi_i)}Z_f^*\frac{\sin\Omega_1 T}{\Omega_1}e^{-i\eta_1 T}$$
$$\left.\left.+i\lambda\sin\frac{\theta_f}{2}\cos\frac{\theta_i}{2}e^{-\frac{i}{2}(\varphi_f+\varphi_i)}Z_i\frac{\sin\Omega_1 T}{\Omega_1}e^{-i\eta_1 T}\right]\right\}, \tag{53}$$

where

$$\eta_2 = \chi(k^2+3k+2) + k\left[\omega_c+\beta_2\right] - \frac{k}{2}\left[\beta_1-\beta_2\right] - \frac{1}{2}(m-l)(\omega_c+\beta_1) - \frac{1}{2}(m_1-l_1)(\omega_c+\beta_1) - \frac{1}{2}\chi(2k+3)(m-l) - \frac{1}{2}\chi(m-l)^2, \tag{54}$$

$$\Delta_2 = -\omega_a - k\left[\beta_1-\beta_2\right] - (m-l)(\omega_c+\beta_1) - \chi(2k+3)(m-l) - \chi(m-l)^2, \tag{55}$$

and

$$\Omega_2 = \sqrt{\frac{\Delta_2^2}{4} - \varpi_{lm}^2}. \tag{56}$$

The θ, φ components is allowed to vary only in the limited domains $[0, 2\pi]$, $[0, 4\pi]$ respectively. This fact enables us to submit the physical system to periodic boundary conditions along this direction. To treat this part, we follow the standard method and add to the angles θ and φ a period $2\pi n$ and $4\pi n$ to give a description of this periodicity.

The propagator (53) relative to our particular case is finally.

$$K(f,i;T) = \sum_{n=-\infty}^{\infty} K\left(Z_f, \theta_f + 2n\pi, \varphi_f + 4n\pi; Z_i, \Omega_i; T\right) = K(f,i;T) \tag{57}$$

Our problem is then resolved.

We can calculate the energy spectrum and the corresponding bi-orthonormal basis functions.

4 The Bi-Orthonormal Basis and Eigenstate of the Pseudo-Hermitian Hamiltonian

Let us now eliminate the coherent states by computing the transition amplitudes between the proper states of the spin. We take as an example the matrix element:

$$K_{\uparrow\uparrow}(z_f, z_i; T) = \langle\uparrow \left| K(z_f, z_i; T) \right| \uparrow\rangle. \tag{58}$$

Using the completeness relations this amplitude becomes:

$$K_{\uparrow\uparrow}(z_f, z_i; T) = \frac{1}{2\pi}\int d\cos(\theta_f) d\varphi_f \frac{1}{2\pi}\int d\cos(\theta_i) d\varphi_i \times \times \langle\uparrow \left|\Omega_f\right\rangle K\left(z_f, \Omega_f, z_i, \Omega_i; T\right) \langle\Omega_i \left|\uparrow\right\rangle, \tag{59}$$

where

$$\langle\uparrow\left|\Omega_f\right\rangle = \cos\frac{\theta_f}{2}e^{-\frac{i}{2}\varphi_f}, \qquad and \qquad \langle\Omega_i|\uparrow\rangle = \cos\frac{\theta_i}{2}e^{+\frac{i}{2}\varphi_i}. \tag{60}$$

Then integrating over polar angles we obtain the propagator [16]:

$$K_{\uparrow\uparrow}\left(Z_f, Z_i; T\right) = e^{-\frac{|z_f|^2+|z_i|^2}{2}}\sum_{k=0}^{\infty}\frac{\left(Z_f^* Z_i\right)^k}{k!}\left(\cos\Omega_1 T - i\frac{\Delta_1}{2\Omega_1}\sin\Omega_1 T\right)e^{-i\eta_1 T}. \tag{61}$$

The other matrix elements of propagator are obtained in an analogous way.

In order to extract the wavefunctions as well as the energy spectrum it is more convenient to use the basis $|l\rangle$, where l is the occupancy number related to $|Z\rangle$ through:

$$|Z\rangle = \exp\left(-\frac{|Z|^2}{2}\right)\sum_{l=0}^{\infty}\frac{Z^l}{\sqrt{l!}}|l\rangle\,. \tag{62}$$

Then the evolution operator is:

$$e^{-iHT} = \begin{pmatrix}\Lambda_{\uparrow\uparrow} & \Lambda_{\uparrow\downarrow}\\ \Lambda_{\downarrow\uparrow} & \Lambda_{\downarrow\downarrow}\end{pmatrix}, \tag{63}$$

which is related to $K\left(Z_f; Z_i; T\right)$ through:

$$e^{-iHT} = \int\frac{d^2 Z_f}{\pi}\frac{d^2 Z_i}{\pi}\left|Z_f\right\rangle K\left(Z_f; Z_i; T\right)\langle Z_i|\,. \tag{64}$$

Performing the integrations yields the matrix elements of the evolution operator [13, 14]:

$$\Lambda_{\uparrow\uparrow} = \sum_{k=0}^{\infty}e^{-i\eta_1 T}\left(\cos\Omega_1 T - i\frac{\Delta_1}{2\Omega_1}\sin\Omega_1 T\right)|k\rangle\langle k|\,, \tag{65}$$

$$\Lambda_{\downarrow\uparrow} = -i\lambda\sum_{k=0}^{\infty}\sqrt{k+1}e^{-i\eta_1 T}\frac{\sin\Omega_1 T}{\Omega_1}|k+l-m\rangle\langle k|\,, \tag{66}$$

$$\Lambda_{\uparrow\downarrow} = +i\lambda\sum_{k=0}^{\infty}\sqrt{k+1}e^{-i\eta_1 T}\frac{\sin\Omega_1 T}{\Omega_1}|k\rangle\langle k+l-m|\,, \tag{67}$$

$$\Lambda_{\downarrow\downarrow} = \sum_{k=0}^{\infty}e^{-i\eta_1 T}\left(\cos\Omega_1 T + i\frac{\Delta_1}{2\Omega_1}\sin\Omega_1 T\right)|k+l-m\rangle\langle k+l-m|\,. \tag{68}$$

The bi-orthonormal basis of states can be deduced by comparing with the spectral decomposition:

$$U = e^{-iHT} = \sum_{k=0}^{\infty} \left(e^{-iTE_+^k} \left|\psi_1^k\right\rangle \left\langle\Gamma_1^k\right| + e^{-iTE_-^k} \left|\psi_2^k\right\rangle \left\langle\Gamma_2^k\right| \right), \tag{69}$$

the bi-orthonormal basis of states can be deduced. They become equal to

$$\left|\psi_1^k\right\rangle = \frac{1}{\Omega_1} \begin{pmatrix} -\Omega_1 - \frac{\Delta_1}{2} \\ -\varpi_{ml} \end{pmatrix}. \quad \left|\Gamma_1^k\right\rangle = \begin{pmatrix} +\frac{1}{2} \\ -\frac{1}{2}\frac{\Delta_1}{2\varpi_{ml}} + \frac{\Omega_1}{2\varpi_{ml}} \end{pmatrix}, \tag{70}$$

$$\left|\psi_2^k\right\rangle = \frac{1}{\Omega_1} \begin{pmatrix} \Omega_1 - \frac{\Delta_1}{2} \\ -\varpi_{ml} \end{pmatrix}. \quad \left|\Gamma_2^k\right\rangle = \begin{pmatrix} -\frac{1}{2} \\ -\frac{1}{2}\frac{\Delta_1}{2\varpi_{ml}} - \frac{\Omega_1}{2\varpi_{ml}} \end{pmatrix}, \tag{71}$$

$$E_k^{\pm} = \eta_1 \pm \sqrt{\frac{\Delta_1^2}{4} - \varpi_{lm}^2}. \tag{72}$$

And the metric is given by definition

$$\left|\Gamma_1^k\right\rangle = \eta \left|\psi_1^k\right\rangle, \ \left|\Gamma_2^k\right\rangle = \eta \left|\psi_2^k\right\rangle, \qquad \text{hence} \qquad \eta = P\sigma_z. \tag{73}$$

We observe that these eigenstates are also eigenstates of the operator $P\sigma_z$ as:

$$P\sigma_z \left|\psi_{1,2}^k\right\rangle = (-1)^k \left|\psi_{1,2}^k\right\rangle. \tag{74}$$

Thus we have real eigenvalues when the symmetry $\left(\left[H, P\sigma_z\right] = 0\right)$ is not broken [12].

In the case where the influence of Stark shift and the nonlinear Kerr cavity are absent it is clear that the calculus is simplify to those obtained by [12, 13]. which are confirms our calculations. The same physical features can thus be obtained and discussed again as has been done by [12]. But the advantage of this alternative formulation is that the biorthonormal eigenvectors with the corresponding eigenvalues arise naturally in this formulation, and one can deduce the symmetry $P\sigma_z$ of the system considered and also this formulation can generalized it to other systems.

5 Conclusion

Using the path-integral formalism and the coherent-states approach we explicitly calculated the metric of the pseudo-Hermitian Hamiltonian and its bi-orthonormal basis of states and the corresponding eigenvalues. We computed the propagator related to our system in a series form which, for this case, is summed up exactly. and we have shown that under some conditions the energy eigenvalues for this system are

real. Note that this conditions arise naturally in this formalism. Finally note that by this approach we also can treat the non-hermitian hamiltonian for a modulated Jaynes-Cummings model with PT symmetry.

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Exceptional Points in a Non-Hermitian Extension of the Jaynes-Cummings Hamiltonian

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Abstract We consider a generalization of the non-Hermitian $\mathcal{PT}$ symmetric Jaynes-Cummings Hamiltonian, recently introduced for studying optical phenomena with time-dependent physical parameters, that includes environment-induced decay. In particular, we investigate the interaction of a two-level fermionic system (such as a two-level atom) with a single bosonic field mode in a cavity. The states of the two-level system are allowed to decay because of the interaction with the environment, and this is included phenomenologically in our non-Hermitian Hamiltonian by introducing complex energies for the fermion system. We focus our attention on the occurrence of exceptional points in the spectrum of the Hamiltonian, clarifying its mathematical and physical meaning.

1 Introduction

Quantum systems whose time evolution can be described by effective non-Hermitian Hamiltonians have been considered since a long time, for example in the framework of irreversible statistical mechanics or for describing decaying unstable systems

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[1]. Originally introduced to describe phenomenologically these important physical systems, non-Hermitian Hamiltonians have been initially used overlooking the well-known contradictions related to their compatibility with the basic principles of quantum mechanics [2].

In recent years, it has been considered in the literature the possibility to describe realistic physical systems using non-Hermitian Hamiltonians whose eigenvalues are real [3–6]. This is mathematically meaningful because requiring Hermiticity is a sufficient but not necessary condition to have a real spectrum and a unitary time evolution. In fact, recently, it has been shown that non-Hermitian Hamiltonians with $\mathcal{PT}$ (Parity-Time) symmetry can have a real eigenvalue spectrum [4, 7, 8]. The same happens for non-Hermitian but pseudo-symmetric Hamiltonians [9], where the $\mathcal{PT}$ symmetry is replaced by a more abstract condition. This new approach has produced several important results in the theory of quantum open systems, quantum optics, balanced gain-loss systems, for example, both from theoretical and experimental point of view (see for example [10] and references therein).

A key point of this topic is to understand what happens when a $\mathcal{PT}$ symmetry breaking occurs in a Hamiltonian describing a physical system. As recently investigated (see for example [11]), this may for example happen when one or more physical parameters in the Hamiltonian assume specific values in the complex plane. In more general terms, this aspect is linked to a wider problem addressed in non-Hermitian operator theory, that is the theory of exceptional points (EPs), term introduced in the literature by Kato [12]. Many physical problems are described by Hamiltonians $H(\lambda)$ which manifest dependence on a parameter λ linked to quantities accessible in the experimental setting. Generally, the spectrum $E_n(\lambda)$ and eigenfunctions $|\psi_n(\lambda)\rangle$ of $H(\lambda)$ are analytic functions of λ. It can occur that, for specific complex values of λ, two or more energy levels are equal and the corresponding eigenstates coalesce into a single state. It should be emphasized that, in the case of non-Hermitian Hamiltonians, this condition is very different from that of degeneracy common in quantum mechanics. In the presence of EPs, in fact, the coalescence of eigenstates causes the collapse of the subspace dimension to one. Because of this circumstance, the eigenstate no longer forms a complete basis and this has very intriguing consequences. For example, $\mathcal{PT}$ symmetry is broken [13]. Moreover, EPs may play a very important role in several physical systems, for example in a photonic crystal slab where their presence has been shown to be connected with peaks of reflectivity [10].

In this paper, we shall consider a non-Hermitian generalization of the well-known Jaynes-Cummings (JC) Hamiltonian and investigate the occurrence of EPs in its spectrum. The Jaynes-Cummings model describes a two-level atom interacting with a mode of the quantized electromagnetic field in a cavity [14]; it has been extensively investigated in the literature, in particular in quantum optics. Very recently, we have generalized this model to the non-Hermitian but PT-symmetric case, in order to simulate a time-dependent modulation of the frequency of the two-level-atom or of the cavity mode in the presence of gain-loss [15]. We have also expressed the effective non-Hermitian Jaynes-Cummings Hamiltonian, having an imaginary coupling constant, in terms of pseudo-bosons and pseudo-fermions [16, 17], discussing

also relevant mathematical and physical aspects of this extension of the Hamiltonian [15].

In this paper we focus our analysis on the occurrence of EPs in the spectrum of this extended Jaynes-Cummings Hamiltonian when the decay of the atomic states is allowed due to the interaction with the environment, highlighting the main effects they have on the behavior of the system. In order to make more general our analysis, we have modified the part of the Hamiltonian relative to the two-level system taking as a basis the analysis done in [18], where the authors study nonadiabatic couplings in decaying systems, showing that EPs can influence time-asymmetric quantum-state-exchange mechanism.

The role played by the Jaynes-Cummings model has been crucial to the development of quantum optics and cavity electrodynamics, from both theoretical and experimental points of view [19]. Thus, our extension of the model can shed further light on the dynamics of open optical systems, usually described in terms of non-Hermitian Hamiltonians. Our analysis to elucidate the structure of the exceptional points of the spectrum of the deformed Jaynes-Cummings non-Hermitian Hamiltonian, can be relevant to understand the role of these points in the dynamics of physical systems, such as optical systems, that can be realized in the laboratory. Also, our analysis widens the scenario of applications of the pseudo-bosons and pseudo-fermions formalism.

This paper is organized as follows. In Sect. 2 we introduce our generalized Jaynes-Cummings model allowing the decay of the atomic states; in Sect. 3 we calculate exactly the spectrum and the eigenstates of H; in Sect. 4, we discuss the formation of exceptional points in the extended Jaynes-Cummings model; Sect. 5 is dedicated to the discussions of our results and to our conclusive remarks.

2 The Non-Hermitian Jaynes-Cummings Hamiltonian

The non-Hermitian extension of the Jaynes-Cummings Hamiltonian we are considering, written in terms of pseudo-bosons and pseudo-fermions, is

$$H = H_{GMM} + \hbar\omega Dd + \epsilon dC + \epsilon^* Dc. \tag{1}$$

where ω is the frequency of the boson field (a single cavity mode, for example), ϵ is the boson-fermion coupling constant; c, C and d, D are respectively the pseudo-bosons and pseudo-fermions satisfying the following commutation and anticommutation rules [16, 17]

$$\begin{aligned} [d \otimes \mathbb{1}_f, D \otimes \mathbb{1}_f] &= \mathbb{1}_b \otimes \mathbb{1}_f = \mathbb{1}, \\ \{\mathbb{1}_b \otimes c, \mathbb{1}_b \otimes C\} &= \mathbb{1}, \end{aligned} \tag{2}$$

while all the other commutators are zero. Our operators act on the Hilbert space $\mathcal{H} := \mathcal{H}_b \otimes \mathcal{H}_f$, where $\mathcal{H}_f = \mathbb{C}^2$ (fermionic sector) and $\mathcal{H}_b$ is infinite dimensional (bosonic sector); ϵ indicates the coupling constant. The term H_{GMM} in (1) (GMM stands for Gilary, Mailybaev and Moiseyev), originally introduced in [18] and studied later in [20], has the following form:

$$H_{GMM} = \begin{pmatrix} \epsilon_1 - i\Gamma_1 & \nu_0 \\ \nu_0 & \epsilon_2 - i\Gamma_2 \end{pmatrix}, \tag{3}$$

where Γ_1 and Γ_2 are positive quantities, ϵ_1 and ϵ_2 are real quantities, and ν_0 is complex-valued. This term is an extension of the usual atomic term of the Jaynes-Cummings Hamiltonian and includes possibility of decay of the two atomic states to other states, for example due to the coupling with an environment with a continuous energy spectrum [1]. The quantities Γ_1 and Γ_2 can be related to such phenomenological decay rates.

As shown in [20], H_{GMM} admits a (double) pseudo-fermions representation, and it can be written as $H_{GMM} = \hbar\omega_0 N_f + \rho\,\mathbb{1}$ where $N_f = Cc$ and

$$c = \begin{pmatrix} \alpha_{11} & \alpha_{12} \\ -\alpha_{11}^2/\alpha_{12} & -\alpha_{11} \end{pmatrix}, \quad C = \begin{pmatrix} \beta_{11} & \beta_{12} \\ -\beta_{11}^2/\beta_{12} & -\beta_{11} \end{pmatrix}, \tag{4}$$

$$\begin{cases} \hbar\omega_0^{\pm}\gamma_{\pm} = \nu_0, \\ \alpha_{\pm} = \frac{1}{2\nu_0}\left(-\Delta\epsilon + i\Delta\Gamma \mp \sqrt{(-\Delta\epsilon + i\Delta\Gamma)^2 + 4\nu_0^2}\right), \\ \beta_{\pm} = \frac{1}{2\nu_0}\left(-\Delta\epsilon + i\Delta\Gamma \pm \sqrt{(-\Delta\epsilon + i\Delta\Gamma)^2 + 4\nu_0^2}\right), \\ \rho_{\pm} = \frac{1}{2}\left(\tilde{\epsilon} - i\Gamma \pm \sqrt{(-\Delta\epsilon + i\Delta\Gamma)^2 + 4\nu_0^2}\right), \end{cases} \tag{5}$$

being $\alpha = \frac{\alpha_{11}}{\alpha_{12}}$, $\beta = \frac{\beta_{11}}{\beta_{12}}$, $\gamma_{\pm} = \alpha_{12}\beta_{11} - \alpha_{11}\beta_{12} = \alpha_{12}\beta_{12}(\beta_{\pm} - \alpha_{\pm})$, $\Delta\epsilon = \epsilon_2 - \epsilon_1$, $\Delta\Gamma = \Gamma_2 - \Gamma_1$, $\tilde{\epsilon} = \epsilon_2 + \epsilon_1$ and $\Gamma = \Gamma_2 + \Gamma_1$. We see that we have two possible solutions (the *plus* solution and the *minus* solution) and that both solutions admit two free parameters. For instance, choosing α_+ above, implies that α_{11} is fixed if we first fix α_{12}. Hence, for each given choice of α_{12} we have a different solution for c. It should be noted that the following condition for the pseudo-fermions existence (see [20]),

$$-\gamma_{\pm}^2 = \alpha_{12}\beta_{12}, \tag{6}$$

must be satisfied, otherwise H_{GMM} can be expressed as standard fermionic operator ($C = c^{\dagger}$) or it cannot be diagonalized. Since $\gamma_{\pm} = \alpha_{12}\beta_{12}(\beta_{\pm} - \alpha_{\pm})$ and $\gamma_{\pm}^2 = -\alpha_{12}\beta_{12}$, we find that, whichever $\alpha_{\pm} \neq \beta_{\pm}$, by taking

$$\alpha_{12}\beta_{12} = \frac{-\nu_0^2}{(-\Delta\epsilon + i\Delta\Gamma)^2 + 4\nu_0^2},$$

the condition (6) is satisfied. On the other hand, this is not possible if $\alpha_\pm = \beta_\pm$, that is $(-\Delta\epsilon + i\Delta\Gamma)^2 = -4\nu_0^2$; in this case the eigenvalues of H_{GMM} coalesce to the value $\frac{1}{2}(\tilde{\epsilon} - i\Gamma)$. Notice that all the above conditions lead to the link of ω_0 with the parameters defining H_{GMM}, as the following condition must be satisfied to ensure that (6) is valid:

$$\hbar\omega_0^\pm = \pm\sqrt{4\nu_0^2 + (-\Delta\epsilon + i\Delta\Gamma)^2}. \tag{7}$$

Notice that this in general means that $\omega_0^\pm$ are complex quantities. To simplify the treatment we restrict here to the principal square root. This relation will prove to be very important in the following because it highlights that the formation of EPs depends on the phenomenological parameters Γ_1 and Γ_2, justifying their introduction in Hamiltonian (1).

3 Eigenstates and Eigenvalues of H

With a simple extension of the procedure discussed in [15] (see also [19]) we can rewrite H in a diagonal form. For that, we first introduce a global non self-adjoint number operator, analogous to the total-excitations-number operator,

$$N = Dd + Cc,$$

and the map defined as

$$T = \exp\{-\theta(4|\epsilon|^2 N)^{-1/2}(\epsilon dC + \epsilon^* Dc)\}, \tag{8}$$

where θ is the operator defined by $\sin\theta = -(4|\epsilon|^2 N)^{1/2}\Delta^{-1}$, and $\cos\theta = -\delta\Delta^{-1}$, where $\delta = \hbar(\omega_0 - \omega)$ is the detuning between the energies of the two fields. By defining the *dressed* operators $\hat{C} = TCT^{-1}$, $\hat{c} = TcT^{-1}$, $\hat{D} = TDT^{-1}$, $\hat{d} = TdT^{-1}$ it is easy to check that they are tensor products of pseudo-bosonic and pseudo-fermionic operators satisfying themselves commutation rules analogous to (2), and the Hamiltonian H can be written in a diagonal form as:

$$H = \left(\hbar\omega - \hat{\Delta}\right)\left(\hat{C}\hat{c} - \frac{1}{2}\right) + \hbar\omega\hat{D}\hat{d} + \left(\frac{\hbar\omega_0}{2} + \rho\right)\mathbb{1}. \tag{9}$$

Following the general procedures used for the pseudo-fermions and pseudo-bosons operators in [16], we can construct the eigenvectors of H and $H^\dagger$ in the framework of deformed canonical commutation relations and canonical anti-commutation relations. We know that two non-zero vectors $\hat{\varphi}_0$ and $\hat{\psi}_0$ do exist in $\mathcal{H}_b$ such that, if

$\hat{\eta}_0$ and $\hat{\mu}_0$ are two vectors of the fermionic Hilbert space $\mathcal{H}_f$ annihilated respectively by $\hat{c}$ and $\hat{C}^\dagger$, we have

$$\left(\hat{d}\otimes\hat{\mathbb{1}}_f\right)\hat{\Phi}_{0,0}=\left(\hat{\mathbb{1}}_b\otimes\hat{c}\right)\hat{\Phi}_{0,0}=0, \tag{10}$$

as well as

$$\left(\hat{D}^\dagger\otimes\hat{\mathbb{1}}_f\right)\hat{\Psi}_{0,0}=\left(\hat{\mathbb{1}}_b\otimes\hat{C}^\dagger\right)\hat{\Psi}_{0,0}=0, \tag{11}$$

where $\hat{\Phi}_{0,0}:=\hat{\varphi}_0\otimes\hat{\eta}_0$ and $\hat{\Psi}_{0,0}:=\hat{\psi}_0\otimes\hat{\mu}_0$. As already pointed out in [17, 21], it is convenient to assume that $\hat{\varphi}_0$ and $\hat{\psi}_0$ belong to a dense domain $\mathcal{D}$ of $\mathcal{H}_b$, which is left stable under the action of d_α, D_α, and their adjoint. As for $\hat{\eta}_0$ and $\hat{\mu}_0$, these vectors surely exist in $\mathcal{H}_f$ and belong to the domain of all the (pseudo-fermionic) operators involved into the game, as one can easily deduce from the fact that $\mathcal{H}_f$ is a finite dimensional vector space. If such a $\mathcal{D}$ exists, then we can use the two vacua $\hat{\Phi}_{0,0}$ and $\hat{\Psi}_{0,0}$ to construct two different sets of vectors, $\mathcal{F}_{\hat{\Phi}}:=\{\hat{\Phi}_{n,k},\ n\geq 0,\ k=0,1\}$ and $\mathcal{F}_{\hat{\Psi}}:=\{\hat{\Psi}_{n,k},\ n\geq 0,\ k=0,1\}$, all belonging to $\mathcal{D}\otimes\mathcal{H}_f$, as follows:

$$\begin{aligned}\hat{\Phi}_{n,k}&=\left(\frac{1}{\sqrt{n!}}\hat{D}_\alpha^n\otimes\hat{C}_\alpha^k\right)\hat{\Phi}_{0,0},\\&=\left(\frac{1}{\sqrt{n!}}\hat{D}_\alpha^n\hat{\varphi}_0\right)\otimes\left(\hat{C}_\alpha^k\hat{\eta}_0\right)=\hat{\varphi}_n\otimes\hat{\eta}_k\end{aligned} \tag{12}$$

and

$$\begin{aligned}\hat{\Psi}_{n,k}&=\left(\frac{1}{\sqrt{n!}}\hat{d_\alpha^\dagger}^n\otimes\hat{c_\alpha^\dagger}^k\right)\hat{\Psi}_{0,0}\\&=\left(\frac{1}{\sqrt{n!}}\hat{d_\alpha^\dagger}^n\hat{\psi}_0\right)\otimes\left(\hat{c^\dagger}_\alpha^k\hat{\mu}_0\right)=\hat{\psi}_n\otimes\hat{\mu}_k,\end{aligned} \tag{13}$$

with obvious notations, where $n=0,1,2,\ldots$ and $k=0,1$. It is now easy to check that

$$H\hat{\Phi}_{n,k}=E_{n,k}\hat{\Phi}_{n,k},\qquad H^\dagger\hat{\Psi}_{n,k}=E_{n,k}^*\hat{\Psi}_{n,k}, \tag{14}$$

where the eigenvalues are

$$E_{n,k}=\hbar\omega n+\frac{\hbar\omega_0}{2}+\rho+\left[\hbar\omega-\left(\delta^2+4|\epsilon|^2(n+k)\right)^{1/2}\right]\left(k-\frac{1}{2}\right). \tag{15}$$

Also, if the normalization of $\hat{\Phi}_{0,0}$ and $\hat{\Psi}_{0,0}$ is chosen in such a way that $\langle\hat{\Phi}_{0,0},\hat{\Psi}_{0,0}\rangle=1$, then

$$\langle\hat{\Phi}_{n,k},\hat{\Psi}_{m,l}\rangle=\langle\hat{\varphi}_n,\hat{\psi}_m\rangle_{\mathcal{H}_b}\langle\hat{\eta}_k,\hat{\mu}_l\rangle_{\mathcal{H}_f}=\delta_{n,m}\delta_{l,k}\,. \tag{16}$$

Here $\langle.,.\rangle_{\mathcal{H}_b}$ and $\langle.,.\rangle_{\mathcal{H}_f}$ are respectively the scalar products in $\mathcal{H}_b$ and in $\mathcal{H}_f$.

4 Exceptional Points Formation

In this section we investigate the formation of exceptional points in our extended Jaynes-Cummings Hamiltonian. It is convenient to introduce the analogous pseudo-structures given by the conditions (10–13) for the non diagonal form (1) of our Hamiltonian. As before, we can also define the two set of vectors, $\mathcal{F}_\Phi := \{\Phi_{n,k},\ n \geq 0,\ k = 0, 1\}$ and $\mathcal{F}_\Psi := \{\Psi_{n,k},\ n \geq 0,\ k = 0, 1\}$, all belonging to $\mathcal{D} \otimes \mathcal{H}_f$, as follows:

$$\Phi_{n,k} = \left(\frac{1}{\sqrt{n!}} D_\alpha^n \otimes C_\alpha^k\right) \Phi_{0,0} = \left(\frac{1}{\sqrt{n!}} D_\alpha^n \varphi_0\right) \otimes \left(C_\alpha^k \eta_0\right) = \varphi_n \otimes \eta_k,$$
$$\Psi_{n,k} = \left(\frac{1}{\sqrt{n!}} d_\alpha^{\dagger n} \otimes c_\alpha^{\dagger k}\right) \Psi_{0,0} = \left(\frac{1}{\sqrt{n!}} d_\alpha^{\dagger n} \psi_0\right) \otimes \left(c^{\dagger k}_\alpha \mu_0\right) = \psi_n \otimes \mu_k,$$

and, as usual,

$$\left(d \otimes \hat{\mathbb{1}}_f\right) \Phi_{0,0} = \left(\mathbb{1}_b \otimes c\right) \Phi_{0,0} = 0, \tag{17}$$
$$\left(D^\dagger \otimes \mathbb{1}_f\right) \Psi_{0,0} = \left(\mathbb{1}_b \otimes C^\dagger\right) \Psi_{0,0} = 0, \tag{18}$$

and

$$\langle \Phi_{n,k}, \Psi_{m,l} \rangle = \delta_{n,m} \delta_{l,k}. \tag{19}$$

It is easy to check that, in terms of the vectors given above, the eigenvalues of H and $H^\dagger$ can be rewritten in order to satisfy the following conditions:

$$H\left(\Phi_{n-1,1} + \lambda_n^\pm \Phi_{n,0}\right) = E_n^\pm \left(\Phi_{n-1,1} + \lambda_n^\pm \Phi_{n,0}\right), \tag{20}$$
$$H^\dagger \left(\Psi_{n-1,1} + \xi_n^\pm \Psi_{n,0}\right) = E_n^{\pm *} \left(\Psi_{n-1,1} + \xi_n^\pm \Psi_{n,0}\right), \tag{21}$$

where

$$E_n^\pm = \hbar\omega\left(n - \frac{1}{2}\right) + \frac{\hbar\omega_0}{2} + \rho \pm \frac{\left(\delta^2 + 4|\epsilon|^2 n\right)^{1/2}}{2},$$

and

$$\lambda_n^\pm = \frac{-\delta \pm (\delta^2 + 4|\epsilon|^2 n)^{1/2}}{2\epsilon\sqrt{n}}, \xi_n^\pm = \frac{-\delta^* \pm \left((\delta^*)^2 + 4|\epsilon|^2 n\right)^{1/2}}{2\epsilon\sqrt{n}}.$$

For each n, we have $E_n^+ = E_{n,0}$ and $E_n^- = E_{n-1,1}$. It thus follows from (14) and (21) that

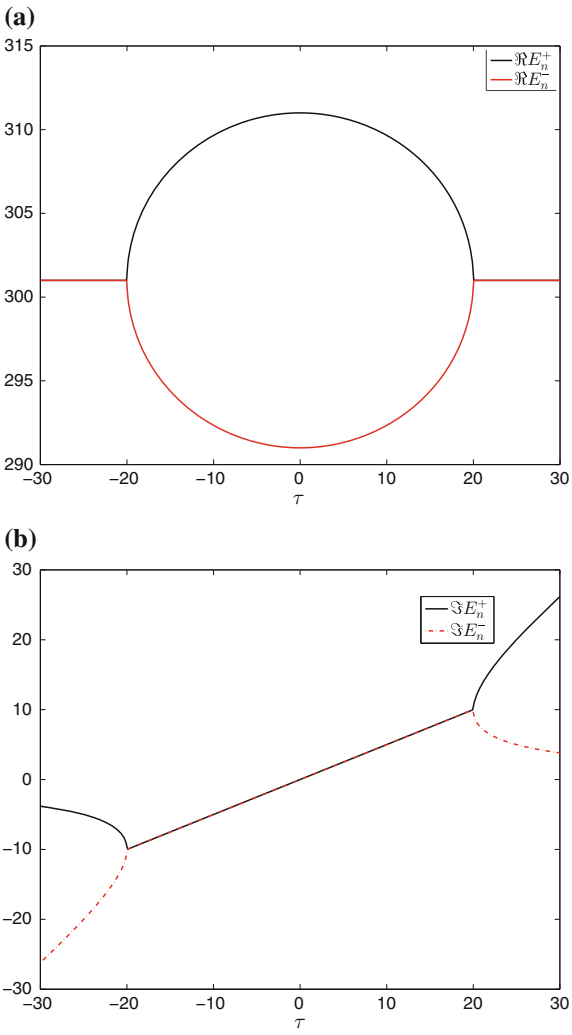

Fig. 1 Real (**a**) and imaginary (**b**) parts of the eigenvalues $E_n^{\pm}$ for $n = 100$ as function of the parameter $\tau = -i(\hbar\omega_0 - \hbar\omega)$. Other parameters are $\epsilon = 1$, $\rho = 1$, $\omega = 3$; units are such that $\hbar = 1$. At the EPs $\tau = \pm 20$ eigenvalues coalesce so that $E_n^+ = E_n^-$

$$\hat{\Phi}_{n,0} = g_{\hat{\Phi}}^{n,0}\left(\Phi_{n-1,1} + \lambda_n^+ \Phi_{n,0}\right), \hat{\Phi}_{n,0} = g_{\hat{\Psi}}^{n,0}\left(\Psi_{n-1,1} + \xi_n^+ \Psi_{n,0}\right),$$
$$\hat{\Phi}_{n-1,1} = g_{\hat{\Phi}}^{n-1,1}\left(\Phi_{n-1,1} + \lambda_n^- \Phi_{n,0}\right), \hat{\Psi}_{n-1,1} = g_{\hat{\Psi}}^{n-1,1}\left(\Psi_{n-1,1} + \xi_n^- \Psi_{n,0}\right),$$

being g_Φ, g_Ψ appropriate normalization constants given by the bi-orthogonality conditions (16).

If we now consider the case in which $\delta^2 + 4|\epsilon|^2 n = 0$, then $E_n^+ = E_n^-$, $\lambda_n^+ = \lambda_n^-$. Therefore, the couples of vectors $\hat{\Phi}_{n,0}$, $\hat{\Phi}_{n-1,1}$ and $\hat{\Psi}_{n,0}$, $\hat{\Psi}_{n-1,1}$ being proportional,

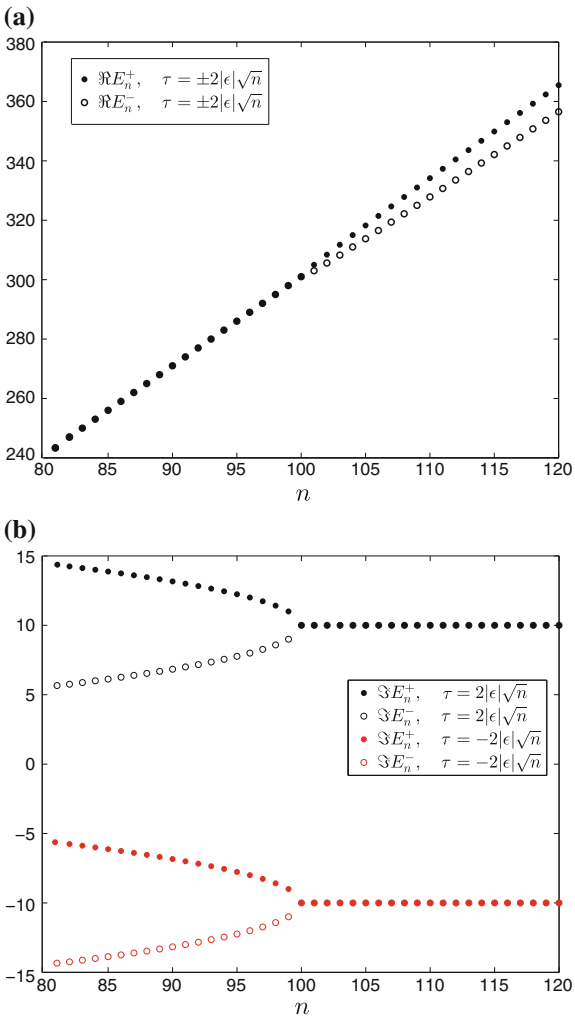

Fig. 2 Real (**a**) and imaginary (**b**) parts of the eigenvalues $E_n^{\pm}$ as function of the parameter n for $\tau = i(\hbar\omega_0 - \hbar\omega)$ (*black lines*) and $\tau = -i(\hbar\omega_0 - \hbar\omega)$ (*red lines*). Other parameters are $\epsilon = 1$, $\rho = 1$, $\omega = 3$; units are such that $\hbar = 1$. At $n = 100$ the EPs are formed, and eigenvalues coalesce so that $E_n^+ = E_n^-$

are linearly dependent. This condition implies that δ is purely imaginary, so that $\hbar(\omega_0 - \omega) = i\tau$ with $\tau = \tau^{\pm} = \pm 2|\epsilon|\sqrt{n}$. Varying τ leads to the situation shown in Fig. 1 for $n = 100$. For $\tau < \tau^-$ and $\tau > \tau^+$, the eigenvalues E_n^+, E_n^- relative to the n-excitation subspace have same real parts and different imaginary parts. For $\tau^- \leq \tau \leq \tau^+$, the eigenvalues have different real parts and the same imaginary parts. At $\tau = \tau^{\pm}$ the eigenvalues coalesce to the value $\hbar\omega\left(n - \frac{1}{2}\right) + \frac{\hbar\omega_0}{2} + \rho$; also, due to the presence of two branch points in $\tau^{\pm}$ for $E_n^{\pm}(\tau)$, we obtain that encircling the points $\tau^{\pm}$ in the complex plane interchanges the two eigenvalues. In fact considering an arbitrary closed loop $s^{\pm}(\theta) = \tau^{\pm} + re^{i\theta}$ around $\tau^{\pm}$ leads to $E_n^{\pm}(s(0)) = E_n^{\mp}(s(2\pi))$.

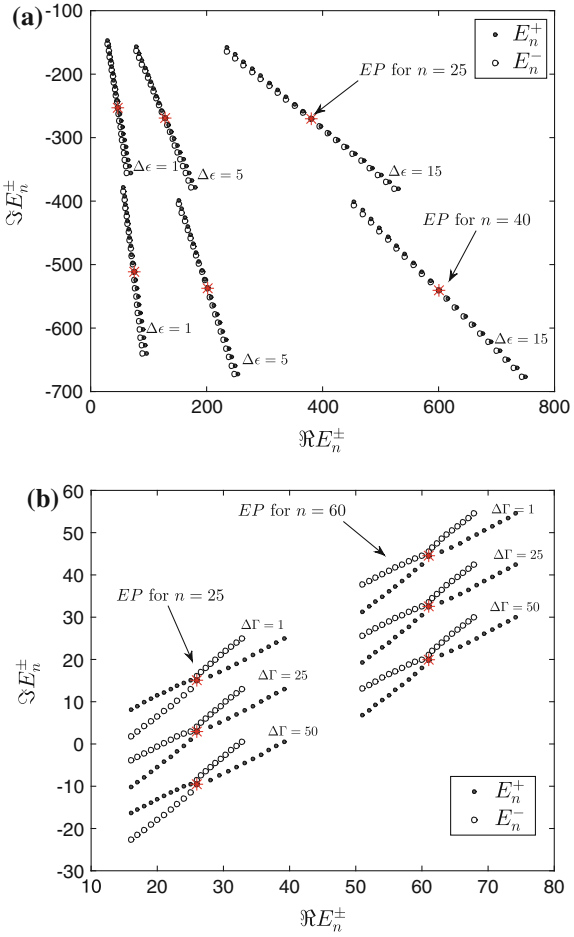

Fig. 3 Eigenvalues $E_n^\pm$ in the complex plane for various values of n. In **a** eigenvalues are obtained by taking $\nu_0 = 1, \epsilon_1 = 0.5, \Gamma_1 = 0, \Gamma_2 = 1$, $\omega_0 = \sqrt{4 + (\Delta\epsilon + i)^2}$, $\rho = 0.5(1 + \Delta\epsilon - i + \sqrt{4 + (\Delta\epsilon + i)^2})$ and $\omega = \sqrt{4 + (\Delta\epsilon + i)^2} - 2i\sqrt{\tilde{n}}$, for $\tilde{n} = 25$ and $\tilde{n} = 40$, ϵ_2 is varied according to the chosen value of $\Delta\epsilon$. In **b** eigenvalues are obtained by taking $\epsilon_1 = \epsilon_2 = 0.5, \Gamma_1 = 0, \omega = 1 + i$, $\nu_0 = 0.5\sqrt{(1 + i - 2i\sqrt{\tilde{n}})^2 - (i\,\Delta\Gamma^2)}, \omega_0 = 1 + 3i\sqrt{\tilde{n}}, \rho = 0.5(2 - i\,\Delta\Gamma + 3i\sqrt{n})$, for $\tilde{n} = 25$ and $\tilde{n} = 60$, Γ_2 is varied according to the chosen value of $\Delta\Gamma$. At the EPs, the eigenvalues coalesce, marked in the plots by the *red* $*$

It is worth noting that at $\tau = \tau^\pm$ the condition $\lambda_n^+ = \lambda_n^- = -\frac{\delta}{2|\epsilon|\sqrt{n}}$ leads to the vanishing of the scalar products $\langle \hat{\Phi}_{n,0}, \hat{\Psi}_{n,0} \rangle$ and $\langle \hat{\Phi}_{n-1,1}, \hat{\Psi}_{n-1,1} \rangle$. In fact

$$\langle \hat{\Phi}_{n,0}, \hat{\Psi}_{n,0} \rangle = g_{\hat{\Phi}}^{n,0*} g_{\hat{\Psi}}^{n,0} \left(\langle \Phi_{n-1,1}, \Psi_{n-1,1} \rangle - \frac{\tau^2}{4|\epsilon|^2 n} \langle \Phi_{n,0}, \Psi_{n,0} \rangle \right) = 0, \qquad (22)$$

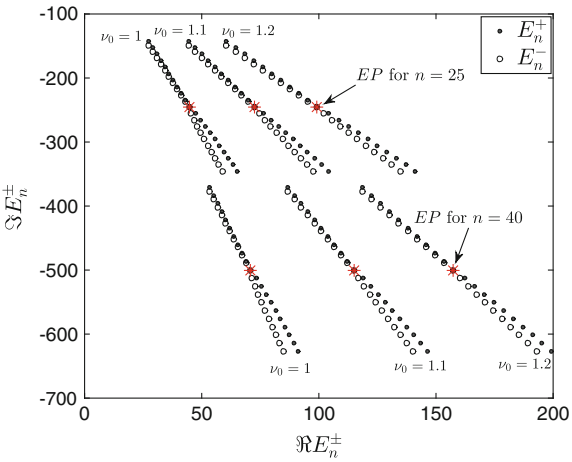

Fig. 4 Eigenvalues $E_n^{\pm}$ in the complex plane for various values of ν_0 and n. Parameters are $\epsilon_1 = \epsilon_2 = 0.5$, $\Gamma_1 = 0$, $\Gamma_2 = 1$,$\omega = 1 + 1i$, $\omega_0 =$, $\rho = 0.5(1 - i1 + \omega_0)$, $\omega = \sqrt{4 + (\Delta\epsilon + i1)^2} - 2i\sqrt{\tilde{n}}$, for $\tilde{n} = 25$ and $\tilde{n} = 40$. At the EPs the eigenvalues coalesce, marked in the plot by the *red* $*$

because $\tau^{\pm} = \pm 2|\epsilon|\sqrt{n}$. Analogously $\langle \hat{\Phi}_{n-1,1}, \hat{\Psi}_{n-1,1} \rangle = 0$. These conditions are typical of the EPs formation at $\tau^{\pm}$, [22]. Figure 2 shows that only for $n = 100$, for our particular choice of parameters, $E_n^+ = E_n^-$, so that the related eigenstates coalesce. More important, our results show that at the EPs the pseudo-structure in terms of pseudo-fermions and pseudo-bosons operator is no more valid. In fact it has been shown that, in presence of an EP, the coefficients defining the operators c and C, see (4), cannot satisfy the necessary condition (6) (see [20]).

Notice that through (7), we obtain that the EPs formation is compatible only with the following choices of ω

$$\hbar\omega^{\pm} = \pm\sqrt{4\nu_0^2 + (-\Delta\epsilon + i\,\Delta\Gamma)^2} - i\tau, \tag{23}$$

where it is evident that EPs form only for an appropriate choice of ν_0 and of the relative differences $\Delta\epsilon$, $\Delta\Gamma$ of the parameters $\epsilon_{1,2}$ and $\Gamma_{1,2}$ in (1), which is related to ω and ω_0. It must be emphasized that by manipulating parameters present in the Hamiltonian (1), it is possible to change the position of the EPs in the complex plane. In Figs. 3 and 4 we show the eigenvalues $E_n^{\pm}$ in the complex plane by varying respectively $\Delta\epsilon$, $\Delta\Gamma$ and ν_0. This opens up the prospects of a kind of engineering of EPs in order to exploit their impact on the dynamics of the physical system in which they appear. For example, this can be obtained by appropriately changing the decay rates Γ_1 and Γ_2 (see [23] and references therein).

5 Conclusions and Perspectives

In this paper we have considered the formation of exceptional points in a non-Hermitian Jaynes-Cummings Hamiltonian, that generalizes the Hamiltonian of a two-level atom interacting with a single cavity field mode to the case in which dissipation and decay are phenomenologically included.

The results obtained in this paper show the exceptional points identified in the non-Hermitian Jaynes-Cummings Hamiltonian (1), have the same structure obtained in [24, 25].

From a mathematical point of view, this is due to the fact that, for a two-level system, the eigenvalues contain in their mathematical expression a square root as that of a second-degree algebraic equation. The collapse of the eigenvalues and the formation of EPs depend on the vanishing of the square-root argument for specific values of the physical parameters involved. On the other hand, the interchange properties of the eigenvalues when EPs are encircled can be interpreted as an effect due to the branch points of the square root when analyzed as a function in the complex plane. Also, encircling EPs causes the switch of the eigenfunctions, showing that their relative phases are not rigid. From a physical point of view, this behavior can be interpreted as a manifestation of the capability of the system to align itself with the environment to which it is coupled (see also [25]).

The main novelties introduced in this paper concern with the analysis of the exceptional points for the spectrum of a non-Hermitian Jaynes-Cummings Hamiltonian expressed in terms of a mixture of pseudo-fermions and pseudo-bosons (previous analysis were focused on EPs in non-Hermitian pseudo-fermionic operators, [20]). Thus, the application range of this theory on pseudo-particles is here extended. We wish to stress that the existence of a pseudo-structure is deeply related to the existence of EPs: in fact, as we have shown in Sect. 4, the spontaneous generation of the EPs implies that the biorthogonality condition (16), which characterizes the pseudo-structure we have introduced, is no more satisfied. This is expected, since a pseudofermionic or pseudobosonic structure is intrinsically connected with the existence of non coincident eigenvalues. Moreover, the *deformed* Jaynes-Cummings model analyzed in [15] and in this paper, could be used to further investigate the role played by EPs on interaction between atomic systems and the electromagnetic field, including damping or amplifying processes, which is of fundamental importance in quantum optics.

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$\mathscr{D}$–Deformed and SUSY-Deformed Graphene: First Results

F. Bagarello and M. Gianfreda

Abstract We discuss some mathematical aspects of two particular deformed versions of the Dirac Hamiltonian for graphene close to the Dirac points, one involving $\mathscr{D}$-pseudo bosons and the other supersymmetric quantum mechanics. In particular, in connection with $\mathscr{D}$-pseudo bosons, we show how biorthogonal sets arise, and we discuss when these sets are bases for the Hilbert space where the model is defined, and when they are not. For the SUSY extension of the model we show how this can be achieved and which results can be obtained.

1 Introduction

Because of its properties graphene is quite interesting both for mathematical and for physical reasons, as well as for its concrete applications, due to its mechanical and electrical properties. Because of this, it has been intensely studied in recent years [1, 2].

Graphene is a two-dimensional configuration of carbon atoms organized in a hexagonal honeycomb structure (Fig. 1). The hexagonal arrangement of carbon atoms can be decomposed into two interpenetrating sublattices of carbon atoms related by inversion symmetry. The low-energy band structure of graphene can be approximated as cones located at two inequivalent Brillouin zone corners called the Dirac points K and K'. (There are six Dirac points in total, but only two are worth considering due to the periodicity of the momenta in the Brillouin zone.) At each cone the two-dimensional energy dispersion relation is analogous to that of relativistic, massless fermions. Corresponding to the K point, the electron dynamics is then described by

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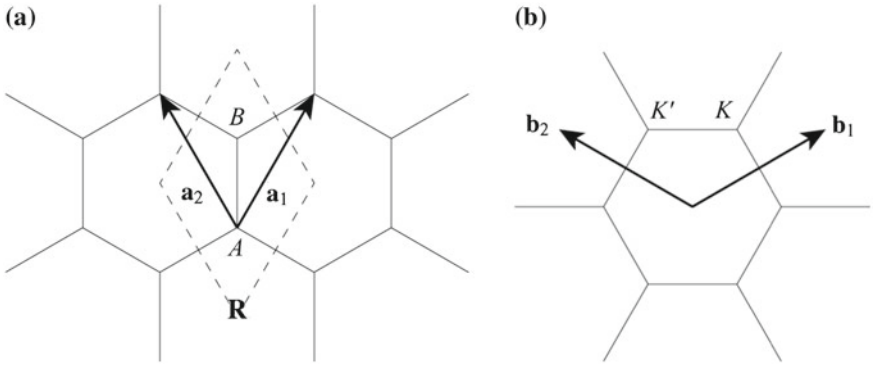

Fig. 1 **a** A honeycomb lattice consists of a unit cell of two sites. The location of each cell is denoted by a two-dimensional vector $\mathbf{R}$. The vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ denote the shifts from the unit cell to the neighboring unit cells, so that the neighboring cells are located at $\mathbf{R}+\mathbf{a}_1$ and $\mathbf{R}+\mathbf{a}_2$. A and B denotes each of the two atoms in a unit cell (namely the sublattices). **b** The first Brillouin zone of the honeycomb lattice. The upper and lower energy bands touch at the K and K' points. The vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ are the reciprocal vectors of $\mathbf{a}_1$ and $\mathbf{a}_2$ in the momentum space

a Dirac Hamiltonian. The dynamics corresponding to the K point provides all of the informations about the model, since the point K' is obtained under mirror reflection of K.

Some years ago [3], a noncommutative extension of the original model was proposed, and some consequences were deduced. As a matter of fact, this extension only implied the appearance of one overall multiplicative constant in the final formulas, leaving almost all the other aspects of the model essentially unchanged. In particular, the Hamiltonian of the system still stays self-adjoint. Here, also in view of the recent success on what is nowadays called *PT-quantum mechanics* [4], we analyze a different deformation of the original Hamiltonian leading to different statistics and to non self-adjoint Hamiltonians. This will be achieved using the so-called $\mathscr{D}$-pseudo bosonic operators [5, 6], for which biorthogonal sets, intertwining operators, bounded or unbounded metrics, and so on, play a relevant role.

Also, in the second part of this paper we consider a different deformation, related to what is called *supersymmetric quantum mechanics* (SUSY-QM) [7], and we show that some interesting features also appear in the model, in connection with such a deformation.

This article is organized as follows: in the next section we briefly review the self-adjoint version of the model, and some of its main mathematical characteristics. In Sect. 3 we introduce our first deformed version of the model, the one related to pseudo-bosons, and we consider the consequences of this deformation. In Sect. 4 we consider the SUSY-related deformation, while our conclusions are given in Sect. 5. To keep the paper self-contained, we give in Appendix 1 some useful results on $\mathscr{D}$-pseudo bosons, while Appendix 2 contains some results on the SUSY deformed version of the model, for some particular values of the parameters involved.

2 The Self-adjoint Model

We consider a layer of graphene in an external constant magnetic field along z: $\mathbf{B} = B\hat{e}_3$. $\mathbf{B}$ can be deduced, adopting the symmetric gauge, from a vector potential $\mathbf{A} = \frac{B}{2}(-y, x, 0)$, and $\mathbf{B} = \nabla \wedge \mathbf{A}$. The Hamiltonian for the two Dirac points K and K' can be written as [2]

$$H_D = \begin{pmatrix} H_K & 0 \\ 0 & H_{K'} \end{pmatrix}, \tag{1}$$

where, in units $\hbar = c = 1$, we have

$$H_K = v_F \begin{pmatrix} 0 & p_x - ip_y + \frac{eB}{2}(y + ix) \\ p_x + ip_y + \frac{eB}{2}(y - ix) & 0 \end{pmatrix}. \tag{2}$$

The operator $H_{K'}$ is just the matrix transpose of H_K: $H_{K'} = H_K^T$. Here x, y, p_x and p_y are the canonical, self-adjoint, two-dimensional position and momentum operators: $[x, p_x] = [y, p_y] = i\mathbb{1}$, all the other commutators being zero. $\mathbb{1}$ is the identity operator in $\mathscr{H} := \mathscr{L}^2(\mathbb{R}^2)$. The factor v_F is the so-called Fermi velocity. The scalar product in $\mathscr{H}$ will be denoted as $\langle ., . \rangle$.

Let us now introduce $\xi = \sqrt{\frac{2}{eB}}$, and the following canonical operators:

$$X = \frac{1}{\xi}x, \quad Y = \frac{1}{\xi}y, \quad P_X = \xi p_x, \quad P_Y = \xi p_y.$$

These operators can be used to define two different pairs of bosonic operators: we first put $a_X = \frac{X+iP_X}{\sqrt{2}}$ and $a_Y = \frac{Y+iP_Y}{\sqrt{2}}$, and then

$$A_1 = \frac{a_X - ia_Y}{\sqrt{2}}, \quad A_2 = \frac{a_X + ia_Y}{\sqrt{2}}. \tag{3}$$

The following commutation rules are satisfied:

$$[a_X, a_X^\dagger] = [a_Y, a_Y^\dagger] = [A_1, A_1^\dagger] = [A_2, A_2^\dagger] = \mathbb{1}, \tag{4}$$

the other commutators being zero. In terms of these operators, H_K appears particularly simple. Indeed we find:

$$H_K = \frac{2iv_F}{\xi} \begin{pmatrix} 0 & A_2^\dagger \\ -A_2 & 0 \end{pmatrix}. \tag{5}$$

It is evident that $H_K = H_K^\dagger$, which of course implies also that $H_{K'} = H_{K'}^\dagger$. It is also clear that neither H_K nor $H_{K'}$ depends on A_1 and $A_1^\dagger$, so that their eigenstates are expected to show a manifest degeneracy. And this is in fact what we easily deduce now, following [3]. Let $e_{0,0} \in \mathscr{H}$ be the nonzero vacuum of A_1 and A_2: $A_1 e_{0,0} =$

$A_2 e_{0,0} = 0$. Then we introduce, in standard fashion,

$$e_{n_1,n_2} = \frac{1}{\sqrt{n_1! n_2!}} (A_1^\dagger)^{n_1} (A_2^\dagger)^{n_2} e_{0,0}, \tag{6}$$

and the set $\mathscr{E} = \left\{e_{n_1,n_2},\ n_j \geq 0\right\}$. $\mathscr{E}$ is an orthonormal (o.n.) basis for $\mathscr{H}$. It appears to be the o.n. basis of a two-dimensional harmonic oscillator. To deal with H_K, it is convenient to work in a different Hilbert space, the direct sum of $\mathscr{H}$ with itself, $\mathscr{H}_2 = \mathscr{H} \oplus \mathscr{H}$:

$$\mathscr{H}_2 = \left\{ f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, \quad f_1, f_2 \in \mathscr{H} \right\}.$$

In $\mathscr{H}_2$ the scalar product $\langle ., . \rangle_2$ is defined as

$$\langle f, g \rangle_2 := \langle f_1, g_1 \rangle + \langle f_2, g_2 \rangle\,, \tag{7}$$

and the squared norm is $\|f\|_2^2 = \|f_1\|^2 + \|f_2\|^2$, for all $f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$, $g = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}$ in $\mathscr{H}_2$. Introducing now the vectors

$$e^{(1)}_{n_1,n_2} = \begin{pmatrix} e_{n_1,n_2} \\ 0 \end{pmatrix}, \quad e^{(2)}_{n_1,n_2} = \begin{pmatrix} 0 \\ e_{n_1,n_2} \end{pmatrix}, \tag{8}$$

the set $\mathscr{E}_2 := \{e^{(k)}_{n_1,n_2},\ n_1, n_2 \geq 0,\ k = 1, 2\}$ is an o.n. basis for $\mathscr{H}_2$. This means, among other things, that $\mathscr{E}_2$ is complete in $\mathscr{H}_2$: the only vector $f \in \mathscr{H}_2$ which is orthogonal to all the vectors of $\mathscr{E}_2$ is the zero vector. In view of applications to graphene, it is more convenient to use a different o.n. basis of $\mathscr{H}_2$, the set $\mathscr{V}_2 = \{v^{(k)}_{n_1,n_2},\ n_1, n_2 \geq 0,\ k = \pm\}$, where

$$v^{(+)}_{n_1,0} = v^{(-)}_{n_1,0} = e^{(1)}_{n_1,0} = \begin{pmatrix} e_{n_1,0} \\ 0 \end{pmatrix}. \tag{9}$$

Quite often we will simply call this vector $v_{n_1,0}$. Moreover (i.e., if $n_2 \geq 1$), we have

$$v^{(\pm)}_{n_1,n_2} = \frac{1}{\sqrt{2}} \begin{pmatrix} e_{n_1,n_2} \\ \mp i e_{n_1,n_2-1} \end{pmatrix} = \frac{1}{\sqrt{2}} \left(e^{(1)}_{n_1,n_2} \mp i e^{(2)}_{n_1,n_2-1} \right). \tag{10}$$

It is easy to check that these vectors are mutually orthogonal, normalized in $\mathscr{H}_2$, and complete. Hence, $\mathscr{V}_2$ is an o.n. basis for $\mathscr{H}_2$, as stated before. This is not surprising, since its vectors are indeed the eigenvectors of H_K:

$$H_K v_{n_1,0} = 0, \quad H_K v^{(+)}_{n_1,n_2} = E^{(+)}_{n_1,n_2} v^{(+)}_{n_1,n_2}, \quad H_K v^{(-)}_{n_1,n_2} = E^{(-)}_{n_1,n_2} v^{(-)}_{n_1,n_2}, \tag{11}$$

where $E^{(\pm)}_{n_1,n_2} = \pm \frac{2v_F}{\xi} \sqrt{n_2}$. More compactly, we can simply write $H_K v^{(\pm)}_{n_1,n_2} = E^{(\pm)}_{n_1,n_2}$ $v^{(\pm)}_{n_1,n_2}$. We see explicitly that the eigenvalues have an infinite degeneracy in n_1, which

can be removed by using the angular momentum. We will not consider this aspect here, since it is not relevant for us.

Of course, both $\mathscr{E}_2$ and $\mathscr{V}_2$ can be used to produce two different resolutions of the identity. Indeed we have

$$\sum_{n_1,n_2=0}^{\infty}\sum_{k=1}^{2}\left\langle e^{(k)}_{n_1,n_2},f\right\rangle_2 e^{(k)}_{n_1,n_2}=\sum_{n_1,n_2=0}^{\infty}\sum_{k=\pm}\left\langle v^{(k)}_{n_1,n_2},f\right\rangle_2 v^{(k)}_{n_1,n_2}=f, \tag{12}$$

for all $f\in\mathscr{H}_2$.

Remark: Of course, what we have seen so far can be easily adapted to the analysis of $H_{K'}$, since this is simply the transpose of H_K.

3 The Non-self-adjoint Model

The starting point of our analysis is a $\mathscr{D}$ pseudo-bosonic deformation of the Hamiltonian H_K in (5), see Appendix 1. This is a first possible alternative to what is suggested, for instance, in [3], where the authors extend the same Hamiltonian by considering noncommutative variables of a special kind, instead of the original ones. From our point of view, the one considered here is more interesting, since the deformation proposed in [3] did not cause any particular difference in the mathematical structure of the resulting model. In particular, their *new* Hamiltonian turns out to be self-adjoint, and differs from the one in (5) only for an overall multiplication parameter. The aim of this section is to show how the different deformation we propose here, on the other hand, produces several differences with the original model, at least on the mathematical level.

We start with two pairs of operators $(a_j, b_j), j = 1, 2$, acting on $\mathscr{H}$ and satisfying the $\mathscr{D}$ pseudo-bosonic commutation rules

$$a_jb_kf-b_ka_jf=\delta_{j,k}f, \tag{13}$$

for all $f\in\mathscr{D}$. Here $\mathscr{D}$ is a suitable dense subset of $\mathscr{H}$, which we assume to be invariant under the action of a_j, b_j, and their adjoints. Quite often, in the following, we will rewrite commutation rules like this in the following convenient way: $[a_j, b_k] = \delta_{j,k}\,\mathbb{1}$, $j, k = 1, 2$, with the implicit agreement that both sides must be applied to vectors of $\mathscr{D}$. Moreover, we have $[a_1, a_2] = [b_1, b_2] = 0$.

Mimicking H_D in (1), we consider now the following Hamiltonian:

$$h_D=\begin{pmatrix} h_K & 0\\ 0 & h_{K'}\end{pmatrix},$$

where

$$h_K = \frac{2iv_F}{\xi}\begin{pmatrix} 0 & b_2 \\ -a_2 & 0 \end{pmatrix},$$

while, as before, $h_{K'}$ is just its transpose: $h_{K'} = h_K^T$. It is clear that h_K coincides with H_K if $b_2 = a_2^\dagger$, but not otherwise. To find the eigensystem of h_K we observe that

$$h_K^2 = \frac{4v_F^2}{\xi^2}\begin{pmatrix} \hat{n}_2 & 0 \\ 0 & \mathbb{1} + \hat{n}_2 \end{pmatrix},$$

where $\hat{n}_j = b_j a_j$, $j = 1, 2$ are the pseudo-bosonic number operators. They are non-self-adjoint, since $\hat{n}_j^\dagger = a_j^\dagger b_j^\dagger$ coincides with $\hat{n}_j$ only if $b_j = a_j^\dagger$. Still, see Appendix 1, it is quite easy to find their eigenvectors and to show that the related eigenvalues are the natural numbers including zero, $\mathbb{N}_0$. This happens to be true if a minimal set of Assumptions, extending to two dimensions those given in Appendix 1, are satisfied. To begin with, we assume that a nonzero vector $\varphi_{0,0}$ exists in $\mathscr{D}$ such that $a_1\varphi_{0,0} = a_2\varphi_{0,0} = 0$. Under this assumption, using the invariance of the set $\mathscr{D}$ under the action of b_1 and b_2, we conclude that all the vectors

$$\varphi_{n_1,n_2} = \frac{1}{\sqrt{n_1!n_2!}} b_1^{n_1} b_2^{n_2}\varphi_{0,0},$$

$n_j \in \mathbb{N}_0$, belong to $\mathscr{D}$ and are eigenstates of $\hat{n}_j$: $\hat{n}_j\varphi_{n_1,n_2} = n_j\varphi_{n_1,n_2}$. Moreover, the following raising and lowering properties are satisfied:

$$b_1\varphi_{n_1,n_2} = \sqrt{n_1+1}\,\varphi_{n_1+1,n_2}, \quad b_2\varphi_{n_1,n_2} = \sqrt{n_2+1}\,\varphi_{n_1,n_2+1},$$

as well as

$$a_1\varphi_{n_1,n_2} = \sqrt{n_1}\,\varphi_{n_1-1,n_2}, \quad a_2\varphi_{n_1,n_2} = \sqrt{n_2}\,\varphi_{n_1,n_2-1},$$

with the agreement that $\varphi_{-1,n_2} = \varphi_{n_1,-1} \equiv 0$. Once again, these equations are all well posed because of the invariance of $\mathscr{D}$ under the action of all the operators involved.

Going back to the eigenvectors of h_K, it is clear that if some nonzero vector η satisfies $h_K\eta = E\eta$, then η must also satisfy the (somewhat easier) eigenvalue equation $h_k^2\eta = E^2\eta$. This equation, because of what we have just observed for $\mathscr{D}$-PBs, is satisfied if $E^2 = \frac{4v_F^2 n_2}{\xi^2}$ and if $\eta = \gamma\begin{pmatrix} \varphi_{n_1,n_2} \\ \alpha\varphi_{n_1,n_2-1} \end{pmatrix}$. Here γ is a normalization constant, while α is a complex quantity still to be fixed by requiring that η also solves the original eigenvalue equation, $h_K\eta = E\eta$.

Using the lowering and raising equations above, we end up with the following result:

$$h_K\eta^{(\pm)}_{n_1,n_2} = E^{(\pm)}_{n_1,n_2}\eta^{(\pm)}_{n_1,n_2}, \tag{14}$$

where

$$\eta^{(\pm)}_{n_1,n_2} = \gamma^{(\pm)}_{n_1,n_2} \begin{pmatrix} \varphi_{n_1,n_2} \\ \mp i\,\varphi_{n_1,n_2-1} \end{pmatrix}, \quad E^{(\pm)}_{n_1,n_2} = \pm \frac{2v_F}{\xi}\sqrt{n_2} \tag{15}$$

for all $n_1, n_2 \geq 0$. Again $\varphi_{n_1,-1} \equiv 0$. The normalizing factors $\gamma^{(\pm)}_{n_1,n_2}$ still have to be fixed. We see that, apart these factors, the general expression of these eigenvectors are quite similar to those we obtained in the previous section, see (10). This is not surprising, since the $\mathscr{D}$-PBs keep several of the characteristics of ordinary bosonic operators. However, this is only partially true. In fact, for instance, the vectors $\eta^{(\pm)}_{n_1,n_2}$ are not mutually orthogonal in $\mathscr{H}_2$, since the φ_{n_1,n_2} are not orthogonal in $\mathscr{H}$. Also, the set $\mathscr{F}_\eta = \{\eta^{(\pm)}_{n_1,n_2},\ n_1, n_2 \geq 0\}$, is not necessarily a basis for $\mathscr{H}_2$. Similar features have been deduced in several models in the literature [6]. Yet, since they correspond to different eigenvalues, they turn out to be linearly independent in $\mathscr{H}_2$: any finite linear combination of these vectors can be zero if and only if all the coefficients are zero.

Due to the fact that $h_K \neq h_K^\dagger$, it is now interesting to see what can be said for $h_K^\dagger$. We start assuming that a non zero vacuum $\Psi_{0,0}$ of $b_1^\dagger$ and $b_2^\dagger$ exists in $\mathscr{D}$: $b_1^\dagger\Psi_{0,0} = b_2^\dagger\Psi_{0,0} = 0$. Of course, since $b_j^\dagger \neq a_j$ we do not expect that $\Psi_{0,0}$ and $\varphi_{0,0}$ do coincide, even if this could happen, for some particular choices of the pseudo-bosonic operators [8].

Using the invariance of $\mathscr{D}$ under the action of $a_1^\dagger$ and $a_2^\dagger$, we can construct the following vectors, all belonging to $\mathscr{D}$:

$$\Psi_{n_1,n_2} = \frac{1}{\sqrt{n_1!n_2!}} a_1^{\dagger n_1} a_2^{\dagger n_2} \Psi_{0,0},$$

$n_j \in \mathbb{N}_0$, and the set $\mathscr{F}_\Psi = \{\Psi_{n_1,n_2},\ n_1, n_2 \in \mathbb{N}_0\}$. These vectors are eigenstates of $\hat{n}_j^\dagger$: $\hat{n}_j^\dagger \Psi_{n_1,n_2} = n_j \Psi_{n_1,n_2}$. Therefore, it is easy to see that, if the normalization of $\varphi_{0,0}$ and $\Psi_{0,0}$ is chosen in such a way $\langle \varphi_{0,0}, \Psi_{0,0} \rangle = 1$ holds, we have

$$\langle \varphi_{n_1,n_2}, \Psi_{m_1,m_2} \rangle = \delta_{n_1,m_1}\delta_{n_2,m_2}. \tag{16}$$

The vectors Ψ_{n_1,n_2} can be used now to construct, in analogy with the $\eta^{(\pm)}_{n_1,n_2}$, the eigenvectors of $h_K^\dagger$. We have

$$h_K^\dagger \Phi^{(\pm)}_{n_1,n_2} = E^{(\pm)}_{n_1,n_2} \Phi^{(\pm)}_{n_1,n_2}, \tag{17}$$

where

$$\Phi^{(\pm)}_{n_1,n_2} = \tilde{\gamma}^{(\pm)}_{n_1,n_2} \begin{pmatrix} \Psi_{n_1,n_2} \\ \mp i\,\Psi_{n_1,n_2-1} \end{pmatrix}, \tag{18}$$

for all $n_1, n_2 \geq 0$. As before $\Psi_{n_1,-1} \equiv 0$. The normalizing factor $\tilde{\gamma}^{(\pm)}_{n_1,n_2}$ must be chosen, together with $\gamma^{(\pm)}_{n_1,n_2}$, in such a way that

$$\left\langle \eta^{(k)}_{n_1,n_2}, \Phi^{(l)}_{m_1,m_2} \right\rangle_2 = \delta_{n_1,m_1}\delta_{n_2,m_2}\delta_{k,l}, \tag{19}$$

where $n_1, n_2, m_1, m_2 \in \mathbb{N}_0$, $k, l = \pm$. This is satisfied if $\overline{\gamma_{n_1,0}}\tilde{\gamma}_{n_1,0} = 1$ and if, for $n_2 \geq 1$, $2\overline{\gamma_{n_1,n_2}}^{(\pm)}\tilde{\gamma}^{(\pm)}_{n_1,n_2} = 1$. For simplicity we choose $\gamma_{n_1,0} = \tilde{\gamma}_{n_1,0} = 1$, and $\gamma_{n_1,n_2} = \tilde{\gamma}_{n_1,n_2} = \frac{1}{\sqrt{2}}$, for $n_2 \geq 1$. Now, calling $\mathscr{F}_\Phi = \{\Phi^{(\pm)}_{n_1,n_2},\ n_1, n_2 \geq 0\}$, this set is biorthogonal to $\mathscr{F}_\eta$ and, under suitable conditions that we will discuss below, produces, together with $\mathscr{F}_\eta$, a resolution of the identity:

$$\sum_{n_1,n_2=0}^{\infty}\sum_{k=\pm}\left\langle \eta^{(k)}_{n_1,n_2}, f\right\rangle_2 \Phi^{(k)}_{n_1,n_2} = \sum_{n_1,n_2=0}^{\infty}\sum_{k=\pm}\left\langle \Phi^{(k)}_{n_1,n_2}, f\right\rangle_2 \eta^{(k)}_{n_1,n_2} = f, \tag{20}$$

for all $f \in \mathscr{H}_2$, or for some subset of $\mathscr{H}_2$. In fact, it is not hard to check that these equalities hold in all of $\mathscr{H}_2$ if, for instance, $\mathscr{F}_\eta$ and $\mathscr{F}_\Phi$ are biorthogonal Riesz bases while, in other situations, they are only true in suitable subspaces of $\mathscr{H}_2$.

3.1 A Slight Refinement of the Framework

It has been shown in [6] that, under suitable conditions, mostly related to the unboundedness of the operators involved in the game, pseudo-bosonic operators are related to truly bosonic creation and annihilation operators by some similarity map. This motivates our next step. In this section we assume that (a_j, b_j) are related to the operators $(A_j, A_j^\dagger)$ introduced in Sect. 2 by means of an operator S which we assume to be self-adjoint and invertible, not necessarily bounded or with bounded inverse. Moreover we assume that S and S^{-1} both map $\mathscr{D}$ into itself. Hence, our working hypothesis is that

$$a_j f = SA_j S^{-1} f, \quad b_j f = SA_j^\dagger S^{-1} f, \tag{21}$$

for all $f \in \mathscr{D}, j = 1, 2$.

Remark: It is worth noticing that the right hand sides of these equalities make sense whenever $\mathscr{D}$ is also invariant under the action of $A_j^\sharp$, because, for instance, since $f \in \mathscr{D}$, $S^{-1}f \in \mathscr{D}$ as well. Therefore, $A_j^\sharp S^{-1} f \in \mathscr{D}$, hence $SA_j^\sharp S^{-1} f \in \mathscr{D}$. This is in agreement with the fact that both $a_j f$ and $b_j f$ belong to $\mathscr{D}$.

We can now compute the adjoint of a_j and b_j which turn out to satisfy the following equalities:

$$a_j^\dagger f = S^{-1} A_j^\dagger S f, \quad b_j^\dagger f = S^{-1} A_j S f,$$

for all $f \in \mathscr{D}, j = 1, 2$. Then, by induction on n_1 and n_2, one can prove that the sets $\mathscr{E}$, $\mathscr{F}_\varphi$ and $\mathscr{F}_\Psi$ are related by S in the following way:

$$\varphi_{n_1,n_2} = Se_{n_1,n_2}, \quad \Psi_{n_1,n_2} = S^{-1}e_{n_1,n_2}, \tag{22}$$

for all $n_1, n_2 \in \mathbb{N}_0$. Then we can prove the following

Proposition 1 *(1) Assume S and S^{-1} are both bounded. Then $\mathscr{F}_\varphi$ and $\mathscr{F}_\Psi$ are biorthogonal Riesz bases in $\mathscr{H}$.*

(2) Assume that S or S^{-1}, or both, are unbounded. Then $\mathscr{F}_\varphi$ and $\mathscr{F}_\Psi$ are biorthogonal $\mathscr{D}$-quasi bases.

Proof (1) This is essentially the definition of Riesz basis, recalling that $\mathscr{E}$ is an o.n. basis for $\mathscr{H}$.

(2) Let $f, g \in \mathscr{D}$. Then

$$\langle f, g\rangle = \left\langle S^{-1}f, Sg\right\rangle = \sum_{n_1,n_2=0}^{\infty} \left\langle S^{-1}f, e_{n_1,n_2}\right\rangle \left\langle e_{n_1,n_2}, Sg\right\rangle$$

$$= \sum_{n_1,n_2=0}^{\infty} \left\langle f, S^{-1}e_{n_1,n_2}\right\rangle \left\langle Se_{n_1,n_2}, g\right\rangle = \sum_{n_1,n_2=0}^{\infty} \left\langle f, \Psi_{n_1,n_2}\right\rangle \left\langle \varphi_{n_1,n_2}, g\right\rangle.$$

Analogously one can prove that $\langle f, g\rangle = \sum_{n_1,n_2=0}^{\infty} \left\langle f, \varphi_{n_1,n_2}\right\rangle \left\langle \Psi_{n_1,n_2}, g\right\rangle$. Hence, see (A.71), $\mathscr{F}_\varphi$ and $\mathscr{F}_\Psi$ are $\mathscr{D}$-quasi bases. Biorthogonality is obvious.

It is now useful to introduce the operator $S_2 = \begin{pmatrix} S & 0 \\ 0 & S \end{pmatrix}$, acting on $\mathscr{H}_2$. Of course, S_2 can be inverted and its inverse is $S_2^{-1} = \begin{pmatrix} S^{-1} & 0 \\ 0 & S^{-1} \end{pmatrix}$. Also, we call $\mathscr{D}_2$ the following dense subset of $\mathscr{H}_2$:

$$\mathscr{D}_2 = \left\{ f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, f_1, f_2 \in \mathscr{D} \right\}.$$

It turns out that $\mathscr{D}_2$ is stable under the action of S_2 and S_2^{-1}, as well as of all the two-by-two matrices with entries which are polynomials in $a_j^\sharp$ and $b_j^\sharp$. Moreover, with our previous choice of normalization, we have

$$\eta^{(\pm)}_{n_1,n_2} = S_2 \nu^{(\pm)}_{n_1,n_2}, \quad \Phi^{(\pm)}_{n_1,n_2} = S_2^{-1} \nu^{(\pm)}_{n_1,n_2}, \tag{23}$$

for all $n_1, n_2 \geq 0$. Now, the nature of $\mathscr{F}_\eta$ and $\mathscr{F}_\Phi$ is driven by the nature of S_2 which, in turns, is driven by S itself. In fact, given an operator X on $\mathscr{H}$ and the operator X_2 on $\mathscr{H}_2$ defined as $X_2 = \begin{pmatrix} X & 0 \\ 0 & X \end{pmatrix}$, it is easy to check that X is bounded in $\mathscr{H}$ if and only if X_2 is bounded in $\mathscr{H}_2$.

Then it is easy to extend Proposition 1:

Proposition 2 *(1) Assume S and S^{-1} are both bounded. Then $\mathcal{F}_\eta$ and $\mathcal{F}_\Phi$ are biorthogonal Riesz bases in $\mathcal{H}_2$.*

(2) Assume that S or S^{-1}, or both, are unbounded. Then $\mathcal{F}_\eta$ and $\mathcal{F}_\Phi$ are biorthogonal $\mathcal{D}_2$-quasi bases.

The proof is not particularly different from that of the previous Proposition, and will not be given here. Let us now introduce two operators Θ_η and Θ_Φ as follows:

$$D(\Theta_\eta) = \left\{ f \in \mathcal{H}_2 : \sum_{n_1,n_2,k} \left\langle \eta^{(k)}_{n_1,n_2}, f \right\rangle_2 \eta^{(k)}_{n_1,n_2} \in \mathcal{H}_2 \right\},$$

$$D(\Theta_\Phi) = \left\{ g \in \mathcal{H}_2 : \sum_{n_1,n_2,k} \left\langle \Phi^{(k)}_{n_1,n_2}, g \right\rangle_2 \Phi^{(k)}_{n_1,n_2} \in \mathcal{H}_2 \right\},$$

and

$$\Theta_\eta f = \sum_{n_1,n_2,k} \left\langle \eta^{(k)}_{n_1,n_2}, f \right\rangle_2 \eta^{(k)}_{n_1,n_2}, \quad \Theta_\Phi f = \sum_{n_1,n_2,k} \left\langle \Phi^{(k)}_{n_1,n_2}, f \right\rangle_2 \Phi^{(k)}_{n_1,n_2}, \tag{24}$$

for all $f \in D(\Theta_\eta)$ and $g \in D(\Theta_\Phi)$. Then

Lemma 1 *If S and S^{-1} are bounded in $\mathcal{H}$ then $D(\Theta_\eta) = D(\Theta_\Phi) = \mathcal{H}_2$, and $\Theta_\eta = S_2$, $\Theta_\Phi = S_2^{-1}$.*

On the other hand, if S or S^{-1}, or both, are unbounded, neither $D(\Theta_\eta)$ nor $D(\Theta_\Phi)$ need to coincide with $\mathcal{H}_2$. However, they are both dense in $\mathcal{H}_2$. In fact, let us introduce the sets $\mathcal{L}_\Phi = \text{linear span}\{\Phi^{(\pm)}_{n_1,n_2}\}$ and $\mathcal{L}_\eta = \text{linear span}\{\eta^{(\pm)}_{n_1,n_2}\}$. These sets are dense in $\mathcal{H}_2$ at least if both $\mathcal{F}_\eta$ and $\mathcal{F}_\Phi$ are complete[1] in $\mathcal{H}_2$. We will always assume completeness of the sets $\mathcal{F}_\varphi$ and $\mathcal{F}_\Psi$ in $\mathcal{H}$, which in turns implies completeness of $\mathcal{F}_\eta$ and $\mathcal{F}_\Phi$ in $\mathcal{H}_2$, since, in our knowledge, this has always been observed in all the examples discussed in the literature so far.

A straightforward computation shows that $a_j f = S^2 b_j^\dagger S^{-2} f$, for all $f \in \mathcal{D}$ and $j = 1, 2$. Hence [5], $(a_j, b_j^\dagger)$ are S^{-2}-conjugate. And in fact, in agreement with [5], we can easily check that $\Psi_{n_1,n_2} = S^{-2}\varphi_{n_1,n_2}$ for all $n_1, n_2 \geq 0$. Of course, S^{-2} is positive. These results can be easily extended to $\mathcal{H}_2$, by introducing

$$a = \begin{pmatrix} a_1 & 0 \\ 0 & a_2 \end{pmatrix}, \quad b = \begin{pmatrix} b_1 & 0 \\ 0 & b_2 \end{pmatrix}.$$

In fact we can check that $(a, b^\dagger)$ are S_2^{-2} conjugate and, therefore, $\Phi^{(\pm)}_{n_1,n_2} = S_2^{-2}\eta^{(\pm)}_{n_1,n_2}$, for all $n_1, n_2 \geq 0$. Finally, it is a simple consequence of what we have discussed so far

[1] We remind that, for a non o.n. set, being complete is *less* than being a basis. In the mathematical and physical literature it is easy to find examples of sets which are complete in a certain Hilbert space, but which are not bases. Examples are given in [6].

that Θ_η and Θ_Φ behave as intertwining operators between h_K and $h_K^\dagger$ in the following sense:

$$\left(\Theta_\Phi h_k - h_K^\dagger \Theta_\Phi\right) \eta^{(\pm)}_{n_1,n_2} = 0, \quad \left(h_k \Theta_\eta - \Theta_\eta h_K^\dagger\right) \Phi^{(\pm)}_{n_1,n_2} = 0 \tag{25}$$

These equalities can be extended clearly respectively to $\mathscr{L}_\eta$ and $\mathscr{L}_\Phi$, but not, in general, to all of $\mathscr{H}_2$.

Remark: As discussed in the literature on PT quantum mechanics [4], the operators Θ_η and Θ_Φ could be used to define new scalar products in $\mathscr{H}_2$ (see also [6]). However, this aspect of the model is not interesting for us here and will not be considered further in this paper.

3.2 Some Explicit Choices of $\mathscr{D}$-PBs

We consider now some explicit choices of the operator S in (21) and discuss what happens in two cases. In the first case, we take an unbounded operator S. This will produce biorthogonal sets which are not bases, but appear to be quasi-bases on some suitable dense subset of $\mathscr{H}$. After this we will consider the case in which S is bounded, so that $\mathscr{F}_\varphi$ and $\mathscr{F}_\Psi$ are biorthogonal Riesz bases, and we discuss also possible extensions of this particular choice.

3.2.1 A Shift Map

Let us consider the unitary operator $D_j(z_j) = \exp\left\{\overline{z_j} A_j - z_j A_j^\dagger\right\}$, with $j = 1, 2$ and z_j a complex variable. Then, let us put $D(\underline{z}) = D_1(z_1)D_2(z_2) = D_2(z_2)D_1(z_1)$. This is still unitary. It is well known that they act as shift operators on the A_j and $A_j^\dagger$:

$$D(\underline{\gamma})A_j D^{-1}(\underline{\gamma}) = A_j + \gamma_j, \quad D(\underline{\nu})A_j^\dagger D^{-1}(\underline{\nu}) = A_j^\dagger + \overline{\nu_j}.$$

Now, it has been shown in [9] that, calling $a_j = A_j + \gamma_j$ and $b_j = A_j^\dagger + \overline{\nu_j}$, these can be written as in (21):

$$\begin{cases} a_j = V(\underline{\gamma}, \underline{\nu})A_j V^{-1}(\underline{\gamma}, \underline{\nu}), \\ b_j = V(\underline{\gamma}, \underline{\nu})A_j^\dagger V^{-1}(\underline{\gamma}, \underline{\nu}), \end{cases} \tag{26}$$

where

$$V_j(\gamma_j, \nu_j) = e^{\frac{1}{2}\gamma_j(\overline{\nu}_j - \overline{\gamma}_j)} e^{(\overline{\nu}_j A_j - \gamma_j A_j^\dagger)}, \quad V(\underline{\gamma}, \underline{\nu}) = V_1(\gamma_1, \nu_1)V_2(\gamma_2, \nu_2).$$

This allows us to identify S in (21) with the operator $V(\underline{\gamma}, \underline{\nu})$, which is unbounded with unbounded inverse. Now, defining the following dense subspace of $\mathscr{H}$,

$$\mathscr{D} = \left\{f(x_1, x_2) \in \mathscr{S}(\mathbb{R}^2), \text{ such that } e^{k_1 x_1 + k_2 x_2} f(x_1, x_2) \in \mathscr{S}(\mathbb{R}^2), \ \forall k_1, k_2 \in \mathbb{C}\right\},$$

we can prove the following results, most of which are just simple applications of what has already been proved in [9]:

1. $\mathscr{D}$ is stable under the action of $a_j^\sharp$ and $b_j^\sharp$.
2. $\mathscr{D}$ contains the vacuum states $\varphi_{0,0}$ of (a_1, a_2), $\Psi_{0,0}$ of $(b_1^\dagger, b_2^\dagger)$, and $e_{0,0}$ of (A_1, A_2).
3. As a simple consequence of these facts, defining the vectors φ_{n_1,n_2}, Ψ_{n_1,n_2} and e_{n_1,n_2} as shown before, and the related sets $\mathscr{F}_\varphi$, $\mathscr{F}_\Psi$ and $\mathscr{E}$, they are all in $\mathscr{D}$. Also, $\mathscr{E}$ is an o.n. basis for $\mathscr{H}$.
4. Since $\varphi_{n_1,n_2} = V(\underline{\gamma}, \underline{\nu})e_{n_1,n_2}$ and $\Psi_{n_1,n_2} = N_\Psi V(\underline{\nu}, \underline{\gamma})e_{n_1,n_2}$, with N_Ψ a normalization factor ensuring that $\langle \varphi_{0,0}, \Psi_{0,0}\rangle = 1$, the sets $\mathscr{F}_\varphi$, $\mathscr{F}_\Psi$ are not Riesz bases. This follows from the unboundedness of the operator $V(\underline{\gamma}, \underline{\nu})$.
5. $\mathscr{F}_\varphi$, $\mathscr{F}_\Psi$ are not even bases. Still, they are $\mathscr{D}$-quasi bases.

Calling now [9],

$$\Theta(\underline{\gamma}, \underline{\nu}) = \prod_{j=1}^{2} e^{|\gamma_j|^2 - |\nu_j|^2} e^{A_j(\overline{\gamma}_j - \overline{\nu}_j)} e^{A_j^\dagger(\gamma_j - \nu_j)},$$

which is proportional to the operator $V(\underline{\gamma}, \underline{\nu})$, it is clear that $\Theta(\underline{\gamma}, \underline{\nu})$ is unbounded, with unbounded inverse, positive on $\mathscr{D}$, and maps $\mathscr{F}_\varphi$ into $\mathscr{F}_\Psi$: $\Psi_{n_1,n_2} = \Theta(\underline{\gamma}, \underline{\nu})\varphi_{n_1,n_2}$. Moreover, $(a_j,\ b_j^\dagger)$ turn out to be $\Theta(\underline{\gamma}, \underline{\nu})$-conjugate: $a_j f = \Theta^{-1}(\underline{\gamma}, \underline{\nu})b_j\Theta(\underline{\gamma}, \underline{\nu})f$, for all $f \in \mathscr{D}$, and for the same f we conclude that $N_j f = \Theta^{-1}(\underline{\gamma}, \underline{\nu})N_j^\dagger\Theta(\underline{\gamma}, \underline{\nu})f$.

As Proposition 2 shows, similar results can be deduced for $\mathscr{H}_2$, introducing first $\mathscr{D}_2$, S_2 and the other operators needed in our framework.

Remark: From a physical point of view, our present deformation of the model just corresponds to going from the Hamiltonian in (2) to

$$h_K = v_F \begin{pmatrix} 0 & p_x - ip_y + \frac{eB}{2}(y + ix) + \frac{2i}{\xi}\overline{\nu_2} \\ p_x + ip_y + \frac{eB}{2}(y - ix) - \frac{2i}{\xi}\gamma_2 & 0 \end{pmatrix} = H_k + \delta h_K,$$

where

$$\delta h_K = v_F \begin{pmatrix} 0 & \frac{2i}{\xi}\overline{\nu_2} \\ -\frac{2i}{\xi}\gamma_2 & 0 \end{pmatrix}.$$

The Hamiltonian h_K is manifestly not self-adjoint, if δh_K is not zero or if $\nu_2 \neq \gamma_2$. Moreover, the eigenvectors of h_K and of $h_K^\dagger$ are shifted versions of the functions $e_{n_1,n_2}(x, y)$. It is interesting to stress that the presence of ν_2 and γ_2 in the Hamiltonian does not change the values of the eigenvalues, which are still real.

3.2.2 A Bounded Transformation

Let P be an orthogonal projection on $\mathscr{H}$: $P = P^\dagger = P^2$, and let us define the bounded operator $S := \mathbb{1} + iP$, already introduced in [10]. This operator is invertible and the

inverse is $S^{-1} = \mathbb{1} - \frac{i+1}{2} P$, which is also bounded. Hence, defining $\varphi_{n_1,n_2} := S e_{n_1,n_2}$ and $\Psi_{n_1,n_2} = (S^{-1})^\dagger e_{n_1,n_2}$, the sets $\mathscr{F}_\varphi = \{\varphi_{n_1,n_2}\}$ and $\mathscr{F}_\Psi = \{\Psi_{n_1,n_2}\}$ are biorthogonal Riesz bases. We consider here the simplest situation, i.e. that in which P is just the projector on $e_{0,0}$: $Pf = \langle e_{0,0}, f\rangle e_{0,0}$, for all $f \in \mathscr{H}$. In Dirac notation, $P = |e_{0,0}\rangle\langle e_{0,0}|$. Then $\varphi_{n_1,n_2} = e_{n_1,n_2}$ if n_1 or n_2, or both, are different from zero. On the other hand, we find that $\varphi_{0,0} = (1+i)e_{0,0}$. Analogously we find that $\Psi_{0,0} = \frac{1+i}{2} e_{0,0}$, while all the other vectors Ψ_{n_1,n_2} again coincide with the e_{n_1,n_2}. Hence, because of the really simple choice of P, going from the original basis to the two Riesz bases corresponds just to a change of normalization in the first vector.

Despite of this simplicity, the form of h_K appears to be significantly different from the original Hamiltonian H_K. In fact, since $A_2 Pf = PA_2^\dagger f = 0$ for all $f \in \mathscr{H}$, it is easy to check that $a_2 f = A_2 f + i\langle e_{0,1}, f\rangle e_{0,0}$ and that $b_2 f = A_2^\dagger f - \frac{i+1}{2}\langle e_{0,0}, f\rangle e_{0,1}$, for all $f \in \mathscr{H}$. This means that h_K can be rewritten as follows:

$$h_K = \frac{2iv_F}{\xi}\begin{pmatrix} 0 & A_2^\dagger - \frac{i+1}{2}|e_{0,1}\rangle\langle e_{0,0}| \\ -\left(A_2 + i|e_{0,0}\rangle\langle e_{0,1}|\right) & 0 \end{pmatrix} = H_K + \delta h_K,$$

where

$$\delta h_K = \frac{2iv_F}{\xi}\begin{pmatrix} 0 & -\frac{i+1}{2}|e_{0,1}\rangle\langle e_{0,0}| \\ -i|e_{0,0}\rangle\langle e_{0,1}| & 0 \end{pmatrix}.$$

With respect to the previous example, which only involve two different translations in the off diagonal terms of H_K, this Hamiltonian looks maybe more interesting, at least mathematically, since the breaking of the hermiticity is due to the presence of two different rank one operators out of the main diagonal.

It is not hard to imagine how this example can be generalized. In fact, it is enough to replace P as introduced here with a different projection operator $P_u f = \langle u, f\rangle u$, where u is some (finite) normalized linear combination of the vectors of $\mathscr{E}$. In this case what we expect is that the form of δh_K, and those of $\mathscr{F}_\varphi$ and $\mathscr{F}_\Psi$, become more complicated. In particular, the off diagonal terms of δh_K should be replaced by some finite linear combination of rank one operators $|e_{n_1,n_2}\rangle\langle e_{m_1,m_2}|$, for suitable n_j and m_j.

We hope to return on the physical meaning of this and similar transformations in some future paper.

4 The SUSY-QM Framework

Since the end of the nineteenth century, the Darboux method [11] for constructing pairs of systems connected through an isospectrality condition has been a widely used tool in mathematics and mathematical physics (see, for instance, [12] and references therein). Isospectral deformations and the factorization method have been considered, among others, also in the context of quantum mechanics [13]. Nowadays, they

represent the fundamental issues underlying the so-called Supersymmetric Quantum Mechanics (SUSY-QM). In particular, the possibility of arranging the Schrödinger Hamiltonian operators into isospectral pairs (SUSY partners) has been noticed by Witten in [14] and, since then, the SUSY-QM framework attracted the attention of several researchers, and an exhaustive classification of factorizable potentials is now available.

Another input in this respect has been represented by a work of Mielnik [15], who used a factorization through which the general SUSY partner for the oscillator was found by considering the general, rather than a particular, solution to the Riccati type equation underlying the problem. Right after, the technique was applied by Fernandez [16] for devising a one-parameter family of new exactly solvable radial potentials isospectral to the hydrogen-like radial one. All the forthcoming developments generated a revival of interest for the factorization method and for related algebraic methods. Among the others, SUSY-QM partners of time-dependent quadratic Hamiltonian unitarily linked to stationary spectral problems have been treated in [17]. Another remarkable aspect is that an intriguing consequence of the application of a Darboux transformation of first order to the problem of a stationary quantum particle subjected to a given potential stands into the subtraction from the energy spectrum of its lowest level [18]. Even more appealing, the application of higher order Darboux transformations introduces flexibility in the way the energy spectrum can be managed [19]. Because of that, the devising of quantum systems with somewhat pre-planned features is widely stimulated.

Because of these reasons, in this section we briefly discuss a possible SUSY-related extension of the Hamiltonian in (5), extension which somehow complements the one discussed in the previous section. For the reader's convenience, we briefly recall in the next section a few facts on SUSY-QM and then apply these results to graphene.

4.1 First Order SUSY-QM

The main idea underlying the SUSY-QM framework is the use of inverse factorization of a given Hamiltonian operator to define a new Hamiltonian operator. That is, one deals with two Hamiltonians

$$H_i(x) = -\frac{1}{2}\frac{d^2}{dx^2} + V_i(x) \quad i = 0, 1 \tag{27}$$

factorized as

$$H_0(x) + k = AA^\dagger + \epsilon, \quad H_1(x) = A^\dagger A + \epsilon, \tag{28}$$

where k and ϵ are constants and $A(x)$ is a first order differential operator

$$A(x) = \frac{1}{\sqrt{2}}\left[\frac{d}{dx} + \alpha(x)\right]. \tag{29}$$

The operator $A(x)$ is also called *intertwining operator*, as it links the two Hamiltonians through the relation[2]

$$H_1 A^\dagger = A^\dagger (H_0 + k)\,. \tag{33}$$

The intertwining relation (33) implies a constraint for $\alpha(x)$ in the form of a Riccati-type equation. In the case where the starting Hamiltonian is the one dimensional harmonic oscillator, $V_0(x) = \frac{x^2}{2}$, the Riccati equation satisfied by $\alpha(x)$ is

$$x^2 = \alpha'(x) + \alpha^2(x) + 2\gamma, \qquad \gamma = \epsilon - k, \tag{34}$$

and the isospectral potential is

$$V_1(x) = \frac{\alpha^2(x)}{2} - \frac{\alpha'(x)}{2} + \epsilon. \tag{35}$$

Equation (34) can be turned into a confluent hypergeometric equation after two changes of variables. First we set

$$\alpha(x) = \frac{u'(x)}{u(x)}, \tag{36}$$

so that (34) becomes

$$-u''(x) + x^2\, u(x) = 2\,\gamma\, u(x), \tag{37}$$

and then we introduce another variable,

$$u(x) = e^{-\frac{x^2}{2}} h(x), \tag{38}$$

that satisfies the equation

$$h''(x) - 2xh'(x) + (2\gamma - 1)h(x) = 0, \tag{39}$$

---

[2] In order to connect the intertwining technique with the supersymmetric quantum mechanics introduced by Witten [14], we should define the standard SUSY algebra

$$[Q_i,\, H_{SS}] = 0, \quad \{Q_i\,,\, Q_j\} = \delta_{ij} H_{SS}, \quad i, j = 1, 2, \tag{30}$$

where $[.\,,\,.]$ and $\{.\,,\,.\}$ represent the commutator and the anticommutator, in the following way

$$Q = \begin{pmatrix} 0 & 0 \\ A & 0 \end{pmatrix}, \quad Q^\dagger = \begin{pmatrix} 0 & A^\dagger \\ 0 & 0 \end{pmatrix}, \tag{31}$$

$$Q_1 = \frac{Q^+ + Q}{\sqrt{2}}, \quad Q_2 = \frac{Q^+ - Q}{\sqrt{2}\,i}, \quad H_{SS} = \begin{pmatrix} H^+ = A\,A^\dagger & 0 \\ 0 & H_- = A^\dagger A \end{pmatrix}. \tag{32}$$

.

whose solution is

$$h(x) = c_1\, F_{1,1}\left(\frac{2\gamma}{4},\, \frac{1}{2},\, x^2\right) + c_2\, x\, F_{1,1}\left(\frac{2\gamma}{4} + \frac{1}{2},\, \frac{3}{2},\, x^2\right). \tag{40}$$

In Appendix 2 we discuss a particular class of solutions for $\gamma = -p - \frac{1}{2}$.

For a fixed value of γ , the *superpotential* function

$$\alpha(x) = -x + \frac{h'(x)}{h(x)} \tag{41}$$

defines therefore the new class of potentials $V_1(x)$

$$V_1(x) = \frac{x^2}{2} + \frac{h'^2(x) - 2\,x\,h'(x)\,h(x)}{h^2(x)} + 2\,\epsilon - k \tag{42}$$

that depends on four parameters $(c_1,\, c_2,\, k,\, \epsilon)$.

If ψ_+ is eigenstate of H^+ with eigenvalue E_+,

$$A\,A^\dagger\,\psi^+ = E^+\psi^+, \tag{43}$$

by multiplying to the left equation (43) by $A^\dagger$, we have

$$H^-\psi^- = E^+\psi^-, \tag{44}$$

where we have defined $\psi^- = A^+\psi^+$. That is, ψ^- is an eigenstate of H^- with eigenvalue E^+. If $\psi_0^{(n)}$ are eigenstates of $H_0 = \frac{1}{2}(x^2 - \frac{d}{dx}^2)$ with eigenvalues $E_n = n + \frac{1}{2},\, n = 0,\, 1,\, 2\ldots$, the states

$$\psi_1^{(n)} = \frac{A^\dagger\psi_0^{(n)}}{\sqrt{E_n + k - \epsilon}} \tag{45}$$

are normalized eigenstates of H_1 with eigenvalues $E_n + k$. Since the annihilation operator A depends on the standard Harmonic oscillator annihilation operator a according to

$$A(x) = a(x) + \frac{1}{\sqrt{2}}\left(\frac{h'(x)}{h(x)} - 2x\right), \tag{46}$$

then

$$A(x) = \frac{1}{\sqrt{2}}\frac{h'(x)}{h(x)} - a(x), \quad A^\dagger(x) = \frac{1}{\sqrt{2}}\frac{h'(x)}{h(x)} - a^\dagger(x), \tag{47}$$

and the eigenstates of the Hamiltonian H_1 are linked each to the others via

$$\psi_1^{(n)} = \frac{1}{2\sqrt{E_n + k - \epsilon}} \frac{h'(x)}{h(x)} \psi_0^{(n)} - \frac{\sqrt{n}}{\sqrt{E_n + k - \epsilon}} \psi_0^{(n)}. \tag{48}$$

Moreover, if $\psi_+^{(0)}$ is the ground state for H_+, it solves the first order differential equation $A\,\psi_+^{(0)} = 0$, so that the state

$$\psi_+^{(0)} = e^{-\int_0^x \alpha_\gamma(x_1)\,dx_1} = \frac{e^{\frac{x^2}{2}}}{h(x)} \tag{49}$$

is another eigenstate of H_1 with eigenvalue ϵ. Of course, for being well-defined, the solutions $h(x)$ need to be selected among those without zeros. Hence, the SUSY spectral problem is solved in terms of the eigenstates

$$\left\{\psi_+^{(0)},\ \psi_1^{(n)}\right\}_{n=0,1,2...} \tag{50}$$

with eigenvalues

$$\{\epsilon,\ E_n + k\}_{n=0,1,2...}\,. \tag{51}$$

4.2 SUSY Deformation of the Graphene Hamiltonian

The objective here is to find a isospectral deformation of the Hamiltonian defined in (5),

$$H_K^2 = \begin{pmatrix} A_2^\dagger A_2 & 0 \\ 0 & A_2 A_2^\dagger \end{pmatrix}. \tag{52}$$

(To simplify the notation we are omitting here and in the following the multiplicative factor $\frac{2v_F}{\xi}$). We can write the creation and annihilation operators $(A_2,\ A_2^\dagger)$ in terms of a new position coordinate, $X = \frac{1}{\sqrt{2}}(x + iy)$, as

$$A_2 = \frac{1}{\sqrt{2}}\left(X + \partial_X\right), \quad A_2^\dagger = \frac{1}{\sqrt{2}}\left(X - \partial_X\right). \tag{53}$$

If we call $H_0 = \frac{1}{2}(X^2 - \partial_X^2)$, we can see that

$$A_2^\dagger A_2 = H_0 - \frac{1}{2}, \quad A_2 A_2^\dagger = H_0 + \frac{1}{2}, \tag{54}$$

so that

$$A_2 A_2^\dagger = A_2^\dagger A_2 + 1. \tag{55}$$

The SUSY procedure can be applied here by introducing the superpotential α that satisfies (34) in the variable X. The standard creation-annihilation operators $(A_2,\ A_2^\dagger)$ are now deformed into the new operators

$$B_2 = \frac{1}{\sqrt{2}}\,(\alpha + \partial_X)\,, \quad B_2^\dagger = \frac{1}{\sqrt{2}}\,(\alpha - \partial_X) \tag{56}$$

such that

$$B_2\,B_2^\dagger \neq B_2^\dagger\,B_2 + k, \quad k = constant. \tag{57}$$

The new class of Hamiltonians isospectral to the Hamiltonian (52) can be constructed in the following form[3]

$$H_B = \begin{pmatrix} B_2^\dagger\,B_2 + \epsilon = H_1 & 0 \\ 0 & B_2\,B_2^\dagger + \epsilon = H_0 + k \end{pmatrix}. \tag{58}$$

By using the o.n. basis of the two dimensional harmonic oscillator e_{n_1,n_2} introduced in (6), we can define the vectors

$$\phi_{n_1,\,n_2} = \begin{pmatrix} \phi^+_{n_1,\,n_2} \\ \phi^-_{n_1,\,n_2} \end{pmatrix}, \quad \phi^+_{n_1,\,n_2} = \frac{B_2^\dagger\,e_{n_1,n_2}}{\sqrt{E_{n_2} + k - \epsilon}}, \quad \phi^-_{n_1,\,n_2} = e_{n_1,n_2}. \tag{59}$$

Since

$$H_1\,\phi^+_{n_1,\,n_2} = (E_{n_2} + k)\,\phi^+_{n_1,\,n_2}, \quad H_0\,\phi^-_{n_1,\,n_2} = E_{n_2}\,\phi^-_{n_1,\,n_2}, \tag{60}$$

we end up with the following result

$$H_B\,\phi_{n_1,\,n_2} = (E_{n_2} + k)\,\phi_{n_1,\,n_2}, \tag{61}$$

The new ground state is

$$\phi^{(0)}_{n_1\,n_2} = \begin{pmatrix} \psi^{(0)}_+ \\ 0 \end{pmatrix}, \quad H_B\,\phi^{(0)}_{n_1,\,n_2} = \epsilon\,\phi^{(0)}_{n_1,\,n_2}, \tag{62}$$

where $\psi^{(0)}_+$ is defined in (50).

Summarizing, as result of the SUSY deformation of the Hamiltonian H_k^2 defined in (52), we have obtained the new Hamiltonian H_B in (58), whose eigenvectors are $\{\phi^{(0)},\ \phi_{n_1,\,n_2}\}$ and eigenspectrum $\{\epsilon,\ E_{n_2} + k\}$. For $k = 0$, H_B is isospectral to H_k^2, in addition, its spectrum includes another eigenstate $\phi^{(0)}_{n_1\,n_2}$ with eigenvalue ϵ. We

[3]Note that (36) defining the superpotential $\alpha(X)$ can be expressed as a partial differential equation in the original variables (x, y):

$$x^2 + 2\,i\,x\,y - y^2 = \sqrt{2}\,\partial_x\,\alpha(x, y) - \sqrt{2}\,i\,\partial_y\,\alpha(x, y) + 2\,\alpha(x, y)^2 + 4\gamma.$$

.

hope to come back to the physical implications of this SUSY-deformed version of graphene in a future paper.

Remark: A step further can be done to perform a SUSY deformation of the Hamiltonian discussed in Sect. 3,

$$h_K^2 = \begin{pmatrix} \hat{n} & 0 \\ 0 & \mathbb{1} + \hat{n} \end{pmatrix}, \tag{63}$$

where $\hat{n} = b\,a$ and $[a,\ b] = 1$, but $b \neq a^\dagger$. The SUSY procedure results now in the following Hamiltonian

$$H_{PB} = \begin{pmatrix} \tilde{b}\,\tilde{a} + \epsilon = \tilde{H}_1 & 0 \\ 0 & \tilde{a}\tilde{b} + \epsilon = H_0 + k \end{pmatrix}. \tag{64}$$

Under the assumptions that $\tilde{a}$ and $\tilde{b}$ are first order differential operators in the variable x of the form $\tilde{a} = i\partial_x + \beta(x)$ and $\tilde{b} = i\partial_x - \beta(x)$, along with the constraint

$$x^2 = -i\beta'(x) - \beta^2(x) + \epsilon - k, \tag{65}$$

the isospectral potential can be written in terms of $\beta(x)$ as

$$\tilde{V}_1(x) = i\beta'(x) - \beta^2(x) - \epsilon, \tag{66}$$

and considerations regarding the spectrum and eigenstates of (64) are exactly the same as in the previous case (58).

5 Conclusions and Perspectives

We have discussed two alternative extensions of the graphene Hamiltonian close to the Dirac points. In particular, the first pseudo-bosonic deformed version leaves the eigenvalues unchanged, but it modifies significantly the eigenvectors of the Hamiltonian and of its adjoint, and their mathematical properties. The second deformation, arising from SUSY-QM, looks less friendly from the point of view of the explicit computations, but still produces interesting mathematics and, hopefully, interesting physics. However, the analysis of the possible physical consequences of the deformations considered here are postponed to a future paper.

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Appendix 1: $\mathscr{D}$-pseudo-bosons

We briefly review here a few facts and definitions about $\mathscr{D}$-PBs. More details can be found in [5, 6].

Let $\mathscr{H}$ be a given Hilbert space with scalar product $\langle .,. \rangle$ and related norm $\|.\|$. Let further a and b be two operators on $\mathscr{H}$, with domains $D(a)$ and $D(b)$ respectively, $a^\dagger$ and $b^\dagger$ their adjoints, and let $\mathscr{D}$ be a dense subspace of $\mathscr{H}$ such that $a^\sharp \mathscr{D} \subseteq \mathscr{D}$ and $b^\sharp \mathscr{D} \subseteq \mathscr{D}$, where $x^\sharp$ is x or $x^\dagger$. Of course, $\mathscr{D} \subseteq D(a^\sharp)$ and $\mathscr{D} \subseteq D(b^\sharp)$.

Definition 1 The operators (a, b) are called $\mathscr{D}$-pseudo bosonic ($\mathscr{D}$-pb) if, for all $f \in \mathscr{D}$, we have

$$a\,b\,f - b\,a\,f = f. \tag{A.67}$$

Our working assumptions are the following:

Assumption $\mathscr{D}$-pb 1. There exists a non-zero $\varphi_0 \in \mathscr{D}$ such that $a\,\varphi_0 = 0$.

Assumption $\mathscr{D}$-pb 2. There exists a non-zero $\Psi_0 \in \mathscr{D}$ such that $b^\dagger\,\Psi_0 = 0$.

Then, if (a, b) satisfy Definition 1, it is obvious that $\varphi_0 \in D^\infty(b) := \cap_{k\geq 0} D(b^k)$ and that $\Psi_0 \in D^\infty(a^\dagger)$, so that the vectors

$$\varphi_n := \frac{1}{\sqrt{n!}}\, b^n \varphi_0, \quad \Psi_n := \frac{1}{\sqrt{n!}}\, a^{\dagger n} \Psi_0, \tag{A.68}$$

$n \geq 0$, can be defined and they all belong to $\mathscr{D}$ and, as a consequence, to the domains of $a^\sharp$, $b^\sharp$ and $N^\sharp$, where $N = ba$. We further introduce $\mathscr{F}_\Psi = \{\Psi_n,\ n \geq 0\}$ and $\mathscr{F}_\varphi = \{\varphi_n,\ n \geq 0\}$.

It is now simple to deduce the following lowering and raising relations:

$$\begin{cases} b\,\varphi_n = \sqrt{n+1}\varphi_{n+1}, & n \geq 0, \\ a\,\varphi_0 = 0, \quad a\varphi_n = \sqrt{n}\,\varphi_{n-1}, & n \geq 1, \\ a^\dagger \Psi_n = \sqrt{n+1}\Psi_{n+1}, & n \geq 0, \\ b^\dagger \Psi_0 = 0, \quad b^\dagger \Psi_n = \sqrt{n}\,\Psi_{n-1}, & n \geq 1, \end{cases} \tag{A.69}$$

as well as the following eigenvalue equations: $N\varphi_n = n\varphi_n$ and $N^\dagger \Psi_n = n\Psi_n$, $n \geq 0$. In particular, as a consequence of these last equations, choosing the normalization of φ_0 and Ψ_0 in such a way $\langle \varphi_0, \Psi_0 \rangle = 1$, we deduce that

$$\langle \varphi_n, \Psi_m \rangle = \delta_{n,m}, \tag{A.70}$$

for all $n, m \geq 0$. The third assumption we introduced in [5] is the following:

Assumption $\mathscr{D}$-pb 3. $\mathscr{F}_\varphi$ is a basis for $\mathscr{H}$.

This is equivalent to the request that $\mathscr{F}_\Psi$ is a basis for $\mathscr{H}$ [6]. In particular, if $\mathscr{F}_\varphi$ and $\mathscr{F}_\Psi$ are Riesz bases for $\mathscr{H}$, we have called our $\mathscr{D}$-PBs *regular*. Since this

assumption is rarely satisfied in concrete models, we introduced in [5] a weaker version of Assumption $\mathscr{D}$-pb 3: for that, let $\mathscr{G}$ be a suitable dense subspace of $\mathscr{H}$. Two biorthogonal sets $\mathscr{F}_\eta = \{\eta_n \in \mathscr{G},\ g \geq 0\}$ and $\mathscr{F}_\Phi = \{\Phi_n \in \mathscr{G},\ g \geq 0\}$ have been called *$\mathscr{G}$-quasi bases* if, for all $f, g \in \mathscr{G}$, the following holds:

$$\langle f, g\rangle = \sum_{n\geq 0} \langle f, \eta_n\rangle \langle \Phi_n, g\rangle = \sum_{n\geq 0} \langle f, \Phi_n\rangle \langle \eta_n, g\rangle . \tag{A.71}$$

Is is clear that, while Assumption $\mathscr{D}$-pb 3 implies (A.71), the reverse is false. However, if $\mathscr{F}_\eta$ and $\mathscr{F}_\Phi$ satisfy (A.71), we still have some (weak) form of resolution of the identity. Now Assumption $\mathscr{D}$-pb 3 is replaced by the following:

Assumption $\mathscr{D}$-pbw 3. For some subspace $\mathscr{G}$ dense in $\mathscr{H}$, $\mathscr{F}_\varphi$ and $\mathscr{F}_\Psi$ are $\mathscr{G}$-quasi bases.

To refine further the structure, let us assume there exists a self-adjoint, invertible, operator Θ, which, together with Θ^{-1}, leaves $\mathscr{D}$ invariant: $\Theta\mathscr{D} \subseteq \mathscr{D}$, $\Theta^{-1}\mathscr{D} \subseteq \mathscr{D}$. Then we say that $(a, b^\dagger)$ are $\Theta-$conjugate if $af = \Theta^{-1} b^\dagger \Theta f$, for all $f \in \mathscr{D}$. One can prove that, if $\mathscr{F}_\varphi$ and $\mathscr{F}_\Psi$ are $\mathscr{D}$-quasi bases for $\mathscr{H}$, then the operators $(a, b^\dagger)$ are $\Theta-$conjugate if and only if $\Psi_n = \Theta\varphi_n$, for all $n \geq 0$. Moreover, if $(a, b^\dagger)$ are $\Theta-$conjugate, then $\langle f, \Theta f\rangle\rangle 0$ for all non zero $f \in \mathscr{D}$.

We refer to [6] for more results on $\mathscr{D}$-PBs.

Appendix 2: A Class of Potentials Isospectral to H_0

In this Appendix we briefly discuss a particular class of isospectral potential to the Harmonic oscillator Hamiltonian, given by the choice of the parameter γ in the confluent hypergeometric equation (39). Its solution will be expressed in terms of combinations of Hermite and Pseudo-Hermite polynomials [20].

For $\gamma = -\frac{1}{2} - p$, (40) becomes

$$h_p(x) = c_1 F_{1,1}\left(\frac{1+p}{2},\ \frac{1}{2},\ x^2\right) + c_2\, x\, F_{1,1}\left(\frac{2+p}{2},\ \frac{3}{2},\ x^2\right). \tag{A.72}$$

It is simple to show that

$$F_{1,1}\left(\frac{1+p}{2},\ \frac{1}{2},\ x^2\right) = \frac{\sqrt{\pi}}{2^p\ \Gamma\left(\frac{1+p}{2}\right)} \frac{d^p}{dx^p} e^{x^2}, \tag{A.73}$$

$$x\, F_{1,1}\left(\frac{2+p}{2},\ \frac{3}{2},\ x^2\right) = \frac{\sqrt{\pi}}{2^p p\ \Gamma\left(\frac{p}{2}\right)} \frac{d^p}{dx^p} \left(e^{x^2} \mathrm{Erf}\,(x)\right) \tag{A.74}$$

for p even, and

$$F_{1,1}\left(\frac{1+p}{2},\,\frac{1}{2},\,x^2\right)=\frac{\sqrt{\pi}}{2^p\,\Gamma\left(\frac{1+p}{2}\right)}\frac{d^p}{dx^p}\left(e^{x^2}\mathrm{Erf}(x)\right), \tag{A.75}$$

$$x\,F_{1,1}\left(\frac{2+p}{2},\,\frac{3}{2},\,x^2\right)=\frac{\sqrt{\pi}}{2^p p\,\Gamma\left(\frac{p}{2}\right)}\frac{d^p}{dx^p}\left(e^{x^2}\right), \tag{A.76}$$

for p odd. Equation (A.72) thus becomes

$$\begin{aligned}
h_{p_{even}}(x)&=\frac{\sqrt{\pi}}{2^p\,\Gamma\left(\frac{1+p}{2}\right)}\left(c_1\frac{d^p}{dx^p}e^{x^2}+c_2\frac{\Gamma\left(\frac{p+1}{2}\right)}{2\,\Gamma\left(\frac{p}{2}+1\right)}\frac{d^p}{dx^p}\left(e^{x^2}\mathrm{Erf}(x)\right)\right),\\
h_{p_{odd}}(x)&=\frac{\sqrt{\pi}}{2^p p\,\Gamma\left(\frac{p}{2}\right)}\left(c_2\frac{d^p}{dx^p}e^{x^2}+c_1\frac{\Gamma\left(\frac{p}{2}\right)}{\Gamma\left(\frac{1+p}{2}\right)}\frac{d^p}{dx^p}\left(e^{x^2}\mathrm{Erf}(x)\right)\right).
\end{aligned} \tag{A.77}$$

In view of the relations

$$\frac{d^p}{dx^p}e^{x^2}=e^{x^2}\mathscr{H}_p(x), \tag{A.78}$$

$$\frac{d^p}{dx^p}\left(e^{x^2}\mathrm{Erf}(x)\right)=e^{x^2}\mathrm{Erf}(x)\,\mathscr{H}_p(x)+\frac{2}{\sqrt{\pi}}\mathscr{P}_p(x), \tag{A.79}$$

Equation (A.77) can be cast as

$$\begin{aligned}
h_{p_{even}}(x)&=\left(c_1+c_2\frac{\Gamma\left(\frac{p+1}{2}\right)}{2\,\Gamma\left(\frac{p}{2}+1\right)}\mathrm{Erf}(x)\right)e^{x^2}\mathscr{H}_p(x)+c_2\frac{\Gamma\left(\frac{p+1}{2}\right)}{\sqrt{\pi}\,\Gamma\left(\frac{p}{2}+1\right)}\mathscr{P}_p(x),\\
h_{p_{odd}}(x)&=\left(c_2+c_1\frac{\Gamma\left(\frac{p}{2}\right)}{\Gamma\left(\frac{1+p}{2}\right)}\mathrm{Erf}(x)\right)e^{x^2}\mathscr{H}_p(x)+c_1\frac{2\,\Gamma\left(\frac{p}{2}\right)}{\sqrt{\pi}\,\Gamma\left(\frac{1+p}{2}\right)}\mathscr{P}_p(x),
\end{aligned} \tag{A.80}$$

where $\mathscr{H}_p(x)$ are defined as the Pseudo-Hermite polynomials [20] and $\mathscr{P}_p(x)$ are linear combination of the standard Hermite polynomials $H(x)$,

$$\mathscr{P}_p(x)=\sum_{k=1}^{p}(-1)^{k-1}\binom{p}{k}\sum_{i=0}^{p-k}\frac{2^i(p-k)!(p-1-i)!}{i!(p-k-i)!(p-1-2i)!}H_{p-1-2i}(x). \tag{A.81}$$

The polynomials $\mathscr{P}_p(x)$ are nodeless polynomials of degree $(p-1)$, odd/even if p is even/odd.[4] Remark that $\frac{d^p}{dx^p}\left(e^{x^2}\text{Erf}(x)\right)$ is nodeless for odd p, but it has a singularity at $x=0$ for even p, while $\frac{d^p}{dx^p}\left(e^{x^2}\right)$ is nodeless for even p, but it has a singularity at $x=0$ for odd p. The formulas above contain the classes of isospectral potentials discussed in the literature. For instance, the Mielink's result of [15] is recovered for $\epsilon=\frac{1}{2}$, $k=1$ and $p=0$ with the choice $c_2=1$ and $c_1=C_0^M$,

$$\alpha^M_{-\frac{1}{2}}(x)=x+\frac{e^{-x^2}}{C_0^M+\frac{\sqrt{\pi}}{2}\text{Erf}(x)} \tag{A.82}$$

(that (41) with $C_0^M=\frac{C_1}{C_2}$). Rational nodeless solutions are obtained for $c_2=0$ and even p, while they present a singularity in $x=0$ for odd p,

$$\begin{aligned} h_p(x)&=\frac{\sqrt{\pi}}{2^p\,\Gamma\left(\frac{1+p}{2}\right)}c_1e^{x^2}\mathscr{H}_p(x)\quad(\text{p even}),\\ h_p(x)&=\frac{\sqrt{\pi}}{2^p p\,\Gamma\left(\frac{p}{2}\right)}c_2e^{x^2}\mathscr{H}_p(x)\quad(\text{p odd}), \end{aligned} \tag{A.83}$$

the case of the class of solutions $\phi_p(x)=e^{\frac{x^2}{2}}(-i)^p\mathscr{H}_p(ix)$ recently discussed in [20] is recovered with the choice of the constants $c_1=\frac{2^p\,\Gamma\left(\frac{1+p}{2}\right)}{\sqrt{\pi}}$, $c_2=0$ for even values of p and $c_2=\frac{2^p\,p\,\Gamma\left(\frac{p}{2}\right)}{\sqrt{\pi}}$, $c_1=0$ for odd values of p. In particular, for even p

$$h_{2m}(x)=\frac{\sqrt{\pi}}{2^{2m}\,\Gamma\left(\frac{1+2m}{2}\right)}c_1e^{x^2}\mathscr{H}_{2m}(x) \tag{A.84}$$

and the isospectral Hamiltonian is

$$H_1(x)=-\frac{1}{2}\frac{d^2}{dx^2}+\frac{x^2}{2}+\frac{\mathscr{H}_{2m}'^2-\mathscr{H}_{2m}''\mathscr{H}_{2m}}{\mathscr{H}_{2m}^2}+k-1 \tag{A.85}$$

with ground state $\psi_+(x)=C_0\frac{e^{\frac{x^2}{2}}}{h_p(x)}=C_0\frac{e^{-\frac{x^2}{2}}}{\mathscr{H}_p(x)}$, where $C_0=\left[\frac{(2m)!2^m}{\sqrt{\pi}}\right]^{\frac{1}{2}}$ is a normalization constant. The spectrum obtained by selecting only the odd eigenstates of the harmonic oscillator is given by

[4]Examples are: $\mathscr{P}_1(x)=1$, $\mathscr{P}_2(x)=2x$, $\mathscr{P}_3(x)=4(1+x^2)$, $\mathscr{P}_4(x)=4(5x+2x^3)$, $\mathscr{P}_5(x)=8(4+9x^2+2x^4)$, and so on.

$$\psi_1^{(j)} = \left(\frac{2j+2}{2j+\frac{3}{2}+k-\epsilon}\right)^{\frac{1}{2}} \psi_0^{(2j+2)} + (4j+3+2k-2\epsilon)^{-\frac{1}{2}} \frac{\mathscr{H}'_{2m}(x)}{\mathscr{H}_{2m}(x)} \psi_0^{(2j+1)} \tag{A.86}$$

with eigenvalues $(2j+\frac{3}{2}+k)$ for $j=0,1\ldots,\ m=0,1\ldots,\ (k,\epsilon)\in\mathbb{R}$.

Another example is found in [21], where the authors studied the one-dimensional quantum system described by the potential

$$V_1^C(x) = \frac{x^2}{2} + \frac{4(2x^2-1)}{(2x^2+1)^2}. \tag{A.87}$$

It correspond to the choice $\epsilon=-\frac{3}{2},\ k=1, p=2,\ c=1,\ c_2=0$. The ground state $\psi_+ = \frac{2}{\sqrt{\pi}}\frac{e^{-\frac{x^2}{2}}}{(1+2x^2)}$ is well defined and the eigenstates $\psi_1^{(n)}$ with eigenvalues $(n+\frac{3}{2})$ are obtained for all n

$$\psi_1^{(n)} = \left(\frac{n+1}{n+3}\right)^{\frac{1}{2}} \psi_0^{(n+1)} + (2n+6)^{-\frac{1}{2}} \frac{4x}{1+2x^2}\psi_0^{(n)},\ n=0,1\ldots \tag{A.88}$$

The rational (odd p) and transcendental (even p) potentials obtained for $c_1=0$ possess a singularity in $x=0$,

$$h_p(x) = c_2\,|x|\,F_{1,1}\left(\frac{2+p}{2},\ \frac{3}{2},\ x^2\right), \tag{A.89}$$

$$\alpha_p(x) = \frac{1}{x} - x + \frac{2(p+2)}{3}x\frac{F_{1,1}\left[2+\frac{p}{2},\frac{5}{2},x^2\right]}{F_{1,1}\left[1+\frac{p}{2},\frac{3}{2},x^2\right]}. \tag{A.90}$$

The eigenstates of the isospectral Hamiltonian H_1 are then well defined only for odd values of the quantum number n. An example of such a rational and singular solution is given by the radial part ($l=1$) of the three-dimensional harmonic oscillator, recovered for $\epsilon=-\frac{1}{2},\ k=1\,(p=1),\ c_1=0,\ c_2=1$.[5] The hamiltonian

$$H_1(x) = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{x^2}{2} + \frac{1}{x^2} \tag{A.91}$$

[5]The spectral problem $\left(-\frac{1}{2}\frac{d^2}{dx^2}+\frac{x^2}{2}+\frac{1}{x^2}\right)\phi^{(n)} = \left(2n+\frac{5}{2}\right)\phi^{(n)}$ has solutions $\phi^{(n)} = \left(\frac{2\Gamma(n+1)}{\Gamma\left(\frac{5}{2}+n\right)}\right)^{\frac{1}{2}} x^2 e^{-\frac{x^2}{2}} L_n^{\frac{3}{2}}(x^2)$, where $L_n^a(x)$ are the generalized Laguerre polynomials.

isospectral to $H_0 + 1$, has eigenstates

$$\psi_1^{(n)} = \left(\frac{n+1}{n+2}\right)^{\frac{1}{2}} \psi_0^{(n+1)} + \frac{1}{x\sqrt{2n+4}}\psi_0^{(n)}, n = 1, 2 \ldots \tag{A.92}$$

but, to in order to avoid divergences, we have to consider only the ones corresponding to odd values of n

$$\psi_1^{(j)} = \left(\frac{2j+2}{2j+3}\right)^{\frac{1}{2}} \psi_0^{(2j+2)} + \frac{1}{x\sqrt{4j+6}}\psi_0^{(2j+1)}, \; j = 0, 1, 2 \ldots \tag{A.93}$$

with spectrum $2j + 5/2$.

Before concluding the section, it is in order to point out that it is simple to extend the previous results to the case $\Gamma = \frac{1}{2} + p$, in that it merely coincides with the same problem for $u_\gamma(x)$ up to the change of variable $y = ix$. Therefore, the general solution would be simply

$$\begin{aligned} u_p^-(x) = e^{\frac{x^2}{2}} & \left(c_1 \frac{1+(-1)^p}{2} \frac{\sqrt{\pi}}{2^p \, \Gamma\left(\frac{1+p}{2}\right)} + c_2 \frac{1-(-1)^p}{2} \frac{\sqrt{\pi}}{2^p \, p \, \Gamma\left(\frac{p}{2}\right)} \right) \frac{d^p}{dx^p} e^{-x^2} \\ & - \imath \, e^{\frac{x^2}{2}} \left(c_1 \frac{1-(-1)^p}{2} \frac{\imath\sqrt{\pi}}{2^p \Gamma\left(\frac{1+p}{2}\right)} + c_2 \frac{1+(-1)^p}{2} \frac{\sqrt{\pi}}{2^{p+1} \Gamma\left(\frac{2+p}{2}\right)} \right) \\ & \times \frac{d^p}{dx^p} \left(e^{-x^2} \mathrm{Erf}(-x) \right). \end{aligned}$$

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Localised Nonlinear Modes in the *PT*-Symmetric Double-Delta Well Gross-Pitaevskii Equation

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Abstract We construct exact localised solutions of the *PT*-symmetric Gross-Pitaevskii equation with an attractive cubic nonlinearity. The trapping potential has the form of two δ-function wells, where one well loses particles while the other one is fed with atoms at an equal rate. The parameters of the constructed solutions are expressible in terms of the roots of a system of two transcendental algebraic equations. We also furnish a simple analytical treatment of the linear Schrödinger equation with the *PT*-symmetric double-δ potential.

1 Introduction

We consider the Gross-Pitaevskii equation,

$$i\,\Psi_t + \Psi_{xx} - V(x)\Psi + g|\Psi|^2\Psi = 0, \tag{1}$$

with $g \geq 0$ and the *PT*-symmetric potential

$$V(x) = U(x) + iW(x), \qquad U(-x) = U(x), \quad W(-x) = -W(x). \tag{2}$$

The system (1)–(2) was employed to model the dynamics of the self-gravitating boson condensate trapped in a confining potential $U(x)$. The imaginary coefficient

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iW accounts for the particle leakage—in the region where $W(x) < 0$—and the compensatory injection of atoms in the region where $W(x) > 0$ [1, 2].

The same equation was used to describe the stationary light beam propagation in the self-focusing Kerr medium. In the optical context, t stands for the scaled propagation distance while Ψ is the complex electric-field envelope. The real part of the potential (U) is associated with the refractive index guiding, while the imaginary part (W) gives the optical gain and loss distribution [3].

We are interested in localised solutions of this equation, that is, solutions with the asymptotic behaviour $\Psi(x,t) \to 0$ as $x \to \pm\infty$. We also require that

$$\int_{-\infty}^{\infty} |\Psi|^2 dx = 1. \tag{3}$$

In the context of leaking condensate with injection, the normalisation condition (3) implies that the total number of particles in the condensate is kept at a constant level.

In this study, we consider stationary solutions of the form $\Psi(x,t) = \psi(x)e^{i\kappa^2 t}$, where κ^2 is real and the spatial part of the eigenfunction obeys

$$-\psi_{xx} + V(x)\psi - g\psi|\psi|^2 = -\kappa^2\psi. \tag{4}$$

Assuming that the potential satisfies $V(x) \to 0$ as $x \to \pm\infty$, the coefficient κ^2 has to be taken positive. For definiteness, we choose the real quantity κ to be positive as well. Equation (4) will be solved under the normalisation constraint

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1, \tag{5}$$

stemming from the condition (3).

Our study will be confined to the PT-symmetric solutions of equation (4), that is, solutions satisfying

$$\psi(-x) = \psi^*(x). \tag{6}$$

Typically, stationary solutions supported by PT-symmetric potentials can be brought to the form (6) by a suitable constant phase shift.

With an eye to the forthcoming study of the jamming anomaly [4], we consider a PT-symmetric potential of the special form:

$$V(x) = -(1 - i\gamma)\delta(x + L/2) - (1 + i\gamma)\delta(x - L/2). \tag{7}$$

Here $\gamma \geq 0$ and $L > 0$. The $V(x)$ is an idealised potential consisting of two infinitely deep wells. The right-hand well is leaking particles, while its left-hand counterpart is injected with atoms at an equal constant rate γ.

Previous analyses of the double-delta cubic Gross-Pitaevskii equation focused mainly on the situation with no gain or loss—that is, on the potential (7) with $\gamma = 0$. Using a combination of analytical and numerical tools, Gaididei, Mingaleev and Christiansen [5] demonstrated the spontaneous breaking of the left-right symmetry by localised solutions. Subsequently, Jackson and Weinstein [6] performed geometric analysis of the symmetry breaking and classified the underlying bifurcations of stationary solutions. Besides the absence of gain and loss, the mathematical setting of [6] was different from our present problem in that the normalisation condition (3) was not imposed there.

Studies of the *PT*-symmetric model with $\gamma \neq 0$ were pioneered by Znojil and Jakubský who analysed the linear Schrödinger equation with point-like gain and loss (but no wells) on a finite interval [7, 8]. The double-well potential (7) was proposed by Uncu and Demiralp [9] whose paper also focussed on the linear equation—yet on the infinite line. Cartarius and Wunner [2, 10] considered both linear and nonlinear Gross-Pitaevskii model. The numerical study of [2, 10] identified a branch of localised nonlinear modes bifurcating from eigenfunctions of the linear operator in (4).

In this contribution, we get an analytical handle on the *PT*-symmetric double-δ problem, linear and, most importantly, nonlinear. In the linear situation (equation (4) with $g = 0$) we provide a mathematical interpretation and verification of the numerics reported in [2, 10]. In the nonlinear case ($g \neq 0$), the analytical consideration allows us to advance beyond the numerical conclusions of the previous authors. In particular, we demonstrate the existence of infinite families of localised solutions with multiple humps and dips between the two potential singularities.

2 Linear Schrödinger Equation with Complex Double-δ Well Potential

Relegating the analysis of the full nonlinear equation (4), (7) to the subsequent sections, here we consider its linear particular case ($g = 0$). The normalised eigenfunction pertaining to the eigenvalue $-\kappa^2$ is given by

$$\psi(x) = \begin{cases} \frac{e^{i\phi}+e^{\kappa L-i\phi}}{2\sqrt{N}} e^{\kappa x}, & x \leq -L/2; \\ \frac{\cosh(\kappa x+i\phi)}{\sqrt{N}}, & -L/2 \leq x \leq L/2; \\ \frac{e^{-i\phi}+e^{\kappa L+i\phi}}{2\sqrt{N}} e^{-\kappa x}, & x \geq L/2. \end{cases}$$

Here κ is a positive root of the transcendental equation [2, 9, 10]

$$e^{-2\kappa L} = \frac{\gamma^2 + (2\kappa - 1)^2}{\gamma^2 + 1}, \tag{8}$$

while ϕ and N are readily expressible through κ. The secular equation (8) was solved numerically in [2, 10]. Here, we analyse it without resorting to the help of computer.

To this end, we express γ as an explicit function of κ:

$$\gamma^2 = \frac{4\kappa(1-\kappa)}{1-e^{-2\kappa L}} - 1. \tag{9}$$

Instead of evaluating eigenvalues κ as the parameter $\gamma > 0$ is varied, we identify the range of positive κ where the function $\gamma^2(\kappa)$ is positive. We prove the following

Proposition 1 *Regardless of the value of L, there is a finite interval of κ where $\gamma^2 > 0$. When $L < 2$, the interval is $0 < \kappa < \kappa^{(b)}$, and when $L > 2$, the interval is $\kappa^{(a)} < \kappa < \kappa^{(b)}$. Here $\kappa^{(a)}$ and $\kappa^{(b)}$ are dependent on L, with $0 < \kappa^{(a)} < \kappa^{(b)} < 1$.*

Proof The inequality $\gamma^2 > 0$ amounts to $k_1 < \kappa < k_2$, where the endpoints of the interval (k_1, k_2) also depend on κ:

$$k_1(\kappa) = \frac{1-e^{-\kappa L}}{2}, \quad k_2(\kappa) = \frac{1+e^{-\kappa L}}{2}.$$

If $L < 2$, the quantity $k_1(\kappa)$ is smaller than κ for all $\kappa > 0$. If, on the other hand, $L > 2$, the graph of the function $y = k_1(\kappa)$ lies above $y = \kappa$ in the interval $0 \le \kappa < \kappa^{(a)}$ and below $y = \kappa$ in the interval $\kappa^{(a)} < \kappa < \infty$. Here $\kappa^{(a)} = \kappa^{(a)}(L)$ is the (unique) root of the equation $k_1(\kappa) = \kappa$.

On the other hand, the function $k_2(\kappa)$ is greater than κ when $0 < \kappa < \kappa^{(b)}$ and smaller than κ when $\kappa > \kappa^{(b)}$. Here $\kappa^{(b)} = \kappa^{(b)}(L)$ is the root of the equation $k_2(\kappa) = \kappa$. (There is a unique root for all $L > 0$.)

Note that in the range of the L values where the root $\kappa^{(a)}$ exists—that is, in the region $L > 2$—we have $\kappa^{(a)} < \kappa^{(b)}$. Since $\kappa_2(1) < 1$, we have $\kappa^{(b)} < 1$. □

Our next result concerns the number of eigenvalues arising for various γ. Again, instead of counting branches of the function $\kappa(\gamma)$, we identify regions of monotonicity of the inverse function, $\gamma(\kappa)$. These are separated by the points of local extrema (stationary points).

Proposition 2 *When $L < 1$, the function $\gamma(\kappa)$ is monotonically decreasing as κ changes from 0 to $\kappa^{(b)}$, with $\kappa^{(b)}$ defined above. When $L > 1$, the function $\gamma(\kappa)$ has a single local maximum at $\kappa = \kappa_c$ (where $\kappa_c < \kappa^{(b)}$).*

Proof Stationary points of the function $\gamma^2(\kappa)$ are given by zeros of

$$\frac{d\gamma^2}{d\kappa} = \frac{(1-2\kappa)}{2\kappa L \sinh^2(L\kappa)} [f(\kappa) - g(\kappa)], \tag{10}$$

where

$$f = \frac{e^{2L\kappa}-1}{2L\kappa}, \quad g = \frac{1-\kappa}{1-2\kappa}.$$

We consider (10) for $0 < \kappa < 1$. (Note that $\kappa = 1/2$ is not a zero of $d\gamma^2/d\kappa$.) When $1/2 < \kappa < 1$, the function g is strictly negative; hence stationary points may only lie in the interval $0 < \kappa < 1/2$.

Assume, first, that $L < 1$ and expand $f(\kappa)$ and $g(\kappa)$ in powers of κ:

$$f = 1 + \sum_{n=1}^{\infty} f_n \kappa^n, \quad f_n = \frac{(2L)^n}{(n+1)!} \tag{11}$$

$$g = 1 + \sum_{n=1}^{\infty} g_n \kappa^n, \quad g_n = 2^{n-1}. \tag{12}$$

The series (11) converges in the entire complex plane of κ while the series (12) converges in the disc $|\kappa| < 1/2$. Noting that $f_n < g_n$ for all n, we conclude that $f(\kappa) < g(\kappa)$ for all $0 < \kappa < 1/2$. Equation (10) implies then that for any $L < 1$, the function $\gamma^2(\kappa)$ decreases monotonically as κ changes from 0 to 1.

Let now $L > 1$. The values of f and g at the origin are equal while their slopes are not:

$$\left.\frac{df}{d\kappa}\right|_{\kappa=0} = L, \quad \left.\frac{dg}{d\kappa}\right|_{\kappa=0} = 1.$$

Consequently, the graph of $f(\kappa)$ lies above the graph of $g(\kappa)$ as long as κ remains sufficiently close to the origin. At the opposite end of the interval, that is, in the vicinity of $\kappa = 1/2$, the graph of $g(\kappa)$ lies above $f(\kappa)$. Therefore the equation $f(\kappa) = g(\kappa)$ has (at least one) root κ_c in the interval $0 < \kappa < 1/2$. This root emerges from the point $\kappa = 0$ as soon as L becomes greater than 1.

To show that no additional stationary points can emerge as L is further increased, assume the contrary—assume that a pair of stationary points is born as L passes through a critical value L_* (where $L_* > 1$). At the bifurcation value $L = L_*$, the newborn stationary points are equal; we denote them κ_*. When $L = L_*$, the equality

$$\left.\frac{df}{d\kappa}\right|_{\kappa=\kappa_*} = \left.\frac{dg}{d\kappa}\right|_{\kappa=\kappa_*} \tag{13}$$

should be fulfilled along with

$$f(\kappa_*) = g(\kappa_*). \tag{14}$$

Solving the system (13), (14) yields $L_* = (1 - 2\kappa_*)^{-1}$. This can be written as

$$L_* = 1 + q, \tag{15}$$

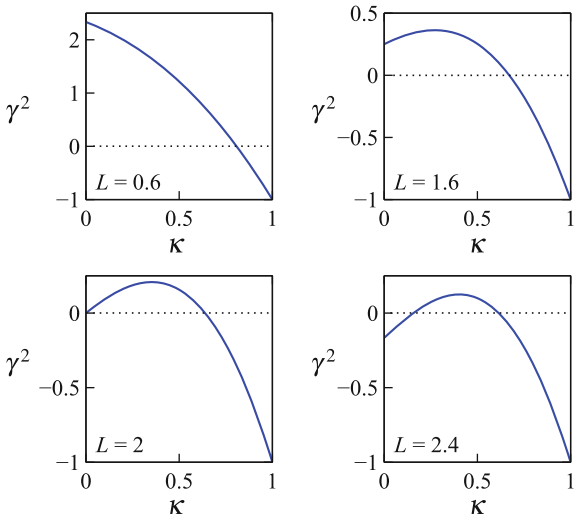

Fig. 1 The function (9) plotted for several representative values of L. In the interval of κ where $\gamma^2 \geq 0$, the function gives the square of the gain-loss coefficient. The inverse function $\kappa(\gamma^2)$ is obtained simply by flipping the part of the graph with $\gamma^2 \geq 0$ about the $\gamma^2 = \kappa$ line (see Fig. 2)

where we have defined $q = 2\kappa_* L_*$. Making use of (15), equation (14) becomes

$$\frac{e^q - 1}{q} = 1 + \frac{q}{2}.$$

Expanding the left-hand side in powers of q one can readily check that it is greater than the right-hand side for any $q > 0$; hence the above equality can never be satisfied. This proves that the stationary point κ_c of the function $\gamma^2(\kappa)$ is single.

Since $d\gamma^2/d\kappa|_{\kappa=0} > 0$, the stationary point κ_c is a maximum. □

The above propositions are illustrated by Fig. 1 which shows $\gamma^2(\kappa)$ with $L < 1$ (a); $1 < L < 2$ (b); $L = 2$ (c), and $L > 2$ (d).

Our conclusions are sufficient to determine the shape of the inverse function, $\kappa(\gamma)$. When $L < 1$, there is a single positive branch of $\kappa\ (\gamma)$ which decays, monotonically, as γ is increased from zero to γ_0 (Fig. 2a). As γ reaches γ_0, the quantity κ drops to zero and the eigenvalue $-\kappa^2$ collides with the continuous spectrum. Since $\gamma^2(0) = 2/L - 1$, we can obtain the critical value of γ exactly: $\gamma_0 = \gamma(0) = \sqrt{2/L - 1}$.

When L is taken between 1 and 2, the function $\kappa\ (\gamma)$ has two branches (Fig. 2b). Along the monotonically decreasing branch, κ drops from $\kappa^{(b)}$ to κ_c as γ is raised from 0 to γ_c. In addition, there is a monotonically increasing branch with $\gamma_0 < \gamma < \gamma_c$. Here, κ grows from 0 to κ_c as γ is increased from γ_0 to γ_c. The two eigenvalues merge and become complex as γ is raised through γ_c.

Finally, when $L \geq 2$, the monotonically decreasing and increasing branch of $\kappa(\gamma)$ exist over the same interval $0 < \gamma < \gamma_c$ (Fig. 2c, d). As γ grows from 0 to γ_c, one branch of κ grows from $\kappa^{(a)}$ to κ_c whereas the other one decreases from $\kappa^{(b)}$ to κ_c.

These conclusions are in agreement with the numerical results of [2, 10].

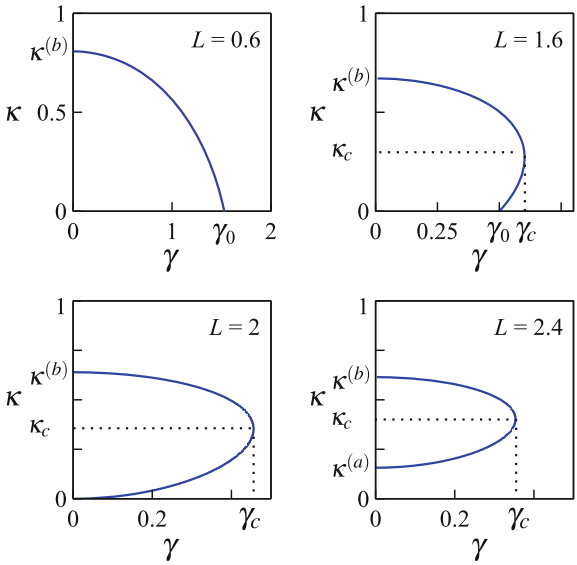

Fig. 2 Positive roots of (8) versus the gain-loss coefficient γ, for several representative values of L

3 *PT*-Symmetric Gross-Pitaevskii Equation with Variable-Depth Wells

Proceeding to the nonlinear situation ($g \neq 0$), it is convenient to transform the stationary equation (4) to

$$\varphi_{\tau\tau} + \lambda\,[\delta(\tau + T) + \delta(\tau - T)]\,\varphi - i\eta[\delta(\tau + T) - \delta(\tau - T)]\varphi + 2\varphi|\varphi|^2 = \varphi, \tag{16}$$

with

$$\tau = \kappa x, \quad T = \kappa\frac{L}{2}, \quad \varphi = \sqrt{\frac{g}{2}}\frac{\psi}{\kappa}, \quad \lambda = \frac{1}{\kappa}, \quad \eta = \frac{\gamma}{\kappa}.$$

Here $\eta \geq 0$, $\lambda > 0$, and $T > 0$. In equation (16) the chemical potential has been normalised to unity at the expense of making the well depths, λ, variable. The normalisation constraint (5) acquires the form

$$\int_{-\infty}^{\infty} |\varphi|^2 d\tau = \frac{\lambda}{2}g, \tag{17}$$

while the symmetry condition (6) translates into

$$\varphi^*(\tau) = \varphi(-\tau). \tag{18}$$

Consider a solution $\varphi(\tau)$ of the equation (16) and denote $N = \int |\varphi|^2 d\tau$ the corresponding number of particles. The number of particles is a function of λ, η and T: $N = N(\lambda, \eta, T)$. Setting g to a particular value, the constraint (17) defines a two-dimensional surface in the (λ, η, T) space:

$$\frac{1}{\lambda} N(\lambda, \eta, T) = \frac{g}{2}.$$

For any fixed L, the "nonlinear eigenvalue" $\kappa = \lambda^{-1}$ becomes an (implicit) function of γ:

$$\kappa N\left(\frac{1}{\kappa}, \frac{\gamma}{\kappa}, \frac{\kappa L}{2}\right) = \frac{g}{2}.$$

The purpose of our study is to construct the solution $\varphi(\tau)$ and determine this function.

It is fitting to note here that the equation (4) with $g = 0$ can also be transformed to the form (16)—where one just needs to drop the cubic term. In this case, the number of particles is not fixed though; that is, the constraint (17) does not need to be satisfied. The relation between κ and γ—equation (8)—arises as a secular equation for an eigenvalue problem.

4 Particle Moving in a Mexican-Hat Potential

In the external region $|\tau| \geq T$, the PT-symmetric solutions with the boundary conditions $\varphi(\pm\infty) = 0$ have the form

$$\begin{aligned} \varphi(\tau) &= e^{-i\chi} \operatorname{sech}(\tau + \mu), \quad \tau \leq -T; \\ \varphi(\tau) &= e^{i\chi} \operatorname{sech}(\tau - \mu), \quad \tau \geq T. \end{aligned} \tag{19}$$

Here μ is an arbitrary real value, positive or negative, determining the amplitude of φ, and χ is an arbitrary real phase. The solution $\varphi(\tau)$ in the internal region $|\tau| \leq T$ will be matched to the values of (19) at the endpoints $\tau = \pm T$:

$$\varphi(\pm T) = e^{\pm i\chi} \operatorname{sech}(\mu - T). \tag{20}$$

Integrating (16) across the singularities and using (19) once again, we obtain the matching conditions for the derivatives as well:

$$\begin{aligned} \dot{\varphi}|_{\tau=T-0} &= e^{i\chi} \operatorname{sech}(\mu - T)[i\eta + \lambda + \tanh(\mu - T)], \\ \dot{\varphi}|_{\tau=-T+0} &= e^{-i\chi} \operatorname{sech}(\mu - T)[i\eta - \lambda - \tanh(\mu - T)]. \end{aligned} \tag{21}$$

Here the overdot stands for the differentiation with respect to τ.

To construct the solution between $-T$ and T it is convenient to interpret the modulus and the phase of φ as polar coordinates of a particle on the plane,

$$\varphi = re^{i\theta},$$

and the coordinate τ as time. The newtonian particle moves in the radial-symmetric mexican hat-shaped potential $U(r) = \frac{1}{2}(r^4 - r^2)$. Hence the angular momentum

$$\ell = \dot{\theta} r^2 \tag{22}$$

and the energy

$$\mathscr{E} = \frac{\dot{r}^2}{2} + U_{\text{eff}}(r), \quad U_{\text{eff}} = \frac{\ell^2}{2r^2} + \frac{r^4 - r^2}{2} \tag{23}$$

are conserved. The effective potential for the radial motion is shown in Fig. 3a.

The particle starts its motion at time $\tau = -T$ and ends at $\tau = T$. The boundary conditions follow from (20) and (21):

$$r(\pm T) = \operatorname{sech}(\mu - T), \tag{24}$$

$$\dot{r}(-T) = -\dot{r}(T) = -(\lambda + \xi)\operatorname{sech}(\mu - T), \tag{25}$$

$$\theta(\pm T) = \pm\chi, \tag{26}$$

$$\dot{\theta}(\pm T) = \eta, \tag{27}$$

where

$$\xi = \tanh(\mu - T).$$

The parameter ξ satisfying $\lambda + \xi > 0$ requires a negative initial velocity, $\dot{r}(-T) < 0$, and $\lambda + \xi < 0$ corresponds to an outward initial motion: $\dot{r}(-T) > 0$.

Equations (22) and (27) imply that the conserved angular momentum has a positive value:

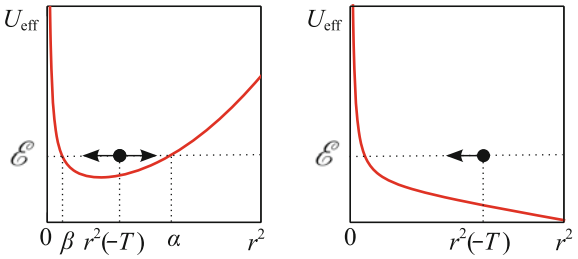

Fig. 3 The *left panel* shows $U_{\text{eff}}(r)$, the effective potential of radial motion defined in (23). *Two arrows* indicate two possible directions of motion of the fictitious particle. Whether the particle starts with a positive or negative radial velocity, it will run into a turning point. Dropping the quartic term from (23) gives the effective potential for the linear equation (*right panel*). This time the turning point will only be run into if $\dot{r}(-T) < 0$

$$\ell = \eta\,\mathrm{sech}^2(\mu - T) \tag{28}$$

and so θ grows as τ varies from $-T$ to T. (Hence $\chi > 0$.) The energy of the particle is found by substituting (24)–(25) in (23):

$$\mathscr{E} = \frac{1}{2}(1-\xi^2)\left[(\lambda+\xi)^2 - \xi^2 + \eta^2\right]. \tag{29}$$

Since the energy (23) includes the square of $\dot{r}$ but not $\dot{r}$ itself, the information about the initial direction of motion becomes lost in the expression (29). In fact, by using the value of energy instead of the boundary condition (25) we are acquiring spurious solutions. These solutions have the wrong sign of $\dot{r}(\tau)$ as $\tau \to -T+0$ and do not satisfy (25). Fortunately we remember that the sign of $\dot{r}|_{\tau\to -T+0}$ should be opposite to that of $\lambda+\xi$. This simple rule will be used to filter out the spurious roots in Sect. 7.

The radial trajectory $r(\tau)$ for a PT-symmetric solution satisfying (18) should be described by an even function and the trajectory should have a turning point at $\tau = 0$: $\dot{r}(0) = 0$. The separable equation (23) has two even solutions,

$$r_A^2(\tau) = (\alpha-\beta)\mathrm{cn}^2\left(\sqrt{2\alpha+\beta-1}\,\tau, k\right) + \beta \tag{30}$$

and

$$r_B^2(\tau) = (\alpha-\beta)\mathrm{cn}^2\left(K - \sqrt{2\alpha+\beta-1}\,\tau, k\right) + \beta. \tag{31}$$

The Jacobi-function solutions (30) and (31) are parametrised by two parameters, α and β, where $\alpha \geq \beta \geq 0$ and $\alpha+\beta > 1$. These are related to ℓ and $\mathscr{E}$ via

$$\ell^2 = \alpha\beta(\alpha+\beta-1), \tag{32}$$

$$2\mathscr{E} = (\alpha+\beta)(\alpha+\beta-1) - \alpha\beta. \tag{33}$$

The elliptic modulus k is given by

$$k^2 = \frac{\alpha-\beta}{2\alpha+\beta-1},$$

and $K(k)$ in (31) is the complete elliptic integral of the first kind. Eliminating ℓ between (28) and (32), and $\mathscr{E}$ between (29) and (33) we get

$$\eta^2(1-\xi^2)^2 = \alpha\beta(\alpha+\beta-1), \tag{34}$$

$$(1-\xi^2)(\lambda^2+\eta^2+2\lambda\xi) = (\alpha+\beta)(\alpha+\beta-1) - \alpha\beta. \tag{35}$$

The solution r_A is maximum-centred and r_B is minimum-centred (see Fig. 4).

For the purposes of our study, it is convenient to have a relation between α, β, and ξ not involving the gain-loss parameter. Eliminating η^2 between (34) and (35)

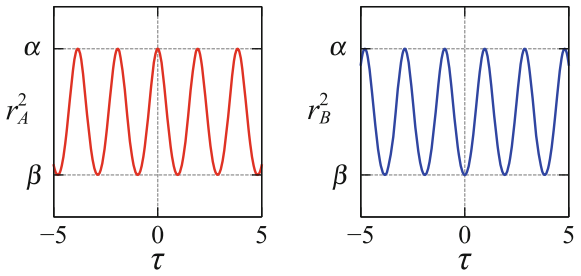

Fig. 4 Two even solutions of equation (23). **a** The maximum-centred solution, equation (30). **b** The minimum-centred solution, equation (31). In both panels $\alpha = 2$ and $\beta = 0.5$

we obtain

$$(\lambda + \xi)^2 = S^2, \tag{36}$$

where

$$S^2 = \frac{(\alpha+\beta)(\alpha+\beta-1)-\alpha\beta}{1-\xi^2} - \frac{\alpha\beta(\alpha+\beta-1)}{(1-\xi^2)^2} + \xi^2. \tag{37}$$

The structural relation (36)–(37) will prove useful in what follows.

5 Boundary Conditions and Normalisation Constraint

The boundary conditions (24) give a transcendental equation

$$\beta + (\alpha - \beta)\mathrm{cn}^2\,(y, k) = 1 - \xi^2, \tag{38a}$$

for the r_A and

$$\beta + (\alpha - \beta)\mathrm{cn}^2\,(K - y, k) = 1 - \xi^2 \tag{38b}$$

for the r_B solution. Here

$$y = \sqrt{2\alpha + \beta - 1}\,T.$$

Note that there is a simple correspondence between equations (38a) and (38b). Namely, if we assume that α, β and ξ in (38a) and (38b) are given, and denote $\widetilde{y}$ the value of y satisfying (38b), then $y = K - \widetilde{y}$ will satisfy (38a).

The linear ($g = 0$) Schrödinger equation (4) with the potential (7) corresponds to the newtonian particle moving in the effective potential without the quartic barrier at large r. In this case the particle can only run into a turning point if $\dot{r}(-T) < 0$ (see Fig. 3b). On the other hand, when the quartic barrier is present, the particle will turn no matter whether $\dot{r}(-T)$ is negative or positive (Fig. 3a).

Consider, first, the solution $r_A(\tau)$ and assume that $\dot{r}(-T) > 0$. The simplest trajectory satisfying the boundary conditions (24)–(25) describes the particle starting with a positive radial velocity at $\tau = -T$, reaching the maximum $r^2 = \alpha$ at $\tau = 0$ and returning to the starting point at $\tau = T$. We use T_0 to denote the corresponding

return time, T. Coexisting with this solution are longer trajectories that reach the maximum $r^2 = \alpha$ not once but $2n + 1$ times ($n \geq 1$), namely, at $\tau = 2m\Theta$, where

$$\Theta = \frac{K(k)}{\sqrt{2\alpha + \beta - 1}} \tag{39}$$

is the half-period of the function $\mathrm{cn}^2(\sqrt{2\alpha + \beta - 1}\tau, k)$ and $m = 0, \pm 1, \pm 2, ..., \pm n$. These trajectories have the same values of α and β (the same apogee and perigee) but different return times, $T = T_0 + 2n\Theta$. Since the trajectory reaches its apogee $2n + 1$ times and pays $2n$ visits to its minimum value of $r^2 = \beta$, we are referring to these solutions as $(2n + 1)$-hump, $2n$-dip nonlinear modes.

In contrast to these, the r_A solution with $\dot{r}(-T) < 0$ will be visiting its minimum $2n$ times ($n \geq 1$), at $\tau = (1 - 2n)\Theta$, ...$(2n - 1)\Theta$, but will only pay $2n - 1$ visits to its maximum. These trajectories will be classified as $2n$-dip, $(2n - 1)$-hump modes. The corresponding return times are $T = 2n\Theta - T_0$.

Turning to the minimum-centred solutions, we consider trajectories with $\dot{r}(-T) < 0$ first. The simplest r_B solution describes the particle starting with a negative velocity at $\tau = -T$, reaching its perigee $r^2 = \beta$ at $\tau = 0$ and returning to the starting point at $\tau = T$, where $T = \Theta - T_0$ and T_0 was introduced above. The r_B solutions with more bounces visit the minimum r not once but $2n + 1$ times ($n \geq 1$), at $\tau = 2m\Theta$, $m = 0, \pm 1, ..., \pm n$. The corresponding return time is $T = (2n + 1)\Theta - T_0$. With their $2n + 1$ local minima and $2n$ maxima, these solutions are referred to as the $(2n + 1)$-dip, $2n$-hump nonlinear modes.

Finally, the r_B solution with $\dot{r}(-T) > 0$ reaches its apogee $2n$ times ($n \geq 1$), that is, at $\tau = (2m + 1)\Theta$, with $m = -n - 1, ..., n$. The return time is $T = T_0 + (2n - 1)\Theta$. The trajectory pays $2n - 1$ visits to its minimum value of $r^2 = \beta$; hence we classify this solution as the $2n$ hump, $(2n - 1)$-dip modes.

For the fixed α and β, the return time T_0 is given by the smallest positive root of (38a). (Note that $T_0 < \Theta$.) Other roots of this equation are $T_0 + 2\Theta$, $T_0 + 4\Theta$, ..., and $2\Theta - T_0$, $4\Theta - T_0$, ... On the other hand, the smallest positive root of (38b) is $\Theta - T_0$, with other roots being $3\Theta - T_0$, $5\Theta - T_0$, ..., and $T_0 + \Theta$, $T_0 + 3\Theta$, ...

The normalised return time

$$\frac{T}{\Theta} = \frac{y}{K(k)} \tag{40}$$

provides a simple tool for the identification of the nonlinear mode. Indeed, an r_A solution with T/Θ between $2n$ and $2n + 1$ has $2n + 1$ humps, $2n$ dips and $\dot{r}(-T) > 0$. On the other hand, an r_A solution with T/Θ between $2n - 1$ and $2n$ has $2n$ dips, $2n - 1$ humps and $\dot{r}(-T) < 0$. Similarly, an r_B solution will have $2n$ humps, $2n - 1$ dips, and $\dot{r}(-T) > 0$—if T/Θ lies between $2n - 1$ and $2n$, or $2n + 1$ dips, $2n$ humps, and $\dot{r}(-T) < 0$—if T/Θ is between $2n$ and $2n + 1$.

Evaluating the number of particles

$$N = \int_{-\infty}^{-T} \operatorname{sech}^2(\tau + \mu)d\tau + \int_{-T}^{T} r_A^2 d\tau + \int_{T}^{\infty} \operatorname{sech}^2(\tau - \mu)d\tau$$

and substituting in the normalisation constraint (17), the constraint is transformed into

$$\zeta_A(\alpha, \beta, y, \lambda) = \xi, \tag{41}$$

where the function ζ_A is defined by

$$\zeta_A = \frac{\alpha + \beta - 1}{\sqrt{2\alpha + \beta - 1}} y - 1 + \frac{g}{4}\lambda - \sqrt{2\alpha + \beta - 1}\, E\left[\operatorname{am}(y)\right]. \tag{42}$$

Here $E[\operatorname{am}(y)] = E[\operatorname{am}(y), k]$ is the incomplete elliptic integral of the second kind,

$$E[\operatorname{am}(y), k] = \int_0^{\operatorname{am}(y)} \sqrt{1 - k^2 \sin^2\theta}\, d\theta = \int_0^{y} \operatorname{dn}^2(w, k) dw,$$

and $\operatorname{am}(y)$ is the elliptic amplitude. (To simplify the notation, we omit the dependence on the elliptic modulus k in (42).)

A similar procedure involving the solution r_B yields

$$\zeta_B(\alpha, \beta, y, \lambda) = \xi, \tag{43}$$

where we have introduced

$$\zeta_B = \frac{\alpha + \beta - 1}{\sqrt{2\alpha + \beta - 1}} y - 1 + \frac{g}{4}\lambda - \sqrt{2\alpha + \beta - 1}\left\{E\left(\frac{\pi}{2}\right) - E\left[\operatorname{am}(K - y)\right]\right\}. \tag{44}$$

Here $E(\pi/2) = E(\pi/2, k)$ is the complete elliptic integral of the second kind.

Note that unlike the pair of equations (38a) and (38b), the normalisation constraints (41) and (43) are not related by the transformation $y = K - \widetilde{y}$. Therefore, the solution of the system (38b)+(43) cannot be reduced to solving (38a)+(41). The "r_A" and "r_B" systems have to be considered independently.

6 Reduction to the Linear Schrödinger Equation

Before proceeding to the analysis of the systems (38a)+(41) and (38b)+(43), it is instructive to verify that the transcendental equation (8) for the linear Gross-Pitaevskii equation is recovered as the $g \to 0$ limit of (38b).

Assume that κ is fixed and g is varied in the stationary Gross-Pitaevskii equation (4). When g is small, the solution of (4) bifurcating from the solution of the corresponding *linear* Schrödinger equation remains of order 1. The corresponding solution φ of equation (16) will then have to be of order $g^{1/2}$. This means, in particular, that for all $|\tau| \geq T$, the "outer" solution (19) will have to approach zero as $g \to 0$. In order to have

$$\int_T^\infty \mathrm{sech}^2(\tau - \mu) d\tau \to 0 \quad \text{as } g \to 0,$$

one has to require that $\tanh(\mu - T) \to -1$ as $g \to 0$. Defining σ by

$$\mathrm{sech}^2(\mu - T) = \sigma^2 g, \quad \sigma = O(1), \tag{45}$$

the quantity $\xi = \tanh(\mu - T)$ will have the following asymptotic behaviour:

$$\xi = -1 + \frac{\sigma^2}{2} g + O(g^2).$$

Letting

$$\alpha = 1 + \mathscr{A}_1 g + \mathscr{A}_2 g^2 + \cdots, \quad \beta = \mathscr{B}_1 g + \mathscr{B}_2 g^2 + \cdots$$

and substituting these expansions in (34) and (35) gives

$$\mathscr{A}_1 = A\sigma^2, \quad \mathscr{B}_1 = B\sigma^2,$$

where

$$A = \lambda^2 - 2\lambda + \eta^2, \quad B = -\frac{1}{2} A + \frac{1}{2}\sqrt{A^2 + 4\eta^2}. \tag{46}$$

Turning to the transcendental equation (38b), we note that the elliptic modulus of the Jacobi cosine tends to 1 as $g \to 0$:

$$k^2 = 1 - (\mathscr{A}_1 + 2\mathscr{B}_1) g + \cdots$$

In this limit, the elliptic function approaches a hyperbolic sine:

$$\mathrm{cn}(K - y, k) = k' \sinh y + O(k'^3), \quad k'^2 = 1 - k^2.$$

In equation (38b), $y = \sqrt{2\alpha + \beta - 1}\, T$. With $\sqrt{2\alpha + \beta - 1} = 1 + O(g)$, the transcendental equation reduces to

$$B + (A + 2B) \sinh^2 T = 1. \tag{47}$$

Substituting for A and B from (46), equation (47) gives

$$e^{-4T} = \frac{(\lambda - 2)^2 + \eta^2}{\lambda^2 + \eta^2}. \tag{48}$$

Transforming to $\gamma = \eta/\lambda$, $\kappa = 1/\lambda$ and $L = 2\lambda T$, we recover the transcendental equation (8).

Finally, we consider the normalisation constraint (43). As $k \to 1$, the elliptic integral of the second kind has the following asymptotic behaviour:

$$E\left(\frac{\pi}{2}\right) - E\left[\mathrm{am}(K - y)\right] = k'^2 \int_0^y \frac{du}{\mathrm{dn}^2(u, k)} = \frac{k'^2}{2}\left(y + \frac{\sinh 2y}{2}\right) + O\left(k'^4\right).$$

Making use of this expansion, we reduce equation (43) to

$$2 - 2AT + \sqrt{A^2 + 4\eta^2}\sinh(2T) = \frac{\lambda}{\sigma^2}. \tag{49}$$

Given λ, η and T, equation (49) furnishes the coefficient σ in the relation (45). The relation (45), in turn, determines the amplitude of the solution φ corresponding to the nonlinearity parameter g.

7 Transcendental Equations

In this section we assume that L, the distance between the potential wells in the original Gross-Pitaevskii equation (4), and g, the coefficient of the nonlinearity, are fixed. On the other hand, the gain-loss coefficient γ and the "nonlinear eigenvalue" κ (and hence the scaling factor $\lambda = \kappa^{-1}$, the scaled gain-loss $\eta = \gamma\kappa^{-1}$, and the dimensionless well-separation distance $2T = \kappa L$) are allowed to vary. The parameter ξ—the parameter defining the amplitude of the nonlinear mode—has not been fixed either.

Substituting ξ from the normalisation constraint (41) to the boundary condition (38a) we obtain a transcendental equation

$$\zeta_A^2 + \beta + (\alpha - \beta)\mathrm{cn}^2 y - 1 = 0 \tag{50a}$$

for the parameters of the r_A solution. In a similar way, substituting from (43) to (38b) we obtain an equation

$$\zeta_B^2 + \beta + (\alpha - \beta)\mathrm{cn}^2\left(K - y\right) - 1 = 0 \tag{50b}$$

for the solution r_B. Note that the functions ζ_A and ζ_B, defined in (42) and (44), depend on λ as a parameter.

Substituting ξ from the constraint (41) to the structural relation (36) gives another transcendental equation for the maximum-centred nonlinear mode:

$$(\lambda + \zeta_A)^2 - S_A^2 = 0. \tag{51a}$$

Here we are using a new notation S_A for the combination that was previously denoted S and given by (37). In a similar way, substituting ξ from (43) to (36) gives an equation for the minimum-centred (the r_B) solution:

$$(\lambda + \zeta_B)^2 - S_B^2 = 0, \tag{51b}$$

where the same combination S (defined in (37)) has been renamed S_B. (We are using two different notations for the same combination in order to be able to set the variable S to two different values later.) Like equations (50a) and (50b) before, equations (51a) and (51b) include λ as a parameter.

Eliminating $1 - \xi^2$ from the expression (37) by means of the boundary condition (38a), we specify S_A:

$$S_A^2 = \frac{(\alpha+\beta)(\alpha+\beta-1)-\alpha\beta}{\beta+(\alpha-\beta)\mathrm{cn}^2 y} - \frac{\alpha\beta(\alpha+\beta-1)}{\left[\beta+(\alpha-\beta)\mathrm{cn}^2 y\right]^2} + 1 - \beta - (\alpha-\beta)\mathrm{cn}^2 y. \tag{52a}$$

In order to specify S_B, we use the boundary condition (38b) instead:

$$S_B^2 = \frac{(\alpha+\beta)(\alpha+\beta-1)-\alpha\beta}{\beta+(\alpha-\beta)\mathrm{cn}^2\,(K-y)} - \frac{\alpha\beta(\alpha+\beta-1)}{\left[\beta+(\alpha-\beta)\mathrm{cn}^2\,(K-y)\right]^2} + 1 - \beta - (\alpha-\beta)\mathrm{cn}^2\,(K-y)\,. \tag{52b}$$

The system (50a), (51a) with ζ_A as in (42) and S_A as in (52a), is a system of two equations for two parameters of the solution r_A (the "A-system"). For the given L, g and λ, the A-system has one or several roots (α_n, β_n).

Not all roots define the Gross-Pitaevskii solitons though; some roots are spurious. To filter the spurious roots out, we use the simple rule formulated in Sect. 4. First, we calculate the normalised return time (40) and establish whether $2n < T/\Theta < 2n+1$ or $2n-1 < T/\Theta < 2n$ for some natural n. The former situation corresponds to $\dot{r}(-T) > 0$ and the latter to $\dot{r}(-T) < 0$. Evaluating the amplitude parameter ξ by means of (42), we then discard the roots with the sign of $\lambda + \xi$ coincident with the sign of $\dot{r}(-T)$.

Having thus validated the genuine roots for a range of λ values, we can use (38a) to express $1 - \xi^2$ through $\alpha(\lambda)$ and $\beta(\lambda)$, and then employ equation (34) to obtain $\eta(\lambda)$. Transforming from λ and η to $\kappa = 1/\lambda$ and $\gamma = \eta/\lambda$, we arrive at

$$\gamma_A(\kappa) = \frac{\sqrt{\alpha\beta(\alpha+\beta-1)}\kappa}{\beta + (\alpha-\beta)\mathrm{cn}^2\left(\sqrt{2\alpha+\beta-1}\kappa L/2\right)}. \tag{53a}$$

The transcendental system (50b), (51b), (44), (52b) (the "B-system") is not equivalent to the A-system and has to be solved independently. Having determined the roots $\alpha(\lambda)$, $\beta(\lambda)$ and validated them in the same way as we did with the A-roots before, we obtain an analogue of the formula (53a):

$$\gamma_B(\kappa) = \frac{\sqrt{\alpha\beta(\alpha+\beta-1)}\kappa}{\beta + (\alpha-\beta)\mathrm{cn}^2\left(K - \sqrt{2\alpha+\beta-1}\kappa L/2\right)}. \tag{53b}$$

The curve $\gamma(\kappa)$—or, equivalently, $\kappa(\gamma)$—will constitute the central result of our analysis. Each root (α_n, β_n) of the A- or B-system will contribute a branch to this curve. Before presenting the $\kappa(\gamma)$ relationships for various L and g, we note a useful symmetry of the A- and B-systems.

8 The Dip- and Hump-Adding Transformation

Consider the r_A solution and assume (α, β) is a root of the system (50a), (51a), (42), (52a) with parameters g, T and λ. The A-system with shifted parameters

$$\tilde{T} = T + 2\Theta, \quad \tilde{\lambda} = \lambda, \quad \tilde{g} = g + \Delta g,$$
$$\Delta g = \frac{8}{\lambda}\left[\sqrt{2\alpha+\beta-1}E - \frac{\alpha+\beta-1}{\sqrt{2\alpha+\beta-1}}K\right], \tag{54}$$

will have the same root (α, β). Here Θ is given by (39), while $K = K(k)$ and $E = E(k)$ are the complete elliptic integrals of the first and second kind, respectively.

The mapping (54) adds two units to the normalised return time T/Θ: $T/\Theta \to T/\Theta + 2$. Therefore (54) adds two humps and two dips to the A-mode with $2n$ dips and $2n \pm 1$ humps. Note that the expression in the square brackets in (54) is equal to $\int_0^\Theta r_A^2 d\tau$; hence $\Delta g > 0$ for any α and β. Therefore the map generates an infinite sequence of nonlinearity strengths g, $g + \Delta g$, $g + 2\Delta g$, ... supporting hump-centred nonlinear modes with an increasing number of lateral crests.

Turning to the B-solution and the system (50b), (51b), (44), (52b), the same mapping (54) transforms this system into itself. As a result of the application of the mapping (54), the B-solution with $2n$ humps and $2n \pm 1$ dips acquires two new humps and two new dips. The expression in the square brackets in (54) equals $\int_0^\Theta r_B^2 d\tau$; hence we have $\Delta g > 0$ in the case of the B solution as well. As with the A-solution before, the map (54) generates an infinite sequence of multicrest (yet dip-centred) modes.

9 *PT*-Symmetric Localised Nonlinear Modes

The A- and B-system of two transcendental equations were solved numerically. We employed a path-following algorithm with a newtonian iteration to obtain the root (α, β) as κ was varied with g and L fixed. The initial guess for the continuation process was provided either by the analysis of intersecting graphs of two simultaneous equations on the (α, β)-plane, or by transplanting a known root to a different set of g and L by means of the mapping (54).

Figure 5a traces a branch of the B-modes on the (γ, κ)-plane. Here, the parameters ($L = 2.2$ and $g = 1$) correspond to Fig. 1a in [2]. These are nonlinear modes with exactly one dip—at $x = 0$. The spatial structure of the mode is illustrated by Fig. 6a.

As it was established numerically in [2] and corroborated analytically in Sect. 6, the modes making up this branch are nonlinear deformations of the eigenfunctions of the linear Schrödinger equation (equation (4) with $g = 0$). This kinship is clearly visible in Fig. 6a where the nonlinear ($g = 1$) mode is plotted next to the normalized linear ($g = 0$) eigenfunction with the same value of γ.

In contrast to the above B branch, the A-modes exist only when g exceeds a certain finite threshold; these have no relation to the $g = 0$ eigenfunctions. A single-humped A-mode is exemplified by Fig. 6b, with the corresponding $\kappa(\gamma)$ branch appearing in Fig. 5b.

Finally, the bottom panels of Figs. 5 and 6 correspond to nonlinear modes with multiple humps and dips. The $\kappa(\gamma)$ curve in Fig. 5c pertains to a B-mode with three dips and two humps between the potential wells. This branch results by the κ-continuation from a root (α_0, β_0) of the B-system with κ equal to some κ_0 and

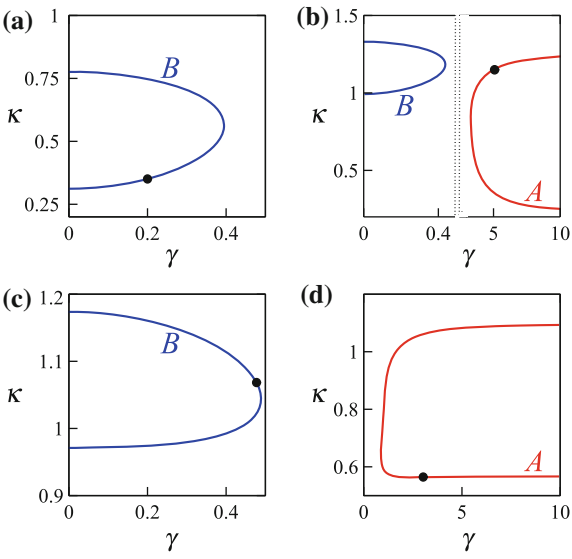

Fig. 5 "Nonlinear eigenvalues" κ versus the gain-loss coefficient γ for several sets of g and L. The *red curves* correspond to the A- and the *blue* ones to the B-modes. Solutions marked by the *black dots* are shown in Fig. 6. In these plots, $g = 1$, $L = 2.2$ (**a**); $g = 5$, $L = 2$ (**b**); $g \approx 12.12$, $L \approx 8.26$ (**c**); $g \approx 12.38$, $L \approx 9.35$ (**d**). Note a break in the horizontal axis in (**b**)

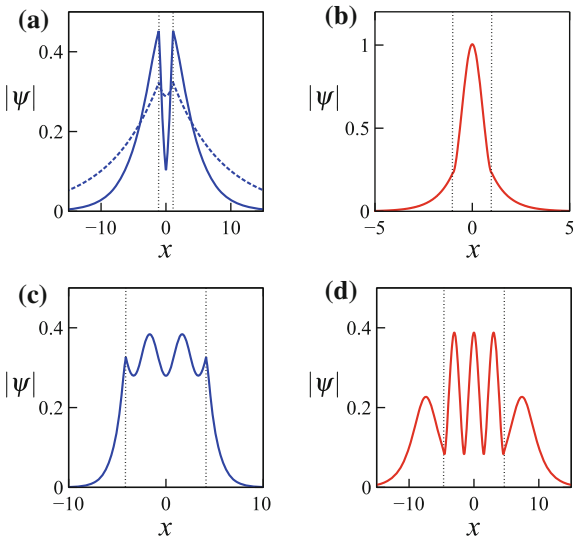

Fig. 6 *Solid curves* depict nonlinear localised modes at representative points along the $\kappa(\gamma)$ curves. (These points are marked by *black dots* in the corresponding panels of Fig. 5.) The B-modes are shown in *blue* and the A-modes in *red*. *Vertical dotted lines* indicate the positions of the potential wells. The *dashed curve* in (**a**) renders the eigenfunction of the equation (4) with $g = 0$ where L and γ are set equal to the L and γ of the nonlinear mode shown in the same panel. Note that the three-hump mode in (**d**) has four and not two local minima inside the $(-L, L)$ interval. The two lateral dips are pressed close to the wells but are nevertheless discernible by zooming in

g, T obtained by a once-off application of the map (54). A typical nonlinear mode arising along this branch is shown in Fig. 6c.

Figure 5d traces a branch of the multi-hump A-modes. Solutions on this branch have three humps and four dips situated between the wells; an example is in Fig. 6d. The starting point for the branch was suggested by the graphical analysis of the equations making up the A-system.

10 Summary and Conclusions

The double-δ well potential, where one well gains and the other one loses particles, furnishes one of the simplest Gross-Pitaevskii models employed in the studies of boson condensates. However the information on its nonlinear modes is scarce and based entirely on numerical solutions. The purpose of this contribution was to formulate an *analytical* procedure for the construction of localised nonlinear modes.

We started with the linear Schrödinger equation with the PT-symmetric double-delta well potential and provided a simple analytical classification of its bound states.

In the nonlinear situation, our procedure reduces the construction of localised modes to finding roots of a system of two simultaneous algebraic equations involving

elliptic integrals and Jacobi functions. We have classified the nonlinear modes under two broad classes: those with a maximum of $|\psi|$ at the centre and those centred on a minimum of $|\psi|$. Accordingly, there are transcendental systems of two types (referred to as the A- and B-systems). Our construction procedure is supplemented with an "identification" algorithm allowing to relate the number of crests and troughs of the nonlinear mode to the root of the transcendental system. We have established a correspondence between localised modes in systems with different distances between the wells and different nonlinearity strengths.

Our procedure has been illustrated by the construction of branches of A- and B-modes for several values of g and L.

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Exactly Solvable Wadati Potentials in the *PT*-Symmetric Gross-Pitaevskii Equation

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Abstract This note examines Gross-Pitaevskii equations with PT-symmetric potentials of the Wadati type: $V = -W^2 + iW_x$. We formulate a recipe for the construction of Wadati potentials supporting exact localised solutions. The general procedure is exemplified by equations with attractive and repulsive cubic nonlinearity bearing a variety of bright and dark solitons.

1 Introduction

A mean-field description of bosons with pairwise interaction is furnished by the Gross-Pitaevskii equation. In the one-dimensional geometry, the equation reads

$$i\Psi_t + \Psi_{xx} - V(x)\Psi + g\Psi|\Psi|^2 = 0. \tag{1}$$

In this contribution, we will be concerned with the Gross-Pitaevskii equations featuring complex potentials $V(x)$ [1, 2]. In quantum physics, complex potentials provide a simple means to account for the inelastic scattering of particles as well as for the loading of particles in an open system [3, 4]. The x-intervals with $\mathrm{Im}\, V(x) > 0$

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and Im $V(x) < 0$ correspond to the gain and loss of particles, respectively. When the gain exactly compensates the loss, that is, when V obeys the symmetry

$$V^*(x) = V(-x), \tag{2}$$

the potential is referred to as the parity-time (PT-) symmetric [5].

The nonlinear Schrödinger equation (1) with a PT-symmetric potential (2) is also used in the paraxial nonlinear optics [6]. In the optics context, t and x stand for the longitudinal and transverse coordinates, and $V(x)$ models the complex refractive index [7].

Stimulated by the interest from the atomic physics and optics, a number of exactly-solvable Gross-Pitaevskii equations was identified, both within and outside the PT-symmetric variety. The list includes periodic complex potentials [8, 9]; the PT-symmetric Scarff II [6, 10] and Rosen-Morse II potentials [11], as well as a PT-symmetric double-well superposition of a quadratic and a gaussian [12].

This contribution deals with potentials of the form

$$V(x) = -W^2 + iW_x, \tag{3}$$

where $W(x)$ is a real function (called the *potential base* below), with $W(x) \to$ const as $|x| \to \infty$. Wadati was apparently the first author who noted the relevance of potentials (3) for the PT-symmetric quantum mechanics [13].[1] For the purposes of this study, we will be referring to (3) as the Wadati potentials.

We consider the standing-wave solutions $\Psi(x,t) = \psi(x)e^{i\kappa^2 t}$, where κ^2 is real while the spatial part of the eigenfunction obeys the stationary equation

$$-\psi_{xx} + V(x)\psi - g\psi|\psi|^2 = -\kappa^2\psi. \tag{4}$$

In the linear case ($g = 0$), the stationary Schrödinger equation with the potential (3) and eigenvalue $-\kappa^2$ can be mapped onto the Zakharov-Shabat spectral problem, with the potential $W(x)$ and eigenvalue $i\kappa$ [18–20]. This correspondence allows one to obtain complex Schrödinger potentials with an entirely real spectrum from the real Zakharov-Shabat potentials whose entire discrete spectrum is pure imaginary. Potentials of the latter type are abundant—in fact, all Zakharov-Shabat eigenvalues of any single-peaked real potential $W(x)$ are pure imaginary [21, 22]. An example of a multihump potential with an entirely imaginary discrete spectrum is given by the modified Korteweg-de Vries multisoliton [23].

In the nonlinear domain, the Gross-Pitaevskii equations with Wadati potentials enjoy an equally exceptional status. In the context of systems with gain and loss, the PT-symmetric Wadati potentials are unique among all PT-symmetric potentials in that they support continuous families of *asymmetric* solitons [24]. This feature has

[1] Yet these have not been unheard of before. For instance, the potentials (3) appear in the context of supersymmetry [14–16] and have applications in subatomic physics (where they were utilized for the modeling of neutrino oscillations [17]).

an analogue outside the realm of PT-symmetric systems. Namely, unlike the generic non-PT symmetric potentials, the PT-asymmetric Wadati potentials bear continuous families of stable nonlinear modes [22, 25]. (Generic non-PT symmetric complex potentials can only support isolated dissipative solitons rather than continuous families of those [26].) These unique attributes of the Wadati potentials stem from the fact that the stationary nonlinear Schrödinger equation (4) with V as in (3) has an x-independent invariant [25].

Finally, it is fitting to note that the Wadati potentials support constant-density waves. This property has been used to study the modulational instability within the Gross-Pitaevskii equations with complex potentials [27].

In this contribution we propose a new procedure for the systematic construction of exactly solvable Wadati potentials. Here, we restrict ourselves to the PT-symmetric case, that is, to the even functions $W(x)$.

Our approach is formulated in Sects. 2 and 4 for the attractive ($g > 0$) and repulsive ($g < 0$) boson gas, respectively. The general procedure for the attractive nonlinearity is exemplified by two Wadati potentials with exact bright solitons (Sect. 3). In the repulsive-gas situation, we construct potentials bearing exact lump and bubble solutions (Sect. 5). Finally, Sect. 6 presents a Wadati potential generating a stationary flow of the condensate.

2 General Procedure: Attractive Nonlinearity

We start with the attractive nonlinearity, $g > 0$, and assume that the potential has been gauged so that $W_x \to 0$ as $|x| \to \infty$. Our main interest is in localised solutions; these obey

$$|\psi(x)| \to 0, \ |\psi_x(x)| \to 0 \quad \text{as } |x| \to \infty. \tag{5}$$

The boundary conditions (5) require that $\kappa^2 > 0$. We let $\kappa > 0$, for definiteness.

It is convenient to cast the equation (4) in the form

$$u_{zz} + (A^2 - iA_z)u + 2u|u|^2 = u, \tag{6}$$

where

$$A(z) = \frac{W(x)}{\kappa}, \quad u(z) = \sqrt{\frac{g}{2}}\frac{\psi(x)}{\kappa}, \quad z = \kappa x.$$

The boundary conditions (5) translate into

$$|u(z)| \to 0, \ |u_z| \to 0 \quad \text{as } |z| \to \infty. \tag{7}$$

Central to our approach is the observation that the equation (6) can be written as a first-order system

$$u_z - iAu + v = 0,$$
$$v_z + iAv - 2u|u|^2 + u = 0.$$

The polar decomposition

$$u = ae^{i\theta}, \quad v = be^{i\chi},$$

where $a > 0, 0 \le \theta < 2\pi$ and $b^2 > 0, 0 \le \chi < \pi$, takes this system to

$$a_z = -b\cos\mu, \tag{8a}$$
$$b_z = a(2a^2 - 1)\cos\mu, \tag{8b}$$
$$(\theta_z - A)a = -b\sin\mu, \tag{8c}$$
$$(\chi_z + A)b = a(1 - 2a^2)\sin\mu, \tag{8d}$$

where we have introduced the angle

$$\mu(z) = \chi(z) - \theta(z).$$

An immediate consequence of (8a)–(8b) is a conservation law

$$a^2\left(1 - a^2\right) = b^2 + C,$$

where C is a constant. Equation (8c), along with the boundary conditions (7) and the fact that A remains bounded as $|z| \to \infty$, gives $b\sin\mu \to 0$. On the other hand, (8a) implies $b\cos\mu \to 0$. Taken together, these two results lead us to conclude that $b \to 0$ as $|z| \to \infty$ and so $C = 0$:

$$a^2\left(1 - a^2\right) = b^2. \tag{9}$$

With the relation (9) in place, equation (8a) can be integrated to give

$$a = \mathrm{sech}(\Phi - \Phi_0), \quad b = \mathrm{sech}(\Phi - \Phi_0)\tanh(\Phi - \Phi_0), \tag{10}$$

where

$$\Phi(z) = \int_0^z \cos\mu(s)ds,$$

and Φ_0 is a constant of integration. The remaining two equations, (8c) and (8d), can be solved for θ and A:

$$\theta = -\frac{\mu}{2} - \frac{1}{2}\int \frac{a^3}{b}\sin\mu dz, \tag{11}$$
$$A = -\frac{\mu_z}{2} + \frac{a}{2b}\left(2 - 3a^2\right)\sin\mu. \tag{12}$$

The seed function $\cos\mu(z)$ can be chosen arbitrarily. Once $\mu(z)$ has been chosen, the first equation in (10) gives $a(z)$ while (11) together with the second equation in (10) produce $\theta(z)$. The corresponding potential base function $A(z)$ is given by (12).

In this contribution we confine ourselves to the seed functions whose integrals $\Phi(z)$ are bounded (from above or from below) over the whole line. Assuming, for definiteness, that $\Phi(z)$ is bounded from below and choosing the constant Φ_0 to satisfy

$$\Phi_0 < \inf_{-\infty<z<\infty} \Phi(z),$$

we will ensure that $\Phi(z) - \Phi_0 > 0$ and the function $b(z)$ in (10) is bounded away from zero. Then the quotient $a(z)/b(z)$ in (11) and (12) will be nonsingular:

$$\left|\frac{a}{b}\right| = \operatorname{cotanh}|\Phi(z) - \Phi_0| < \infty.$$

A simple class of suitable $\Phi(z)$ consists of even functions bounded by their value at the origin.

Finally, equation (10) implies that the solution will only be localised (that is, satisfy the boundary conditions (7)) if the integral $\int_{-\infty}^{\infty} \cos\mu\, ds$ diverges. This means that $\cos\mu(z)$ should either remain nonzero as $|z| \to \infty$ (for example, tend to a nonzero constant), or decay to zero—but no faster than z^{-1}.

3 Pulse-Like Solitons: Two Simple Examples

As our first example we take the seed function of the form

$$\cos\mu(z) = \frac{\sinh z}{\sqrt{\sinh^2 z + \cos^2\alpha}}, \tag{13}$$

where $0 \le \alpha < \pi/2$ is a parameter. The corresponding integral

$$\Phi(z) - \Phi_0 = \operatorname{Arctanh}\sqrt{1 - \sin^2\alpha\,\operatorname{sech}^2 z} \tag{14}$$

is even and monotonically growing from $\operatorname{Arctanh}(\cos\alpha)$ to infinity as z varies from 0 to ∞. We have chosen Φ_0 so as to simplify (14).

Equations (10), (11), and (12) give the potential base function

$$A = \frac{3}{2}\cos\alpha\,\operatorname{sech} z, \tag{15}$$

as well as the absolute value and phase of the soliton:

$$a = \sin\alpha\,\operatorname{sech} z, \quad \theta = \frac{1}{2}\cos\alpha\,\arctan(\sinh z)\,. \tag{16}$$

The Wadati potential $-A^2 + iA_z$ with A as in (15) belongs to the class of PT-symmetric potentials considered by Musslimani et al. [6], and equations (16) constitute the corresponding soliton solution.

Our second example is equally simple—yet new. This time the seed function is

$$\cos\mu(z) = \frac{1}{\sqrt{1+z^2}},$$

with the integral

$$\Phi(z) = \operatorname{Arctanh}\frac{z}{\sqrt{1+z^2}}.$$

The function $\Phi(z)$ grows without bound as z changes from zero to infinity. Letting $\Phi_0 = 0$ and making use of (10), (11), and (12) we arrive at the base

$$A(z) = 1 - \frac{2}{1+z^2}$$

and the corresponding PT-symmetric complex Wadati potential:

$$-A^2 + iA_z = -1 + \frac{4z(z+i)}{(z^2+1)^2}. \tag{17}$$

The localised nonlinear mode, or the soliton, supported by this potential is also given by a rational function:

$$u(z) = \frac{1-iz}{1+z^2}. \tag{18}$$

(We remind the reader that z is a real coordinate in (17) and (18).)

The potential (17) and the soliton (18) are depicted in Fig. 1.

4 Repulsive Nonlinearity and Nonvanishing Backgrounds

Turning to the Gross-Pitaevskii equation with repulsion (equation (4) with $g < 0$), we focus on solitons in the constant-density condensate, that is, localised solutions satisfying the nonvanishing boundary conditions at infinity:

$$|\psi(x)|^2 \to \rho_0, \ |\psi_x(x)| \to 0 \quad \text{as } |x| \to \infty. \tag{19}$$

Assuming that the potential has been gauged so that $W(x) \to 0$ as $|x| \to \infty$, the conditions (19) require $\kappa^2 = g\rho_0 < 0$. Scaling the dependent and independent variables as in

$$A(z) = \lambda W(x), \quad u(z) = \sqrt{-\frac{g}{2}}\lambda\psi(x), \quad z = \frac{x}{\lambda},$$

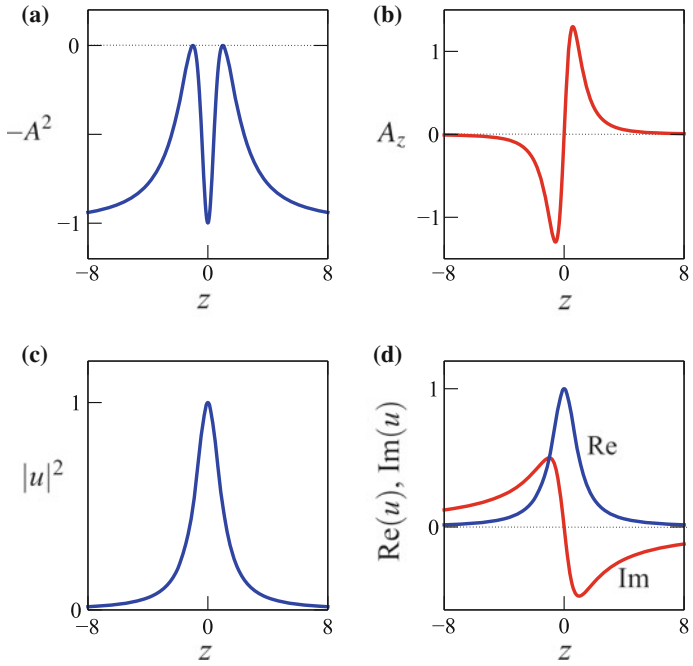

Fig. 1 *Top row* The real (**a**) and imaginary (**b**) part of the rational-function *PT*-symmetric potential (17). *Bottom row* The modulus squared of the corresponding localised nonlinear mode (**c**) and its real and imaginary part (**d**)

with $\lambda = \sqrt{-2/\kappa^2} > 0$, the equation (4) becomes

$$u_{zz} + (A^2 - iA_z)u - 2u|u|^2 = -2u, \tag{20}$$

while the nonvanishing boundary conditions are reduced to

$$|u|^2 \to 1, \ |u_z|^2 \to 0 \quad \text{as } |z| \to \infty. \tag{21}$$

The equation (20) can be written as a first-order system

$$u_z - iAu + v = 0, \tag{22}$$

$$v_z + iAv + 2u|u|^2 - 2u = 0. \tag{23}$$

In the same way as the system (8a)–(8b) gave rise to the conservation law (9), the system (22)–(23) implies

$$b = \pm(1 - a^2), \tag{24}$$

where we have introduced the polar decomposition

$$u = ae^{i\theta}, \quad v = be^{i\chi},$$

and used the boundary conditions (21) together with the fact that $A \to 0$ at infinity. In (24), the top sign corresponds to solutions with $a \leq 1$ while the bottom sign pertains to those with $a \geq 1$.

Letting $\mu(z) = \chi(z) - \theta(z)$ and making use of the conservation law (24) we obtain the modulus and phase of the solution in the sector $a \leq 1$:

$$a = -\tanh(\Phi - \Phi_0), \quad \theta = -\frac{\mu}{2} - \int \frac{(a^2+1)}{2a} \sin\mu \, dz. \tag{25}$$

Here

$$\Phi(z) = \int_0^z \cos\mu(s) ds,$$

as before. The Wadati potential bearing the solution (25) is based on the function

$$A = -\frac{\mu_z}{2} + \frac{(1-3a^2)}{2a} \sin\mu. \tag{26}$$

In the sector $a \geq 1$, the potential base and solution are given by

$$A = -\frac{\mu_z}{2} + \frac{(3a^2-1)}{2a} \sin\mu;$$
$$a = \operatorname{cotanh}(\Phi - \Phi_0), \quad \theta = -\frac{\mu}{2} + \int \frac{(a^2+1)}{2a} \sin\mu \, dz.$$

5 Lumps and Bubbles in a Homogeneous Condensate

Consider, first, the case $a \leq 1$ and let

$$\cos\mu(z) = -\frac{\sinh z}{\sqrt{\sinh^2 z + \cos^2\alpha}}, \tag{27}$$

where $0 \leq \alpha < \pi/2$ is a parameter. (This is a negative of the seed function (13) employed in the attractive case.) Using the integral

$$\Phi(z) - \Phi_0 = -\operatorname{Arctanh}\sqrt{1 - \sin^2\alpha \operatorname{sech}^2 z},$$

equation (26) provides the potential base:

$$A = \frac{3\cos\alpha}{2}\,\mathrm{sech}\, z. \tag{28}$$

Equations (25) give the corresponding solution:

$$u = (\cos\alpha\,\mathrm{sech}\, z + i\tanh z)(\mathrm{sech}\, z + i\tanh z)^{\sigma}, \quad \sigma = \frac{\cos\alpha}{2}. \tag{29}$$

The quantity $|u|^2$ has a dip at the origin:

$$|u|^2 = 1 - \sin^2\alpha\,\mathrm{sech}^2 z.$$

Therefore, (29) describes a bubble—a localised rarefaction in a homogeneous background density.[2]

In the sector $a \geq 1$, choosing

$$\cos\mu = \frac{\sinh z}{\sqrt{\sinh^2 z + \cosh^2\beta}}, \quad \Phi - \Phi_0 = \mathrm{Arccoth}\sqrt{1 + \sinh^2\beta\,\mathrm{sech}^2 z},$$

with β a real parameter, $0 \leq \beta < \infty$, gives rise to the potential base

$$A = \frac{3\cosh\beta}{2}\mathrm{sech}\, z \tag{30}$$

and the solution

$$u = (\cosh\beta\,\mathrm{sech}\, z + i\tanh z)(\mathrm{sech}\, z + i\tanh z)^{\sigma}, \quad \sigma = \frac{\cosh\beta}{2}.$$

This time the quantity $|u|^2$ has a maximum at the origin,

$$|u|^2 = 1 + \sinh^2\beta\,\mathrm{sech}^2 z,$$

and so the solution describes a lump—a localised domain of compression in a condensate of uniform density.

Note that the potential base (28) can be formally obtained from (30) by letting $\beta = i\alpha$. Therefore the bubble- and lump-like solitons form a seamless one-parameter family.

[2]In nonlinear dynamics, the *bubble* refers to a particular class of nontopological solitons with nontrivial boundary conditions [28, 29]. In contrast to the strict mathematical terminology, we use this word in a broad physical sense here—as a synonym of a hole in the constant-density condensate. The optical equivalent of the condensate bubble is *dark soliton*.

6 Solitons in a Stationary Flow

In the boson-condensate interpretation of solutions to the equation (6), the function $J(z) = a^2\theta_z$ represents the superfluid current. Physically, of interest are stationary flows, that is, solutions with $J(z)$ approaching nonzero values as $z \to \pm\infty$. In this section we construct Wadati potentials supporting the stationary flow of condensate.

The lump and the bubble solitons from the previous section are characterised by the zero current at infinity. To construct exact solutions with a nonzero stationary current, we modify the seed function (27) by introducing an additional parameter:

$$\cos\mu = -\sin\varphi\,\frac{\sinh y}{\sqrt{\sinh^2 y + \cos^2\alpha}}, \quad y = \sin(\varphi)z.$$

Here $0 < \varphi \le \pi/2$. The integral of the seed is

$$\Phi(z) = -\mathrm{Arctanh}\sqrt{1 - \sin^2\alpha\,\mathrm{sech}^2 y} + \Phi_0.$$

The corresponding PT-symmetric Wadati potential is generated by the base function

$$A(z) = \frac{3(\sin^2\alpha - \sin^2\varphi) - 2\cos^2\varphi\cosh^2 y}{2\cosh y\sqrt{\cos^2\varphi\sinh^2 y + \cos^2\alpha}}. \tag{31}$$

The absolute value of the corresponding solution has a simple form,

$$a(z) = \sqrt{1 - \sin^2\alpha\,\mathrm{sech}^2 y}, \tag{32a}$$

and the phase gradient is given by

$$\theta_z = \frac{(\sin^2\varphi - \sin^2\alpha)(\sin^2\alpha - 3\cosh^2 y) - 2\cos^2\varphi\cosh^4 y}{2\cosh y\left(\cosh^2 y - \sin^2\alpha\right)\sqrt{\cos^2\varphi\sinh^2 y + \cos^2\alpha}}. \tag{32b}$$

When $\varphi \neq \pi/2$, the solution represents a stationary flow:

$$J|_{z\to\pm\infty} = -\cos\varphi \neq 0.$$

Varying φ we can generate potential-solution pairs with negative currents ranging from -1 to 0. (Inserting a minus in front of the right-hand side in (31) and (32b) produces pairs with positive currents.)

An example of the potential generated by the base function (31) and the corresponding nonlinear mode are shown in Fig. 2.

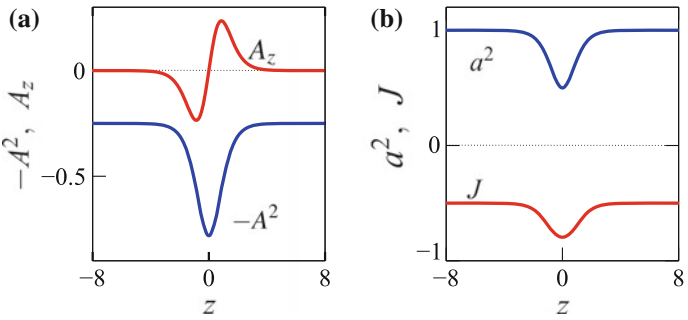

Fig. 2 **a** The real (*blue*) and imaginary (*red*) part of the PT-symmetric Wadati potential generated by the base function (31). **b** The corresponding nonlinear mode (32a, 32b). Shown is the condensate density a^2 and the superfluid current $J = a^2\theta_z$. In these plots, $\alpha = \pi/4$ and $\varphi = \pi/3$

7 Concluding Remarks

Due to their unique properties, Gross-Pitaevskii equations with the Wadati potentials are of particular interest in PT-symmetric theories. Accordingly, it would be desirable to have a sufficiently diverse and ample collection of *exactly-solvable* Wadati potentials—these would serve as testing grounds for realistic physical models and starting points for perturbation expansions. The purpose of this contribution was to show how one can generate broad classes of PT-symmetric Wadati potentials along with exact localised solutions of the associated Gross-Pitaevskii equations.

The crux of our method lies in the ability to write the nonlinear second-order equation with a Wadati potential, as a symmetric system of two first-order equations. The potential function of this first-order system is nothing but the base function of the Wadati potential of the original second-order equation.

A practically-minded reader may naturally wonder what is the advantage of our approach over a simple reverse engineering, where the potential $V(x)$ is reconstructed from a postulated localised solution of equation (4):

$$V(x) = \frac{\psi_{xx}}{\psi} + g|\psi|^2 - \kappa^2. \tag{33}$$

The answer is that the back-engineered potential (33) will generally *not* be of the Wadati variety.

In contrast, our method constructs the *base function* first. Only after the base $W(x)$ has been constructed does one proceed to form the potential $V = -W^2 + iW_x$. Thus the resultant potential is Wadati by construction.

We have exemplified this procedure by constructing several exactly solvable PT-symmetric Wadati potentials for the attractive and repulsive Gross-Pitaevskii equations. In the case of the attractive ("focussing") cubic nonlinearity, the expression (15) reproduces the base function known in literature while the rational potential (17)

is new. In the repulsive ("defocussing") situation, the bases (28) and (30) constitute a continuous family of Wadati potentials supporting solitons over a nonvanishing background (lumps and bubbles). To the best of our knowledge, these potential-solution pairs are also new. Finally, we have constructed an exactly-solvable PT-symmetric potential supporting bubble-like solitons in a stationary flow of the superfluid. The corresponding potential base function is in (31).

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The EMM and the Spectral Analysis of a Non Self-adjoint Hamiltonian on an Infinite Dimensional Hilbert Space

Natalia Bebiano and João da Providência

Abstract The Equation of Motion Method is used in the spectral analysis of a non self-adjoint bosonic Hamiltonian acting on an infinite dimensional Hilbert space. The presented operator has real eigenvalues and can be diagonalized when it is expressed in terms of pseudo-bosons, which do not behave as ordinary bosons under the adjoint transformation, but obey the Weil-Heisenberg commutation relations.

1 Introduction

In conventional formulations of non-relativistic quantum mechanics, the Hamiltonian operator is self-adjoint. However, certain relativistic extensions of quantum mechanics lead to the consideration of non self-adjoint Hamiltonian operators with a real spectrum. This motivated an intense research activity, both on the physical and mathematical level (see, e.g. [1–9] and their references).

Throughout, we shall use synonymously the terms Hermitian and self-adjoint.

Let $\mathscr{D}$ be a certain domain, dense in a Hilbert space $\mathscr{H}$, endowed with an inner product $\langle , \rangle$. Let $a, b, a^*, b^* : \mathscr{D} \to \mathscr{D}$, be bosonic operators. We recall that, conventionally, a, b are said to be *annihilation operators*, while a^*, b^* are *creation operators*. It is worth noticing that these operators are unbounded. Moreover, a, b and of their adjoints satisfy the commutation rules (CR's),

$$[a, a^*] = [b, b^*] = \mathbf{1}, \tag{1}$$

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where $\mathbf{1}$ is the identity operator on $\mathscr{H}$. (This means that $aa^*f - a^*af = bb^*f - b^*bf = f$ for any $f \in \mathscr{D}$.) Furthermore,

$$[a, b^*] = [b, a^*] = [a^*, b^*] = [a, b] = 0. \tag{2}$$

As it is well-known, the canonical commutation relations (1) and (2) characterize an algebra of Weil-Heisenberg (W-H). Moreover, the existence of a vector $\Phi_0 \in \mathscr{D}$, a so-called *vacuum state*, satisfying,

$$a\Phi_0 = b\Phi_0 = 0,$$

is postulated. The set of vectors

$$\{\Phi_{m,n} = a^{*m}b^{*n}\Phi_0 : \ m, n \geq 0\}, \tag{3}$$

constitutes a basis of $\mathscr{H}$, that is, every vector in $\mathscr{H}$ can be uniquely expressed in terms of this vector system, which is *complete*, since 0 is the only vector orthogonal to all its elements.

The main goal of this note is to investigate spectral properties of a certain non self-adjoint operator which is expressed as a quadratic combination of bosonic operators.

2 Non Self-adjoint Operator and the EMM

We are concerned with bosonic operators $a_i^*, a_j, \ i, j = 1, \ldots N$, which, as usual, act on an infinite dimensional Hilbert space $\mathscr{H}$. Ordinary bosons obey the Weil-Heisenberg commutation relations,

$$[a_i, a_j^*] = \delta_{ij}\mathbf{1}, \quad [a_i^*, a_j^*] = 0, \quad [a_i, a_j] = 0, \quad i, j = 1, \ldots, N,$$

where δ_{ij} denotes the Kronecker symbol (δ_{ij} equals 1 for $i = j$ and 0 otherwise). Let us consider the non self-adjoint Hamiltonian

$$H = \sum_{i,j=1}^{N} \left(A_{ij}a_i^*a_j + \frac{1}{2}B_{ij}a_i^*a_j^* - \frac{1}{2}B_{ij}a_ia_j \right), \tag{4}$$

where $A = (A_{ij}), \ B = (B_{ij})$ are real symmetric matrices of size $N \times N$. In order to determine the eigenvalues of H, we use the equation of motion method (EMM). We investigate the condition

$$\left[H, \sum_{i=1}^{N}(X_ia_i^* - Y_ia_i) \right] = \lambda \sum_{i=1}^{N}(X_ia_i^* - Y_ia_i), \tag{5}$$

with λ a complex parameter and $[X, Y] = XY - YX$ denoting, as usually, the commutator of X and Y. From (5), we get the block matrix equation

$$\begin{bmatrix} A & B \\ B & -A \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix} = \lambda \begin{bmatrix} X \\ Y \end{bmatrix} \tag{6}$$

where $X = (X_i)$, $Y = (Y_i)$ are column matrices with N entries. Since the block matrix

$$M = \begin{bmatrix} A & B \\ B & -A \end{bmatrix}$$

is real symmetric, its eigenvalues λ are real. From (6), it follows that

$$\begin{bmatrix} A & B \\ B & -A \end{bmatrix} \begin{bmatrix} Y \\ -X \end{bmatrix} = -\lambda \begin{bmatrix} Y \\ -X \end{bmatrix},$$

so, if λ is an eigenvalue of (6), so is $-\lambda$.Thus, the eigenvalues appear in pairs of symmetric real numbers. Let us consider a set of orthogonal eigenvectors of (6). Let

$$\begin{bmatrix} X^{(r)} \\ Y^{(r)} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} Y^{(r)} \\ -X^{(r)} \end{bmatrix}$$

be the eigenvectors corresponding to the eigenvalues $\lambda_r > 0$ and $-\lambda_r$, respectively. Since they are associated to distinct eigenvalues, they are orthogonal. Orthogonality implies

$$\begin{aligned} X^{(r)T} X^{(s)} + Y^{(r)T} Y^{(s)} &= \delta_{rs}, \\ Y^{(r)T} X^{(s)} - X^{(r)T} Y^{(s)} &= 0. \end{aligned}$$

These orthogonality relations are matricially expressed as

$$\begin{bmatrix} X^{(s)T} & Y^{(s)T} \end{bmatrix} \begin{bmatrix} X^{(r)} \\ Y^{(r)} \end{bmatrix} = \delta_{rs}, \quad \begin{bmatrix} X^{(s)T} & Y^{(s)T} \end{bmatrix} \begin{bmatrix} Y^{(r)} \\ -X^{(r)} \end{bmatrix} = 0,$$

$$\begin{bmatrix} Y^{(s)T} & -X^{(s)T} \end{bmatrix} \begin{bmatrix} X^{(r)} \\ Y^{(r)} \end{bmatrix} = 0, \quad \begin{bmatrix} Y^{(s)T} & -X^{(s)T} \end{bmatrix} \begin{bmatrix} Y^{(r)} \\ -X^{(r)} \end{bmatrix} = \delta_{rs},$$

or, compactly, as

$$\begin{bmatrix} \mathscr{X} & -\mathscr{Y} \\ \mathscr{Y} & \mathscr{X} \end{bmatrix}^T \begin{bmatrix} \mathscr{X} & -\mathscr{Y} \\ \mathscr{Y} & \mathscr{X} \end{bmatrix} = I_{2N},$$

where I_{2N} is the $2N \times 2N$ identity matrix and

$$\mathscr{X} = \left[X^{(1)} \ \ldots \ X^{(N)}\right], \quad \mathscr{Y} = \left[Y^{(1)} \ \ldots \ Y^{(N)}\right] \in M_N,$$

the algebra of $N \times N$ real matrices. The matrix

$$\begin{bmatrix} \mathscr{X} & \mathscr{Y} \\ -\mathscr{Y} & \mathscr{X} \end{bmatrix} = \exp \begin{bmatrix} S & T \\ -T & S \end{bmatrix}, \quad S = -S^T, \ \ T = T^T,$$

belongs to a certain subgroup of the real orthogonal group and the matrix

$$\begin{bmatrix} S & T \\ -T & S \end{bmatrix},$$

belongs to a certain sub-algebra of the algebra of the real skew-symmetric matrices. Consider the pseudo-bosons defined as

$$c_r^{\ddagger} = \sum_{i=1}^{N} (X_i^{(r)} a_i^* - Y_i^{(r)} a_i), \quad c_r = \sum_{i=1}^{N} (Y_i^{(r)} a_i^* + X_i^{(r)} a_i), \quad r, s = 1, \ldots, N. \tag{7}$$

Although $c_r^{\ddagger} \neq c_r^*$, pseudo-bosons obey the Weil-Heisenberg commutation relations,

$$[c_r, c_s^{\ddagger}] = \delta_{rs} \mathbf{1}, \quad [c_r^{\ddagger}, c_s^{\ddagger}] = 0, \quad [c_r, c_s] = 0, \quad r, s = 1, \ldots, N,$$

where $\mathbf{1}$ is the identity on $\mathscr{H}$. The expressions (7) may be inverted, using the orthogonality relations, as

$$a_i^* = \sum_{r=1}^{N} (X_i^{(r)} c_r^{\ddagger} + Y_i^{(r)} c_r), \quad a_i = \sum_{r=1}^{N} (-Y_i^{(r)} c_r^{\ddagger} + X_i^{(r)} c_r).$$

From these expressions, we obtain

$$H = \sum_{i=1}^{N} \sum_{r=1}^{N} \lambda_r Y_i^{(r)2} \mathbf{1} + \sum_{r=1}^{N} \lambda_r c_r^{\ddagger} c_r.$$

The eigenvectors of H are of the form

$$\Psi_{n_1, \ldots, n_N} = c^{\ddagger n_1} \cdots c^{\ddagger n_N} \Psi_0,$$

where Ψ_0 is such that

$$c_1 \Psi_0 = 0, \ldots, c_N \Psi_0 = 0,$$

and the respective eigenvalues are of the form

$$E_{n_1,\ldots,n_N} = \sum_{i=1}^{N}\sum_{r=1}^{N} \lambda_r Y_i^{(r)2} + \sum_{r=1}^{N} n_r \lambda_r,$$

so that

$$H\Psi_{n_1,\ldots,n_N} = E_{n_1,\ldots,n_N}\Psi_{n_1,\ldots,n_N}.$$

Similarly, the eigenvectors of

$$H^* = \sum_{i,j=1}^{N}\left(A_{ij}a_i^* a_j - \frac{1}{2}B_{ij}a_i^* a_j^* + \frac{1}{2}B_{ij}a_i a_j\right).$$

are given by

$$\Psi'_{n_1,\ldots,n_N} = c^{*n_1}\cdots c^{*n_N}\Psi'_0,$$

where Ψ'_0 is such that

$$c_1^{\ddagger *}\Psi'_0 = 0, \ldots, c_N^{\ddagger *}\Psi'_0 = 0.$$

The eigenvalues of H and H^* coincide. The associated eigenvector systems are biorthogonal:

$$\langle \Psi'_{n_1,\ldots,n_N}, \Psi_{m_1,\ldots,m_N}\rangle = n_1!\cdots n_N!\delta n_1 m_1\cdots\delta n_N m_N\langle\Psi'_0, \Psi_0\rangle.$$

Next, the existence of the vacua vectors Ψ_0 and Ψ'_0 is discussed. The real skew-symmetric matrix

$$\begin{bmatrix} S & T \\ -T & S \end{bmatrix},$$

induces the operator

$$\mathscr{S} = -\frac{1}{2}\sum_{i,j=1}^{N}\left(s_{ij}(a_i^* a_j + a_j a_i^*) + t_{ij}a_i^* a_j^* + t_{ij}a_i a_j\right), \quad (s_{ij}) = S,\ (t_{ij}) = T$$

which satisfies

$$\mathrm{e}^{\mathscr{S}} a_r^* \mathrm{e}^{-\mathscr{S}} = c_r^\ddagger = \sum_{i=1}^{N} (X_i^{(r)} a_i^* - Y_i^{(r)} a_i),$$

$$\mathrm{e}^{\mathscr{S}} a_r \mathrm{e}^{-\mathscr{S}} = c_r = \sum_{i=1}^{N} (Y_i^{(r)} a_i^* + X_i^{(r)} a_i), \quad r, s = 1, \ldots, N.$$

By definition, we shall consider

$$\mathscr{D} = \left\{ \sum_{n_1,\ldots,n_N} z_{n_1,\ldots,n_N} \, a^{*\,n_1} \cdots a^{*\,n_N} \, \Phi_0 : z_{n_1,\ldots,n_N} \in \mathbb{C}, \; n_i \geq 0 \right\},$$

where the sum is finite. Some considerations are in order. We observe that a_j^* and a_j map $\mathscr{D}$ into $\mathscr{D}$ and that $\mathscr{S}^n \Phi_0 \in \mathscr{D}$, $0 \leq n \in \mathbf{Z}$, where $\Phi_0 \in \mathscr{D}$ is the vacuum of the operators a_i, i.e. a vector such that

$$a_1 \Phi_0 = 0, \ldots, a_N \Phi_0 = 0,$$

whose existence is postulated. It follows that

$$\Psi_0 = \mathrm{e}^{\mathscr{S}} \Phi_0, \quad \Psi_0' = \mathrm{e}^{-\mathscr{S}} \Phi_0.$$

Consider the series expansion

$$\sum_{n=0}^{\infty} \frac{(\gamma \mathscr{S})^n}{n!} \Phi_0, \quad \gamma = \pm 1.$$

The following question naturally arises: does it converge? Can we ensure that Ψ_0 belongs to $\mathscr{H}$? This point must be investigated on a case by case basis. In the next section it is considered for a specific example in which these questions are affirmatively answered.

The following remark is in order. The spectral analysis of a non self-adjoint Hamiltonian quadratic in bosonic operators should be preceded by the spectral analysis of its self-adjoint part. Recall that a self-adjoint Hamiltonian quadratic in bosonic operators may not have a real spectrum, as is the case of the self-adjoint operator

$$x^2 + \frac{\mathrm{d}^2}{\mathrm{d}x^2} : \mathscr{D} \to \mathscr{D},$$

which does not have real eigenvalues. Indeed, for instance,

$$\left(x^2 + \frac{\mathrm{d}^2}{\mathrm{d}x^2} \right) \mathrm{e}^{i\,x^2/2} = i\, \mathrm{e}^{i\,x^2/2}.$$

Notice that $e^{i\,x^2/2} \notin \mathscr{H}$, because $\langle e^{i\,x^2/2}, e^{i\,x^2/2}\rangle = +\infty$. In general, a non self-adjoint Hamiltonian may have a real spectrum and a system of eigenvectors only if the spectrum of its self-adjoint part is real. Only then its system of eigenvectors will be biorthogonal to the system of eigenvectors of the adjoint Hamiltonian.

3 Example

As a simple illustrative example of application of the EMM developed in the previous section, we consider the Hamiltonian in (4) for case N even and with

$$A = \bigoplus_{i=1}^{N/2} A_i, \quad B = \bigoplus_{i=1}^{N/2} B_i,$$

where

$$A_i = \begin{bmatrix} \alpha_i & 0 \\ 0 & \alpha_i \end{bmatrix}, \quad B_i = \begin{bmatrix} 0 & \beta_i \\ \beta_i & 0 \end{bmatrix}, \quad \alpha_i, \beta_i > 0.$$

The EMM condition $[H, Z] = \lambda Z$, for

$$Z = X_1 a_1^* + X_2 a_2^* - Y_1 a_1 - Y_2 a_2 + \cdots + X_{N-1} a_{N-1}^* + X_N a_N^* - Y_{N-1} a_{N-1} - Y_N a_N,$$

by this order, leads to the real symmetric matrix

$$M = \bigoplus_{i=1}^{N/2} \begin{bmatrix} \alpha_i & 0 & 0 & \beta_i \\ 0 & \alpha_i & \beta_i & 0 \\ 0 & \beta_i & -\alpha_i & 0 \\ \beta_i & 0 & 0 & -\alpha_i \end{bmatrix}, \tag{8}$$

whose positive eigenvalues are as follows

$$\lambda_1 = \lambda_2 = \sqrt{\alpha_1^2 + \beta_1^2},\ \lambda_3 = \lambda_4 = \sqrt{\alpha_2^2 + \beta_2^2},\ \ldots,\ \lambda_{N-1} = \lambda_N = \sqrt{\alpha_{N/2}^2 + \beta_{N/2}^2}.$$

Notice that α_i and $\pm\beta_i$ are the eigenvalues of the blocks A_i and B_i, respectively. In terms of pseudo-bosonic operators, which are determined by the eigenvectors of (8) associated to positive and negative eigenvalues, H is given by

$$H = \sum_{r=1}^{N/2} \left(\sqrt{\alpha_r^2 + \beta_r^2} - \alpha_r + \sqrt{\alpha_r^2 + \beta_r^2} \left(c_{2r-1}^{\ddagger} c_{2r-1} + c_{2r}^{\ddagger} c_{2r} \right) \right).$$

For

$$\mathscr{S} = \theta_1(a_1^* a_2^* + a_1 a_2) + \theta_2(a_3^* a_4^* + a_3 a_4) + \cdots + \theta_{N/2}(a_{N-1}^* a_N^* + a_{N-1} a_N),$$

where $-\pi/2 \leq \theta_i \leq \pi/2$, $i = 1, \ldots, N/2$, we obtain

$$\begin{aligned}
&\mathrm{e}^{\mathscr{S}} \left(\sqrt{\alpha_1^2 + \beta_1^2}(a_1^* a_1 + a_2 a_2^*) + \cdots + \sqrt{\alpha_{N/2}^2 + \beta_{N/2}^2}(a_{N-1}^* a_{N-1} + a_N a_N^*) \right) \mathrm{e}^{-\mathscr{S}} \\
&= \sqrt{\alpha_1^2 + \beta_1^2} \cos 2\theta_1 (a_1^* a_1 + a_2 a_2^*) + \cdots + \sqrt{\alpha_{N/2}^2 + \beta_{N/2}^2} \cos 2\theta_{N/2} (a_{N-1}^* a_{N-1} + a_N a_N^*) \\
&+ \sqrt{\alpha_1^2 + \beta_1^2} \sin 2\theta_1 (a_1 a_2 - a_1^* a_2^*) + \cdots + \sqrt{\alpha_{N/2}^2 + \beta_{N/2}^2} \sin 2\theta_{N/2} (a_{N-1} a_N - a_{N-1}^* a_N^*)
\end{aligned}$$

Taking

$$\tan 2\theta_1 = -\frac{\beta_2}{\alpha_2}, \ \ldots, \ \tan 2\theta_{N/2} = -\frac{\beta_{N/2}}{\alpha_{N/2}},$$

we find

$$\begin{aligned}
&\mathrm{e}^{\mathscr{S}} \left(\sqrt{\alpha_1^2 + \beta_1^2}(a_1^* a_1 + a_2 a_2^*) + \cdots + \sqrt{\alpha_{N/2}^2 + \beta_{N/2}^2}(a_{N-1}^* a_{N-1} + a_N a_N^*) \right) \mathrm{e}^{-\mathscr{S}} \\
&= \alpha_1(a_1^* a_1 + a_2 a_2^*) + \beta_1(a_1^* a_2^* - a_1 a_2) + \cdots \\
&+ \alpha_{N/2}(a_{N-1}^* a_{N-1} + a_N a_N^*) + \beta_{N/2}(a_{N-1}^* a_N^* - a_{N-1} a_N).
\end{aligned}$$

We have shown that the desired transformation is given by $e^{\mathscr{S}}$.

Recall that $\Phi_0 \in \mathscr{D}$ is the vacuum of the operators a_i, $i = 1 \ldots, N$. Next we prove that $\langle \mathrm{e}^{\mathscr{S}} \Phi_0, \mathrm{e}^{\mathscr{S}} \Phi_0 \rangle < \infty$, so that the groundstate eigenvector of H is $\mathrm{e}^{\mathscr{S}} \Phi_0 \in \operatorname{span} \mathscr{D} = \mathscr{H}$. Indeed, it may be checked that the vector $\mathrm{e}^{\mathscr{S}} \Phi_0$ and the vector

$$\begin{aligned}
\Xi_0 &= \exp(\tan\theta_1 \, a_1^* a_2^* + \cdots + \tan\theta_{N/2} \, a_{N-1}^* a_N^*) \Phi_0 \\
&= \sum_{n_1=1}^{\infty} \cdots \sum_{n_{N/2}=1}^{\infty} \frac{\tan^{n_1}\theta_1}{n_1!} \cdots \frac{\tan^{n_{N/2}}\theta_{N/2}}{n_{N/2}!} a_1^{*n_1} a_2^{*n_1} \cdots a_{N-1}^{*n_{N/2}} a_N^{*n_{N/2}} \, \Phi_0
\end{aligned}$$

may differ only by a numerical factor. Notice that

$$c_i \, \mathrm{e}^{\mathscr{S}} \Phi_0 = c_i \, \Xi_0 = 0, \ i = 1, \ldots, N.$$

Actually, $\mathrm{e}^{\mathscr{S}} \Phi_0$ reduces to Ξ_0 by a convenient rearrangement of the series. Now,

$$\tan\theta_i = \alpha_i/\beta_i - \sqrt{1 + (\alpha_i/\beta_i)^2},$$

so that $\tan^2\theta_i < 1$, and

$$\langle \Xi_0, \Xi_0 \rangle = \prod_{i=1}^{N/2} \sum_{n=0}^{\infty} \tan^{2n}\theta_i = \prod_{i=1}^{N/2} (1 - \tan^2\theta_i)^{-1} < \infty.$$

It follows that $\Xi_0 \in \mathscr{H}$. We observe that the geometric series $\sum_{n=0}^{\infty} \tan^{2n}\theta_i$ with ratio $\tan^2\theta_i < 1$, converges in the interior of the unitary disc.

4 Discussion

In Sect. 2, a non self-adjoint Hamiltonian, which is expressed as a quadratic combination of bosonic operators, is investigated. Its eigenvalues and eigenvectors have been determined with the help of a real symmetric matrix M of size $2N \times 2N$, where N is the number of bosonic states, that is determined by the EMM. The investigated Hamiltonian has a system of eigenvectors expressed in terms of the creation and annihilation operators of pseudo-bosons, which is biorthogonal to the system of eigenvectors of the adjoint Hamiltonian, constructed in terms of pseudo-bosonic operators acting on the associated vacuum state.

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Bessel Sequences, Riesz-Like Bases and Operators in Triplets of Hilbert Spaces

Giorgia Bellomonte

Abstract Riesz-like bases for a triplet of Hilbert spaces are investigated, in connection with an analogous study for more general rigged Hilbert spaces performed in a previous paper. It is shown, in particular, that every ω-independent, complete (total) Bessel sequence is a (strict) Riesz-like basis in a convenient triplet of Hilbert spaces. An application to non self-adjoint Schrödinger-type operators is considered. Moreover, some of the simplest operators we can define by them and their dual bases are studied.

1 Introduction

A Riesz basis of a Hilbert space $\mathcal{H}$ is a sequence $\{\xi_n\}$ of elements of $\mathcal{H}$ that are transformed into an orthonormal basis of $\mathcal{H}$ by some bounded operator with bounded inverse. Riesz bases can also be viewed as *frames* [1–3]; i.e., there exist positive numbers c, C such that

$$c\|\xi\|^2 \leq \sum_{n=1}^{\infty} |\langle \xi | \xi_n \rangle|^2 \leq C\|\xi\|^2, \quad \forall \xi \in \mathcal{H}. \tag{1}$$

What distinguishes a frame from a Riesz basis is its minimality, i.e., once one of its elements is dropped out it ceases to be a frame.

In [4] it was studied a possible extension of the notion of Riesz basis of a Hilbert space to rigged Hilbert spaces, by introducing what we called *Riesz-like* bases, the main difference relying on the fact that the operator transforming $\{\xi_n\}$ into an orthonormal basis need not to be bounded. A motivation for this generalization stems from the following considerations.

Let us assume that $\{\xi_n\}$ is a sequence of vectors of $\mathcal{H}$ for which there exists an unbounded closed linear operator T, with dense domain $D(T)$ and bounded inverse

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T^{-1}, such that $\xi_n \in D(T)$, for every $n \in \mathbb{N}$ and the sequence $\{T\xi_n\}$ is an orthonormal basis for $\mathcal{H}$. In this case we can endow $D(T) \subset \mathcal{H}$ with a new inner product

$$\langle \xi \,|\eta\rangle_{+1} := \langle T\xi \,|T\eta\rangle\,, \quad \xi, \eta \in D(T)$$

which makes it into a Hilbert space denoted by $\mathcal{H}_{+1}$. Since $T^{-1} \in \mathcal{B}(\mathcal{H})$, the C*-algebra of linear bounded operators in $\mathcal{H}$, it follows that $c\|\xi\| \leq \|\xi\|_{+1}$, for some $c > 0$ and for every $\xi \in \mathcal{H}$, then $\mathcal{H}$ can be identified with a subspace of the conjugate dual $\mathcal{H}_{+1}^{\times}$ of $\mathcal{H}_{+1}$. This space, in turn, is isomorphic to the completion of $\mathcal{H}$ with respect to the norm induced by the inner product $\langle \cdot\,|\cdot\rangle_{-1}$ defined by

$$\langle \xi \,|\eta\rangle_{-1} := \left\langle T^{*-1}\xi \,\middle|\, T^{*-1}\eta \right\rangle, \quad \xi, \eta \in \mathcal{H}.$$

Thus, we put $\mathcal{H}_{-1} := \mathcal{H}_{+1}^{\times}$. Hence, the sequence $\{\xi_n\}$ and the operator T (which is bounded from $\mathcal{H}_{+1}$ into $\mathcal{H}$, but unbounded in $\mathcal{H}$!) automatically *generate* a Gelfand triplet of Hilbert spaces $\mathcal{H}_{+1} \subseteq \mathcal{H} \subseteq \mathcal{H}_{-1}$, which is a typical example of a *rigged Hilbert space* and we will call $\{\xi_n\}$ a (strict) Riesz-like basis.

A second motivation comes from the so called *Pseudo-Hermitian Quantum Mechanics*. This recent development of Quantum Mechanics deals with non self-adjoint Hamiltonians that often can be made into self-adjoint operators by some (generalized) similarity transformation (see, e.g., [5–8]).

Assume, in fact, that H is a closed operator in Hilbert space whose dense domain $D(\mathsf{H})$ is regarded as a Hilbert space $\mathcal{H}_{\mathsf{H}}$ with the graph norm $\|\cdot\|_{\mathsf{H}}$. As we will see in Sect. 2.1, this automatically produces a rigged Hilbert space. Assume that H_{sa} is a self-adjoint operator in $\mathcal{H}$ with discrete spectrum and, for simplicity, that each eigenvalue $\lambda_k \in \mathbb{R}$ has multiplicity 1. Let ψ_k be an eigenvector corresponding to λ_k. Then $\{\psi_k\}$ is an orthonormal basis for $\mathcal{H}$. Assume that there exists a bounded operator $T : \mathcal{H}_{\mathsf{H}} \to \mathcal{H}$, invertible and with bounded inverse $T^{-1} : \mathcal{H} \to \mathcal{H}_{\mathsf{H}}$ such that

$$\left\langle \mathsf{H}\xi \,\middle|\, T^{\dagger}\eta \right\rangle = \langle T\xi \,|\mathsf{H}_{sa}\eta\rangle\,, \quad \forall \xi \in \mathcal{H}_{\mathsf{H}},\ \eta \in D(\mathsf{H}_{sa}) \text{ s. t. } T^{\dagger}\eta \in \mathcal{H}. \tag{2}$$

Put $\xi_k = T^{-1}\psi_k$, for every k. Then, the set $\{\xi_k\}$ is a Riesz-like basis for $\mathcal{H}_{\mathsf{H}}$ and an easy computation shows that, for every $\eta \in D(\mathsf{H}_{sa})$, such that $T^{\dagger}\eta \in \mathcal{H}$

$$\left\langle \mathsf{H}\xi_n \,\middle|\, T^{\dagger}\eta \right\rangle = \lambda_n \left\langle \xi_n \,\middle|\, T^{\dagger}\eta \right\rangle.$$

Thus, if $\{\eta \in D(\mathsf{H}_{sa}) : T^{\dagger}\eta \in \mathcal{H}\}$ is dense in $\mathcal{H}$, we get $\mathsf{H}\xi_n = \lambda_n\xi_n$, for every n. Hence H has a family of eigenvectors that are mapped by T into the elements of an orthonormal basis of $\mathcal{H}$. It should be noticed that the operator T need not be bounded as an operator in $\mathcal{H}$. This situation is of interest because of the existence of physical models whose (non self-adjoint) Hamiltonian cannot be transformed into a self-adjoint one by similarity operators that are bounded, with bounded inverse [9].

The paper is organized as follows. In Sect. 2 we recall basic notions as that of rigged Hilbert space (RHS), of operators on a RHS, of Schauder basis and of (strict) Riesz-like basis and recall some results given in [4] about (strict) Riesz-like bases.

In Sect. 3 we prove that every ω-independent, complete (total) Bessel sequence is a strict Riesz-like basis in a convenient triplet of Hilbert spaces. Furthermore, we consider an example of application of this result to Schrödinger-type operators. In Sect. 4 we study some operators defined by strict Riesz-like bases and by their dual bases, proving their closedness, their self-adjointness and so on. We also prove that some of them are related by a weak intertwining relation and, moreover, we give a characterization of those which are quasi-Hermitian (this kind of operators are known also as *pseudo-Hermitian* operators in Pseudo-Hermitian Quantum Mechanics).

2 Preliminaries and Basic Aspects

2.1 Rigged Hilbert Spaces and Operators on Them

Let $\mathcal{D}$ be a dense subspace of $\mathcal{H}$. A locally convex topology t on $\mathcal{D}$ finer than the topology induced by the Hilbert norm defines, in standard fashion, a *rigged Hilbert space* (RHS)

$$\mathcal{D}[t] \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{D}^\times[t^\times], \tag{3}$$

where $\mathcal{D}^\times$ is the vector space of all continuous conjugate linear functionals on $\mathcal{D}[t]$, i.e., the conjugate dual of $\mathcal{D}[t]$, endowed with the *strong dual topology* $t^\times = \beta(\mathcal{D}^\times, \mathcal{D})$ and $\hookrightarrow$ denotes a continuous embedding. Since the Hilbert space $\mathcal{H}$ can be identified with a subspace of $\mathcal{D}^\times[t^\times]$, we will systematically read (3) as a chain of topological inclusions: $\mathcal{D}[t] \subset \mathcal{H} \subset \mathcal{D}^\times[t^\times]$. In this paper we will consider only the case where $\mathcal{D}$ itself is a Hilbert space, denoted by $\mathcal{H}_{+1}$, under a norm stronger than that of $\mathcal{H}$. Its conjugate dual is denoted by $\mathcal{H}_{-1}$.

As an example, let us be given a closed operator T with dense domain $D(T)$ in Hilbert space $\mathcal{H}$. Then, a rigged Hilbert space, more precisely a *triplet of Hilbert spaces*, arises in a natural way. Indeed, the domain $D(T)$ with the graph norm $\|\cdot\|_T$ defined by

$$\|\xi\|_T = (\|\xi\|^2 + \|T\xi\|^2)^{1/2} = \|(I + T * T)^{1/2}\xi\|, \quad \xi \in D(T)$$

becomes a Hilbert space, namely $\mathcal{H}_T$. If $\mathcal{H}_T^\times$ denotes the Hilbert space conjugate dual of $\mathcal{H}_T$, then we get the triplet of Hilbert spaces

$$\mathcal{H}_T \subset \mathcal{H} \subset \mathcal{H}_T^\times.$$

If $\mathcal{H}$ and $\mathcal{K}$ are two Hilbert spaces, we will indicate by $\mathcal{B}(\mathcal{H}, \mathcal{K})$ the Banach space of linear bounded operators in $\mathcal{H}$ into $\mathcal{K}$. If $\mathcal{H} = \mathcal{K}$, then, to simplify the notation, we will put $\mathcal{B}(\mathcal{H}, \mathcal{H}) = \mathcal{B}(\mathcal{H})$.

Let $\mathcal{H}_{+1} \subset \mathcal{H} \subset \mathcal{H}_{-1}$ be a triplet of Hilbert spaces. An involution $X \mapsto X^\dagger$ can be introduced in $\mathcal{B}(\mathcal{H}_{+1}, \mathcal{H}_{-1})$ by the equality

$$\left\langle X^\dagger \eta \,|\xi \right\rangle = \overline{\langle X\xi \,|\eta \rangle}, \quad \forall \xi, \eta \in \mathcal{H}_{+1}.$$

Hence $\mathcal{B}(\mathcal{H}_{+1}, \mathcal{H}_{-1})$ is a †-invariant vector space.

2.2 Schauder, Riesz-Like and Strict Riesz-Like Bases

Let $\mathcal{E}[t_\mathcal{E}]$ be a locally convex vector space and $\{\xi_n\}$ a sequence of vectors of $\mathcal{E}$. We adopt the following terminology:

(i) the sequence $\{\xi_n\}$ is *complete* or *total* if the linear span of $\{\xi_n\}$ is dense in $\mathcal{E}[t_\mathcal{E}]$;
(ii) the sequence $\{\xi_n\}$ is ω-*independent* if $\sum_{n=1}^\infty c_n\xi_n = 0$, implies $c_n = 0$, for every $n \in \mathbb{N}$;
(iii) the sequence $\{\xi_n\}$ is a *topological basis* for $\mathcal{E}$ if, for every $\phi \in \mathcal{E}$, there exists a *unique* sequence $\{c_n\}$ of complex numbers such that

$$\phi = \sum_{n=1}^\infty c_n\xi_n, \tag{4}$$

where the series on the right hand side converges in $\mathcal{E}[t_\mathcal{E}]$.
(iv) a topological basis $\{\xi_n\}$ for $\mathcal{E}[t_\mathcal{E}]$ is a *Schauder basis* if the coefficient functionals $\{c_n = c_n(f)\}$, appearing in (4), are $t_\mathcal{E}$-continuous.

If $\{\xi_n\}$ is a topological basis for $\mathcal{E}$, then $\{\xi_n\}$ is ω-*independent* and therefore it consists of linearly independent vectors. Moreover, in Banach spaces, the two notions of topological basis and of Schauder basis do coincide.

In the remainder of the paper the Hilbert space $\mathcal{H}$ will always be meant as a separable one.

Consider a rigged Hilbert space $\mathcal{D}[t] \subset \mathcal{H} \subset \mathcal{D}^\times[t^\times]$ and a Schauder basis $\{\xi_n\}$ for $\mathcal{D}[t]$. Every $f \in \mathcal{D}$ is the sum of a series $\sum_{n=1}^\infty c_n(f)\xi_n$, with uniquely determined, suitable coefficients $c_n(f)$. By the continuity of the linear functionals c_n on $\mathcal{D}[t]$, it follows the existence and the uniqueness of a sequence $\{\zeta_n\} \subset \mathcal{D}^\times$ such that

$$c_n(f) = \overline{\langle \zeta_n \,|f \rangle}, \quad \forall n \in \mathbb{N}, f \in \mathcal{D}.$$

If we take $f = \xi_k$, then $c_n(\xi_k) = \overline{\langle \zeta_n \,|\xi_k \rangle} = \delta_{n,k}$ i.e., the two sequences $\{\xi_n\}$ and $\{\zeta_n\}$ are *biorthogonal*.

The following statements on Schauder bases, given here only for triplet of Hilbert spaces $\mathcal{H}_{+1} \subset \mathcal{H} \subset \mathcal{H}_{-1}$, was proved in [4] for general rigged Hilbert spaces by adapting results given in [2, 10, 11].

Proposition 2.1 *Let $\{\xi_n\}$ be a Schauder basis for $\mathcal{H}_{+1}$. Then there exists a unique sequence $\{\zeta_n\}$ of vectors of $\mathcal{H}_{-1}$ such that*

(i) the sequences $\{\xi_n\}$ *and* $\{\zeta_n\}$ *are biorthogonal;*
(ii) for every $f \in \mathcal{H}_{+1}$,

$$f = \sum_{n=1}^{\infty} \overline{\langle \zeta_n \,|\, f \rangle} \xi_n; \tag{5}$$

(iii) The partial sum operator S_n, *given by*

$$S_n f = \sum_{k=1}^{n} \overline{\langle \zeta_k \,|\, f \rangle} \xi_k, \quad f \in \mathcal{H}_{+1},$$

is continuous from $\mathcal{H}_{+1}$ *into* $\mathcal{H}_{+1}$ *and has an adjoint* $S_n^\dagger$ *everywhere defined in* $\mathcal{H}_{-1}$ *given by*

$$S_n^\dagger \Psi = \sum_{k=1}^{n} \langle \Psi \,|\, \xi_k \rangle \zeta_k, \quad \Psi \in \mathcal{H}_{-1};$$

(iv) the sequence $\{\zeta_n\}$ *is a basis for* $\mathcal{H}_{-1}$ *with respect to the weak topology; i.e., if* $\Psi \in \mathcal{H}_{-1}$ *one has*

$$\langle \Psi \,|\, f \rangle = \left\langle \sum_{k=1}^{\infty} \langle \Psi \,|\, \xi_k \rangle \zeta_k \,|\, f \right\rangle = \sum_{k=1}^{\infty} \langle \Psi \,|\, \xi_k \rangle \, \langle \zeta_k \,|\, f \rangle \,, \quad \forall f \in \mathcal{H}_{+1}. \tag{6}$$

Remark 2.2 Of course, (6) provides a weak expansion for every $h \in \mathcal{H}$; i.e., $h = \sum_{k=1}^{\infty} \langle h \,|\, \xi_k \rangle \zeta_k$, weakly. In particular, for $f \in \mathcal{H}_{+1} \subset \mathcal{H}_{-1}$, (6) gives

$$\|f\|^2 = \sum_{k=1}^{\infty} \langle f \,|\, \xi_k \rangle \, \langle \zeta_k \,|\, f \rangle \,, \quad \forall f \in \mathcal{H}_{+1}$$

so that the series on the right hand side is convergent, for every $f \in \mathcal{H}_{+1}$.

Now we recall the notion of Riesz-like and strict Riesz-like bases we gave in [4] for a rigged Hilbert space $\mathcal{D}[t] \subset \mathcal{H} \subset \mathcal{D}^\times[t^\times]$.

Definition 2.3 A Schauder basis $\{\xi_n\}$ for $\mathcal{D}[t]$ is called a *Riesz-like basis* for $\mathcal{D}[t]$ if there exists a one-to-one continuous operator $T : \mathcal{D}[t] \to \mathcal{H}$ such that $\{T\xi_n\}$ is an orthonormal basis for $\mathcal{H}$.

The range $R(T)$ of T contains the orthonormal basis $\{e_k\}$ with $e_k := T\xi_k$, $k \in \mathbb{N}$, hence $R(T)$ is dense in $\mathcal{H}$.

If $\{\xi_n\}$ is a Riesz-like basis, we can find explicitly the sequence $\{\zeta_n\} \subset \mathcal{H}_{-1}$ of Proposition 2.1. The continuity of T and (5), in fact, imply

$$Tf = \sum_{n=1}^{\infty} \overline{\langle \zeta_n \,|\, f \rangle} T\xi_n = \sum_{n=1}^{\infty} \overline{\langle \zeta_n \,|\, f \rangle} e_n, \quad \forall f \in \mathcal{H}_{+1}.$$

This, in turn, implies that $\overline{\langle \zeta_n \,|\, f \,\rangle} = \langle Tf \,|e_n\,\rangle$, for every $f \in \mathcal{H}_{+1}$. Hence $\zeta_n = T^\dagger e_n$, for every $n \in \mathbb{N}$.

Clearly, for every $n, k \in \mathbb{N}$,

$$\langle \zeta_k \,|\xi_n\,\rangle = \left\langle T^\dagger e_k \,|\xi_n\right\rangle = \langle e_k \,|T\xi_n\,\rangle = \langle e_k \,|e_n\,\rangle = \delta_{k,n}$$

and $T^\dagger T\xi_n = \zeta_n$, for every $n \in \mathbb{N}$. This sequence is called the *dual* sequence.

Let $\{\xi_n\}$ be a Riesz-like basis for $\mathcal{D}[t]$. One can ask what happens if we strengthen the hypotheses on T, e.g. if we suppose that T is onto too and T^{-1} is continuous from $\mathcal{H}$ into $\mathcal{D}[t]$. In other words, let us suppose that the operator T which makes of $\{T\xi_n\}$ an orthonormal basis for $\mathcal{H}$ has a continuous inverse $T^{-1} : \mathcal{H}[\|\cdot\|] \to \mathcal{D}[t]$ (in particular, T^{-1} is a bounded operator in $\mathcal{H}$). We say in this case that $\{\xi_n\}$ is a *strict Riesz-like basis* for $\mathcal{D}[t]$. This assumption has important consequences on the involved topologies. Indeed, as shown in [4, Proposition 3.6]

Proposition 2.4 *If the rigged Hilbert space $\mathcal{D}[t] \subset \mathcal{H} \subset \mathcal{D}^\times[t^\times]$, with $\mathcal{D}[t]$ complete and reflexive, has a strict Riesz-like basis $\{\xi_n\}$ then it is (equivalent to) a triplet of Hilbert spaces $\mathcal{H}_{+1} \subset \mathcal{H} \subset \mathcal{H}_{-1}$. Moreover, $\{\xi_n\}$ is an orthonormal basis for $\mathcal{H}_{+1}$ and the dual sequence $\{\zeta_n\}$ is an orthonormal basis for $\mathcal{H}_{-1}$.*

In other words the rigged Hilbert space is forced to be a triplet of Hilbert spaces. On the other hand, in a triplet of Hilbert spaces $\mathcal{H}_{+1} \subset \mathcal{H} \subset \mathcal{H}_{-1}$, if the operator T which makes of $\{T\xi_n\}$ an orthonormal basis for $\mathcal{H}$ is onto, then T^{-1} is automatically continuous and so the basis $\{\xi_n\}$ is strict.

Remark 2.5 It is clear that, if $\{\xi_n\}$ is a strict Riesz-like basis, then it is an unconditional basis of $\mathcal{H}_{+1}$.

3 Bessel Sequences as Strict-Riesz Like Bases

Now, we will give an answer to the following natural questions: given a sequence $\{\xi_n\} \subset \mathcal{H}$, does there exist a rigged Hilbert space such that $\{\xi_n\}$ is a strict Riesz-like basis for it? Given a sequence $\{\xi_n\} \subset \mathcal{H}$, does there exist a triplet of Hilbert spaces $\mathcal{H}_{+1} \subseteq \mathcal{H} \subseteq \mathcal{H}_{-1}$ such that $\{\xi_n\}$ is an orthonormal basis for $\mathcal{H}_{+1}$?

Let $\{\xi_n\}$ be a Bessel sequence in $\mathcal{H}$, i.e., [11] there exists $C > 0$ such that for every finite sequence of complex numbers $\{c_1, c_2, ...c_n\}$, $n \in \mathbb{N}$,

$$\left\| \sum_{k=1}^{n} c_k \xi_k \right\|^2 \leq C \sum_{k=1}^{n} |c_k|^2 . \tag{7}$$

Let $\{e_n\}$ be an orthonormal basis for $\mathcal{H}$ and define the operator

$$V : \sum_{k=1}^{n} c_k e_k \to \sum_{k=1}^{n} c_k \xi_k . \tag{8}$$

It is clear that V is well-defined and bounded (by (7)) on $\mathcal{G} = \mathsf{span}\{e_n\}$, then it extends to a bounded operator, denoted again by V, to $\mathcal{H}$. Obviously, $Ve_n = \xi_n$, for every $n \in \mathbb{N}$.

We notice that $\{\xi_n\}$ is ω-independent if and only if V, and $\{\xi_n\}$ is complete if and only if V^* is injective. Now we give our main result.

Theorem 3.1 *If $\{\xi_n\}$ is an ω-independent complete Bessel sequence in $\mathcal{H}$, then, for every orthonormal basis $\{e_n\}$ of $\mathcal{H}$, there exists a triplet of Hilbert spaces $\mathcal{K} \subset \mathcal{H} \subset \mathcal{K}^\times$ which has $\{\xi_n\}$ as a strict Riesz-like basis. This triplet is unique up to unitary transformations.*

Proof We maintain the notations of the previous discussion. Let $\{e_n\}$ be an orthonormal basis of $\mathcal{H}$. If $\{\xi_n\}$ is a ω-independent Bessel sequence in $\mathcal{H}$, the operator V defined in (8) is injective on $\mathcal{H}$. Indeed, since $\{e_n\}$ is an orthonormal basis for $\mathcal{H}$, for every $f \in \mathcal{H}$, $f = \lim_{N\to\infty} f_N$, where $f_N = \sum_{n=1}^{N} \langle f \,|e_n\rangle\, e_n \in \mathcal{G}$. It follows that

$$Vf := \lim_{N\to\infty} Vf_N = \lim_{N\to\infty} \sum_{n=1}^{N} \langle f \,|e_n\rangle\, \xi_n = \sum_{n=1}^{\infty} \langle f \,|e_n\rangle\, \xi_n.$$

If $Vf = 0$, then $\langle f \,|e_n\rangle = 0$, for every $n \in \mathbb{N}$. Hence $f = 0$.

Then V has an inverse V^{-1} defined on the range $\mathsf{Ran}(V)$ of V and, since V is bounded, V^{-1} is closed. Moreover, $\{\xi_n\} \subseteq \mathsf{Ran}(V)$, hence, by the completeness of $\{\xi_n\}$, the inverse of the operator V is densely defined. Now, we have

$$\mathsf{Ran}(V) = \left\{ g \in \mathcal{H} : g = \sum_{n=1}^{\infty} c_n \xi_n \text{ with } \sum_{n=1}^{\infty} |c_n|^2 < \infty \right\}.$$

The ω-independence of $\{\xi_n\}$ guarantees the uniqueness of the expansion $g = \sum_{n=1}^{\infty} c_n \xi_n$ of every $g \in \mathsf{Ran}(V)$. Finally, we have

$$V^{-1} g = V^{-1} \left(\sum_{n=1}^{\infty} c_n \xi_n \right) = \sum_{n=1}^{\infty} c_n e_n, \quad \forall g = \sum_{n=1}^{\infty} c_n \xi_n \in \mathsf{Ran}(V).$$

We put, for short, $T := V^{-1}$ and $D(T) = \mathsf{Ran}(V)$. Then T is a closed densely defined operator such that $T\xi_n = e_n$ and has bounded inverse. Then, as we have already seen in Sect. 2.1, a triplet of Hilbert spaces arises in a natural way. More precisely, we get the triplet of Hilbert spaces

$$\mathcal{H}_T \subset \mathcal{H} \subset \mathcal{H}_T^\times$$

where $\mathcal{H}_T = D(T)[\|\cdot\|_T]$ with

$$\|\xi\|_T = (\|\xi\|^2 + \|T\xi\|^2)^{1/2} = \|(I + T^*T)^{1/2}\xi\|, \quad \xi \in D(T)$$

and the sequence $\{\xi_n\}$ is a strict Riesz-like basis for $\mathcal{H}_T$. Now, let us consider two different orthonormal bases $\{e_n\}$ and $\{e'_n\}$ of the Hilbert space $\mathcal{H}$. Then, as it is well-known, there exists a unitary operator $U : \mathcal{H} \to \mathcal{H}$ such that $Ue_n = e'_n$, therefore the two norms $\|\cdot\|_T$ and $\|\cdot\|_{UT}$ coincide and hence the two Hilbert spaces $\mathcal{H}_T$ and $\mathcal{H}_{UT}$ do.

Remark 3.2 If $\{\xi_n\}$ is an ω-independent complete Bessel sequence in $\mathcal{H}$, then, for every orthonormal basis $\{e_n\}$ of $\mathcal{H}$, there exists a (unique) Hilbert space which has $\{\xi_n\}$ as an orthonormal basis since, once the triplet of Hilbert spaces $\mathcal{H}_T \subset \mathcal{H} \subset \mathcal{H}_T^\times$ is at hand (Theorem 3.1), then $\{\xi_n\}$ is an orthonormal basis for $\mathcal{H}_{+1} = D(T)[\|\cdot\|_{+1}]$ and, as a consequence of the uniqueness of $\mathcal{H}_T$, the Hilbert space $\mathcal{H}_{+1}$ (and the triplet), is unique too.

Remark 3.3 If $T = V^{-1}$ is also bounded, then $\{\xi_n\}$ is a Riesz basis for $\mathcal{H}$ and $\mathcal{H}_T$ coincides with $\mathcal{H}$ as a vector space but it carries a different albeit equivalent norm, as stated by the well-known theory of Riesz bases.

Remark 3.4 If $\{\xi_n\}$ is an ω-independent complete Bessel sequence in $\mathcal{H}$, then Theorem 3.1 gives us full information on the possibility of expanding a vector $f \in \mathcal{H}$ in terms of $\{\xi_n\}$: indeed, $\{\xi_n\}$ determines a closed densely defined operator T and every vector f of the domain of T can be expanded uniquely as an unconditionally convergent series $f = \sum_{n=1}^{\infty} c_n \xi_n$, the convergence holds in the graph norm $\|\cdot\|_T$ of $D(T)$, and then in the norm $\|\cdot\|$. Other vectors f of $\mathcal{H}$, by (6), can be obtained by a weakly convergent series $f = \sum_{k=1}^{\infty} \langle f \,|\xi_k\rangle \zeta_k$, $\{\zeta_k\}$ being the dual sequence of $\{\xi_n\}$, in the sense that $\langle f \,|\eta\rangle = \sum_{k=1}^{\infty} \langle f \,|\xi_k\rangle \langle \zeta_k \,|\eta\rangle$, $\forall \eta \in D(T)$.

If T is unbounded, then $0 \in \sigma_c(T^{-1})$, the continuous spectrum of T^{-1}. Some more information on $\{\xi_n\}$ can be obtained just making some assumption on the spectral behaviour of T^{-1}. Assume, for instance, that T^{-1} is compact, then the sequence $\{\xi_n\}$ converges to 0 in the norm of $\mathcal{H}$, being the image of an orthonormal basis through a compact operator. Of course one can go further and require that T^{-1} belongs to some other well-known classes of operators, giving a more accurate description of how fast $\|\xi_n\| \to 0$. For a discussion on this subject see [12].

3.1 An Application

The importance of Theorem 3.1 is that, once we have at hand a non self-adjoint operator H, with purely discrete real spectrum, it is possible to construct the Hilbert space of the system by finding out exactly the closed operator defining an inner product which makes the eigenvectors of H orthonormal. As expected, the inner product of the Hilbert space can be given in terms of the metric operator $Q = T^\dagger T$ which is unbounded as an operator in $\mathcal{H}$, whereas is bounded as an operator in $\mathcal{H}_{+1}$ into $\mathcal{H}_{-1}$ (see Proposition 4.4 in Sect. 4). This change of domain is not a deal by the physical point of view, because the observable of the system are in general unbounded

linear operators defined on a dense set $\mathcal{D}$ of Hilbert space $\mathcal{H}$. As an example of this situation, let us consider the Hilbert space $\mathcal{H} = L^2(\mathbb{R})$ and the Hamiltonian

$$H = -\frac{d^2}{dx^2} + \frac{x^2}{2} - \frac{4x}{1+x^2}\frac{d}{dx} - \frac{2}{1+x^2} = H_0 + V$$

where H_0 is the Hamiltonian operator of the harmonic oscillator and $V = -\frac{4x}{1+x^2}\frac{d}{dx} - \frac{2}{1+x^2}$ (in spite of the notation, the operator V is not a physical potential, since it depends explicitly on the derivative operator). The set of its eigenvectors is $\{\xi_n = \frac{1}{\sqrt{2^n\, n!\sqrt{\pi}}} H_n(x) \frac{e^{-\frac{x^2}{2}}}{1+x^2},\ n \geq 0\}$, where $H_n(x)$ is the nth Hermite polynomial. The vectors ξ_n's do not form a orthonormal basis for $\mathcal{H}$. However, they constitute an ω-independent complete Bessel sequence in $\mathcal{H}$ as we will see in a while. Hence, by Theorem 3.1, there exists a triplet of Hilbert spaces which has $\{\xi_n\}$ as a strict Riesz-like basis and, even more important, there exists a Hilbert space $\mathcal{H}_{+1}$ such that $\{\xi_n\}$ is an orthonormal basis for $\mathcal{H}_{+1}$ and such that $H \in \mathcal{B}(\mathcal{H}_{+1})$ (H is closed and everywhere defined in $\mathcal{H}_{+1}$). Recall that, once we call $N_n = \frac{1}{\sqrt{2^n\, n!\sqrt{\pi}}}$, the set $\{e_n(x) = N_n H_n(x) e^{-\frac{x^2}{2}},\ n \geq 0\}$ is an orthonormal basis of $\mathcal{H}$. Hence the operator T which takes the sequence $\{\xi_n\}$ into $\{e_n\}$ is $T = 1 + x^2$. This is an unbounded continuous operator defined on the dense set $D(T) = \{f \in \mathcal{H} :\ (1+x^2) f \in \mathcal{H}\}$, with bounded inverse: $T^{-1} = \frac{1}{1+x^2}$. The Hamiltonian H is *non self-adjoint* and similar to H_0 by the intertwining operator T, $H = T^{-1} H_0 T$, the eigenvectors of H are transformed into those of H_0 and H and H_0 have the same eigenvalues $\alpha_n = n + \frac{1}{2}$, for every $n \geq 0$ sorted n by n; (in particular, the ground state ξ_0 is transformed in that one of H_0). It remains to show that $\{\xi_n\}$ is an ω-independent complete Bessel sequence in $\mathcal{H}$. Indeed, $\{\xi_n\}$ is a Bessel sequence since there exists $C = \|T^{-1}\| > 0$ such that for every finite sequence of complex numbers $\{c_0, c_1, ...c_n\}$, $n \in \mathbb{N}$,

$$\left\| \sum_{k=0}^{n} c_k \xi_k \right\|^2 = \left\| \sum_{k=0}^{n} c_k T^{-1} e_k \right\|^2 \leq C \sum_{k=0}^{n} |c_k|^2 . \tag{9}$$

They are ω-independent because if

$$\sum_{n=0}^{\infty} c_n \xi_n = 0 = \sum_{n=0}^{\infty} c_n T^{-1} e_n = T^{-1} \left(\sum_{n=0}^{\infty} c_n e_n \right),$$

then it implies $c_n = 0$, for every $n \geq 0$, by the continuity and the injectivity of T^{-1}. Furthermore, they are a complete set because if $f \in \mathcal{H}$ is such that $\langle f \,|\xi_n\rangle = 0$ for every n, then

$$0 = \langle f \,|\xi_n\rangle = \left\langle f \,\middle|\, T^{-1} e_n \right\rangle = \left\langle T^{-1} f \,|e_n \right\rangle = 0$$

which by the injectivity of T^{-1} implies $f = 0$. Notice that, albeit $\{\xi_n = T^{-1}e_n\}$ is an ω-independent complete Bessel sequence in $\mathcal{H}$, it is *not* a Riesz basis for $\mathcal{H}$ because $T = (1 + x^2)$ is an unbounded operator. Now, following what we saw before, the natural space where considering the previous operator H is $\mathcal{H}_{+1} = D(T)[\|\cdot\|_{+1}]$ with $\|\cdot\|_{+1} = \|(1 + x^2)\cdot\|$.

4 Operators Defined by Strict Riesz-Like Bases

In this section some results in [13] are generalized to the case of operators defined in triplets of Hilbert spaces. Furthermore, we will prove some result about the similarity of operators introduced here, and a characterization of those which have real eigenvalues.

Let $\{\xi_n\}$ be a strict Riesz-like basis for the triplet $\mathcal{H}_{+1} \subset \mathcal{H} \subset \mathcal{H}_{-1}$ and $\{\zeta_n\}$ its dual basis. If $\boldsymbol{\alpha} = \{\alpha_n\}$ is a sequence of complex numbers we can formally define, for $f \in \mathcal{H}_{+1}$,

$$A^{\boldsymbol{\alpha}} f = \sum_{n=1}^{\infty} \alpha_n (\xi_n \otimes \overline{\zeta}_n) f = \sum_{n=1}^{\infty} \alpha_n \overline{\langle \zeta_n \,|\, f \rangle} \xi_n \tag{10}$$

$$B^{\boldsymbol{\alpha}} f = \sum_{n=1}^{\infty} \alpha_n (\zeta_n \otimes \overline{\xi}_n) f = \sum_{n=1}^{\infty} \alpha_n \langle f \,|\, \xi_n \rangle \zeta_n. \tag{11}$$

$$R^{\boldsymbol{\alpha}} f = \sum_{n=1}^{\infty} \alpha_n (\xi_n \otimes \overline{\xi}_n) f = \sum_{n=1}^{\infty} \alpha_n \, \langle f \,|\, \xi_n \rangle \, \xi_n \tag{12}$$

$$Q^{\boldsymbol{\alpha}} f = \sum_{n=1}^{\infty} \alpha_n (\zeta_n \otimes \overline{\zeta}_n) f = \sum_{n=1}^{\infty} \alpha_n \overline{\langle \zeta_n \,|\, f \rangle} \zeta_n \tag{13}$$

Of course, these are the simplest operators that can be defined via $\{\xi_n\}$ and $\{\zeta_n\}$.

Remark 4.1 Before going further, a comment is in order. In [14] Balazs introduced the notion of Bessel multipliers (frame multipliers, Riesz multipliers) whose definition is apparently similar to those given above. To be more precise, if $\{\varphi_n\}$, $\{\psi_n\}$ are Bessel sequences respectively in two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, fix $\boldsymbol{m} = \{m_n\}$ a bounded sequence of complex numbers, the Bessel multiplier for the Bessel sequences above is an operator $M : \mathcal{H}_2 \to \mathcal{H}_1$ defined by

$$M = \sum_{n=1}^{\infty} m_n (\varphi_n \otimes \overline{\psi}_n).$$

The main differences with the operators in (10)–(11) is that the two sequences $\{\varphi_n\}$, $\{\psi_n\}$ are not necessarily biorthogonal (in particular, in [14, Corollary 7.5] a necessary

and sufficient condition is given for $\{\varphi_n\}, \{\psi_n\}$ to be biorthogonal), and moreover, as we shall see in a while, we will also deal with possibly unbounded sequences. Thus, the two notions are not directly comparable.

Let $\mathcal{H}_{+1} \subset \mathcal{H} \subset \mathcal{H}_{-1}$ be a triplet of Hilbert spaces and $\{\xi_n\}$ a strict Riesz-like basis for $\mathcal{H}_{+1}$.

Clearly, the operator formally defined by (10) can take values in $\mathcal{H}_{+1}$ or in $\mathcal{H}$ or even in $\mathcal{H}_{-1}$, following the different topologies that make the series on the right hand side convergent. It is clear that, if $f \in \mathcal{H}_{+1}$, then

$$\sum_{n=1}^{\infty} \alpha_n \overline{\langle \zeta_n \,|\, f \rangle} \xi_n \text{ converges in } \mathcal{H}_{-1} \Leftrightarrow \sum_{n=1}^{\infty} \left| \sum_{k=1}^{\infty} \alpha_k \overline{\langle \zeta_k \,|\, f \rangle} \, \langle \xi_k \,|\, \zeta_n \rangle_{-1} \right|^2 < \infty.$$

Since $\langle \xi_k \,|\, \zeta_n \rangle_{-1} = \langle \xi_k \,|\, \xi_n \rangle$, for every $k, n \in \mathbb{N}$, we can conclude that

$$A^{\boldsymbol{\alpha}} f \in \mathcal{H}_{-1} \Leftrightarrow \sum_{n=1}^{\infty} \left| \sum_{k=1}^{\infty} \alpha_k \overline{\langle \zeta_k \,|\, f \rangle} G_{k,n} \right|^2 < \infty.$$

where $(G_{k,n})$ is the Gram matrix of the basis $\{\xi_k\}$; i.e., $G_{k,n} = \langle \xi_k \,|\, \xi_n \rangle$, for $k, n \in \mathbb{N}$. Differently from the standard case, the Gram matrix of $\{\xi_k\}$ need not be bounded.

Similarly, since $\{e_n\}$ is an orthonormal basis in $\mathcal{H}$, we have

$$A^{\boldsymbol{\alpha}} f \in \mathcal{H} \Leftrightarrow \sum_{n=1}^{\infty} \left| \sum_{k=1}^{\infty} \alpha_k \overline{\langle \zeta_k \,|\, f \rangle} \, \langle \xi_k \,|\, e_n \rangle \right|^2 < \infty,$$

where, as before, $e_k = T\xi_k$, $k \in \mathbb{N}$.

Finally, as we shall see in Proposition 4.2,

$$A^{\boldsymbol{\alpha}} f \in \mathcal{H}_{+1} \Leftrightarrow \sum_{k=1}^{\infty} |\alpha_k|^2 |\langle \zeta_k \,|\, f \rangle|^2 < \infty.$$

Of course, analogous considerations can be made for the operators defined in (11), (12) and (13). It is worth remarking that for the operators $B^{\boldsymbol{\alpha}}$ and $R^{\boldsymbol{\alpha}}$ the series on the right hand side of (11), (12) may converge also for some $f \in \mathcal{H}_{-1}$.

Now we examine more closely one of the cases listed above. In particular, we will suppose $A^{\boldsymbol{\alpha}} f \in \mathcal{H}_{+1}$, for every $f \in \mathcal{H}_{+1}$. Under this assumption, let us define

$$\begin{cases} D(A^{\boldsymbol{\alpha}}) = \left\{ f \in \mathcal{H}_{+1}; \sum_{n=1}^{\infty} \alpha_n \overline{\langle \zeta_n \,|\, f \rangle} \xi_n \text{ exists in } \mathcal{H}_{+1} \right\} \\ A^{\boldsymbol{\alpha}} f = \sum_{n=1}^{\infty} \alpha_n \overline{\langle \zeta_n \,|\, f \rangle} \xi_n, \quad f \in D(A^{\boldsymbol{\alpha}}) \end{cases}$$

$$\begin{cases} D(B^{\boldsymbol{\alpha}}) = \left\{ \Psi \in \mathcal{H}_{-1};\ \sum_{n=1}^{\infty} \alpha_n \langle \Psi \,|\xi_n\rangle\, \zeta_n \text{ exists in } \mathcal{H}_{-1} \right\} \\ B^{\boldsymbol{\alpha}}\Psi = \sum_{n=1}^{\infty} \alpha_n \langle \Psi \,|\xi_n\rangle\, \zeta_n,\ \ \Psi \in D(B^{\boldsymbol{\alpha}}) \end{cases}.$$

Then we have the following

$$\begin{aligned} &\mathcal{D}_\xi := \operatorname{span}\{\xi_n\} \subset D(A^{\boldsymbol{\alpha}}); \\ &\mathcal{D}_\zeta := \operatorname{span}\{\zeta_n\} \subset D(B^{\boldsymbol{\alpha}}); \qquad (14) \\ &A^{\boldsymbol{\alpha}}\xi_k = \alpha_k \xi_k,\ \ k = 1, 2, \ldots; \\ &B^{\boldsymbol{\alpha}}\zeta_k = \alpha_k \zeta_k,\ \ k = 1, 2, \ldots. \qquad (15) \end{aligned}$$

Hence, $A^{\boldsymbol{\alpha}}$ and $B^{\boldsymbol{\alpha}}$ are densely defined and have the same eigenvalues. As we will see, if $\alpha_n \in \mathbb{R}$, $\forall n \in \mathbb{N}$, they are one the adjoint of the other.

It worths noting that the operators $(T^\dagger)^{-1}$ and $(T^{-1})^\dagger$ do coincide [15, Remark 3.2].

Before continuing, we recall that if $X : D(X) \subseteq \mathcal{H}_{+1} \to \mathcal{H}_{+1}$ is a closed map and $D(X)$ is dense in $\mathcal{H}_{+1}$, then there exists a closed densely defined map $X^\dagger : D(X^\dagger) \subseteq \mathcal{H}_{-1} \to \mathcal{H}_{-1}$ such that

$$\langle \Phi \,|X\xi\rangle = \left\langle X^\dagger \Phi \,|\xi \right\rangle, \quad \forall \xi \in \mathcal{H}_{+1},\ \Phi \in \mathcal{H}_{-1}.$$

If X is also closed as an operator in $\mathcal{H}$, then its Hilbert adjoint X^* exists and $X^* = X^\dagger_{\restriction D(X^*)}$ where $D(X^*) = \{\phi \in \mathcal{H} :\ X^\dagger\phi \in \mathcal{H}\}$.

Proposition 4.2 *The following statements hold.*

(i) $D(A^{\boldsymbol{\alpha}}) = \left\{ f \in \mathcal{H}_{+1};\ \sum_{n=1}^{\infty} |\alpha_n|^2 |\langle \zeta_n \,| f\rangle|^2 < \infty \right\}$,
$D(B^{\boldsymbol{\alpha}}) = \left\{ \Psi \in \mathcal{H}_{-1};\ \sum_{n=1}^{\infty} |\alpha_n|^2 |\langle \Psi \,|\xi_n\rangle|^2 < \infty \right\}$.

(ii) $A^{\boldsymbol{\alpha}}$ *and* $B^{\boldsymbol{\alpha}}$ *are closed operators respectively in* $\mathcal{H}_{+1}[\|\cdot\|_{+1}]$ *and in* $\mathcal{H}_{-1}[\|\cdot\|_{-1}]$.

(iii) $(A^{\boldsymbol{\alpha}})^\dagger = B^{\overline{\boldsymbol{\alpha}}}$, *where* $\overline{\boldsymbol{\alpha}} = \{\overline{\alpha}_n\}$.

(iv) $A^{\boldsymbol{\alpha}}$ *is bounded in* $\mathcal{H}_{+1}$ *if, and only if,* $B^{\boldsymbol{\alpha}}$ *is bounded in* $\mathcal{H}_{-1}$ *and if, and only if,* $\boldsymbol{\alpha}$ *is a bounded sequence. In particular* $A^{\boldsymbol{1}} = I_{\mathcal{H}_{+1}}$ *and* $B^{\boldsymbol{1}} = I_{\mathcal{H}_{-1}}$, *where* $\boldsymbol{1}$ *is the sequence constantly equals to* 1.

Proof (i): Since $\{\xi_n\}$ is an orthonormal basis for $\mathcal{H}_{+1}$, we have

$$\left\| \sum_{k=n}^{m} \alpha_k \langle \zeta_k \,| f\rangle\, \xi_k \right\|_{+1}^2 = \sum_{k=n}^{m} |\alpha_k|^2 |\langle \zeta_k \,| f\rangle|^2, \quad f \in \mathcal{H}_{+1} \qquad (16)$$

which shows that $f \in D(A^{\boldsymbol{\alpha}})$ if and only if $\sum_{n=1}^{\infty} |\alpha_n|^2 |\langle \zeta_n | f \rangle|^2 < \infty$.

(ii): The proof of this statement can be made by slight modifications of [13, Proposition 2.1 (2)].

(iii): It is easy to show that $B^{\overline{\boldsymbol{\alpha}}} = \sum_{n=1}^{\infty} \overline{\alpha}_n (\zeta_n \otimes \overline{\xi_n}) \subseteq (A^{\boldsymbol{\alpha}})^{\dagger}$. Conversely, let $\Psi \in D((A^{\boldsymbol{\alpha}})^{\dagger})$; then there exists $\Phi \in \mathcal{H}_{-1}$ such that

$$\left\langle \Psi \left| \sum_{n=1}^{\infty} \alpha_n \overline{\langle \zeta_n | f \rangle} \xi_n \right. \right\rangle = \langle \Phi | f \rangle, \quad \forall f \in D(A^{\boldsymbol{\alpha}}).$$

By (14) and (15), $\mathcal{D}_{\xi} \subseteq D(A^{\boldsymbol{\alpha}})$ and $A^{\boldsymbol{\alpha}} \xi_k = \alpha_k \xi_k$, $k = 1, 2, \ldots$. Thus, $\langle \Psi | \alpha_k \xi_k \rangle = \langle \Phi | \xi_k \rangle$, $k = 1, 2, \ldots$. Hence

$$\sum_{k=1}^{\infty} |\alpha_k|^2 |\langle \Psi | \xi_k \rangle|^2 = \sum_{k=1}^{\infty} |\langle \Phi | \xi_k \rangle|^2 = \sum_{k=1}^{\infty} |\langle (T^{-1})^{\dagger} \Phi | e_k \rangle|^2 = \|(T^{-1})^{\dagger} \Phi\|^2 < \infty.$$

This implies that $\Psi \in D(B^{\overline{\boldsymbol{\alpha}}})$.

(iv): Let $\boldsymbol{\alpha}$ be a bounded sequence, then there exists $M > 0$ such that

$$\|A^{\boldsymbol{\alpha}} f\|_{+1} = \left\| \sum_{k=1}^{\infty} \alpha_k \overline{\langle \zeta_k | f \rangle} \xi_k \right\|_{+1} \leq M \left\| \sum_{k=1}^{\infty} \overline{\langle \zeta_k | f \rangle} \xi_k \right\|_{+1},$$

hence $A^{\boldsymbol{\alpha}}$ is bounded in $\mathcal{H}_{+1}$.

In a very similar way one can prove (i), (ii) and (iv) for $B^{\boldsymbol{\alpha}}$. This completes the proof.

Remark 4.3 In [15] Di Bella, Trapani and the author gave a definition of spectrum for continuous operators acting in a rigged Hilbert space $\mathcal{D} \subset \mathcal{H} \subset \mathcal{D}^{\times}$. We refer to that paper for precise definitions and results. So a natural question is: what is the spectrum (in that sense) of the operator $A^{\boldsymbol{\alpha}}$ defined above? Let us assume that the sequence $\boldsymbol{\alpha}$ is bounded, so that $A^{\boldsymbol{\alpha}}$ is a bounded operator in $\mathcal{H}_{+1}$. The analysis is, in this case, particularly simple since, as usual, the set of eigenvalues consists exactly of the α_k's and, if λ does not belong to the closure $\overline{\{\alpha_k; k \in \mathbb{N}\}}$ of the set of eigenvalues, then the inverse of $A^{\boldsymbol{\alpha}} - \lambda I_{\mathcal{H}_{+1}}$ exists as a bounded operator in $\mathcal{H}_{+1}$. Hence, as expected, $\sigma(A^{\boldsymbol{\alpha}}) = \overline{\{\alpha_k; k \in \mathbb{N}\}}$. The situation for $B^{\boldsymbol{\alpha}}$ is analogous.

Let us now consider the operators formally given by (12) and (13). They are, in fact, defined as follows:

$$\begin{cases} D(R^{\boldsymbol{\alpha}}) = \left\{ \Psi \in \mathcal{H}_{-1}; \sum_{n=1}^{\infty} \alpha_n \langle \Psi | \xi_n \rangle \xi_n \text{ exists in } \mathcal{H}_{+1} \right\} \\ R^{\boldsymbol{\alpha}} \Psi = \sum_{n=1}^{\infty} \alpha_n \langle \Psi | \xi_n \rangle \xi_n, \ \Psi \in D(R^{\boldsymbol{\alpha}}) \end{cases}$$

$$\begin{cases} D(Q^{\boldsymbol{\alpha}}) = \left\{ f \in \mathcal{H}_{+1};\ \sum_{n=1}^{\infty} \alpha_n \overline{\langle \zeta_n \,|\, f \rangle} \zeta_n \text{ exists in } \mathcal{H}_{-1} \right\} \\ Q^{\boldsymbol{\alpha}} f = \sum_{n=1}^{\infty} \alpha_n \overline{\langle \zeta_n \,|\, f \rangle} \zeta_n, \ \ f \in D(Q^{\boldsymbol{\alpha}}) \end{cases}.$$

It is clear that

$$\mathcal{D}_\zeta \subset D(R^{\boldsymbol{\alpha}}) \text{ and } R^{\boldsymbol{\alpha}} \zeta_k = \alpha_k \xi_k, \ k = 1, 2, \ldots; \tag{17}$$

$$\mathcal{D}_\xi \subset D(Q^{\boldsymbol{\alpha}}) \text{ and } Q^{\boldsymbol{\alpha}} \xi_k = \alpha_k \zeta_k, \ k = 1, 2, \ldots \tag{18}$$

Hence, $R^{\boldsymbol{\alpha}}$ and $Q^{\boldsymbol{\alpha}}$ are densely defined, and the following results can be established:

Proposition 4.4 *The following statements hold.*

(1) $D(R^{\boldsymbol{\alpha}}) = \left\{ \Psi \in \mathcal{H}_{-1};\ \sum_{n=1}^{\infty} |\alpha_n|^2 |\langle \Psi \,|\, \xi_n \rangle|^2 < \infty \right\} = D(B^{\boldsymbol{\alpha}})$,
$D(Q^{\boldsymbol{\alpha}}) = \left\{ f \in \mathcal{H}_{+1};\ \sum_{n=1}^{\infty} |\alpha_n|^2 |\langle \zeta_n \,|\, f \rangle|^2 < \infty \right\} = D(A^{\boldsymbol{\alpha}})$.

(2) $R^{\boldsymbol{\alpha}}$ *and* $Q^{\boldsymbol{\alpha}}$ *are closed.*

(3) $(R^{\boldsymbol{\alpha}})^\dagger = R^{\overline{\boldsymbol{\alpha}}}$ *and* $(Q^{\boldsymbol{\alpha}})^\dagger = Q^{\overline{\boldsymbol{\alpha}}}$, *where* $\overline{\boldsymbol{\alpha}} = \{\overline{\alpha_n}\}$.

(4) If $\{\alpha_n\} \subset \mathbb{R}$ *(respectively,* $\{\alpha_n\} \subset \mathbb{R}^+$*) then* $R^{\boldsymbol{\alpha}}$ *and* $Q^{\boldsymbol{\alpha}}$ *are self-adjoint (respectively, positive self-adjoint). Furthermore,* $R^{\boldsymbol{\alpha}}$ *is bounded from* $\mathcal{H}_{-1}$ *to* $\mathcal{H}_{+1}$ *if and only if* $Q^{\boldsymbol{\alpha}}$ *is bounded from* $\mathcal{H}_{+1}$ *to* $\mathcal{H}_{-1}$ *and if, and only if,* $\boldsymbol{\alpha}$ *is a bounded sequence.*

(5) If $\boldsymbol{\alpha} = \mathbf{1}$, *where, as before,* $\mathbf{1}$ *denotes the sequence constantly equals to* 1, *then* $R := R^{\mathbf{1}}$ *and* $Q := Q^{\mathbf{1}}$ *are bounded positive self-adjoint operators respectively of* $\mathcal{B}(\mathcal{H}_{-1}, \mathcal{H}_{+1})$ *and of* $\mathcal{B}(\mathcal{H}_{+1}, \mathcal{H}_{-1})$ *and they are inverses of each other, that is* $R = (Q)^{-1}$, *and* $R = T^{-1}(T^{-1})^\dagger$, $Q = T^\dagger T$, *where* $T \in \mathcal{B}(\mathcal{H}_{+1}, \mathcal{H})$ *is the operator such that* $T\xi_n = e_n$, $\forall n \in \mathbb{N}$ *and* $\{e_n\}$ *is an orthonormal basis for* $\mathcal{H}$.

Proof The proof is similar to that of Proposition 4.2 and we omit it.

Remark 4.5 From Proposition 4.4, we see that there exists a bounded invertible, positive self-adjoint operator Q from $\mathcal{H}_{+1}$ into $\mathcal{H}_{-1}$ that maps the strict Riesz-like basis $\{\xi_n\}$ into its dual basis $\{\zeta_n\}$.

Now, recall that $Q = Q^{\mathbf{1}}$ and $R = R^{\mathbf{1}}$, then we have the following

Proposition 4.6 *Let* $\boldsymbol{\alpha} = \{\alpha_n\}$ *be a sequence of complex numbers. The following equalities hold:*

$$\begin{aligned} QA^{\boldsymbol{\alpha}} &= B^{\boldsymbol{\alpha}} Q = Q^{\boldsymbol{\alpha}}, \\ RB^{\boldsymbol{\alpha}} &= A^{\boldsymbol{\alpha}} R = R^{\boldsymbol{\alpha}}. \end{aligned} \tag{19}$$

Proof By Proposition 4.4 we have $D(A^{\boldsymbol{\alpha}}) = D(Q^{\boldsymbol{\alpha}})$ and $D(B^{\boldsymbol{\alpha}}) = D(R^{\boldsymbol{\alpha}})$. Moreover, from Proposition 4.2 and (18), if $f \in D(Q)$

$$Qf \in D(B^{\boldsymbol{\alpha}}) \Leftrightarrow \sum_{n=1}^{\infty} |\alpha_n|^2 |\langle Qf \,|\xi_n\rangle|^2 < \infty$$
$$\Leftrightarrow \sum_{n=1}^{\infty} |\alpha_n|^2 |\langle \zeta_n \,|f\rangle|^2 < \infty \Leftrightarrow f \in D(Q^{\boldsymbol{\alpha}}).$$

Similarly one proves the equality $D(QA^{\boldsymbol{\alpha}}) = D(Q^{\boldsymbol{\alpha}})$. It is easily seen that $QA^{\boldsymbol{\alpha}} f = B^{\boldsymbol{\alpha}} Qf = Q^{\boldsymbol{\alpha}} f$, for every $f \in D(Q^{\boldsymbol{\alpha}})$. The proof of the second equality in (19) is analogous.

Remark 4.7 Equations (19) show that the two operators $A^{\boldsymbol{\alpha}}$ and $B^{\boldsymbol{\alpha}}$ are *similar*, in the sense that Q and R act as intertwining operators, see e.g. [5, Definition 7.3.1]. The intertwining relations between operators have found some recent interest in Quantum Mechanics.

A simple consequence of previous results is the following corollary which generalizes the Theorem by Mostafazadeh[1] in [16] and thus gives a characterization of operators as $A^{\boldsymbol{\alpha}}$ and $B^{\boldsymbol{\alpha}}$ with real eigenvalues. Before continuing we recall the definition of (unbounded) quasi-Hermitian operator (see, e.g. [5, Definition 7.5.1]).

Definition 4.8 A closed operator A, with dense domain $D(A)$ is called *quasi-Hermitian* if there exists a metric operator G, with dense domain $D(G)$ in Hilbert space $\mathcal{H}$ such that $D(A) \subset D(G)$ and

$$\langle A\xi \,|G\eta\rangle = \langle G\xi \,|A\eta\rangle, \quad \xi, \eta \in D(A). \tag{20}$$

If A is a quasi-Hermitian operator on $\mathcal{H}$, then by definition there exists an unbounded metric operator G such that

$$A^{\dagger} G = AG.$$

Corollary 4.9 *Let T be the operator which transforms the strict Riesz-like basis $\{\xi_n\}$ into an orthonormal basis of Hilbert space $\mathcal{H}$. The following statements are equivalent.*

(i) The sequence $\boldsymbol{\alpha} = \{\alpha_n\}$ consists of real numbers.
(ii) $A^{\boldsymbol{\alpha}}$ is quasi-Hermitian, with $G = Q = T^{\dagger}T$.
(iii) $B^{\boldsymbol{\alpha}}$ is quasi-Hermitian, with $G = R = T^{-1}\left(T^{\dagger}\right)^{-1}$.

Proof $(i) \Rightarrow (ii)$ Suppose first that $\{\alpha_n\} \subset \mathbb{R}$, then according to (iii) of Proposition 4.2 $(A^{\boldsymbol{\alpha}})^{\dagger} = B^{\boldsymbol{\alpha}}$. Then we can rewrite the first equality in (19) as

$$QA^{\boldsymbol{\alpha}} = \left(A^{\boldsymbol{\alpha}}\right)^{\dagger} Q,$$

hence $A^{\boldsymbol{\alpha}}$ is quasi-Hermitian, with $G = Q$.

[1] The author in [16] calls the operators involved G-pseudo-Hermitian operators, however they are in fact quasi-Hermitian operators in the original sense of Dieudonné [17], even though unbounded.

$(ii) \Rightarrow (i)$ Let $A^{\boldsymbol{\alpha}}$ be quasi-Hermitian, with $G = Q$ then

$$A^{\boldsymbol{\alpha}} = Q^{-1}\left(A^{\boldsymbol{\alpha}}\right)^{\dagger} Q = T^{-1}(T^{\dagger})^{-1} A^{\boldsymbol{\alpha}} T^{\dagger} T. \tag{21}$$

Put $H_0 := T A^{\boldsymbol{\alpha}} T^{-1}$. It is an easy computation to prove that

$$D\left(T A^{\boldsymbol{\alpha}} T^{-1}\right) = D\left((T^{\dagger})^{-1}\left(A^{\boldsymbol{\alpha}}\right)^{\dagger} T^{\dagger}\right) = \left\{ f \in \mathcal{H};\ \sum_{n=1}^{\infty} |\alpha_n|^2 |\langle f\, |e_n\rangle|^2 < \infty \right\},$$

and from (21) we have

$$T A^{\boldsymbol{\alpha}} T^{-1} = (T^{\dagger})^{-1}\left(A^{\boldsymbol{\alpha}}\right)^{\dagger} T^{\dagger}. \tag{22}$$

Since $D\left((T^{\dagger})^{-1}\left(A^{\boldsymbol{\alpha}}\right)^{\dagger} T^{\dagger}\right) \subseteq D\left(\left(T A^{\boldsymbol{\alpha}} T^{-1}\right)^{\dagger}\right)$ we can conclude that H_0 is symmetric and its eigenvalues are $\{\alpha_n\} \subset \mathbb{R}$.

$(i) \Leftrightarrow (iii)$ is analogous to $(i) \Leftrightarrow (ii)$.

Other operators defined by a strict Riesz-like basis and its dual basis, more precisely *lowering* and *raising* operators, have been considered in [18] to factorize, under opportune hypotheses, the operators $A^{\boldsymbol{\alpha}}$ and $B^{\boldsymbol{\alpha}}$.

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Geometric Aspects of Space-Time Reflection Symmetry in Quantum Mechanics

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Abstract For nearly two decades, much research has been carried out on properties of physical systems described by Hamiltonians that are not Hermitian in the conventional sense, but are symmetric under space-time reflection; that is, they exhibit $\mathscr{P}\mathscr{T}$ symmetry. Such Hamiltonians can be used to model the behavior of closed quantum systems, but they can also be replicated in open systems for which gain and loss are carefully balanced, and this has been implemented in laboratory experiments for a wide range of systems. Motivated by these ongoing research activities, we investigate here a particular theoretical aspect of the subject by unraveling the geometric structures of Hilbert spaces endowed with the parity and time-reversal operations, and analyze the characteristics of $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians. A canonical relation between a $\mathscr{P}\mathscr{T}$-symmetric operator and a Hermitian operator is established in a geometric setting. The quadratic form corresponding to the parity operator, in particular, gives rise to a natural partition of the Hilbert space into two halves corresponding to states having positive and negative $\mathscr{P}\mathscr{T}$ norm. Positive definiteness of the norm can be restored by introducing a conjugation operator $\mathscr{C}$; this leads to a positive-definite inner product in terms of $\mathscr{C}\mathscr{P}\mathscr{T}$ conjugation.

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1 Introduction

The observation that non-Hermitian Hamiltonians possessing a physical symmetry associated with a discrete space-time reflection, known as $\mathscr{P}\mathscr{T}$ invariance, can possess entirely real eigenvalues [1] has generated considerable research outputs for nearly two decades. It is by now well documented that a $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian possesses real eigenvalues if the symmetry is unbroken in the sense that eigenstates of H are also eigenstates of $\mathscr{P}\mathscr{T}$ [2]. A $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian can describe dynamical and probabilistic aspects of closed quantum systems if one augments the Hilbert space with a suitable inner product [3, 4]. A $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian can be replicated in an open system by balancing gain and loss [5–7]. Open systems can have phase transitions associated with the breaking of $\mathscr{P}\mathscr{T}$ symmetry, leading to a range of counterintuitive phenomena that have been observed in laboratory experiments for many different kinds of physical systems [8–15].

For a quantum system having continuous degrees of freedom parity reflection $\mathscr{P}$ has the classical analog $x \to -x$ and $p \to -p$. Time reversal $\mathscr{T}$ generates the transformations $p \to -p$ and $\mathrm{i} \to -\mathrm{i}$. In the case of an open system modeled on a finite-dimensional Hilbert space $\mathscr{P}$ can be interpreted as the interchange of the left and the right sides of the system and $\mathscr{T}$ amounts to interchanging the gain and loss channels. Hence, if the mirror image of the gain channel is a loss channel, then $\mathscr{P}\mathscr{T}$ symmetry can be realized if the strengths of gain and loss are matched exactly. For a closed system characterized by a finite-dimensional matrix Hamiltonian the interpretation of $\mathscr{P}$ is not immediately apparent. Nevertheless, one can augment the Hilbert space with a structure that in a general sense embodies properties of parity reflection. It is then of interest to investigate the mathematical properties of Hilbert spaces endowed with such a structure.

This paper addresses this question by clarifying mathematical, and in particular the geometric aspects of the underlying real Hilbert space endowed with the parity structure. Apart from its intrinsic mathematical appeal, the geometric formalism has led, even in standard Hermitian quantum theory, to discoveries that no other mathematical approach has reproduced (for example, higher-order corrections to the Heisenberg uncertainty relation [16, 17]), or discoveries that come naturally with the geometric formalism (for example, the identification of the measure of entanglement for pure states [18]). In this spirit we develop here a geometric framework that is sufficiently general to admit both standard quantum theory with a Hermitian Hamiltonian as well as extensions of the standard theory. In Sects. 2 and 3 we discuss the underlying mathematical structures and the role of the observables in conventional Hermitian quantum mechanics. In Sects. 4 and 5 we compare these results with the corresponding structures in $\mathscr{P}\mathscr{T}$-symmetric quantum theory. It is well known that the requirement of $\mathscr{P}\mathscr{T}$ invariance alone on the Hamiltonian leads to a state space with an indefinite metric. The crucial observation that we make here is that the parity operator plays the role of an indefinite metric, while the complex structure J of standard quantum mechanics is unaltered in $\mathscr{P}\mathscr{T}$-symmetric quantum theory. This is an attractive complex-analytic feature of $\mathscr{P}\mathscr{T}$-symmetric theory. Proposition 1

states that the $\mathscr{P}\mathscr{T}$ norm of a state is expressible as a difference of the standard Dirac norm of the positive- and negative-parity parts of the state.

Section 6 analyses the properties of $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian operators. Proposition 2 shows that any such Hamiltonian is a product of the parity structure and a Hermitian quadratic form. This leads to a new way to understand the reality of the spectrum of such Hamiltonians; Proposition 3 shows that the energy eigenvalues are necessarily real if the corresponding eigenvectors have nonvanishing $\mathscr{P}\mathscr{T}$ norm. In our geometric scheme Proposition 4 shows that the eigenvalues of such Hamiltonians are either real or occur as complex conjugate pairs [19]. A sufficient condition for the reality of the eigenvalues is then established in Proposition 5.

In Sect. 7 we introduce an additional structure $\mathscr{C}$ that has the interpretation of charge conjugation. This symmetry allows us to construct an alternative inner product on the vector space spanned by the eigenfunctions of the $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian by means of $\mathscr{C}\mathscr{P}\mathscr{T}$ conjugation, thus eliminating states having negative norms. As a consequence, a consistent probabilistic interpretation for a closed system can be assigned to quantum theories described by $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians.

2 Geometry of Hermitian Quantum Mechanics

Before discussing $\mathscr{P}\mathscr{T}$-symmetric quantum theory, it is helpful first to formulate standard quantum mechanics from a perspective that is useful in clarifying the similarities and differences of the two formalisms. In standard quantum theory Hermitian operators play a dual role, namely, as physical observables and as generators of dynamics. To explain the relation between these two roles, we show how to build quantum mechanics, not in terms of the complex Hilbert space with respect to which it is usually formulated, but rather in terms of a more primitive underlying even-dimensional *real* Hilbert space $\mathbb{H}$. By introducing certain structures on $\mathbb{H}$ we arrive at standard quantum theory. Then by considering a related alternative set of structures on $\mathbb{H}$ we arrive at $\mathscr{P}\mathscr{T}$-symmetric quantum theory, and the relationship of the two theories becomes clear.

Using index notation [16, 17, 20–22], we let the real vector ξ^a denote a typical element of $\mathbb{H}$. The real Hilbert space $\mathbb{H}$ is equipped with a positive-definite quadratic form g_{ab} satisfying $g_{ab} = g_{ba}$, and the squared norm of the vector ξ^a is given by $g_{ab}\xi^a\xi^b$. If ξ^a and η^a are elements of $\mathbb{H}$ we define their inner product by $g_{ab}\xi^a\eta^b$.

To recover the apparatus of standard quantum mechanics we require that $\mathbb{H}$ also be endowed with a compatible complex structure, by which we mean a real tensor $J^a{}_b$ whose square is equal to the negative of the identity $J^a{}_c J^c{}_b = -\delta^a{}_b$. The complex structure is compatible with the symmetric quadratic form if g_{ab} satisfies

$$g_{ab} J^a{}_c J^b{}_d = g_{cd} \tag{1}$$

and g_{ab} is said to be J-invariant. The J-invariance condition implies that the tensor

$$\Omega_{ab} = g_{ac} J^{c}_{\ b} \tag{2}$$

is antisymmetric and nondegenerate, and thus defines a *symplectic structure* on $\mathbb{H}$. To verify the antisymmetry of Ω_{ab} we insert (1) into (2): $\Omega_{ba} = g_{bc} J^{c}_{\ a} = g_{de} J^{d}_{\ b} J^{e}_{\ c} J^{c}_{\ a} = -g_{de} J^{d}_{\ b} \delta^{e}_{\ a} = -\Omega_{ab}$.

To verify the nondegeneracy of Ω_{ab} we note that $\Omega^{ab} = g^{ac} g^{cd} \Omega_{cd}$ acts as the required inverse. Indeed, we have $\Omega^{ac} \Omega_{bc} = g^{ae} g^{cf} g_{eh} J^{h}_{\ f} g_{bd} J^{d}_{\ c} = g_{bd} J^{d}_{\ c} J^{a}_{\ f} g^{cf} = \delta^{a}_{\ b}$. In the last step we have used the J-invariance of g^{ab}, which satisfies $J^{a}_{\ c} J^{b}_{\ d} g^{cd} = g^{ab}$. The symplectic structure is also compatible with $J^{a}_{\ b}$ in the sense that $\Omega_{ab} J^{a}_{\ c} J^{b}_{\ d} = \Omega_{cd}$. (This follows because $\Omega_{ab} J^{a}_{\ c} J^{b}_{\ d} = g_{ae} J^{e}_{\ b} J^{a}_{\ c} J^{b}_{\ d} = -g_{ae} \delta^{e}_{\ d} J^{a}_{\ c} = -\Omega_{dc} = \Omega_{cd}$). We then say that Ω_{ab} is J-invariant.

We can now elucidate the structure of standard quantum mechanics. We endow the real Hilbert space $\mathbb{H}$ with a *Hermitian inner product*. If ξ^a and η^a are two real Hilbert space vectors, then their Hermitian inner product, which we write as $\langle \eta | \xi \rangle$ in the usual Dirac notation, is the complex expression

$$\langle \eta | \xi \rangle = \tfrac{1}{2} \eta^a (g_{ab} - \mathrm{i} \Omega_{ab}) \xi^b. \tag{3}$$

Because the symplectic form Ω_{ab} is antisymmetric, the Hermitian norm agrees with the real Hilbertian norm, apart from a factor of two: $\langle \xi | \xi \rangle = \frac{1}{2} g_{ab} \xi^a \xi^b$.

Next, we complexify the Hilbert space $\mathbb{H}$ and denote the result $\mathbb{H}_{\mathbb{C}}$. The elements of $\mathbb{H}_{\mathbb{C}}$ are the complex vectors $\xi^a + \mathrm{i}\eta^b$, where $\xi^a,\ \eta^b \in \mathbb{H}$. With the aid of the complex structure, a real Hilbert space vector ξ^a can be decomposed into complex J-positive and J-negative parts:

$$\xi^a = \xi^a_+ + \xi^a_-, \tag{4}$$

where

$$\xi^a_+ = \tfrac{1}{2}(\xi^a - \mathrm{i} J^a_{\ b} \xi^b) \quad \text{and} \quad \xi^a_- = \tfrac{1}{2}(\xi^a + \mathrm{i} J^a_{\ b} \xi^b). \tag{5}$$

For the case of relativistic fields, where ξ^a is a square-integrable solution of the Klein-Gordon equation defined on a background space-time, this decomposition corresponds to splitting the fields into positive- and negative-frequency parts.

Note that ξ^a_+ and ξ^a_- are complex eigenstates of the $J^a_{\ b}$ operator: $J^a_{\ b} \xi^b_+ = +\mathrm{i} \xi^a_+$ and $J^a_{\ b} \xi^b_- = -\mathrm{i} \xi^a_-$. The Hermitian ($J$-invariance) condition (1) implies that two vectors of the same type (for example, a pair of J-positive vectors) are orthogonal with respect to the metric g_{ab}. Thus, we have $g_{ab} \xi^a_+ \eta^b_+ = 0$ for any pair $\xi^a_+,\ \eta^a_+$ of J-positive vectors, and $g_{ab} \xi^a_- \eta^b_- = 0$ for any pair $\xi^a_-,\ \eta^a_-$ of J-negative vectors.

For a real vector ξ^a it follows from (4) that $\xi^a_- = \overline{\xi^a_+}$. We can also split a complex vector into J-positive and J-negative parts. However, in splitting a *complex* vector $\zeta^a = \zeta^a_+ + \zeta^a_-$ there is no *a priori* relationship between the components ζ^a_+ and ζ^a_-.

Thus, if ζ^a is not real, then $\zeta_-^a \neq \overline{\zeta_+^a}$. The complex conjugate of a J-positive vector is nevertheless a J-negative vector, and vice versa. To be precise, we have $\overline{\zeta_+^a} = \bar{\zeta}_-^a$.

Introducing J-positive and J-negative vectors allows us to express the Dirac inner product (3) in a simplified form, namely, $\langle \eta | \xi \rangle = \eta_-^a g_{ab} \xi_+^b$. The equivalence of (3) and the simplified form is verified by using (1) and the antisymmetry of Ω_{ab}:

$$\begin{aligned}\eta_-^a g_{ab} \xi_+^b &= \tfrac{1}{4}(\eta^a + \mathrm{i} J^a{}_c \eta^c) g_{ab} (\xi^b - \mathrm{i} J^b{}_d \xi^d) \\ &= \tfrac{1}{4}\left(g_{ab} + J^c{}_a J^d{}_b g_{cd}\right) \eta^a \xi^b - \tfrac{1}{4}\mathrm{i}\left(g_{ac} J^c{}_b - J^c{}_a g_{bc}\right) \eta^a \xi^b \\ &= \tfrac{1}{2} \eta^a (g_{ab} - \mathrm{i}\Omega_{ab}) \xi^b .\end{aligned}$$

3 Quantum-Mechanical Observables

We now explain how the observables of standard quantum mechanics are represented in terms of the geometry of the real Hilbert space $\mathbb{H}$. A quantum observable corresponds to a real symmetric J-invariant quadratic form on $\mathbb{H}$; that is, a real tensor F_{ab} satisfying $F_{ab} = F_{ba}$ and $F_{ab} J^a{}_c J^b{}_d = F_{cd}$. The observable corresponding to the identity is g_{ab}, and for the expectation of F in the state ξ^a we write $\langle \xi | F | \xi \rangle / \langle \xi | \xi \rangle = F_{ab} \xi^a \xi^b / g_{ab} \xi^a \xi^b$. In general, for the states ξ^a and η^a, we have $\langle \eta | F | \xi \rangle = \eta_-^a F_{ab} \xi_+^b$. The *operator* associated with the observable F_{ab} is obtained by raising one of the indices with the inverse of the metric: $F^a{}_b = g^{ac} F_{cb}$. From the J-invariance of F_{ab}, when the operator $F^a{}_b$ acts on a J-positive vector, the result is another J-positive vector. Alternative ways to write $\langle \eta | F | \xi \rangle$ are $\eta_-^a g_{ac} F^c{}_b \xi_+^b = F^a{}_c \eta_-^c g_{ab} \xi_+^b$, which expresses the self-adjointness of $F^a{}_b$ with respect to the given inner product.

What are the symmetries of the Hilbert space $\mathbb{H}$? Rotations of $\mathbb{H}$ around the origin are given by orthogonal transformations, that is, the matrix operations $\xi^a \to M^a{}_b \xi^b$ such that $g_{ab} M^a{}_c M^b{}_d = g_{cd}$. Such transformations preserve the norm $g_{ab} \xi^a \xi^b$ of the state ξ^a. The unitary group consists of orthogonal matrices that also leave the symplectic structure invariant: $\Omega_{ab} M^a{}_c M^b{}_d = \Omega_{cd}$.

In the case of an infinitesimal orthogonal transformation $M^a{}_b = \delta^a{}_b + \varepsilon f^a{}_b$, with $\varepsilon^2 \sim 0$, it is easy to verify that $f^a{}_b$ must satisfy $g_{ac} f^c{}_b + g_{bc} f^c{}_a = 0$, from which we deduce that $f^a{}_b$ has the form $f^a{}_b = g^{ac} f_{cb}$, where f_{ab} is antisymmetric. For $M^a{}_b$ to be a unitary operator it is necessary and sufficient that f_{ab} be J-invariant. We thus see that any infinitesimal unitary transformation has the form

$$M^a{}_b = \delta^a{}_b + \varepsilon J^a{}_c F^c{}_b, \tag{6}$$

where $F^a{}_b$ is the operator associated with a standard quantum observable F_{ab}. Indeed, f_{ab} is antisymmetric and J-invariant if and only if it can be expressed as

$$f_{ab} = F_{ac} J^c{}_b, \tag{7}$$

where F_{ab} is symmetric and J-invariant. If $F^a_{\ b}$ is proportional to the identity $g^a_{\ b}$ then (6) corresponds to an infinitesimal phase transformation. Conversely, if $F^a_{\ b}$ is trace-free, then (6) gives an infinitesimal special unitary transformation.

Thus, we see how the *operator* $F^a_{\ b}$ is associated with both the *observable* F_{ab} as well as the infinitesimal unitary transformation $\xi^a \to \xi^a + \varepsilon J^a_{\ b} F^b_{\ c} \xi^c$. The complete trajectory of the unitary transformation associated with the operator $F^a_{\ b}$ can be obtained by exponentiating the infinitesimal transformation and writing

$$\xi^a(t) = \exp\left(t J^b_{\ c} F^c_{\ d} \xi^d \partial_b\right) \xi^a \Big|_{\xi^a = \xi^a(0)},$$

where $\partial_b = \partial/\partial\xi^b$. The differential operator appearing in the exponent can be written as $J^b_{\ c} F^c_{\ d} \xi^d \partial_b = \frac{1}{2}\left(\Omega^{ab}\partial_b F\right)\partial_a$, where $F(\xi) = F_{ab}\xi^a\xi^b$. Thus, the quadratic form $F_{ab}\xi^a\xi^b$ appears as the generator of a Hamiltonian vector field $X^a(\xi) = \partial\xi^a/\partial t$ on $\mathbb{H}$ given by $\partial\xi^a/\partial t = \frac{1}{2}\Omega^{ab}\partial_b F(\xi)$. The trajectory of the one-parameter family of unitary transformations associated with the observable F_{ab} is generated by the Hamiltonian vector field $\frac{1}{2}\Omega^{ab}\partial_b F(\xi)$. If $H(\xi) = H_{ab}\xi^a\xi^b$ denotes the quadratic function on $\mathbb{H}$ associated with the Hamiltonian of a standard quantum system, then the Schrödinger equation is

$$\frac{\partial\xi^a}{\partial t} = \tfrac{1}{2}\Omega^{ab}\partial_b H. \tag{8}$$

We conclude that standard quantum mechanics can be described in terms of the geometry of a real vector space $\mathbb{H}$ equipped with a complex structure $J^a_{\ b}$, a positive definite quadratic form g_{ab}, and a compatible symplectic structure Ω_{ab}. Observables are J-invariant quadratic forms on $\mathbb{H}$, and dynamical trajectories are the symplectic vector field on $\mathbb{H}$ generated by such forms. All these structures are intrinsic to standard quantum theory.

4 Space-Time Reflection Symmetry

In standard quantum theory, we fix the complex tensor $J^a_{\ b}$ on the space $\mathbb{H}$ of real state vectors; the remaining structures, namely, the positive-definite quadratic form g_{ab} and the symplectic structure Ω_{ab}, are then chosen so as to satisfy the compatibility conditions. The compatibility conditions are useful for relativistic fields, that is, when we insist that the creation and annihilation operators satisfy canonical commutation relations [23]. For the quantum theory of a $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian we introduce another quadratic form called *parity* π_{ab} that for certain purposes replaces the metric g_{ab} of the standard theory. The parity operator, whose properties are defined below, can only be introduced if the *complex* dimension of the space of J-positive vectors is even. Hence, the dimensionality of the underlying space of real state vectors associated with $\mathscr{P}\mathscr{T}$-symmetric quantum theory is a multiple of four rather

than two. This is the sense in which $\mathscr{P}\mathscr{T}$ symmetry extends (complex) quantum mechanics further into the complex domain [3].

Let us define the properties of the parity operator $\pi^a{}_b$. In a general sense, this operator represents space reflection and satisfies the conditions of a standard observable in quantum theory discussed in Sect. 3. Therefore, $\pi_{ab} = g_{ac}\pi^c{}_b$ is required to be real and symmetric and to satisfy the J-invariance condition $\pi_{ab}J^a{}_cJ^b{}_d = \pi_{cd}$. This condition is equivalent to the commutation relation $\pi^a{}_cJ^c{}_b = J^a{}_c\pi^c{}_b$. In addition, the parity operator is required to be trace-free,

$$\pi^a{}_a = 0, \tag{9}$$

and to satisfy the orthogonality condition

$$g_{ab}\pi^a{}_c\pi^c{}_b = g_{cd}. \tag{10}$$

Thus, $\pi^a{}_b$ is unitary on the space of J-positive vectors associated with $\mathbb{H}$.

One may relax the trace-free condition (9) to define a generalization of the parity operator [24] on a complex Hilbert space of any dimension. For the physical intuition behind this, recall the case of a coupled pair of waveguides; here, $\mathscr{P}$ swaps the two waveguides. If there are three coupled waveguides, then a $\mathscr{P}$ reflection leaves the middle waveguide intact; there is a degenerate component. If such degeneracies are allowed, the parity operator can be defined in arbitrary dimension. Here, we focus on the nondegenerate case. Conditions (9) and (10) then prevent us from defining a parity structure unless the dimension of the underlying real Hilbert space $\mathbb{H}$ is a multiple of four. In particular, *from the defining conditions of the parity operator half of its eigenvalues are* $+1$ *and the other half are* -1*, and the parity operator is unique up to unitary transformations*. The eigenvalues are ± 1 because π_{ab} is symmetric and the orthogonality condition (10) can be written as

$$\pi^a{}_c\pi^c{}_b = \delta^a{}_b. \tag{11}$$

Since a successive application of space reflection is the identity, if we diagonalize $\pi^a{}_b$, the diagonal entries are ± 1, and the trace-free condition (9) implies that the two signs occur in equal numbers. Suppose that $\mathscr{P}$ and $\mathscr{P}'$ are distinct parity operators. They have the same spectrum, so there exists a unitary transformation from one to the other. Hence, $\pi^a{}_b$ is unique up to unitary equivalence.

In $\mathscr{P}\mathscr{T}$-symmetric quantum theory we keep the real Hilbert space $\mathbb{H}$ and its complex structure $J^a{}_b$ and introduce a new inner-product on $\mathbb{H}$ in terms of the parity operator. The $\mathscr{P}\mathscr{T}$ inner product $\langle\eta\|\xi\rangle$ between the elements ξ^a and η^a in $\mathbb{H}$ is

$$\langle\eta\|\xi\rangle = \tfrac{1}{2}\eta^a(\pi_{ab} - \mathrm{i}\omega_{ab})\xi^b, \tag{12}$$

where ω_{ab} is defined by $\omega_{ab} = \Omega_{ac}\pi^c{}_b$. Equivalently, from (2) we can write $\omega_{ab} = \pi_{ac}J^c{}_b$. Since π_{ab} is an observable in standard quantum mechanics, ω_{ab} is antisymmetric and defines a new symplectic structure on $\mathbb{H}$ that is compatible with the

complex structure $J^a_{\ b}$. One can easily verify the J-invariance condition $\omega_{ab}J^a_{\ c}J^b_{\ d} = \omega_{cd}$ associated with the symplectic structure.

As in standard quantum mechanics, the $\mathscr{P}\mathscr{T}$ inner product (12) can be written in terms of the J-positive and J-negative parts of the vectors ξ^a and η^a. Splitting $\mathbb{H}$ into J-positive and J-negative parts depends on the complex structure $J^a_{\ b}$, and not on the associated quadratic forms. A short calculation then shows that $\langle \eta \| \xi \rangle = \eta^a_- \pi_{ab} \xi^b_+$. Indeed, starting from this equation we have $\eta^a_- \pi_{ab} \xi^b_+ = \frac{1}{4}(\eta^a + \mathrm{i}J^a_{\ c}\eta^c)\pi_{ab}(\xi^b - \mathrm{i}J^b_{\ d}\xi^d)$ by virtue of (5). Then, using the J-invariance of π_{ab} and the antisymmetry of ω_{ab}, we are immediately led back to the inner product (12).

Because of (11), if we adapt the usual convention of writing $\pi^{ab} = g^{ac}g^{bd}\pi_{cd}$, then π^{ab} is the inverse of π_{ab} because $\pi_{ab}\pi^{bc} = \delta_a^{\ c}$. Analogously, the tensor $\omega^{ab} = g^{ac}g^{bd}\omega_{cd}$ satisfies $\omega^{ab} = \pi^{ac}\pi^{bd}\omega_{cd}$ and ω^{ab} is the inverse of ω_{ab}, so $\omega_{ab}\omega^{bc} = \delta_a^{\ c}$. Note also that ω_{ab} is $\mathscr{P}$-invariant because $\pi_a^{\ c}\pi_b^{\ d}\omega_{cd} = \omega_{ab}$.

To summarize these results, in the case of the Hermitian theory we have the compatible structures $(J^a_{\ b}, g_{ab}, \Omega_{ab})$ on $\mathbb{H}$, whereas the $\mathscr{P}\mathscr{T}$-symmetric quantum theory comes equipped with the compatible structures $(J^a_{\ b}, \pi_{ab}, \omega_{ab})$. The key difference between the two theories is that, while g_{ab} is positive definite, π_{ab} is indefinite with the split signature $(+, \cdots, +, -, \cdots, -)$. The $\mathscr{P}\mathscr{T}$ norm (pseudo-norm) of a state ξ^a, which is defined by

$$\langle \xi \| \xi \rangle = \tfrac{1}{2}\pi_{ab}\xi^a\xi^b, \tag{13}$$

can be either positive or negative, and in some cases may also vanish.

We interpret the $\mathscr{P}\mathscr{T}$ norm as follows. Given any real element ξ^a in $\mathbb{H}$ we can split this into its positive and negative parity parts by writing $\xi^a = \xi^a_\oplus + \xi^a_\ominus$, where $\xi^a_\oplus = \frac{1}{2}(\xi^a + \pi^a_{\ b}\xi^b)$ and $\xi^a_\ominus = \frac{1}{2}(\xi^a - \pi^a_{\ b}\xi^b)$. These vectors are eigenstates of the parity operator π_{ab}, satisfying $\pi^a_{\ b}\xi^b_\oplus = \xi^a_\oplus$ and $\pi^a_{\ b}\xi^b_\ominus = -\xi^a_\ominus$. In terms of the projection operators $\Pi^a_{\oplus b} = \frac{1}{2}(\delta^a_{\ b} + \pi^a_{\ b})$ and $\Pi^a_{\ominus b} = \frac{1}{2}(\delta^a_{\ b} - \pi^a_{\ b})$ onto positive- and negative-parity eigenstates, we have

$$\pi^a_{\ b} = \Pi^a_{\oplus b} - \Pi^a_{\ominus b}, \tag{14}$$

where $\Pi^a_{\oplus b}\xi^b = \xi^a_\oplus$ and $\Pi^a_{\ominus b}\xi^b = \xi^a_\ominus$. Furthermore, because $\pi^a_{\ b}$ and $J^a_{\ b}$ commute, the positive-parity component of the J-positive part of a real vector ξ^a agrees with the J-positive part of the positive-parity part of ξ^a, and similarly for other such combinations. We can now establish the following result for the $\mathscr{P}\mathscr{T}$ norm.

Proposition 1 *The squared $\mathscr{P}\mathscr{T}$ norm of a state $\xi^a \in \mathbb{H}$ is the difference between the squared Hermitian norm of the positive-parity part $\xi^a_\oplus$ of the state and that of the negative-parity part $\xi^a_\ominus$ of the state:*

$$\langle \xi \| \xi \rangle = \langle \xi_\oplus | \xi_\oplus \rangle - \langle \xi_\ominus | \xi_\ominus \rangle. \tag{15}$$

Thus, if a state is "more probably" of positive parity, its $\mathscr{P}\mathscr{T}$-norm is positive. Conversely, for a state of "more probably" negative parity, its $\mathscr{P}\mathscr{T}$-norm is negative. The identity (15) follows immediately if we insert (14) into (13).

Finally, we note that if ξ^a and η^a are positive- and negative-parity states, then their standard quantum transition amplitude vanishes: $\langle \xi_\oplus | \eta_\ominus \rangle = 0$. This follows from (3) if we insert $\eta^a_\ominus$ for η^a and $\xi^a_\oplus$ for ξ^a and use the identities $g_{ab}\Pi^a_{\oplus c}\Pi^b_{\ominus d} = 0$ and $\Omega_{ab}\Pi^a_{\oplus c}\Pi^b_{\ominus d} = 0$. The second of these two relations follows from the former because the J-tensor commutes with the parity projection operators.

5 Observables and Symmetries

What are the transformations of $\mathbb{H}$ that preserve the $\mathscr{P}\mathscr{T}$ norm $\pi_{ab}\xi^a\xi^b$? The transformation $\xi^a \to M^a{}_b\xi^b$ preserves the $\mathscr{P}\mathscr{T}$ norm for all $\xi^a \in \mathbb{H}$ if and only if

$$\pi_{ab}M^a{}_cM^b{}_d\xi^c\xi^d = \pi_{ab}\xi^a\xi^b \tag{16}$$

for all ξ^a. In the case of the infinitesimal transformation $M^a{}_b = \delta^a{}_b + \varepsilon f^a{}_c$, (16) holds to first order in ε if and only if

$$\pi_{ab}f^a{}_c\xi^b\xi^c = 0 \tag{17}$$

for all ξ^a, from which we deduce that $f^a{}_b$ must have the form

$$f^a{}_b = \pi^{ac}f_{cb}, \tag{18}$$

where f_{bc} is antisymmetric. As in Sect. 4, π^{ab} denotes the inverse of π_{ab} and satisfies $\pi^{ab}\pi_{bc} = \delta^a{}_c$. Note that π^{ab} is defined unambiguously without reference to g_{ab}.

To verify (18) we argue that if (17) holds for all ξ^a, then $\pi_{ab}f^b{}_c$ is antisymmetric. Writing $\pi_{ab}f^b{}_c = f_{ac}$, we obtain (18) by applying the inverse of π_{ab} to each side. Thus, the infinitesimal pseudo-orthogonal transformations that preserve the $\mathscr{P}\mathscr{T}$ norm are given by $M^a{}_b = \delta^a{}_b + \varepsilon\pi^{ac}f_{cb}$, where f_{ab} is antisymmetric.

We require that the transformation preserve the $\mathscr{P}\mathscr{T}$ symplectic structure ω_{ab}. Because of the compatibility condition this is equivalent to requiring that the complex structure is preserved. We have $\omega_{ab}M^a{}_cM^b{}_d = \omega_{cd} + \varepsilon\left(\omega_{ad}\pi^{ae}f_{ec} + \omega_{cb}\pi^{be}f_{ed}\right)$ to first order in ε. Thus, in order for ω_{ab} to be preserved we require that $\omega_{ad}\pi^{ae}f_{ec} + \omega_{cb}\pi^{be}f_{ed} = 0$. However, since $\omega_{ab} = \pi_{ac}J^c{}_b$, this condition implies that f_{ab} is J-invariant. Because f_{ab} is antisymmetric and J-invariant, it can be written in the form $f_{ab} = F_{ac}J^c{}_b$, where F_{ab} is a J-invariant symmetric quadratic form on $\mathbb{H}$.

We conclude that the general infinitesimal pseudo-unitary transformation preserving π_{ab} and ω_{ab} has the form $M^a{}_b = \delta^a{}_b + \varepsilon\omega^{ac}F_{cb}$, where F_{ab} is a standard quantum observable; it is symmetric and J-invariant. It is interesting to recall (7) and to note that the same J-invariant quadratic forms on $\mathbb{H}$ appear both in standard quantum theory and in $\mathscr{P}\mathscr{T}$-symmetric quantum theory.

Arguments analogous to those in Sect. 3 show that the trajectory of the pseudo-unitary transformation associated with the operator $F^a_{\ b} = \pi^{ac} F_{cb}$ has the form

$$\xi^a(t) = \exp\left(t\omega^{bc} F_{cd} \xi^d \partial_b\right) \xi^a \Big|_{\xi^a = \xi^a(0)},$$

where $\partial_b = \partial/\partial\xi^b$. Thus, if $F(\xi) = F_{ab}\xi^a\xi^b$ is the quadratic function on $\mathbb{H}$ associated with an observable F_{ab}, then the dynamical equation for the corresponding one-parameter family of pseudo-unitary transformations on $\mathbb{H}$ preserves the $\mathscr{PT}$ inner product, and it can be expressed in Hamiltonian form: $\partial\xi^a/\partial t = \frac{1}{2}\omega^{ab}\partial_b F$. This contrasts with (8) for standard quantum mechanics.

6 $\mathscr{PT}$-symmetric Hamiltonian Operators

We now introduce the notion of observables invariant under $\mathscr{PT}$ symmetry and consider the properties of $\mathscr{PT}$-symmetric Hamiltonian operators. Unlike Hermiticity in conventional quantum mechanics, we demand here that the Hamiltonian be invariant under space-time reflection. In ordinary quantum mechanics we require the Hamiltonian operator $H^a_{\ b}$ to be real, $H^a_{\ b} = \bar{H}^a_{\ b}$, and J-invariant, $J^a_{\ b} H^b_{\ c} J^c_{\ d} = H^a_{\ d}$. A Hamiltonian that satisfies these conditions is Hermitian. Here, we keep the J-invariance, but replace the reality condition with another condition that has the physical interpretation of invariance under space-time reflection.

We have introduced the real vector space $\mathbb{H}$ and the complex structure $J^a_{\ b}$ and we have shown that this structure can be augmented in two ways, either by introducing the positive-definite symmetric quadratic form g_{ab} and associated symplectic structure Ω_{ab}, or by introducing the split-signature indefinite form π_{ab} and associated symplectic structure ω_{ab}. Here, we consider either the structure $(J^a_{\ b}, g_{ab}, \Omega_{ab})$ or the structure $(J^a_{\ b}, \pi_{ab}, \omega_{ab})$ (or both). We call the former the g-structure on $\mathbb{H}$ and the latter the π-structure on $\mathbb{H}$. First, we consider those aspects of the $\mathscr{PT}$ symmetry that arise when we only have the π-structure on $\mathbb{H}$. We make no direct use of the parity operator $\pi^a_{\ b} = g^{ac}\pi_{cb}$ for now (because this involves g_{ab}) and we consider only the consequence of introducing a π-structure on $\mathbb{H}$.

Suppose that $\mathbb{H}$ is endowed with a π-structure, and let $H^a_{\ b}$ be a complex operator on $\mathbb{H}_{\mathbb{C}}$. Thus, $H^a_{\ b} = X^a_{\ b} + \mathrm{i}Y^a_{\ b}$, where $X^a_{\ b}$ and $Y^a_{\ b}$ are real. We assume that $H^a_{\ b}$ is J-invariant. Then $H^a_{\ b}$ is invariant under space-time reflection (is $\mathscr{PT}$-symmetric) with respect to the given π-structure, if

$$\pi_{bc}\bar{H}^c_{\ d}\pi^{ad} = H^a_{\ b}. \tag{19}$$

This relation suggests that if we take the complex conjugate of the Hamiltonian followed by a parity transformation, then we recover the original Hamiltonian.

Next, we introduce the notion of a *Hermitian form*. A tensor K_{ab} on $\mathbb{H}_{\mathbb{C}}$ is a Hermitian form if it is J-invariant and satisfies $\bar{K}_{ab} = K_{ba}$. Thus, K_{ab} is a Hermitian

form if $K_{ab} = X_{ab} + \mathrm{i}Y_{ab}$, where X_{ab} and Y_{ab} are real and J-invariant, and X_{ab} is symmetric and Y_{ab} is antisymmetric. Examples of Hermitian forms are $g_{ab} - \mathrm{i}\Omega_{ab}$ and $\pi_{ab} - \mathrm{i}\omega_{ab}$. The following proposition emerges from these definitions.

Proposition 2 *A Hamiltonian operator $H^a_{\ b}$ is $\mathscr{P}\mathscr{T}$-symmetric with respect to the π-structure $(J^a_{\ b}, \pi_{ab}, \omega_{ab})$ if and only if there exists a Hermitian form K_{ab} such that $H^a_{\ b} = \pi^{ac}K_{bc}$.*

To verify Proposition 2 we note that $\pi_{bc}\bar{H}^c_{\ d}\pi^{ad} = \pi_{bc}\pi^{ce}\bar{K}_{de}\pi^{ad} = \delta_b^{\ e}K_{ed}\pi^{ad} = H^a_{\ b}$. Thus, $\mathscr{P}\mathscr{T}$ invariance of a Hamiltonian is an unconventional Hermiticity condition. One can characterize $\mathscr{P}\mathscr{T}$ invariance without reference to any elements of the g-structure on $\mathbb{H}$.

We now turn to the spectrum of the operator $H^a_{\ b}$, still keeping in the context of the π-structure. Because $H^a_{\ b}$ is complex, we must admit the possibility of complex eigenvectors, that is, elements of $\mathbb{H}_{\mathbb{C}}$. We define the $\mathscr{P}\mathscr{T}$ norm as follows: if ϕ^a is an element of $\mathbb{H}_{\mathbb{C}}$, then its $\mathscr{P}\mathscr{T}$ norm is $\pi_{ab}\phi^a\bar{\phi}^b$, which is the sum of the $\mathscr{P}\mathscr{T}$ norms of the real and imaginary parts of ϕ^a.

Proposition 3 *If the $\mathscr{P}\mathscr{T}$ norm of an eigenvector of a $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian is nonvanishing, then the corresponding eigenvalue is real.*

Proof For some possibly complex value of E the vector ϕ^a, which may be complex, satisfies the eigenvalue equation $H^a_{\ b}\phi^b = E\phi^a$. Taking the complex conjugate, we have $\bar{H}^a_{\ b}\bar{\phi}^b = \bar{E}\bar{\phi}^a$. Transvecting each side of these equations with π_{ca}, we get $\pi_{ca}H^a_{\ b}\phi^b = E\pi_{ca}\phi^a$ and $\pi_{ca}\bar{H}^a_{\ b}\bar{\phi}^b = \bar{E}\pi_{ca}\bar{\phi}^a$. Hence, from Proposition 1 we get

$$K_{ab}\phi^b = E\pi_{ab}\phi^b \tag{20}$$

and $\bar{K}_{ab}\bar{\phi}^b = \bar{E}\pi_{ab}\bar{\phi}^b$, and because K_{ab} is a Hermitian form we can replace this with

$$K_{ab}\bar{\phi}^b = \bar{E}\pi_{ab}\bar{\phi}^b. \tag{21}$$

Contracting (20) and (21) with $\bar{\phi}^a$ and ϕ^a and subtracting, we get $(E - \bar{E})\pi_{ab}\phi^a\bar{\phi}^b = 0$, from which Proposition 3 follows. □

Thus, if a $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian has any complex eigenvalues, then the corresponding eigenstates have vanishing $\mathscr{P}\mathscr{T}$ norm. We proceed to augment the vector space $\mathbb{H}$ with the g-structure in addition to the π-structure. Introducing the g-structure allows us to consider the parity operator $\pi^a_{\ b}$. The condition (19) for the invariance under space-time reflection can now be written in the form

$$\pi^a_{\ c}\bar{H}^c_{\ d}\pi^d_{\ b} = H^a_{\ b}. \tag{22}$$

Note that real part of the Hamiltonian has even parity and the imaginary part has odd parity. Therefore, writing $H^a_{\ b} = X^a_{\ b} + \mathrm{i}Y^a_{\ b}$, where $X^a_{\ b}$ and $Y^a_{\ b}$ are real, we get $\pi^a_{\ c}X^c_{\ d}\pi^d_{\ b} = X^a_{\ b}$ and $\pi^a_{\ c}Y^c_{\ d}\pi^d_{\ b} = -Y^a_{\ b}$. Conversely, any such complex operator is invariant under space-time reflection. We then have the following observation on the reality of the energy eigenvalues.

Proposition 4 *Let E be an eigenvalue of a $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian operator $H^a_{\ b}$ with corresponding eigenstate ϕ^a. Then, $\bar{E}$ is also an eigenvalue of $H^a_{\ b}$, for which the associated eigenstate is $\pi^a_{\ b}\bar{\phi}^b$. In particular, if ϕ^a is a simultaneous eigenstate of the $\mathscr{P}\mathscr{T}$ operator, then E is real.*

Proof Consider the eigenvalue equation

$$H^a_{\ b}\phi^b = E\phi^a, \tag{23}$$

where E is an energy eigenvalue, which may or may not be real. Substituting (22) in the right side of (23) gives $\pi^a_{\ c}\bar{H}^c_{\ d}\pi^d_{\ b}\phi^b = E\phi^a$. Taking the complex conjugate, we obtain $\pi^a_{\ c}H^c_{\ d}\pi^d_{\ b}\bar{\phi}^b = \bar{E}\bar{\phi}^a$. We then multiply on the left by the parity operator:

$$H^a_{\ b}\pi^b_{\ c}\bar{\phi}^c = \bar{E}\pi^a_{\ b}\bar{\phi}^b. \tag{24}$$

Thus, if ϕ^a is an energy eigenstate with eigenvalue E, then the state defined by $\pi^a_{\ b}\bar{\phi}^b$ is another energy eigenstate with eigenvalue $\bar{E}$. If, in addition, the energy eigenstate ϕ^a is a simultaneous eigenstate of the $\mathscr{P}\mathscr{T}$ operator, then $\pi^a_{\ b}\bar{\phi}^b = \lambda\phi^a$, where λ is a pure phase. Substituting this into (24) and subtracting the result from (23) gives $\bar{E} = E$. This establishes Proposition 4. □

If an energy eigenstate ϕ^a_i is not a simultaneous eigenstate of $\mathscr{P}\mathscr{T}$, we say that $\mathscr{P}\mathscr{T}$ symmetry is broken. In this case the nonreal eigenvalues E_i form complex conjugate pairs. If the $\mathscr{P}\mathscr{T}$ symmetry is unbroken so that $\{\phi^a_i\}$ are eigenstates of $\mathscr{P}\mathscr{T}$, the corresponding energy eigenvalues are real. Proposition 5 gives a sufficient (but not necessary) condition for the orthogonality of the eigenstates.

Proposition 5 *If the eigenstates $\{\phi^a_i\}$ of a $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian $H^a_{\ b}$ are also eigenstates of $\mathscr{P}\mathscr{T}$, then a sufficient condition for orthogonality of the eigenstates with respect to $\mathscr{P}\mathscr{T}$ inner-product is that the quadratic form $H_{ab} = g_{ac}H^c_{\ b}$ be symmetric.*

Proof Consider for $i \neq j$ a pair of eigenvalue equations $H^a_{\ b}\phi^b_i = E_i\phi^a_i$ and $H^a_{\ b}\phi^b_j = E_j\phi^a_j$. Transvect these equations with $\pi_{ac}\bar{\phi}^c_j$ and $\pi_{ac}\bar{\phi}^c_i$ and subtract:

$$\bar{\phi}^c_j\pi_{ca}H^a_{\ b}\phi^b_i - \bar{\phi}^c_i\pi_{ca}H^a_{\ b}\phi^b_j = \pi_{ab}\left(E_i\phi^b_i\bar{\phi}^a_j - E_j\phi^b_j\bar{\phi}^a_i\right). \tag{25}$$

If the energy eigenstates are eigenstates of the $\mathscr{P}\mathscr{T}$ operator so that $\pi^a{}_b\bar{\phi}^b_i = \phi^a_i$, then $\pi_{ab}\bar{\phi}^b_i = g_{ab}\phi^b_i$. Therefore, the left side of (25) becomes $\phi^c_j g_{ca} H^a{}_b \phi^b_i - \phi^c_i g_{ca} H^a{}_b \phi^b_j = H_{cb}\big(\phi^c_j\phi^b_i - \phi^c_i\phi^b_j\big)$, where $H_{cb} = g_{ca}H^a{}_b$. Hence, the condition $H_{cb} = H_{bc}$ ensures that the right side of (25) vanishes. This establishes Proposition 5. □

Note that the symmetric condition on the complex Hamiltonian H_{ab} is sufficient to ensure the orthogonality of the eigenstates, but it is not necessary.

7 Charge-Conjugation Symmetry

We have shown how to formulate quantum mechanics on a Hilbert space endowed with the structure of space-time reflection symmetry. Owing to the property of the parity structure π_{ab}, we noted that the resulting state space is equipped with an indefinite metric having a split signature; half of the states have positive and half have negative $\mathscr{P}\mathscr{T}$ norm.

In standard quantum mechanics the norm is associated with the probabilistic interpretation of the theory. Therefore, the physical interpretation of the inner product defined in (12) is somewhat ambiguous. To remedy this ambiguity, [3] pointed out the existence of a new symmetry associated with Hamiltonians that are $\mathscr{P}\mathscr{T}$ symmetric (see also [4]). By using this symmetry, which has an interpretation similar to that of charge conjugation, it is possible to introduce a new inner product on the vector space $\mathbb{H}_{\mathbb{C}}$ spanned by the eigenstates of $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians such that all the eigenstates have positive-definite norm. With the aid of this symmetry the probabilistic aspects of quantum theory are restored. We refer to this symmetry as charge conjugation in a broad sense, and introduce here briefly the properties of the symmetry associated with the 'charge' operator $C^a{}_b$. We make the following observation.

Proposition 6 *Let $H^a{}_b$ be a $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian operator. If the $\mathscr{P}\mathscr{T}$ symmetry is not broken, the energy eigenvalues are real. Let $\{\phi^a_n\}$ denote a set of normalized eigenstates of $H^a{}_b$. Then, the $\mathscr{P}\mathscr{T}$ inner product between a pair of energy eigenstates is $\langle\phi_m\|\phi_n\rangle = g_{ab}\phi^a_n\phi^b_m$.*

The $\mathscr{P}\mathscr{T}$ inner product between a pair of states is given by $\pi_{ab}\phi^a_n\bar{\phi}^b_m$; then, the above equation follows from Proposition 3, which states that in unbroken $\mathscr{P}\mathscr{T}$ symmetry ϕ^a_n is an eigenstate of the $\mathscr{P}\mathscr{T}$ operator. Thus, we have $\pi_{ab}\phi^a_n\bar{\phi}^b_m = g_{ac}\pi^c{}_b\phi^a_n\bar{\phi}^b_m = g_{ac}\phi^a_n\phi^b_m$. Because the $\mathscr{P}\mathscr{T}$ norm of the energy eigenstates are real, the real part of ϕ^a_n is orthogonal to its imaginary part with respect to g_{ab}.

Next, we normalize energy eigenstates according to $\phi^a_n \to \phi^a_n/\big(g_{ab}\phi^a_n\phi^b_n\big)^{1/2}$ and assume, in what follows, that ϕ^a_n is normalized. Then, according to the discussion of Sect. 4, exactly half of the normalized energy eigenstates have $\mathscr{P}\mathscr{T}$ norm $+1$, and the remaining half have $\mathscr{P}\mathscr{T}$ norm -1. We order the levels so that

$$g_{ab}\phi^a_m\phi^b_n = (-1)^n\delta_{nm}. \tag{26}$$

With these conventions, we define the charge conjugation operator $C^a_{\ b}$. First, $C^a_{\ b}$ is $\mathscr{P}\mathscr{T}$-symmetric; thus, there exists a positive Hermitian form L_{ab} satisfying $\bar{L}_{ab} = L_{ba}$ such that $C^a_{\ b} = \pi^{ac}L_{bc}$. Second, $C^a_{\ b}$ commutes with the Hamiltonian $H^a_{\ b}$, so the eigenstates $\{\phi^a_n\}$ of $H^a_{\ b}$ are simultaneous eigenstates of $C^a_{\ b}$. Third, the eigenvalues of $C^a_{\ b}$ are given by $C^a_{\ b}\phi^b_n = (-1)^n\phi^a_n$, where ϕ^a_n satisfies (26). Thus, $C^a_{\ b}$ commutes with the Hamiltonian $H^a_{\ b}$ and its eigenvalues are precisely the $\mathscr{P}\mathscr{T}$ norm of the corresponding eigenstates. Hence, $C^a_{\ b}$ is involutary, $C^a_{\ b}C^b_{\ c} = \delta^a_{\ c}$, and trace-free, so $C^a_{\ a} = 0$. In the infinite-dimensional context, $\mathscr{C}$ has a position-space representation [3, 4] $\mathscr{C} = \sum_n \phi_n(x)\phi_n(y)$, which is similar to the position-space representation for the parity operator $\mathscr{P} = \sum_n (-1)^n\phi_n(x)\phi_n(-y)$. [Here, $\{\phi_n(x)\}$ are eigenfunctions of the $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian.]

Having defined the operator $C^a_{\ b}$, we introduce on the vector space $\mathbb{H}_{\mathbb{C}}$ the following inner product. If $\xi^a, \eta^a \in \mathbb{H}_{\mathbb{C}}$, their inner product $\langle\xi\,|\eta\rangle$ is defined by

$$\langle\xi\,|\eta\rangle = g_{ac}C^c_{\ b}\pi^b_{\ d}\eta^a\bar{\xi}^d. \tag{27}$$

In particular, $\langle\phi_n|\phi_m\rangle = g_{ac}C^c_{\ b}\pi^b_{\ d}\phi^a_m\bar{\phi}^d_n = g_{ac}C^c_{\ b}\phi^a_m\phi^b_n = (-1)^n g_{ab}\phi^a_m\phi^b_n = \delta_{nm}$. Thus, (27) defines a positive-definite inner product between elements of $\mathbb{H}_{\mathbb{C}}$. Here, to simplify notation, we make no distinction between the Dirac inner product defined in (3) and the inner product (27) with respect to the $\mathscr{C}\mathscr{P}\mathscr{T}$ conjugation. This is because (27) is a natural extension of (3); when the prescribed Hamiltonian is Hermitian, (27) reduces to the conventional Dirac inner product (3). We emphasize that the charge operator $C^a_{\ b}$ introduced here is not the conventional charge-conjugation operator (cf. [25]). In conventional Hermitian quantum theory, the commutation relation between the charge operator $\mathscr{C}$ and the parity operator $\mathscr{P}$ is $\mathscr{C}\mathscr{P} = (-1)^N\mathscr{P}\mathscr{C}$, where N is the Fermion number. Hence, these operators commute for Bosons and anticommute for Fermions. The operators $\mathscr{C}$ and $\mathscr{P}$ in this paper are distinct square roots of the identity operator, and when the Hamiltonian is Hermitian, $\mathscr{C}$ becomes identical to $\mathscr{P}$ so that the $\mathscr{C}\mathscr{P}\mathscr{T}$ invariance condition reduces to the Hermiticity requirement [3].

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Mathematical and Physical Meaning of the Crossings of Energy Levels in $\mathscr{P}\mathscr{T}$-Symmetric Systems

Denis I. Borisov and Miloslav Znojil

Abstract Unavoided crossings of the energy levels due to a variation of a real parameter are studied. It is found that after the quantum system in question passes through one of its energy-crossing points *alias* Kato's exceptional points (EP), its physical interpretation may *dramatically* change even when the crossing energies themselves do not complexify. The anomalous physical phase-transition mechanism of the change is revealed, attributed to the EP-related mathematics and illustrated via several exactly solvable matrix toy models.

1 Introduction

One-parametric quantum Hamiltonians $\tilde{H}(\lambda)$ are most often assumed self-adjoint inside a real interval of $\lambda \in \mathscr{D}_{(physical)}$. This implies that an unavoided crossing of energy levels is either excluded or "incidental", i.e., resulting from a symmetry. The centrally symmetric harmonic oscillator with energies $\tilde{E}_{n,\ell} \sim 4n + 2\ell + 3$ where $n = 0, 1, \ldots$ and $\ell = 0, 1, \ldots$ may be recalled as the best known illustration of the incidental degeneracy due to which one has $\tilde{E}_{n+1,0} = \tilde{E}_{n,2}$, etc.

The exclusion of degeneracy accompanied by the well known tendency of eigenvalues to avoid each other may be illustrated via the following four by four tilded matrix

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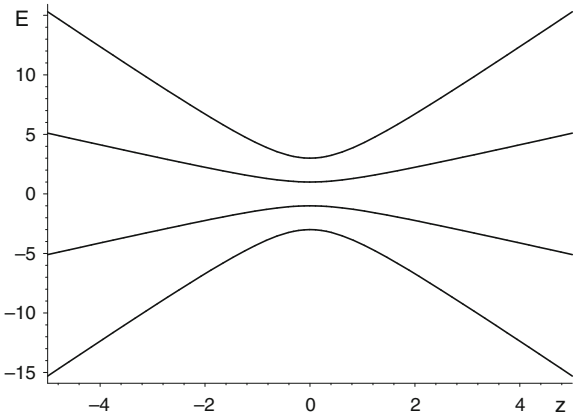

Fig. 1 Repulsion of levels for Hermitian Hamiltonian (1)

$$\tilde{H}^{(4)}(z) = \begin{bmatrix} -3 & \sqrt{3}z & 0 & 0 \\ \sqrt{3}z & -1 & 2z & 0 \\ 0 & 2z & 1 & \sqrt{3}z \\ 0 & 0 & \sqrt{3}z & 3 \end{bmatrix} = \left[\tilde{H}^{(4)}(z)\right]^{\dagger}. \tag{1}$$

This model without incidental symmetries nicely illustrates a "mutual repulsion" of eigenvalues (cf. Fig. 1).

1.1 Crossings of Energies in $\mathscr{P}\mathscr{T}$-Symmetric Models

Incidental energy-level crossings also occur for multiple non-Hermitian Hamiltonians exhibiting parity-times-time-reversal (a.k.a. $\mathscr{P}\mathscr{T}$, i.e., nonlinear) symmetry (cf. review paper [1] or recent papers [2, 3]). One of the simplest illustrations is provided by the generalized radial harmonic oscillator Hamiltonian of [4], i.e., by the non-selfadjoint ordinary differential operator

$$H^{(HO)}(\alpha, c) = -\frac{d^2}{dx^2} + x^2 - 2ic\,x + \frac{\alpha^2 - 1/4}{(x - ic)^2}, \quad x \in (-\infty, \infty) \tag{2}$$

defined in $L^2(\mathbb{R})$ and possessing all of its energy eigenvalues in closed form,

$$E = E_{(n,q)} = 4n + 2 - 2q\alpha + c^2, \quad n = 0, 1, \ldots, \quad q = \pm 1. \tag{3}$$

These quantities are real along the whole real line of α (we may ignore here the role of the inessential second parameter $c \neq 0$). The unavoided energy-level crossings abound. At all of the integer couplings $\alpha = m - n$ they have the form of degeneracies $E_{(m,1)} = E_{(n,-1)}$.

1.2 Exceptional Points

Tentatively, one could conjecture that in the context of crossing of levels the linear and nonlinear symmetries might have played a similar role. A deeper study of solvable models reveals that it is not so. A number of decisive differences emerges. First of all, Hermitian Hamiltonians exhibiting a linear symmetry remain diagonalizable at the crossing point. In our non-Hermitian model (2), in contrast, all of the energy-degeneracy parameters $\alpha = m - n$ are "exceptional points" (EP; the concept was introduced by Kato [5]) at which the Hamiltonian *ceases* to be diagonalizable (see [4] for details). For this reason the model *does not* admit the standard physical probabilistic interpretation at any energy-crossing value of $\alpha = m - n = \alpha^{(EP)}$. In contrast to their Hermitian analogues, operators $H^{(HO)}(\alpha^{(EP)}, c)$ *cannot* consistently describe a quantum system. This means that the physics which is controlled by a parameter may change abruptly at the EP horizon [6].

The argument may further be strengthened when one recalls the finite-dimensional and non-Hermitian $\mathscr{P}\mathscr{T}$-symmetric toy-models of [7]. Their four-by-four sample

$$H^{(4)}(z) = \begin{bmatrix} -3 & \sqrt{3}z & 0 & 0 \\ -\sqrt{3}z & -1 & 2z & 0 \\ 0 & -2z & 1 & \sqrt{3}z \\ 0 & 0 & -\sqrt{3}z & 3 \end{bmatrix} \neq \left[H^{(4)}(z)\right]^{\dagger} \tag{4}$$

differs from (1) just by the inversion of the signs in the lower diagonal. The new model is also solvable yielding equidistant spectrum $E_n(z) = d_n\sqrt{1-z^2}$ with coefficients $d_0 = -3$, $d_1 = -1$, $d_2 = 1$ and $d_3 = 3$. These energies are only real for $|z| \leq 1$ (cf. Fig. 2). The two points $z_{coll.} = \pm 1$ of the collision of the eigenvalues become exceptional in the sense of Kato, $z_{coll.} = z^{(EP)}$. At these parameters the eigenvectors cease to form a complete basis. This means that also mathematics changes abruptly at the EP horizon.

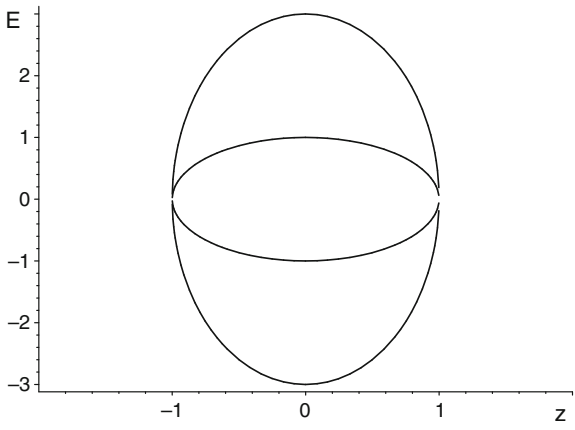

Fig. 2 Attraction of levels for non-Hermitian Hamiltonian (4)

One of the most characteristic generic features of finite-dimensional non-Hermitian Hamiltonians exhibiting $\mathscr{P}\mathscr{T}$ symmetry lies in an effective *attraction* between eigenvalues. For model (4), in particular, the four half-hyperbolas of Fig. 1 become replaced by four half-ellipses of Fig. 2 (matched in two ellipses). The whole spectrum is complex at all $z < -1$ and $z > 1$. A priori, no space seems left for a real crossing of the levels. Other toy models must be sought.

2 Ad Hoc Physical Hilbert Spaces

Our forthcoming considerations will be motivated by all of the latter observations. We feel addressed by the apparent lack of suitable (i.e., preferably, non-numerical) N by N matrix examples which would exhibit an unavoided energy-level crossing phenomenon (without complexifications) and which would admit a consistent probabilistic quantum-mechanical interpretation, i.e., an explicit construction of some standard physical Hilbert space $\mathscr{H}^{(S)}$ of quantum states. Our interest in models with $N < \infty$ was also co-evoked by the technical complexity of the latter task in the case of $N = \infty$ [8–10].

2.1 The Concept of Metric Operator Θ

A given diagonalizable Hamiltonian with real spectrum may be found non-Hermitian when considered in an unphysical Hilbert space $\mathscr{H}^{(F)}$. In the notation of [11] the superscript stands here for *both* "false" and "favored" *alias* "friendly". The most straightforward amendment of the situation may be mediated by the replacement of the unphysical Hilbert space by a physical one, $\mathscr{H}^{(F)} \to \mathscr{H}^{(S)}$. This replacement is being realized by the mere change of the inner product,

$$\langle\psi_1|\psi_2\rangle^{(F)} \ \to \ \langle\psi_1|\psi_2\rangle^{(S)} = \langle\psi_1|\Theta|\psi_2\rangle^{(F)} \tag{5}$$

where symbol Θ denotes the so called inner-product-metric operator [12].

The main idea of the recipe is that for a given Hamiltonian with real spectrum which appeared non-Hermitian in $\mathscr{H}^{(F)}$ (we will write $H \neq H^\dagger$) we may achieve, via a suitable choice of metric, its Hermiticity in $\mathscr{H}^{(S)}$ (we will define $H^\ddagger = \Theta^{-1}H^\dagger\Theta$ and write $H = H^\ddagger$). The assignment of the Hermitizing metric Θ to a given Hamiltonian H is not unique [12]. This ambiguity may play the role of a new freedom in quantum model-building.

From an opposite perspective, a unique choice of physical metric Θ enables us to decide whether a given candidate for an observable is acceptable (i.e., Hermitian in given $\mathscr{H}^{(S)}$) or not. Any change of the metric would induce the change of the set of the operators of observables, i.e., of the whole physical meaning and interpretation of

the quantum system in question. This idea will form a background of our forthcoming considerations.

2.2 Constructive Specification of Eligible Metrics

The concrete specification and practical use of metric Θ must take into consideration its necessary mathematical properties [12]. Firstly, in a setting valid for all observables, the generator H of the time evolution of wave functions must be Hermitian in $\mathscr{H}^{(S)}$, i.e.,

$$\sum_{k=1}^{N} \left[H_{jk}^{\dagger}\, \Theta_{kn} - \Theta_{jk}\, H_{kn} \right] = 0, \quad j, n = 1, 2, \ldots, N, \quad N = \dim \mathscr{H}^{(F,S)} \leq \infty. \tag{6}$$

Although H may be non-Hermitian in $\mathscr{H}^{(F)}$ (though not necessarily—see [13]), the spectrum must be real in a suitable physical domain $\mathscr{D}$ of a multiplet of parameters $\boldsymbol{\lambda}$. Inside this domain, our preselected Hamiltonian $H = H(\boldsymbol{\lambda})$ must be also diagonalizable [14]. For the sake of non-triviality of our considerations, we shall also assume the non-emptiness of the EP boundary, $\partial\mathscr{D} \neq \emptyset$.

The spectrum of H is often postulated non-degenerate, discrete and bounded from below. This is a technical condition which may easily be satisfied whenever one works with Hilbert spaces $\mathscr{H}^{(F)}$ of a finite dimension $N < \infty$. In such a case one may construct the (complete) set of N eigenstates $|\Xi_j\rangle$ of the F-space-conjugate operator $H^{\dagger}(\boldsymbol{\lambda})$,

$$H^{\dagger}\, |\Xi_n\rangle = E_n\, |\Xi_n\rangle, \quad n = 0, 1, \ldots, N-1. \tag{7}$$

Following [15], we finally define the general metric as the following sum

$$\Theta = \Theta(H, \boldsymbol{\kappa}) = \sum_{j=0}^{N-1} |\Xi_j\rangle\, \kappa_n\, \langle \Xi_j|. \tag{8}$$

The practically unrestricted variability of the optional parameters $\kappa_j > 0$ represents just the well known degree of freedom of the theory.

2.3 $N = 2$ Illustration

In a two-by-two-matrix illustration using real Hilbert space $\mathscr{H}^{(F)} = \mathbb{R}^2$, the Hamiltonian-simulating matrix

$$H = H^{(2)}(\lambda) = \begin{pmatrix} 0 & 1 \\ 1+\lambda & 0 \end{pmatrix}, \quad \lambda > -1 \tag{9}$$

is exclusively Hermitian at $\lambda = 0$ but it possesses manifestly real and non-degenerate eigenvalues $E_\pm = \pm\sqrt{1+\lambda}$ at any $\lambda > -1$. We may recall (8) and define the general metric

$$\Theta = \Theta^{(S)}(\lambda, b) = \begin{pmatrix} 1+\lambda & b \\ b & 1 \end{pmatrix}, \quad -\sqrt{1+\lambda} < b < \sqrt{1+\lambda} \tag{10}$$

with two positive eigenvalues $\theta_\pm = 1 + \lambda/2 \pm \sqrt{b^2 + \lambda^2/4}$. This enables us to declare *the same* Hamiltonian matrix (9) Hermitian in *all* Hilbert spaces $\mathscr{H}^{(S)}$ numbered by parameter b.

3 Four-State Non-Hermitian Toy Model

Practical applications of nontrivial metrics Θ suffer from a scarcity of their supply [16]. Up to rare exceptions [17] a restriction of attention to *finite* Hilbert-space dimensions $N < \infty$ seems necessary. In a search for insight, the use of the smallest Ns admitting non-numerical results seems particularly rewarding. Let us start, therefore, from the choice of $N = 4$.

3.1 Energies

Illustrative Hamiltonian (4) was designed as an example in which the spontaneous breakdown of $\mathscr{PT}$-symmetry proceeds exclusively via complexifications of the energies [7]. Such a model would be unsuitable for our present purposes. Fortunately, in the light of our more recent methodical studies [3, 18] it appeared that many methodical advantages of the family of N by N models of [7] (like the reality of spectrum or its non-numerical tractability) may be shared by simpler, albeit more-parametric models in which the main diagonal is allowed to vanish. After we picked up the first nontrivial two-parametric element

$$H = H^{(4)}(\alpha, \beta) = \begin{bmatrix} 0 & -1+\beta & 0 & 0 \\ -1-\beta & 0 & -1+\alpha & 0 \\ 0 & -1-\alpha & 0 & -1+\beta \\ 0 & 0 & -1-\beta & 0 \end{bmatrix} \tag{11}$$

of this family (cf. [18]), we discovered that it may offer the service.

The potentially observable bound-state energies of model (11) coincide with the four real roots of secular equation

$$E^4 + \left(\alpha^2 - 3 + 2\,\beta^2\right) E^2 + 1 - 2\,\beta^2 + \beta^4 = 0. \tag{12}$$

These energies occur in pairs $E_{\pm,\varepsilon} = \pm\sqrt{Z_\varepsilon}$ numbered by $\varepsilon = \pm$ where the symbol Z_ε denotes two easily written roots of a quadratic equation. Inside the closure of the physical parametric domain $\mathscr{D}$ these roots must be non-negative.

From the secular equation one immediately deduces the double degeneracy $E \to 0$ of one of the pairs of the eigenenergies in the limit of $\beta^2 \to 1$. Under this constraint the complete quadruple degeneracy $E_{\pm,\pm} \to 0$ takes place in the second limit of $\alpha^2 \to 1$. Still, the exact knowledge of the energies

$$E_{\pm,\pm} = \pm\tfrac{1}{2}\sqrt{6 - 2\,\alpha^2 - 4\,\beta^2 \pm 2\,\sqrt{\alpha^4 - 6\,\alpha^2 + 4\,\alpha^2\beta^2 + 5 - 4\,\beta^2}}$$

offers more insight than expected.

3.2 A Reparametrization

In terms of new variables $A = 1 - \alpha^2$, $B = 1 - \beta^2$ and $C = A + 4B$ the previous formula becomes more transparent,

$$2\,E_{\pm,\pm} = \pm\sqrt{A + C \pm 2\,\sqrt{AC}} = \pm\sqrt{(\sqrt{A} \pm \sqrt{C})^2} = \pm\sqrt{A} \pm \sqrt{C}. \tag{13}$$

The reparametrization clarifies the root-complexification nature of the lines $A = 0$ and $C = 0$. More precisely, formula (13) indicates that the set of the potentially physical parameters A and B or C yielding the real spectrum of energies is specified by the two elementary inequalities $A \geq 0$ and $C \geq 0$ in the $A - B$ plane (cf. Fig. 3).

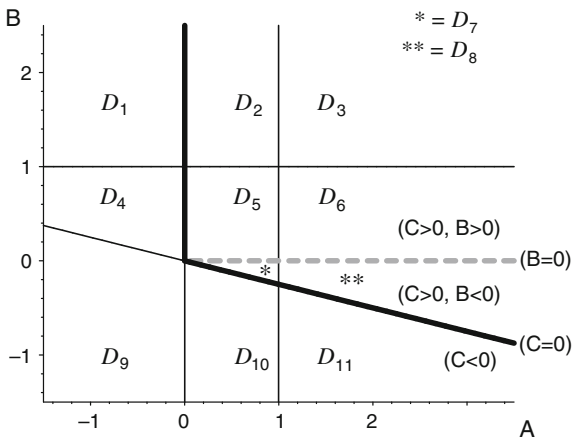

Fig. 3 The $A - B$ plane of reparametrized Hamiltonian (11). After exemption of the *dashed line*, the *points* inside the *thick-line-bounded upper-right* wedge specify the unitary dynamical regime

After a return to the old parameters $\alpha = \sqrt{1-A}$ and $\beta = \sqrt{1-B}$, our new $N = 4$ matrix (11) would cease to be real in the whole $A - B$ plane. This slightly redefines the model. Keeping this in mind let us further recall Fig. 3 and separate the $A - B$ plane of parameters into eleven subdomains while noticing that

- in the usual matrix sense, i.e., inside the most common complex vector space $\mathscr{H}^{(F)} \equiv \mathbb{C}^4$ endowed with trivial metric $\Theta^{(F)} = I$, our (possibly, complex) Hamiltonian (11) is manifestly Hermitian just in the single subdomain $\mathscr{D}_3$;
- our four by four Hamiltonian is a real matrix with real spectrum just in the two simply connected subdomains of parameters $\mathscr{D}_5$ and $\mathscr{D}_7$;
- the spectrum is real inside the closure of the union $\overline{\mathscr{D}_2 \cup \mathscr{D}_3 \cup \mathscr{D}_5 \cup \mathscr{D}_6 \cup \mathscr{D}_7 \cup \mathscr{D}_8}$ of six subdomains.

In Fig. 3 the two thick EP half-lines with $A = 0$ and $C \geq 0$ or with $C = 0$ and $A \geq 0$ play the role of the boundaries of stability of the system (let us call them "quantum horizons of the first kind"). Beyond these horizons the energies complexify and cease to be observable.

The most elementary illustration of this most common form of quantum phase transition is provided by Fig. 4 where we varied parameter A along a line connecting the unphysical subdomain $\mathscr{D}_4$ with its most conventional physical neighbor $\mathscr{D}_5$. Once we choose a nonvanishing second parameter $B = 1/50$ we obtained a generic picture in which the two separate degenerate energies are unfolding in parallel.

With the decrease of $B > 0$ the degenerate energies get closer to each other. In the limit one arrives at an exceptional, double-degeneracy scenario with $A = B = 0$. The spectrum in the vicinity is sampled in Fig. 5. One moves there along the path with $B = A$ so that the system passes through the origin in a way connecting the physical region $\mathscr{D}_5$ with the twice-forbidden unphysical subdomain $\mathscr{D}_9$. Obviously, one could now reinterpret a return to the pattern of Fig. 4 as a consequence of perturbation due to which the upper and lower doublets get decoupled.

The $B = A$ pass is anomalous because inside the twice-forbidden subdomain $\mathscr{D}_9$ the model happens to have a purely imaginary spectrum. As long as this means that

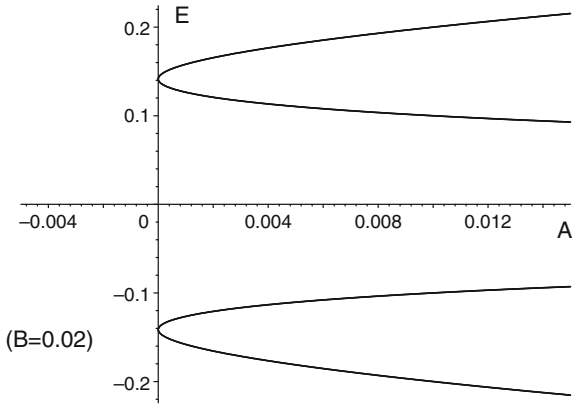

Fig. 4 The spectrum in the vicinity of the $A = 0$ horizon of the first kind

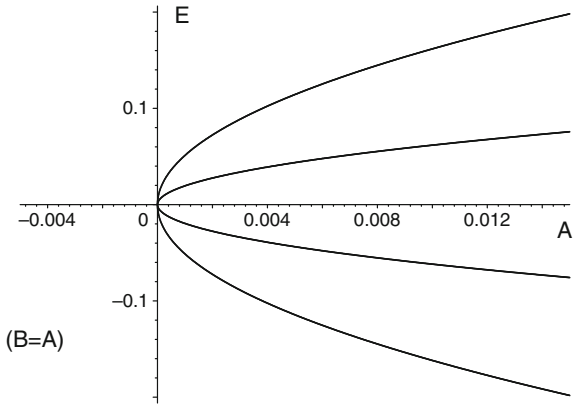

Fig. 5 The confluent-EP scenario at $B = A$

Im $(\mathrm{i}\, E_n) = 0$, one could obtain a potentially measurable spectrum also in subdomain $\mathscr{D}_9$, using simply a premultiplied form $\hat{H} = \mathrm{i}\, H^{(4)}(\alpha, \beta)$ of an after-transition candidate for one of possible physical Hamiltonians in $\mathscr{D}_9$.

4 New Physics Behind the Unavoided Level Crossings

Admitting, in Fig. 3, a further decrease of B below zero while keeping $A \geq 0$ we enter another dynamical regime which opens the possibility of the $C = 0$ EP phase transitions of the first kind. During them one moves, typically, from the physical subdomain $\mathscr{D}_7$ to its unphysical neighbor $\mathscr{D}_{10}$. The parameter-dependence of the spectrum as well as its complexification pattern will be analogous to the ones displayed in Fig. 4.

Along both of the thick EP lines of Fig. 3 the phase transitions between the complex and real spectrum are qualitatively the same (i.e., in our terminology, of the first kind). In both of these cases the degeneracy of a pair of energies at the EP singularity is followed by its subsequent unfolding into unobservable complex eigenvalues. This mechanism is widely known as the so called spontaneous breakdown of $\mathscr{PT}$ symmetry (see also its numerous exactly solvable models in [19]).

What remains unclarified is the physical nature of the other, alternative parameter-changing processes during which a pair of energies would pass through the remaining, dashed $B = 0$ EP line of Fig. 3 *without* getting complexified. We intend to show now that after one crosses such an EP horizon there will emerge good reasons for speaking about an anomalous phase transition "of the second kind".

4.1 The Menu of Metrics

In the light of formula (8) the metric ceases to be positive definite at any EP parameter. Keeping in mind Fig. 3 we may conclude that no positive definite metric Θ can exist

at $A \leq 0$, at $C \leq 0$ and at $B = 0$. Temporarily, let us assume that $A > 0$, $C > 0$ and $B \neq 0$, therefore.

Once we insert Hamiltonian (11) in the implicit linear algebraic definition (6) of the real, symmetric and positive definite metric matrix Θ, we obtain an overdetermined set of 16 equations for 10 unknown matrix elements. As long as formula (8) indicates that there are strictly four free real parameters in the family of solutions, let us pick up the quadruplet of elements $\Theta_{1\,j} = t_j$ with $j = 1, 2, 3, 4$ as free parameters. Next, let us solve the system by the standard elimination technique yielding

$$\Theta_{22} = -\frac{-t_1 + t_1\,\beta - t_3 - t_3\,\alpha}{1+\beta}, \quad \Theta_{23} = \frac{t_2 - t_2\,\alpha + t_4 + t_4\,\beta}{1+\beta}, \quad \Theta_{24} = -\frac{t_3\,(-1+\beta)}{1+\beta}$$

in the second row of the matrix,

$$\Theta_{33} = \frac{t_1 - t_1\,\alpha - t_1\,\beta + t_1\,\beta\alpha + t_3 - t_3\,\alpha^2}{1+\beta+\alpha+\alpha\beta} = \frac{(-t_1 + t_1\,\beta - t_3 - t_3\,\alpha)\,(-1+\alpha)}{(1+\beta)\,(1+\alpha)},$$

$$\Theta_{34} = \frac{t_2\,(1-\alpha-\beta+\alpha\beta)}{1+\beta+\alpha+\alpha\beta} = \frac{t_2\,(-1+\alpha)\,(-1+\beta)}{(1+\beta)\,(1+\alpha)}$$

in the third row and

$$\Theta_{44} = -\frac{t_1\,\left(\alpha\beta^2 - \beta^2 + 2\,\beta - 2\,\alpha\beta + \alpha - 1\right)}{\beta^2 + \alpha\beta^2 + 2\,\beta + 2\,\alpha\beta + 1 + \alpha} = -\frac{t_1\,(-1+\beta)^2\,(-1+\alpha)}{(1+\beta)^2\,(1+\alpha)}$$

in the fourth row of the metric. An exhaustive, general and complete solution is obtained. It would be too space-consuming to display the whole matrix of the eligible metrics in print. Still, its display element by element enables us to discuss some of the most important consequences.

4.2 EP Horizon of the Second Kind

The insertion of $B = 0$ *alias* $\beta = 1$ reduces our Hamiltonian (11) to one-parametric matrix

$$H = H^{(4)}(\alpha, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ -2 & 0 & -1+\alpha & 0 \\ 0 & -1-\alpha & 0 & 0 \\ 0 & 0 & -2 & 0 \end{bmatrix}. \tag{14}$$

One can easily prove that such a matrix possesses two vanishing eigenvalues $E = 0$ but just a single related eigenvector. This means that matrix (14) is non-diagonalizable and that the $B = 0$ line is all composed of exceptional points. The Jordan-block canonical structure of the $B = 0$ Hamiltonian cannot be Hermitized by any metric Θ. Two of the eigenvectors $|\Xi_j\rangle$ in formula (8) coincide in the limit $B \to 0$ so that in

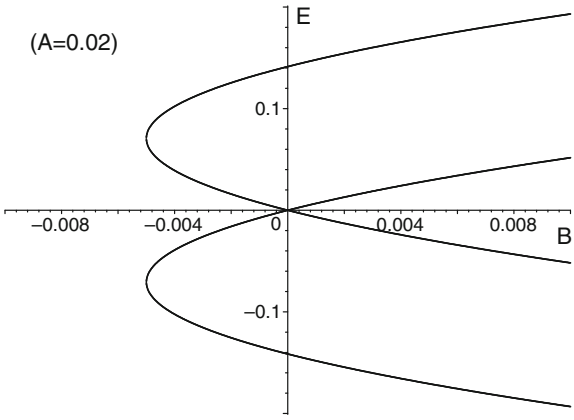

Fig. 6 The unavoided level crossing at $B = 0$ for $A = 1/50$

the same limit, one of the eigenvalues of Θ goes to zero. All of the metric-candidates of the concrete form (8) become non-invertible at $B = 0$.

The B-dependence of the energy levels is such that two of them merge at $B = 0$. In the vicinity of the $B = 0$ singularity (i.e., in our present terminology, along the EP horizon of the second kind) one observes the unavoided level crossing, the concrete form of which is illustrated in Fig. 6. The picture may be complemented by the closed-form construction of the bound-state solutions starting from the small-perturbation version

$$H = H^{(4)}(\alpha, 1-\gamma) = \begin{bmatrix} 0 & -\gamma & 0 & 0 \\ -2+\gamma & 0 & -1+\alpha & 0 \\ 0 & -1-\alpha & 0 & -\gamma \\ 0 & 0 & -2+\gamma & 0 \end{bmatrix}$$

of the original Hamiltonian. A small shift γ in $\beta = 1 - \gamma$ yields an equally small value of $B = 2\gamma + \mathcal{O}(\gamma^2)$ of both signs. The resulting closed form of the pair of the almost-vanishing eigenvalues reads

$$\pm 2E_{\pm,-} = \sqrt{2 - 2\alpha^2 + 8\gamma - 4\gamma^2 - 2\sqrt{\alpha^4 - 8\alpha^2\gamma + 4\alpha^2\gamma^2 - 2\alpha^2 - 4\gamma^2 + 8\gamma + 1}}. \tag{15}$$

One quickly arrives at the required perturbation-expansion description of the crossing phenomenon in the language of Taylor series

$$E_{\pm,-} \approx \pm\left(2 + \alpha^2 + 3/4\,\alpha^4 + \cdots\right)\gamma \mp \left(5 + 13/2\,\alpha^2 + \cdots\right)\gamma^2 \pm \cdots .$$

The change of the sign of the auxiliary small parameter γ may be perceived as a transition between the potentially physical real-spectrum domain $\mathscr{D}_5$ and another, equally acceptable real-spectrum domain $\mathscr{D}_7$.

4.3 Phase Transition of the Second Kind

During the above-mentioned transition, the only suspicious point is $B = 0$ at which the metric ceases to exist. Hence, we have to analyze the B-dependence of the metric near the EP singularity at $B = 0$ in a more explicit representation. Most efficiently, such a task may be simplified when we accept the specific choice of $t_2 = t_3 = t_4 = 0$. Under a symmetrized overall normalization choice of $t_1 \neq 0$ this makes our metric strictly diagonal, with elements

$$\Theta_{11} = \frac{(1+\alpha)\,(1+\beta)}{1-\beta}, \quad \Theta_{22} = 1+\alpha, \quad \Theta_{33} = 1-\alpha, \quad \Theta_{44} = \frac{(1-\alpha)\,(1-\beta)}{1+\beta}.$$

Inside the physical subdomain $\mathscr{D}_5$ of Fig. 3 our diagonal metric is positive definite for all of the real parameters such that $|\alpha| < 1$ and $|\beta| < 1$. Below the EP line $B = 0$ our metric ceases to be positive definite.

As long as we stay inside the physical domain giving real energies (viz., inside subdomain $\mathscr{D}_7$ of Fig. 3) we may put $\beta = 1 + \delta^2$ (where δ is small but real) and check the statement. It gets verified: our diagonal matrix Θ loses the status of metric and becomes converted into the mere indefinite diagonal pseudometric $\mathscr{P}$ which possesses two negative elements and/or eigenvalues,

$$\mathscr{P}_{11} = -\frac{(1+\alpha)\left(2+\delta^2\right)}{\delta^2}, \quad \mathscr{P}_{22} = 1+\alpha, \quad \mathscr{P}_{33} = 1-\alpha, \quad \mathscr{P}_{44} = -\delta^2\,\frac{1-\alpha}{2+\delta^2}.$$

Below the EP line $B = 0$, *any* correct physical metric must necessarily be non-diagonal. The *physics* of the quantum system in question will be *different* in the neighboring physical subdomains $\mathscr{D}_5$ and $\mathscr{D}_7$. The energies remain observable but the set of the admissible operators of observables for parameters inside $\mathscr{D}_5$ will necessarily be different from the set of the operators of observables for parameters which crossed the $B = 0$ line and belong to $\mathscr{D}_7$.

Such a change of physics at $B = 0$ is not as drastic as the truly catastrophic loss of the reality of the energies at the horizons $A = 0$ or $C = 0$. Still, one must speak about phase transition. We propose to call such a change the phase transition of the second kind.

5 Level Crossings Beyond $N = 4$

When addressing conceptual matters we made an ample use, up to now, of the elementary nature of the toy-model secular (12) at $N = 4$. At a few higher matrix dimensions N the determination of the EP horizons is more complicated but still non-numerical. The methods were described in [20] where, for a not too dissimilar class of matrix models, these methods were shown effective up to $N = 11$.

5.1 The Family of Models

The pass of a quantum observable (typically, of Hamiltonian $H(\lambda)$) through a Kato's exceptional point $\lambda^{(EP)}$ leads, typically, to a quantum catastrophe during which certain eigenvalues collide and, subsequently, complexify. The observability status of Hamiltonian $H(\lambda)$ is lost and the critical value of $\lambda = \lambda^{(EP)}$ may be perceived as a point on horizon of quantum stability. In the alternative, eigenvalue-crossing scenario without complexification we reminded the readers that one has to distinguish between the non-EP degeneracy (typical for Hermitian models) and an anomalous, EP-caused degeneracy. In this general theoretical setting [3] we revealed that one may encounter a loss of the system's observability implying a subtler form of the quantum phase transition.

Via the solvable $N = 4$ example we discovered that the mechanism of the anomalous transition is based on the loss of the positivity of the metric at the EP singularity. The Hilbert space (i.e., its inner product, i.e., the set of the eligible operators of observales) changed. Beyond the eigenvalue-collision at $\lambda = \lambda^{(EP)}$ the physical contents of the theory may be entirely different even if the energy spectrum itself stays real.

Whenever the matrix dimensions get too large, the proofs become more and more numerical even when we keep working with the most elementary tridiagonal and finite-dimensional quasi-real matrix Hamiltonians of [18],

$$H^{(N)}(\lambda,\mu,\ldots)=\begin{pmatrix} 2 & -1+\lambda & 0 & \ldots & & \ldots & 0 \\ -1-\lambda & 2 & -1+\mu & 0 & \ldots & & \vdots \\ 0 & -1-\mu & 2 & -1+\nu & 0 & \ldots & \\ \vdots & 0 & -1-\nu & 2 & \ddots & \ddots & \vdots \\ & & \ddots & \ddots & \ddots & -1+\mu & 0 \\ \vdots & & & \ddots & -1-\mu & 2 & -1+\lambda \\ 0 & \ldots & \ldots & 0 & 0 & -1-\lambda & 2 \end{pmatrix}. \tag{16}$$

The kinematics may be perceived as represented by the discrete Laplacean $T = H^{(N)}(0, 0, \ldots)$. The information about the dynamics is carried by the set of $N/2$ couplings.

Our preliminary numerical experiments with the $N > 4$ models of the above class proved encouraging, providing a few new qualitative insights (cf. the next subsection). On the abstract level it was useful that the interaction $V = H - T$ itself was kept minimally non-local and antisymmetric. The choice was further restricted to the matrices which were required $\mathscr{P}\mathscr{T}$-symmetric with respect to the most elementary antidiagonal N by N parity-simulating matrix

$$\mathscr{P} = \mathscr{P}^{(N)} = \begin{bmatrix} 0 & 0 & \dots & 0 & 1 \\ 0 & \dots & 0 & 1 & 0 \\ \vdots & \iddots & \iddots & \iddots & \vdots \\ 0 & 1 & 0 & \dots & 0 \\ 1 & 0 & \dots & 0 & 0 \end{bmatrix} \tag{17}$$

in combination with the time-reversal-simulating antilinear operator $\mathscr{T}$ of matrix transposition.

5.2 Non-Hermitian Quantum Lattice with $N = 6$

The study of the three-parametric $N = 6$ model

$$H = H^{(6)}(\alpha, \beta \cdot \gamma) = \begin{bmatrix} 0 & -1+\gamma & 0 & 0 & 0 & 0 \\ -1-\gamma & 0 & -1+\beta & 0 & 0 & 0 \\ 0 & -1-\beta & 0 & -1+\alpha & 0 & 0 \\ 0 & 0 & -1-\alpha & 0 & -1+\beta & 0 \\ 0 & 0 & 0 & -1-\beta & 0 & -1+\gamma \\ 0 & 0 & 0 & 0 & -1-\gamma & 0 \end{bmatrix} \tag{18}$$

provides an insight into the pattern of possible generalizations. Reparametrizations $A = 1 - \alpha^2$, $G = 1 - \beta^2$ and $B = 1 - \gamma^2$ enable us to establish a connection between the $N = 4$ and $N = 6$ spectra.

- in the "innermost coupling" dynamical regime we find the same no-intersection pattern both in Fig. 4 (where $N = 4$) and in Fig. 7 (where $N = 6$); the same form of the phase transition of the first kind may be expected to survive at all of the higher dimensions $N < \infty$;

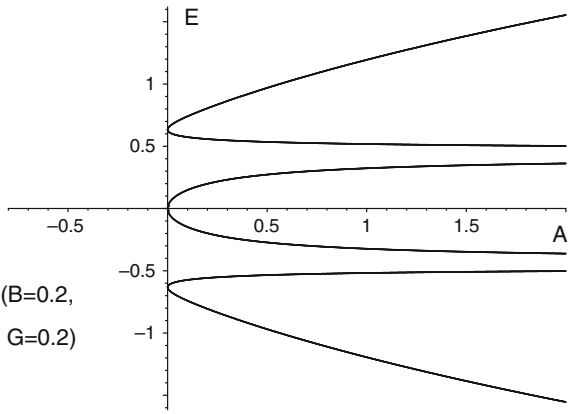

Fig. 7 The $N = 6$ spectrum near the $A = 0$ horizon of the first kind

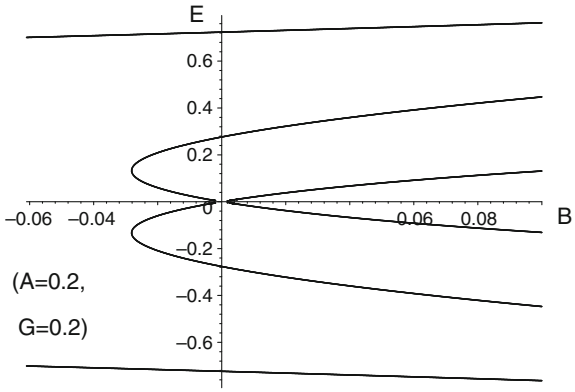

Fig. 8 The unavoided inner-level crossing at $B = 0$ for $N = 6$

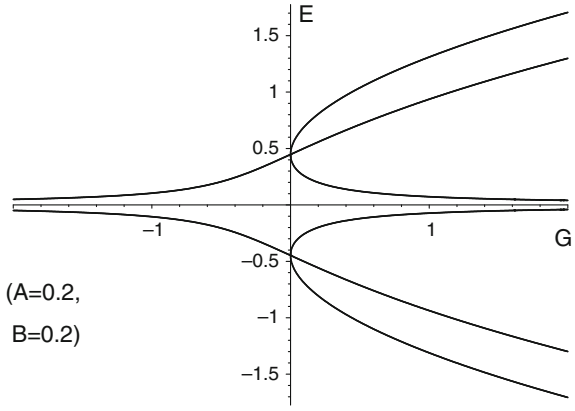

Fig. 9 The $N = 6$ spectrum near the $B = 0$ horizon of the first kind

- in the opposite, "outermost coupling" dynamical regime the inner-level-crossing pattern (which characterizes the phase transition of the second kind) emerges both in Fig. 6 (with $N = 4$) and in Fig. 8 (with $N = 6$); a very similar pattern may be expected at all $N > 6$;
- in the newly emerging "intermediate-coupling" dynamical regime the phase transition of the first kind is expected; in the first nontrivial $N = 6$ example of Fig. 9 the $G = 0$ EP mergers only involve two pairs of levels while the reality of the remaining spectrum is not destroyed. This or similar pattern is also expected to occur at $N > 6$.

6 Conclusions

Let us summarize that in applications of quantum theory the specification of the physical domain $\mathscr{D}$ of parameters may be understood in two ways. A parameter may vary in Hamiltonian $H = H(\lambda)$ itself (*plus*, naturally, in the related physical

Hilbert-space metric) *or* solely in the physical Hilbert space metric (remember that the choice of the Hamiltonian-Hermitizing metric $\Theta = \Theta(\lambda, \kappa)$ is not unique in general [12]).

In the former case people often assume that the pass of the quantum system in question through the EP boundary $\partial\mathscr{D}$ leads to the complexification of some energies so that the unitarity of the evolution is inadvertently lost. In our present paper we considered the second possibility in which the pass through the EP boundary *does not destroy* the reality of the energies.

We imagined that in such a case one must ask the following natural question: "Does this imply that the unitarity of the evolution is preserved?" A nontriviality of this question lies in the fact that after the pass through EP, the very definition of the norm of the wave functions may change.

By means of a constructive analysis of a few solvable models we managed to demonstrate that in some cases when boundary merely separates two disjoint physical subdomains $\mathscr{D}_{\pm}$ the change of the definition of the norm of the wave functions is unavoidable. The value of the norm of a given wave function performs, in general, a jump when crossing such an EP horizon $\partial\mathscr{D}$ of the second kind. In such a dynamical scenario it is necessary to speak about a phase transition of the second kind.

We described the mechanism in more detail. Keeping in mind the popularity of the phase transition of the first kind (during which the change of the metric is accompanied by the necessary change of the effective Hamiltonian) we emphasized the contrast. We introduced the concept of the phase transition of the second kind during which the change of the metric is *not* accompanied by *any* change of the effective Hamiltonian. Subsequently we emphasized that the change of the physics is subtler, mediated merely by the change of the physical Hilbert space, with all of its well known consequences for non-Hamiltonian observables.

In the related literature one often finds the phase transition of the first kind interpreted as a symptom of a spontaneous breakdown of the $\mathscr{P}\mathscr{T}$ symmetry of the system [1]. Via our illustrative examples we demonstrated that the spontaneous breakdown of the $\mathscr{P}\mathscr{T}$ symmetry is not necessary for the existence of quantum phase transition. A "no-complexification" dynamical scenario may exist during which the phase transition does not require any *lasting* loss of $\mathscr{P}\mathscr{T}$ symmetry.

The possibility seems anomalous because after the system passes through the singularity $\lambda^{(EP)}$, the Hamiltonian survives without any changes. The most amazing consequence of the phase transition of the second kind may be seen in the loss of the observability status of multiple operators of observables. The crypto-Hermiticity of many of them will only hold before or after the transition. In any case, the occurrence of the phase transition of *both* kinds will change the physics thoroughly.

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Non-unitary Evolution of Quantum Logics

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Abstract In this work we present a dynamical approach to quantum logics. By changing the standard formalism of quantum mechanics to allow non-Hermitian operators as generators of time evolution, we address the question of how can logics evolve in time. In this way, we describe formally how a non-Boolean algebra may become a Boolean one under certain conditions. We present some simple models which illustrate this transition and develop a new quantum logical formalism based in complex spectral resolutions, a notion that we introduce in order to cope with the temporal aspect of the logical structure of quantum theory.

1 Introduction

Non-Hermitian Hamiltonians [1] find many applications in diverse areas of physics such as for example, optics [2, 3], solid state physics [4], decoherence [5], the quantum to classical limit, and final equilibrium [6]. Decoherence and relaxation times can be defined using non-unitary evolutions, pole theory, and non-Hermitic Hamiltonians [6, 15]. In this work we study the logical properties of quantum systems under the evolution given by a Non-Hermitian Hamiltonian, in order to provide a quantum logical description of the classical limit.

The rigorous formulation of quantum mechanics was achieved after a series of papers by von Neumann, Jordan, Hilbert and Nordheim [16]. Projection operators play a key role in the axiomatization, and this is related to the spectral decomposition

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theorem [17, 18] , which associates a projection valued measure to any quantum observable represented by a self adjoint operator [19]. The set of projection operators can be endowed with an orthomodular (non-Boolean) lattice structure [20, 22] and was named quantum logic [21], in contrast with the distributive structure of classical propositional systems [23]. This approach allows to compare quantum and classical systems by putting them in a common mathematical framework [24]. The quantum logical approach can be also used to provide a solid axiomatic foundation for quantum mechanics, and to explain in an operational way many of important features of the Hilbert space formalism [24, 28]. *But it turns out that the quantum-logical approach has not addressed, up to now, the wholly important problem of characterizing the dynamical transformation in the logic of a system undergoing a decoherence process* [29] *and the reaching of the classical limit*. As was shown in [31], the study of the classical limit offers the possibility of describing the transition from the quantum logic of a quantum system to the Boolean logic characteristic of a classical one. We will continue this line of research in this work by using non-Hermitian time evolutions.

In the standard approach to decoherence [29, 32], the classical limit is reached by the effect of the interaction between the environment and the system. An important model is that of a quantum system interacting with a heat bath of harmonic oscillators. In certain cases, the study of these examples gives rise to quantum Langevin equations (see for example [30]). But there exists an alternative approach, which allows for the possibility of studying the classical limit in terms of the evolution of mean values of relevant sets of observables [34, 41]. According to this framework, it is possible to make an analytical continuation on the energy variable into the lower complex half-plane for any possible Hamiltonian of the system. In general, poles will be found [5, 42], and they can be used to define all possible non-unitary decaying modes with their respective characteristic decaying times, which are proportional to the inverse of the imaginary part of the poles.[1] Poles are complex eigenvalues of the non-Hermitian Hamiltonian H_{eff} which governs the time evolution of the system. Using these characteristic times it is possible to deduce the relaxation time, which turns out to be the inverse of the imaginary part of the pole which lies closest to the real axis. Therefore, it is the largest characteristic time. It is also possible to compute the decoherence time, which turns out to be a function of the imaginary part of the poles and the initial conditions of the system.

The complete description of a quantum system involves non-commutative operators: in the standard approach to quantum mechanics, these are generated by the set of bounded operators $\mathscr{B}(\mathscr{H})$ on a Hilbert space $\mathscr{H}$ [17, 23]. As a consequence, the lattice of quantum properties will be non-distributive [23, 43]. On the other hand, for classical systems, observables are represented by functions over phase space and form a commutative algebra; thus, classical properties are distributive [20, 23]. According to recent works [45, 46], there are certain quantum systems such that,

[1] We do not consider the Khalfin mode since it has an extremely long decaying time [47, 48].

while initially the commutator between two operators can be different from zero, it may tend to zero under the action of certain time evolution operators. In other words, non-Boolean lattices can become Boolean under the action of special time evolutions. On the basis of this observation, in this work, we study the impact of a non unitary evolution on the logical structure of the system by continuing previous works [31]. That is, we study how the logical structure of quantum properties corresponding to relevant observables, becomes essentially Boolean by using an algebraic approach [17].

The paper is organized as follows. In Sect. 2 we review the standard quantum logical formalism. In Sect. 3 we review the Schrödinger and Heisenberg pictures in the standard formalism of quantum mechanics and show that they are not suitable for describing a dynamical interpretation of the logical structure. Next, in Sect. 4, we review the non-Hermitian Hamiltonians approach to quantum theory and show how it can be used to describe the dynamic of logics provided that the Heisenberg picture is used. In Sects. 5 and 6 we present concrete examples of this behavior, the first one with only two different characteristic times, and the other with many of them. We summarize the discussion in Sect. 7 and then present a novel formalism for a dynamical quantum logical approach, based on a generalization of the notion of projective valued measure to the field of complex numbers. Finally, in Sect. 8 we present our conclusions.

2 Classical and Quantum Logics

The state of a classical particle S is completely determined by its position $\mathbf{q}$ and momentum $\mathbf{p}$. Thus, the state can be considered as point $(\mathbf{p}, \mathbf{q})$ in phase space $\mathbb{R}^6$. On the other hand, physical observables are represented as functions over phase space. As an example, consider the energy of the particle $E(\mathbf{p}, \mathbf{q})$. If we now consider an empirically verifiable proposition such as "the energy of the system lies in the interval (a, b)", we can represent it as the set of states of the system which make that proposition true. Similarly, any empirically verifiable property O can be naturally represented as a set of points $\mathscr{O}$ in phase space, i.e., $\mathscr{O} \subset \mathbb{R}^6$. This representation allows to determine if a physical system possesses a given physical property or not: the particle possesses a given property if and only the point $(\mathbf{p}, \mathbf{q})$ representing the state of the particle is included in the set representing that property.

With this assignment between properties and subsets of state space, the logical structure of classical properties gets connected with set theoretical operations. In this way, the conjunction "$\wedge$" of two assertions represented as subsets of phase space can be described as a set theoretical intersection "$\cap$"; the disjunction "$\vee$" as a set theoretical union "$\cup$", and the negation "$\neg$" as the set theoretical complement "$(...)^c$". A partial order relation "$\leq$" (understood as a sort of implication) is given by set theoretical inclusion "$\subseteq$". For technical reasons it is reasonable to restrict to measurable sets of phase space (this is strongly connected with the necessity of computing mean values and probabilities of events) [25, 26]. As is well known,

subsets of a given set, endowed with the logical operations described above form a *Boolean algebra* [23]. A distinctive feature of a Boolean algebra is the *distributive law*, which asserts that for any propositions a and b, we have

$$a = (a \wedge b) \vee (a \wedge \neg b) \tag{1}$$

This is just one of the many properties of Boolean logic, and we put it into the spot, because it will allow us to illustrate the differences with the quantum case.

In quantum mechanics the state of a particle is represented by a trace class positive Hermitian operator of trace one, usually called *density matrix*. Pure states can be represented by one dimensional projection operators or equivalently, as density matrices ρ such that $\rho^2 = \rho$ [17]. In order to establish the algebraic structure underlying the logical propositions associated to a quantum system, let us take a deeper look into the formal structure of quantum mechanics. Physical observables are represented mathematically as self adjoint operators acting on a Hilbert space. What allows physicists to make this connection? The answer lies in the spectral theorem [17, 18], which allows to associate to each self adjoint operator A a *projective valued measure* (PVM), defined as a function from the Borel sets into the set of projection operators of the Hilbert space satisfying

$$\begin{aligned} P : B(\mathbb{R}) &\to \mathscr{P}(\mathscr{H}) \\ &\text{such that} \\ P(\emptyset) &= 0 \\ P(\mathbb{R}) &= \mathbf{1} \\ P(\cup_j (B_j)) &= \sum_j P(B_j), \end{aligned}$$

for any disjoint denumerable family B_j. Also,

$$P(B^c) = \mathbf{1} - P(B) = (P(B))^{\perp}$$

The spectral decomposition theorem allows to put self adjoint operators and PVMs in a one to one correspondence. Despite the mathematical technicalities, these results allow to provide a very clear operational interpretation for observables represented as self adjoint operators as follows. Given an observable A, consider the proposition "the value of A lies in the interval (a, b)" (notice that all empirically testable propositions in quantum mechanics are of this form). Using the PVM associated to A (which we call P_A), the real line interval (a, b) is mapped to a projection operator $P_A(a, b)$. If the state of the system is described by the density matrix ρ, the probability of obtaining the property represented by $P_A(a, b)$ when measuring A is given by the Born rule [49]

$$p(P_A(a, b)) = \mathrm{tr}(\rho P_A(a, b)) \tag{2}$$

In this way, the above mentioned proposition is naturally described by a projection operator. This can be done for any observable and any associated proposition. Thus,

empirically testable propositions in quantum mechanics are represented by the set of projection operators of the Hilbert space. Denote this set by $\mathscr{P}(\mathscr{H})$. As is well known, there is a one to one correspondence between the elements of $\mathscr{P}(\mathscr{H})$ and the set of closed subspaces in the Hilbert space (see for example, Chap. 4.2 of Reference [17]). Thus, we will represent empirical propositions in quantum mechanics interchangeably as closed subspaces or as projection operators. Similarly to classical mechanics, the conjunction of two propositions can be represented as a subspace intersection. In symbols: the conjunction "$\wedge$" of two propositions represented by closed subspaces $\mathbb{S}$ and $\mathbb{T}$ is given by the subspace intersection $\mathbb{S} \cap \mathbb{T}$ (the intersection of two closed subspaces is always a closed subspace). But alike the classical case, it is not possible to take the disjunction "$\vee$" as the union of subspaces: the union of two subspaces will not be in general subspace, and thus, will not be a valid proposition. The solution to this riddle is to represent the disjunction as the closure of the direct sum of the two given subspaces. Implication will be naturally represented by subspace inclusion ($\mathbb{S} \leq \mathbb{T}$ if and only if $\mathbb{S} \subseteq \mathbb{T}$), and negation will be represented by taking the orthogonal complement (with respect to the Hilbert product): $\neg(\mathbb{S}) = (\mathbb{S})^{\perp}$. The main difference with classical mechanics relies in the fact that instead of a collection of subsets of a set (and their canonical operations), we now have a set of closed subspaces of a Hilbert space. In this context, it is important to remark that the set theoretical union and the direct sum of subspaces are very different operations; a similar remark holds for the negation as set theoretical complement and the negation as orthogonal complement of subspaces. Thus, it is to be expected to find important differences between the quantum and classical propositional structures. Indeed, it is immediate to check that the distributive law is no longer valid for arbitrary quantum properties a and b; in fact, we generally have the inequality

$$a \leq (a \wedge b) \vee (a \wedge \neg b) \tag{3}$$

If the above inequality is strict, it is said that we have incompatible properties. From the mathematical point of view, this is a direct consequence of the non-commutativity of the observables involved. Let us take a look at the formal structure of this with more detail. In Reference [23] (Chap. 1, Definition 1.1.3) two observables A and B are said to be compatible if and only if, for every Borel sets Δ and Γ, the projection operators $P_A(\Delta)$ and $P_B(\Gamma)$ satisfy:

$$P_A(\Delta)P_B(\Gamma) = P_A(\Delta)P_B(\Gamma) \tag{4}$$

The above Equation implies that the sub-quantum logic generated by the set of projections (empirical propositions) associated to A and B form a commutative sub-quantum logic. But it is well known that a sub-quantum logic is commutative if and only if it is a distributive lattice (Cf. for example, Proposition 4.16 of Reference [17]; see also Theorem 3.1.2 in Section 3 of [23]). And we will also have that, if $[A, B] \neq 0$, then there will exist propositions associated to A and B that will not satisfy the distributive equality.

3 Schrödinger and Heisenberg Representations

Quantum mechanical dynamics is governed by the time evolution operator

$$U = \exp^{-iHt} \tag{5}$$

where H is the Hamiltonian of the system. As is well known, it is possible to understand such an evolution from two different perspectives: Heisenberg and Schrödinger pictures. In the latter one, a physical system has associated an initial state ρ_0, and any physical magnitude will have associated a self adjoint operator O which remains constant in time. In this case (and assuming that there is no interaction with the environment or any measuring apparatus), the state of the system evolves obeying the following equation

$$\rho(t) = U\rho_0 U^\dagger \tag{6}$$

On the other hand, in the Heisenberg representation, the physical system has associated a state ρ which remains constant in time, while any physical magnitude has associated an initial self adjoint operator $\hat{O}_0$ which changes in time according to the equation

$$O(t) = U^\dagger O_0 U \tag{7}$$

In this way, we have two equivalent formulations of quantum mechanics. The equivalence has its roots in the fact that mean values of physical observables are coincident for each representation

$$\langle O \rangle_{\rho(t)} = \langle O(t) \rangle_\rho \tag{8}$$

In this way, the empirical content of each representation is the same.

From the point of view of the Schrödinger representation, the commutator between two observables is a constant in time: $[O_1, O_2] = O_1 O_2 - O_2 O_1$. This means that in this representation, the compatibility of two observables is a synchronic relation: two observables are compatible or incompatible independently of the temporal evolution. Because of these reasons, if we are trying to study the diachronic character of the logic associated to a quantum system, this representation is not suitable. Notwithstanding, the mean value of an observable can change during time. But, as the Hamiltonian is an Hermitian operator, then, any evolution is unitary. In particular, the mean value of the commutator obeys the unitary time evolution equation

$$\langle [O_1, O_2] \rangle_{\rho(t)} = \langle U^\dagger [O_1, O_2] U \rangle_{\rho_0} \tag{9}$$

From the point of view of the Heisenberg representation we have that, as the observables evolve, the commutator evolves in a unitary way. If we call C to the operator representing the commutator between O_1 and O_2, then

$$[O_1(t), O_2(t)] = C(t) = U^{\dagger} C_0 U \tag{10}$$

In this case, given that the evolution is unitary, it is possible to show that if $C_0 \neq 0 \Longrightarrow C(t) \neq 0$, and on the other hand, $C_0 = 0 \Longrightarrow C(t) = 0$. This means that if two operators are compatible/non-compatible at the beginning, they will remain compatible/non-compatible under the effect of unitary time evolution.

The above considerations show that both the Schrödinger and the Heisenberg representations, if restricted to evolutions modeled by Hermitian self adjoint operators (and thus, unitary evolutions), forces us to a synchronic logic. Notice that a similar analysis could be made for the approach to open quantum system dynamics in the Heisenberg picture [30], but due to reasons of space, we will address this question elsewhere. In this paper we aim to represent time evolution of logics; thus, a natural choice is to change the setting a little bit and use *non-Hermitian* evolution operators. We follow this strategy below presenting some examples first.

4 Quantum Mechanics with Non-Hermitian Hamiltonians in the Heisenberg Representation

In the standard formulation of quantum mechanics the Hamiltonian is a self adjoint operator, and as such, its eigenvalues are real numbers. If we relax this restriction, we win some generality and consequently, a richer dynamics can be described. Indeed, the approach to quantum mechanics based on non-Hermitian operators uses this freedom to obtain a non-unitary evolution [8]. According to the Brussels school, if we consider a non-Hermitian Hamiltonian with complex eigenvalues z_n, then, it is reasonable to describe it using the formula

$$H = \sum_n z_n |z_n\rangle\langle\tilde{z}_n| \tag{11}$$

where $|z_n\rangle$ is an eigenvector of H which, in certain cases, may no longer belong to the traditional Hilbert space, but to the more general *rigged Hilbert space*. $|z_n\rangle$ is the Gamov vector which belongs to the space $\Phi_+^{\times}$ of the Gelfand triplet $\Phi_+^{\times} \supset \mathscr{H} \supset \Phi_+$, and $\langle\tilde{z}_n| \in \Phi_+$ (see [50, 55]). We will denote by $\mathscr{H}_{\mathscr{R}}$ to the rigged Hilbert space associated to $\mathscr{H}$.

The complex energy z_n possesses a real part ω_n and an imaginary part which we conveniently write as $-\frac{1}{2}\gamma_n$. In this way $z_n = \omega_n - i\frac{1}{2}\gamma_n$. The techniques for computing observable quantities in the non-Hermitian setting is similar to that of standard quantum mechanics. The Hamiltonian is introduced in the master equation and the equation is solved. For the case of the time evolution of an eigenstate $|z_n\rangle$ of $\hat{H}$ we obtain a solution analog to that of the standard formalism

$$|z_n(t)\rangle = e^{-i\hat{H}t}|z_n\rangle = e^{-i\omega_n t} e^{-\frac{1}{2}\gamma_n t}|z_n\rangle \tag{12}$$

But we can now clearly see that a time decreasing exponential factor $\exp^{-\frac{1}{2}\gamma_n t}$ comes into stage. This mathematical property allows to study certain physical phenomena for which decaying rates play a central role in a natural way. Some examples of this are the reach of the mechanical equilibrium, quantum decoherence and decaying rates of unstable particles. As is well known, some of these physical processes can be described using open systems interacting with the environment, as for example, the einselection approach to decoherence. But the approach to quantum mechanics based on non-Hermitian operators offers a natural perspective in which these phenomena can be thought of as intrinsic. This alternative offers some computational advantages for certain examples, and at the same time, poses interesting philosophical discussions [31].

As in Sect. 3, we adopt the Heisenberg representation where we can compute the evolution of the commutator between two observables

$$[O_1(t), O_2(t)] = C(t) \tag{13}$$

In this case, given that the evolution is in general non-unitary, the commutator also evolves in a non-unitary way. Some authors (see for example [45, 46]) studied examples of decoherence in the Heisenberg representation. In particular, there are some examples for which the initial commutator between two observables is different from zero. According to what we exposed in Sect. 3, this means that we are dealing with incompatible properties, and as such, it is not possible to measure both observables simultaneously. Notwithstanding, due to the action of decoherence, the final commutator is zero.

$$C(0) \neq 0 \longrightarrow C(t \to \infty) = 0 \tag{14}$$

Our proposal consists in interpreting this process in the following manner: two incompatible properties become compatible. In this work we propose this line of thought to study the time evolution of the logical properties of physical systems in time. In other words, we propose a dynamical perspective of the quantum logical approach. As we will show, this is not only a technical perspective, but involves a radical modification of the logics associated to physical systems: time decaying rates will be included in the propositional system.

It is important to remark at this point that the adoption of non-Hermitian operators may imply the existence of the reverse process:

$$C(0) = 0 \longrightarrow C(t \to \infty) \neq 0 \tag{15}$$

If two observables commute at the beginning of the process, they may become non-commutative as time evolves.

From the quantum logical point of view, these results are very important because they imply that the logical properties associated to a physical system may change in a qualitative way. An example of this is the case of the distributive inequality satisfied by non-compatible quantum properties. As we have seen, such an inequality

is a consequence of the non-commutativity of their associated observables. If the evolution is such that a couple of observables transition from the non-commutative to the commutative case, then the distributive inequality becomes an equality.

$$\begin{aligned} a &\leq (a \wedge b) \vee (a \wedge \neg b) \\ &\Downarrow \\ a &= (a \wedge b) \vee (a \wedge \neg b) \end{aligned} \tag{16}$$

In order to interpret this fact, it is possible to imagine a very simple case in which the two properties are represented each one by a vector. To illustrate, let us suppose that a quantum system has associated the following Hamiltonian

$$H = \omega \left|\omega\right\rangle \left\langle\tilde{\omega}\right| - \frac{i}{2}\gamma \left|\gamma\right\rangle \left\langle\tilde{\gamma}\right| \tag{17}$$

where ω is a real energy and γ is an imaginary energy related to the decaying rate of that mode. On the other hand, let us consider an observable of the form

$$O = \frac{1}{2}\left[(o_1 + o_2)\left|\omega\right\rangle \left\langle\tilde{\omega}\right| + (o_1 - o_2)\left|\omega\right\rangle \left\langle\tilde{\gamma}\right| + (o_1 - o_2)\left|\gamma\right\rangle \left\langle\tilde{\omega}\right| + (o_1 + o_2)\left|\gamma\right\rangle \left\langle\tilde{\gamma}\right|\right] \tag{18}$$

where o_1 and o_2 are the eigenvalues of the given observable. In this case, the commutator between $\hat{H}$ and $\hat{O}$ evolves in such a way that

$$[H(t), O(t)] \propto e^{-\gamma t} \tag{19}$$

In the above expression we can see that the imaginary part of the energy appears in the commutator as the inverse of the characteristic time in an exponential. In this case, for times much bigger than the characteristic time, we can assume that the commutator is zero and that it remains unchanged after that. Then, the commutator between the Hamiltonian and the observable O—which was initially different from zero—vanishes, and thus, the two properties, which were non-compatible at the beginning, become compatible ones. In this case, the evolution of the observables can be interpreted in the following way: the angle between the vectors tends to be smaller when time increases. As far as it is different from zero, the inequality remains, but in the infinite time limit the angle goes to zero, and then, the corresponding observables become commutative. As a consequence, we recover distributivity and a Boolean algebra.

5 An Example with Two Different Characteristic Times

The simple example presented in the previous Section has the virtue of clarifying the mechanism through which a pair of initially non-commuting observables becomes commutative. But it does not offer too many aspects to question further. The case with

more than one characteristic time may offer an interesting variant. Let us suppose then that we have a quantum system with observables O_A, O_B and O_C such that

$$C_{A-B}(t) = [O_A(t), O_B(t)] \propto e^{-\gamma_1 t} \quad \text{and} \quad C_{A-C}(t) = [O_A(t), O_C(t)] \propto e^{-\gamma_2 t} \tag{20}$$

If, starting from this point we define the observable $O_D = O_A + O_B + O_C$, then we have that

$$C_{A-D}(t) = [O_A(t), O_D(t)] = [O_A(t), O_B(t)] + [O_A(t), O_C(t)] \tag{21}$$

follows an evolution in two steps. In order to simplify the description with regard to the non-distributivity we define the functions $f(a, b) = a$ and $g(a, b) = (a \wedge b) \vee (a \wedge \neg b)$. In this way, the equality of (1) can be written as $f(a, b) = g(a, b)$ and the inequality of expression (3) can be written as $f(a, b) \leq g(a, b)$. Then we have that:

1. At the beginning, the commutators are different from zero: $C_{D-A}(t) \neq 0, C_{D-B}(t) \neq 0$ and $C_{D-C}(t) \neq 0$. This means that O_D-O_A, O_D-O_B and O_D-O_C are incompatible. Thus, physical properties a, b, c and d associated to them, will also be incompatible. In this way we have the distributive inequality for the three cases.

$$f(d, a) \leq g(d, a) \quad f(d, b) \leq g(d, b) \quad f(b, c) \leq g(b, c)$$

2. After the passage of the first characteristic time $t_1 = \gamma_1^{-1}$, the first term of (21) disappears, but the commutator between $\hat{O}_A$ and $\hat{O}_D$ remains non-vanishing. This means that a part of the algebra became commutative but the other one did not.

$$f(d, a) \leq g(d, a) \quad f(d, b) = g(d, b) \quad f(b, c) \leq g(b, c)$$

3. Finally, after the second characteristic time $t_2 = \gamma_2^{-1}$, the last term of (21) disappears, and the commutator between O_A and O_D vanishes. In this way, the remaining part of the algebra becomes distributive:

$$f(d, a) = g(d, a) \quad f(d, b) = g(d, b) \quad f(b, c) = g(b, c)$$

The above example shows that the non-unitary evolution transforms incompatible observables in a complex manner. This is just an example, and physical systems of interest may have associated many different characteristic times. For example, in the model of an harmonic oscillator interacting with a bath of harmonic oscillators, we will find infinitely many characteristic times [56]. This situation offers a much more complex dynamic of logics that we will address in future works. But we will give an example in the following Section.

6 Many Different Characteristic Times

In reference [5] we have presented a formalism based on finding the poles of the analytic extension of the mean values. In this paper we consider a system with a Hamiltonian that can be divided in two parts:

$$H = H_0 + V \tag{22}$$

H_0 is supposed to be a known hermitian Hamiltonian (the free Hamiltonian): we know its eigenvalues and eigenvectors. On the other hand V is a perturbation. The total Hamiltonian H is a perturbed Hamiltonian and we can use perturbation theory. This theory tells us that there is a relation between the eigenvectors of the perturbed Hamiltonian $|\tilde{\omega}\rangle$ and the eigenvectors of the non-perturbed Hamiltonian $|\omega\rangle$. This relation is given by the Lippmann-Schwinger equations. To the first order, the equations are [51]

$$\langle\psi|\tilde{\omega}\rangle = \langle\psi|\omega\rangle + \langle\psi| \frac{1}{\omega + i0 - H} V |\omega\rangle$$
$$\langle\tilde{\omega}|\psi\rangle = \langle\omega|\psi\rangle + \langle\tilde{\omega}| \frac{1}{\omega + i0 - H} V |\psi\rangle$$

To solve these equations we need to go to the complex plane and to compute poles and residues. These poles were deeply studied by the Brussels school led by Prigogine (see [57, 60]). The poles can be interpreted as complex energies of the perturbed system. Then, it is possible to build an effective Hamiltonian and we can compute the evolution of the mean values. The result is that the imaginary parts of the poles appear in these mean values as the characteristic times of the exponentials. The mean value can be split in three parts: a constant part, and another part with an exponential decay and a term that is a polynomial decay, known as Khalfin term. But the Khalfin term is very difficult to be detected, and for this reason it can be neglected [5]. So, we obtain

$$(\rho(t)|O_R) \cong (\rho_{R*}|O_R) + \sum_j a_j(t) e^{-\gamma_j t} \tag{23}$$

where ρ_{R*} is the equilibrium state, γ_j are the imaginary part of the poles and functions $a_j(t)$ depends on the observable O_R and the initial condition.

7 A Dynamical Reformulation of Quantum Logic

The discussion posed in this paper calls for a reformulation of the quantum logical formalism in order to take into account the dynamical evolution of logics. In order to achieve this aim, we will modify the notion of projective valued measure presented

in Sect. 2 (cf. 2). Equation (11) gives us an important clue: in such a decomposition, a one dimensional vector is assigned to a complex number. In the standard formalism of quantum mechanics (for discrete spectra), a vector is assigned to each real number in the spectra. This analogy calls for a generalization of the notion of projection valued measure. We define a *complex projection valued measure* (CPVM) as a map from the Borel sets of the complex plane $B(\mathbb{C})$ to the set of projection operators satisfying

$$\begin{aligned} P^{\mathbb{C}} : B(\mathbb{C}) &\to \mathscr{P}(\mathscr{H}) \\ &\text{such that} \\ P^{\mathbb{C}}(\emptyset) &= 0 \\ P^{\mathbb{C}}(\mathbb{C}) &= \mathbf{1} \\ P^{\mathbb{C}}(\cup_j(B_j)) &= \sum_j P^{\mathbb{C}}(B_j), \end{aligned}$$

for any disjoint denumerable family B_j. Also,

$$P^{\mathbb{C}}(B^c) = \mathbf{1} - P^{\mathbb{C}}(B) = (P^{\mathbb{C}}(B))^{\perp}$$

Equation (24) constitute a natural generalization of the notion of PVM (2) to the field of complex numbers. In this way, we postulate that to each non-Hermitian operator H of physical interest we can a assign a CPVM $P_H^{\mathbb{C}}$.

In Sect. 2 we discussed the interpretation of the empirical propositions defined by the spectral theorem in the context of the standard formalism of quantum mechanics. Now we ask for an interpretation of the logical propositions defined by the notion of CPVM associated to a non-Hermitian operator. This can be done in a natural way as follows. Consider a non-Hermitian Hamiltonian H (such as the one in (11)) and a region $R_{a,b,c,d}$ of the complex plane defined by

$$a \leq \Re(z) \leq b \tag{24}$$

$$c \leq \Im(z) \leq d \tag{25}$$

$R_{a,b,c,d}$ is just the Cartesian product between the Borel sets (a, b) and (c, d). Now, consider all the complex eigenvalues $Z_i(R_{a,b,c,d})$ of H which lie inside this region and the associated projection operators $P_i^{z_i}$. The CPVM $P_H^{\mathbb{C}}$ assigns to $R_{a,b,c,d}$ a subspace of $\mathscr{H}_{\mathscr{R}}$ formed by the direct sum of all subspaces associated to each complex eigenvalue: $P_H^{\mathbb{C}}(R_{a,b,c,d}) = \sum_{Z_i \in R_{a,b,c,d}} P_i^{z_i}$.

In order to give a physical interpretation to the above projections as propositions, let us consider the case in which the region involved contains just one eigenvalue z_j with associated eigenprojetor $P_j^{z_j}$. If $z_j = a_j + b_j i$, this proposition is naturally interpreted as: "the observed value of H is a_j and the decaying rate associated to this mode is b_j". All elementary propositions are of this form. The remainder propositions are naturally formed by direct sums and orthogonal complements of the elementary ones. The notions of conjunction, disjunction and orthogonal complement are just the same as in the standard quantum logical approach. In this way, we reach a

(non-Boolean) lattice of projection operators associated to the algebra of non-Hermitian operators. We call this logic $\mathscr{L}^{\mathbb{C}}$. Alike the standard interpretation of the propositions in the von Neumann lattice of projection operators $\mathscr{L}$, which could be termed "static", the propositions of $\mathscr{L}^{\mathbb{C}}$ are interpreted as observed values and decaying rates. In this way, we reach a dynamical version of the of the quantum logical approach.

It is important to remark that our approach allows for a novel quantum logical perspective on the quantum to classical transition. Let us nw turn into the formal aspects of this dynamics. Suppose that the system is initially described by a set observables $\mathbf{V}_0$ generating a von Neumann algebra $\mathscr{V}_0$ (the minimal von Neumann algebra containing $\mathbf{V}_0$). To fix ideas, think of $\mathscr{V}_0$ as the algebra of bounded observables $\mathscr{B}(\mathscr{H})$ for a Hilbert space $\mathscr{H}$; but notice that in principle, it could be a more general von Neumann algebra, i.e., a Type II or Type III factor (depending on the model that we are studying). Under the action of the non-Hermitian evolution $U(t) = \exp^{-iHt}$, $\mathbf{V}_0$ is mapped to the set

$$\mathbf{V}_t = U(t)\mathbf{V}_0 U^{\dagger}(t) \tag{26}$$

As before, $\mathbf{V}_t$ generates an algebra $\mathscr{V}_t$. In this way, the classical limit will be reached if the limiting algebra $\mathscr{V}_\infty$ is a Boolean one. Notice that the formulation of this problem is plagued of subtleties: the question about under which conditions the classical limit is reached can be a hard mathematical problem, which goes far from the scope of this article. Notwithstanding, the examples presented in previous Sections show us that this picture works for cases of interest.

If the process is suitably defined, (26) generates a family of von Neumann algebras

$$\mathscr{F}_{\mathscr{V}_0} = \{\mathscr{V}_t\}_{t\in\mathbb{R}} \tag{27}$$

Notice also that each von Neumann algebra $\mathscr{V}_t$ has associated an orthomodular lattice [17] of projection operators $\mathscr{L}_{\mathscr{V}_t}$. In this way we also have the family of quantum logics

$$\mathscr{F}_{\mathscr{L}_0} = \{\mathscr{L}_{\mathscr{V}_t}\}_{t\in\mathbb{R}} \tag{28}$$

which allow for a quantum logical description of the classical limit process. Notice that the family $\mathscr{F}_{\mathscr{L}_0}$ constitutes a strain of orthomodular lattices, by appealing to the non-Hermitian operator responsible of the non-unitary evolution. If the classical limiting process is successful, the orthomodular lattice $\mathscr{L}_{\mathscr{V}_\infty}$ will be a Boolean one. If we now consider the category of von Neumann algebras and the category of orthomodular lattices, we find a map Φ relating them as follows

$$\begin{array}{ccccccccc}
\mathscr{V}_0 & \longrightarrow & \cdots & \longrightarrow & \mathscr{V}_t & \longrightarrow & \cdots & \longrightarrow & \mathscr{V}_\infty \\
\Phi\downarrow & & & & \downarrow & & & & \downarrow \\
\mathscr{L}_0 & \longrightarrow & \cdots & \longrightarrow & \mathscr{L}_t & \longrightarrow & \cdots & \longrightarrow & \mathscr{L}_\infty
\end{array}$$

It is worth mention again that a structure such as the one described in the above diagram cannot be included in the standard unitary formulation of quantum mechanics.

8 Conclusions

In this paper we addressed the question of how to study the dynamical evolution of quantum logics associated to quantum systems reaching the classical limit. With this aim we have presented a quantum logical approach to the formulation of quantum mechanics based on non-Hermitian operators. This allows us to describe the time evolution of algebras which, being initially non-commutative, become Boolean ones because of the action of a non-unitary time evolution.

This novel perspective allows to describe a family of algebras evolving in time. The starting algebra can be non-Boolean, while the final one (for infinite time) will be Boolean. In this way we presented a quantum logical approach for the reaching of the classical limit, something which was not present in the previous literature. We have shown in Sect. 3 that this was difficult to describe using the standard formalism of quantum mechanics, and thus, a shift to the non-Hermitian Hamiltonians approach was in order. We have described concrete examples of this transition between logics in Sects. 4, 5 and 6.

In Sect. 7 we have introduced the novel notion of *complex projective valued measure* (24), a generalization of the standard notion (2) to the field of complex numbers. This allows us to reinterpret the results of previous sections with a new quantum logical formalism prepared to deal with decaying times associated to physical processes. In this way, we built a family of orthomodular lattices continuously parameterized by time, for which the initial lattice is fully quantum mechanical, but the limiting one is Boolean.

We hope that the ideas presented in this paper can be further developed in order to study the formal aspects of this algebraic approach to decoherence and the classical limit. This could find applications in theories more general than standard quantum theory, such as algebraic relativistic quantum field theory and algebraic quantum statistical mechanics [49].

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A Unifying E2-Quasi Exactly Solvable Model

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Abstract A new non-Hermitian E2-quasi-exactly solvable model is constructed containing two previously known models of this type as limits in one of its three parameters. We identify the optimal finite approximation to the double scaling limit to the complex Mathieu Hamiltonian. A detailed analysis of the vicinity of the exceptional points in the parameter space is provided by discussing the branch cut structures responsible for the chirality when exceptional points are surrounded and the structure of the corresponding energy eigenvalue loops stretching over several Riemann sheets. We compute the Stieltjes measure and momentum functionals for the coefficient functions that are univariate weakly orthogonal polynomials in the energy obeying three-term recurrence relations.

1 Introduction

In addition to the interesting mathematical aspect of enlarging the set of $sl_2(\mathbb{C})$ [1, 2] to E_2-quasi-exactly solvable models [3], the latter type also constitutes the natural framework for various physical applications in optics where the formal analogy between the Helmholtz equation and the Schrödinger equation is exploited [4–13]. Furthermore, a special case of these systems with a specific representation corresponds to the complex Mathieu equation that finds an interesting application in non-equilibrium statistical mechanics, where it corresponds to the eigenvalue equation for the collision operator in a two-dimensional classical Lorentz gas [14, 15].

Here we are mainly concerned with the extension of quasi-exactly solvable models [3, 16–19] to non-Hermitian quantum mechanical systems [20–23] within the above mentioned scheme. So far two different types of E_2-models have been constructed in [3, 24] and the main purpose of this manuscript is to investigate whether

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it is possible to construct a more general model that unifies the two. We show that this is indeed possible by combining the two models and introducing a new parameter into the system that interpolates between the two. In a similar fashion as the previously constructed models, also this one reduces in the double scaling limit to the complex Mathieu equation. As that equation is not fully explored analytically this limit provides an important option to obtain interesting information about the complex Mathieu system. On the other hand, for some applications it may also be sufficient to study an approximate behaviour for some finite values of the coupling constants. For that purpose we identify the parameter for which the general model is the optimal approximation for the complex Mathieu system.

Our manuscript is organized as follows: In Sect. 2 we introduce the general unifying model involving three parameters. We determine the eigenfunctions by solving the standard three-term recurrence relations for the coefficient functions and determine the energy eigenfunction from the requirement that the three-term recurrence relations reduce to a two-term relation. We devote section three to the study of the exceptional points and their vicinities in the parameter space. The explicit branch cut structure is provided that explains the so-called energy eigenvalue loops. In Sect. 4 we compute the central properties of the weakly orthogonal polynomials entering as coefficient functions in the Ansatz for the eigenfunctions, i.e. their norms, the corresponding Stieltjes measure and the momentum functionals. We state our conclusions in Sect. 5.

2 A Unifying E2-Quasi-Exactly Solvable Model

The general notion [1, 2] underlying solvable Hamiltonian systems is that its Hamiltonian operators $\mathcal{H}$ acting on some graded space V_n as $\mathcal{H} : V_n \mapsto V_n$ preserves the flag structure $V_0 \subset V_1 \subset V_2 \subset \cdots \subset V_n \subset \cdots$. A distinction is usually made between exactly and quasi-exactly solvable, depending on whether the structure preservation holds for an infinite or a finite flag, respectively. Here we are concerned with the latter. Lie algebraic versions of Hamiltonians in this context are usually taken to be of $sl_2(\mathbb{C})$-type [1, 2], but as recently proposed [3, 24], they may also be taken to be of a Euclidean Lie algebraic type, thus giving rise to qualitatively new structures.

At present two different types of E_2-quasi-exactly solvable models were identified

$$\mathcal{H}^{(1)}_{E_2} = J^2 + \zeta^2(u^2 - v^2)^2 + 2i\zeta N(u^2 - v^2), \qquad \zeta, N \in \mathbb{R}, \tag{1}$$

$$\mathcal{H}^{(0)}_{E_2} = J^2 + \zeta uvJ + 2i\zeta N(u^2 - v^2), \tag{2}$$

in [3, 24], respectively. Both Hamiltonians are expressed in terms of the E_2-basis operators u, v and J that obey the commutation relations

$$[u, J] = iv, \qquad [v, J] = -iu, \qquad [u, v] = 0. \tag{3}$$

Except for $\mathcal{H}^{(0)}_{E_2}$ at $N = 1/4$, both Hamiltonians are non-Hermitian, but respect the anti-linear symmetry [25] $\mathcal{PT}_3 : J \to J,\ u \to v,\ v \to u,\ i \to -i$ as defined in [10]. For the particular representation $J := -i\partial_\theta$, $u := \sin\theta\ v := \cos\theta$ the $\mathcal{PT}_3$-symmetry is simply $\mathcal{PT}_3 : \theta \to \pi/2 - \theta,\ i \to -i$, such that the invariant vector spaces over $\mathbb{R}$ were defined as

$$V^s_n(\phi_0) := \text{span}\left\{\phi_0\left[\sin(2\theta), i\sin(4\theta), \ldots, i^{n+1}\sin(2n\theta)\right]\Big|\,\theta \in \mathbb{R}, \mathcal{PT}_3(\phi_0) = \phi_0 \in L\right\}, \quad (4)$$

$$V^c_n(\phi_0) := \text{span}\left\{\phi_0\left[1, i\cos(2\theta), \ldots, i^{n}\cos(2n\theta)\right]\big|\,\theta \in \mathbb{R}, \mathcal{PT}_3(\phi_0) = \phi_0 \in L\right\}. \quad (5)$$

In order to construct Hamiltonians that preserve the flag structure one needs to identify the action of the E_2-basis operators and its combinations on these spaces as explained in more detail in [3]. The behaviour found allowed to identify the Hamiltonians $\mathcal{H}^{(1)}_{E_2}$ and $\mathcal{H}^{(0)}_{E_2}$ in (1) and (2) as quasi-exactly solvable. The general structure suggests that there might be a master Hamiltonian that unifies the above Hamiltonians into one preserving the quasi-exact solvability. We demonstrate here that this is possible and study the properties of that model.

Thus we introduce the new Hamiltonian

$$\mathcal{H}(N,\zeta,\lambda) = J^2 + 2(1-\lambda)\zeta uvJ + \lambda\zeta^2(u^2-v^2)^2 + 2i\zeta N(u^2-v^2), \qquad \lambda,\zeta,N \in \mathbb{R}, \quad (6)$$

and demonstrate explicitly that it is indeed E_2-quasi-exactly solvable. First we observe that $\mathcal{H}(N,\zeta,\lambda)$ interpolates between the two models in (1) and (2) by varying λ, since

$$\lim_{\lambda\to 1}\mathcal{H}(N,\zeta,\lambda) = \mathcal{H}^{(1)}_{E_2} \qquad \text{and} \qquad \lim_{\lambda\to 0}\mathcal{H}(2N,\zeta/2,\lambda) = \mathcal{H}^{(0)}_{E_2}. \quad (7)$$

Furthermore, $\mathcal{H}(N,\zeta,\lambda)$ reduces to the complex Mathieu Hamiltonian in the double scaling limit $\lim_{N\to\infty,\zeta\to 0}\mathcal{H}(N,\zeta,\lambda) = \mathcal{H}_{\text{Mat}} = J^2 + 2ig(u^2-v^2)$ for $g := N\zeta < \infty$. We also note that $\mathcal{H}^\dagger(N,\zeta,\lambda) = \mathcal{H}(1-\lambda-N,\zeta,\lambda)$, which implies that $\mathcal{H}(N,\zeta,\lambda)$ is non-Hermitian unless $2N = 1-\lambda$, with free coupling constant $\zeta \in \mathbb{R}$.

Given the structure for the vector spaces in (4) and (5) we now make the following Ansätze for the two fundamental solutions of the corresponding Schrödinger equation $\mathcal{H}_N\psi_N = E\psi_N$

$$\psi^c_N(\theta) = \phi_0\sum_{n=0}^{\infty} i^n c_n P_n(E)\cos(2n\theta), \quad \text{and} \quad \psi^s_N(\theta) = \phi_0\sum_{n=0}^{\infty} i^{n+1} c_n Q_n(E)\sin(2n\theta), \quad (8)$$

where the $\mathcal{PT}_3$-symmetric ground state is taken to be $\phi_0 = e^{\frac{i}{2}\zeta\cos(2\theta)}$ and the constant c_n is $c_n = 1/\zeta^n(N+\lambda)(1+\lambda)^{n-1}\left[(1+N+2\lambda)/(1+\lambda)\right]_{n-1}$ with $(a)_n := \Gamma(a+n)/\Gamma(a)$ denoting the Pochhammer symbol. The constants are chosen conveniently in order to ensure the simplicity of the to be determined nth and $(n-1)$th order polynomials $P_n(E)$, $Q_n(E)$ in the energies E, respectively. Upon substitution into the Schrödinger equation we obtain the three-term recurrence relations

$$P_2 = (E-\lambda\zeta^2-4)P_1 + \mathbf{2}\zeta^2[N-1][N+\lambda]P_0, \tag{9}$$
$$P_{n+1} = (E-\lambda\zeta^2-4n^2)P_n + \zeta^2[N+n\lambda+(n-1)][N-(n-1)\lambda-n]P_{n-1}, \tag{10}$$
$$Q_2 = (E-4-\lambda\zeta^2)Q_1, \tag{11}$$
$$Q_{m+1} = (E-\lambda\zeta^2-4m^2)Q_m + \zeta^2[N+m\lambda+(m-1)][N-(m-1)\lambda-m]Q_{m-1}, \tag{12}$$

for $n = 0, 2, \ldots$ and for $m = 2, 3, 4, \ldots$. Note that a more generic Ansatz for the unifying model involving two independent coupling constants μ, λ in the terms $\mu\zeta uvJ + \lambda\zeta^2(u^2-v^2)^2$ leads to a four term recurrence relation in which the highest term is always proportional to $\mu + 2\lambda - 2$. Thus taking this term to zero with the appropriate choice for μ reduces this to the desired three term relations that may be solved in complete generality as outlined in [3]. The lowest order polynomials are easily computed in a recursive way. Taking $P_0 = 1$ we obtain

$$\begin{aligned}
P_1 &= E-\lambda\zeta^2, \\
P_2 &= \lambda^2\zeta^4 + 2\zeta^2[\lambda-\lambda E+N(\lambda+N-1)] + (E-4)E, \\
P_3 &= -\lambda^3\zeta^6 + \lambda\zeta^4\left(\lambda(2\lambda+3E-13) - 3N^2 - 3(\lambda-1)N + 2\right) + (E-16)(E-4)E \\
&\quad -\zeta^2\left[3\lambda E^2 + E\left(2\lambda^2 - 3N^2 - 3\lambda(N+11) + 3N + 2\right) + 32(\lambda + N(\lambda+N-1))\right],
\end{aligned} \tag{13}$$

and likewise with $Q_1 = 1$ we compute

$$\begin{aligned}
Q_2 &= E-4-\lambda\zeta^2, \\
Q_3 &= \lambda^2\zeta^4 + \zeta^2\left[\lambda(15-2\lambda-2E) + N^2 + (\lambda-1)N - 2\right] + (E-16)(E-4), \\
Q_4 &= -\lambda^3\zeta^6 + \lambda\zeta^4\left[8 + \lambda(8\lambda+3E-38) - 2N^2 - 2(\lambda-1)N\right] + (E-36)(E-16)(E-4) \\
&\quad +\zeta^2\left[-8\left(-12\lambda^2 + 69\lambda + 5\lambda N + 5(N-1)N - 12\right)\right] \\
&\quad +\zeta^2\left[-3\lambda E^2 + 2E\left((47-4\lambda)\lambda + N^2 + (\lambda-1)N - 4\right)\right].
\end{aligned} \tag{14}$$

In both cases we observe the typical feature for quasi-exactly solvable systems that the three term relation can be reset to a two-term relation at a certain level. This is due to the fact that in (10) and (12) the last term vanishes when $m = n = \hat{n} = -(1+N)/(1+\lambda)$ or $m = n = \tilde{n} = (\lambda+N)/(1+\lambda)$. Thus when taking $N = \tilde{n} + (\tilde{n}-1)\lambda$ we find the typical factorization

$$P_{\tilde{n}+\ell} = P_{\tilde{n}}R_\ell \qquad \text{and} \qquad Q_{\tilde{n}+\ell} = Q_{\tilde{n}}R_\ell. \tag{15}$$

The first solutions for the factor R_ℓ are easily found from (10) and (12) to

$$R_1 = E - 4\tilde{n}^2 - \lambda\zeta^2, \tag{16}$$
$$R_2 = (E-4\tilde{n}^2-\lambda\zeta^2)(E-4(\tilde{n}+1)^2-\lambda\zeta^2) - 2\tilde{n}(1+\lambda)^2\zeta^2. \tag{17}$$

Next we compute the energy eigenvalues $E_{\tilde{n}}$ from the constraints $P_{\tilde{n}}(E) = 0$ and $Q_{\tilde{n}}(E) = 0$ for the lowest values of N. For the solutions related to the even fundamental solution in (8) we find

$$N=1: \qquad E_1^c=\lambda\zeta^2, \tag{18}$$

$$N=2+\lambda: \qquad E_2^{c,\pm}=2+\lambda\zeta^2\pm 2\sqrt{1-(1+\lambda)^2\zeta^2}, \tag{19}$$

$$N=3+2\lambda: \qquad E_3^{c,\ell}=\frac{20}{3}+\lambda\zeta^2+\frac{4\hat{\Omega}}{3}e^{\frac{i\pi\ell}{3}}+\frac{1}{3}\left[52-12(1+\lambda)^2\zeta^2\right]e^{-\frac{i\pi\ell}{3}}\hat{\Omega}^{-1}, \tag{20}$$

with $\hat{\Omega}^3:=35+18(\lambda+1)^2\zeta^2+\sqrt{\left[3(\lambda+1)^2\zeta^2-13\right]^3+\left[18(\lambda+1)^2\zeta^2+35\right]^2}$, $\ell=0,\pm 2$.

For the solutions related to the odd fundamental solution in (8) we obtain

$$N=2+\lambda: \qquad E_2^s=4+\lambda\zeta^2, \tag{21}$$

$$N=3+2\lambda: \qquad E_3^{s,\pm}=10+\zeta^2\lambda\pm 2\sqrt{9-(\lambda+1)^2\zeta^2}, \tag{22}$$

$$N=4+3\lambda: \qquad E_4^{s,\ell}=\frac{56}{3}+\lambda\zeta^2+\frac{4\Omega}{3}e^{\frac{i\pi\ell}{3}}+\frac{1}{3}\left[196-12(1+\lambda)^2\zeta^2\right]e^{-\frac{i\pi\ell}{3}}\Omega^{-1}, \tag{23}$$

with $\Omega^3:=143+18\zeta^2(\lambda+1)^2+\sqrt{\left(3\zeta^2(\lambda+1)^2-49\right)^3+\left(18\zeta^2(\lambda+1)^2+143\right)^2}$, $\ell=0,\pm 2$. Solutions for higher order may of course also be obtained, but are rather lengthy and therefore not reported here.

3 Exceptional Points and Their Vicinities

The special point in parameter space where two real energy eigenvalues viewed as functions of the coupling constants merge and subsequently split into a complex conjugate pair is usually referred to as exceptional point [26–29]. In our system these points can be computed in an explicit simple and straightforward manner. Using that by definition the discriminant Δ equals the product of the squares of the differences of all energy eigenvalues E_i for $1\leq i\leq n$, i.e. $\Delta=\prod_{1\leq i<j\leq n}(E_i-E_j)^2$ one obtains the exceptional points from the real zeros of $\Delta(E)$. For practical purposes one may also exploit the fact [3], that the discriminant equals the determinant of the Sylvester matrix. This viewpoint has the advantage that it does not require the computation of all the eigenvalues and is more efficient when the sole purpose is to find the exceptional points. Thus in our case we have to find the real zeros of the discriminants $\Delta_{\tilde{n}}^c$ and $\Delta_{\tilde{n}}^s$ for the polynomials $P_{\tilde{n}}(E)$ and $Q_{\tilde{n}}(E)$, respectively. Extracting overall constant factors κ as $\Delta=\kappa\tilde{\Delta}$, that do not contribute to the zeros, we obtain for the lowest values of $\tilde{n}$

$$\begin{aligned}
\tilde{\Delta}_2^c&=\hat{\zeta}^2-1, \\
\tilde{\Delta}_3^s&=\hat{\zeta}^2-9, \\
\tilde{\Delta}_3^c&=\hat{\zeta}^6-\hat{\zeta}^4+103\hat{\zeta}^2-36, \\
\tilde{\Delta}_4^s&=\hat{\zeta}^6-37\hat{\zeta}^4+991\hat{\zeta}^2-3600, \\
\tilde{\Delta}_4^c&=\hat{\zeta}^{12}+2\hat{\zeta}^{10}+385\hat{\zeta}^8-33120\hat{\zeta}^6+16128\hat{\zeta}^4-732276\hat{\zeta}^2+129600, \\
\tilde{\Delta}_5^s&=\hat{\zeta}^{12}-94\hat{\zeta}^{10}+7041\hat{\zeta}^8-381600\hat{\zeta}^6+6645600\hat{\zeta}^4-78318900\hat{\zeta}^2+158760000,
\end{aligned} \tag{24}$$

where we abbreviated $\hat{\zeta}:=\zeta(1+\lambda)$.

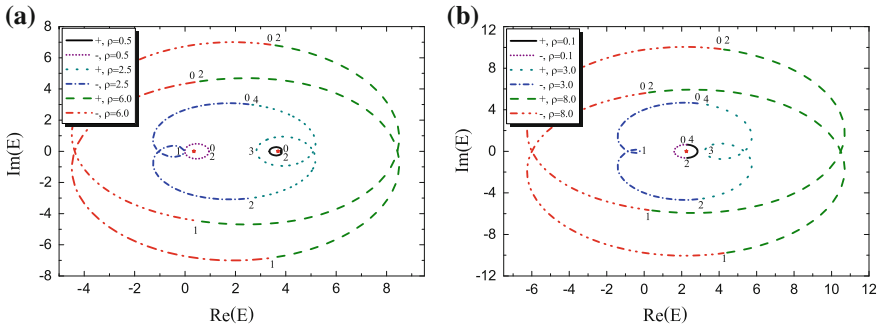

Fig. 1 Energy eigenvalue loops $E_2^{c,\pm}(\tilde{\lambda}+\rho e^{i\pi\phi},\zeta)$ around two real eigenvalues panel (**a**) and around an exceptional point panel (**b**) as functions of ϕ, indicated by the *numbers* on the loops, for fixed value of $\zeta=1/2$ at $\tilde{\lambda}=1/10$ in (**a**) and $\tilde{\lambda}=1$ in (**b**). The energy eigenvalues for $\rho=0$ are distinct in panel **a** as $E_2^{c,-}=0.35$, $E_2^{c,+}=3.70$ and coalesce to an exceptional point in panel **b** as $E_2^{c,-}=E_2^{c,+}=9/4$

There exist many detailed studies about the structures in the coupling constant space in the vicinity of the exceptional points [30–34]. It is evident that when tracing a complex energy eigenvalue E as functions of the coupling constants, λ or ζ in our case, the corresponding path in the energy plane will inevitably pass through various Riemann sheets due to the branch cut structure. As a consequence one naturally generates eigenvalue loops that stretch over several Riemann sheets. This phenomenon is well studied for a large number of models and we demonstrate here that it also occurs in quasi-exactly solvable models. The basic principle can be demonstrated with the square root singularity occurring in $E_2^{c,\pm}$ with branch cuts from $(-\infty,-1-1/\zeta)$ and $(1/\zeta-1,\infty)$. The energy loops are generated by computing $E_2^{c,\pm}(\lambda=\tilde{\lambda}+\rho e^{i\pi\phi},\zeta)$ for some fixed values of ζ, center $\tilde{\lambda}$ and the radius ρ in the λ-plane as functions of ϕ as illustrated in Fig. 1a, b. In panel (a) we simply trace the energy around a point in parameter space that leads to two real eigenvalues. For a small radius ones reaches the starting point by encircling $\tilde{\lambda}$ just once. However, when the radius is increased one needs to surround $\tilde{\lambda}$ twice to reach the starting point and when the radius is increased even further one only needs to surround $\tilde{\lambda}$ once switching, however, between both energy eigenvalues.

Essentially this structure survives when the two eigenvalues merge into an exceptional point. However, since the exceptional point is a branch point we no longer have the option for a closed loop around it produced from only one energy eigenvalue as seen in Fig. 1b.

This behaviour is easily understood from the structure of the branch cuts as depicted in Fig. 2. Whereas for small radii it is possible to encircle for instance the point $\tilde{\lambda}=1/10$ without crossing any branch cut, this is not possible when encircling the exceptional point at $\tilde{\lambda}=1$ where we have to analytically continue from $E_2^{c,-}$ to $E_2^{c,+}$ when crossing a cut. This structure is the same for intermediate radii. For large radii we cross the first cut already at a half circle turn, such that one returns back to the original value already after one complete turn.

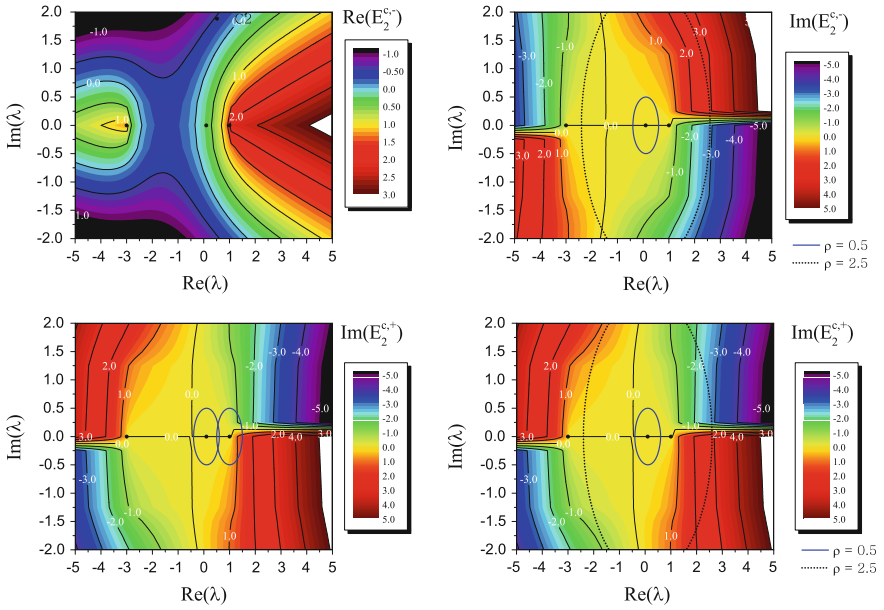

Fig. 2 Energy levels and branch cut structure for $E_2^{c,\pm}$ for fixed $\zeta = 1/2$ as functions of λ. The branch cuts extend to the *left* and *right* from the exceptional points $(-\infty, -3)$ and $(1, \infty)$

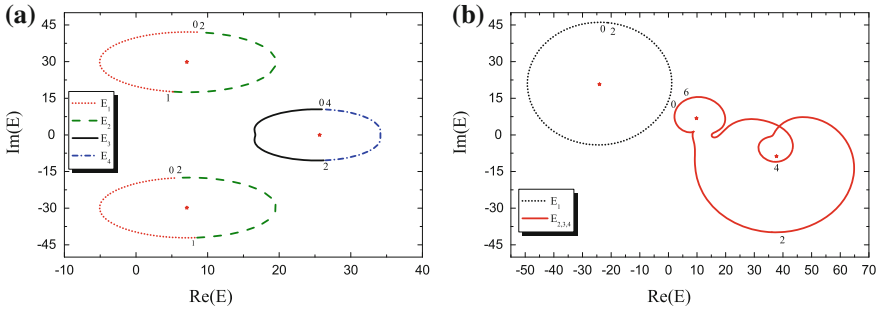

Fig. 3 Energy eigenvalues $E_4^c(\tilde{\lambda} + \rho e^{i\pi\phi}, \zeta)$ as functions of ϕ, indicated by the *numbers* on the loops, for fixed value $\zeta = 1/2$ at $\tilde{\lambda} = 9.5284$ in (**a**) and $\tilde{\lambda} = 5.2562 + i9.9526$ in (**b**). The energy eigenvalues for $\rho = 0$ in panel **a** are $E_4^{c,1} = E_4^{c,2} = 25.6613$, $E_4^{c,3} = (E_4^{c,4})^* = 7.1029 + i29.8106$ and $E_4^{c,1} = E_4^{c,2} = 37.7449 - i8.7611$, $E_4^{c,3} = 9.8103 + i6.7668$, $E_4^{c,4} = -24.0439 + i20.7081$ in panel (**b**). The radii are $\rho = 4.0$ and $\rho = 8.5$ in panels (**a**) and (**b**), respectively

When more eigenvalues are present the structure will be more intricate. Considering for instance a scenario with four eigenvalues in the form of two complex conjugate eigenvalues and an exceptional point, see Fig. 3a, we need to perform again at least two turns in the λ-plane in order to return to the initial position for the energy loops when surrounding an exceptional point. The two complex conjugate eigenvalues may be enclosed with just one turn, albeit we require again different energy eigenvalues

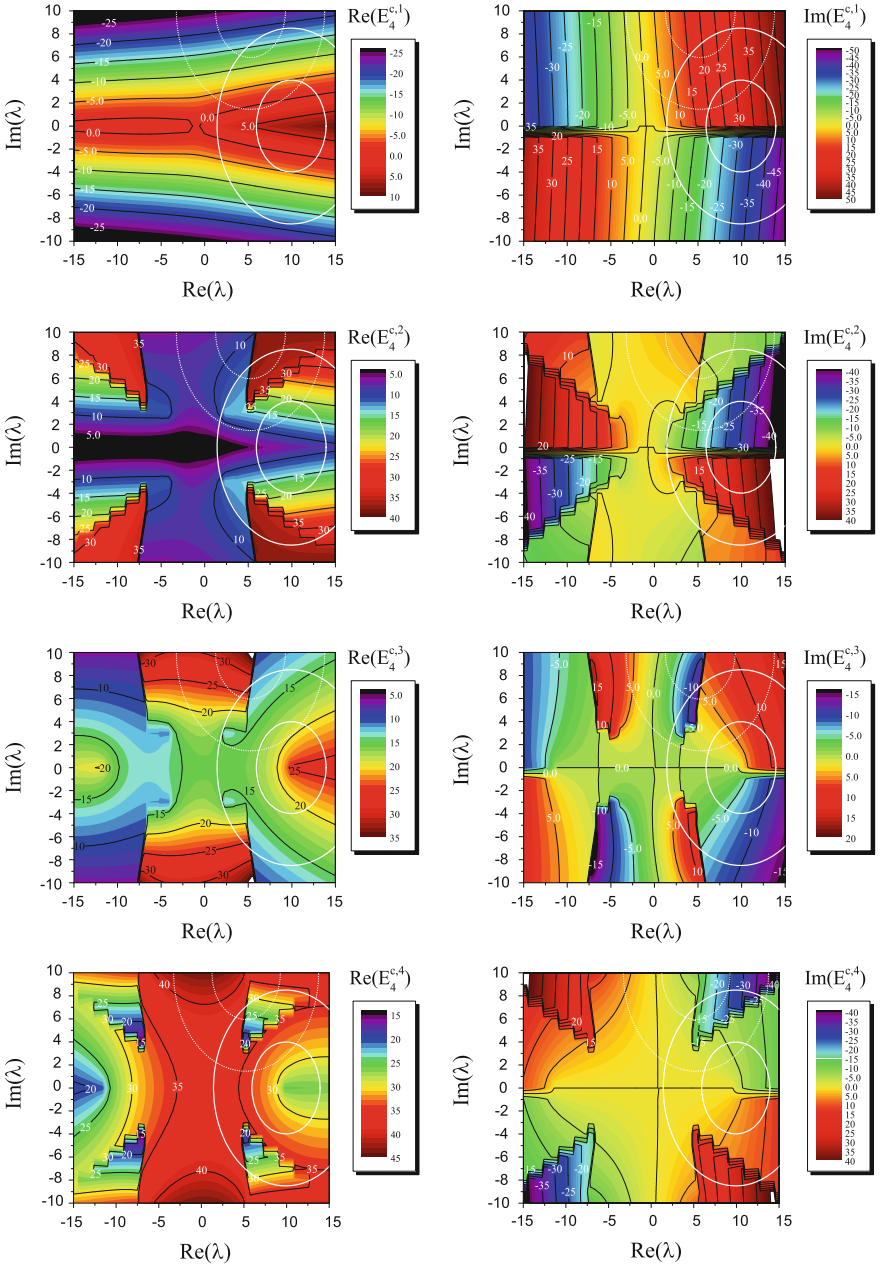

Fig. 4 Energy levels and branch cut structure for $E_2^{c,1,2,3,4}$ for fixed $\zeta = 1/2$ as functions of λ

for this. When enlarging the radius the loops will eventually merge as depicted in Fig. 3b for a situation with a degenerate complex eigenvalue and two complex eigenvalues. We observe that for the given values we have to surround the chosen point at least three times to obtain a closed energy loop surrounding the indicated centers.

In the same manner as for the simpler scenario one may understand the nature of these loops from an analysis of the branch cut structure of the energy as seen in Fig. 4. Tracing the indicated radii at $\rho = 4.0$ and $\rho = 8.5$ in Fig. 4 produces the energy loops in Fig. 3 when properly taking care of the analytic continuation at the branch cuts.

As discussed earlier the Hamiltonian $\mathcal{H}(N, \zeta, \lambda)$ has the interesting property that in the double scaling limit it reduces to the complex Mathieu equation for which only incomplete information is available, especially concerning the locations of the exceptional points. In comparison with the previously analyzed models $\mathcal{H}^{(1)}_{E_2}$ in [3] and $\mathcal{H}^{(0)}_{E_2}$ in [24] we have now the additional parameter λ at our disposal and we may investigate how the complex Mathieu system is approached. In particular we may address the question of whether there exists a value λ for which this is optimal. Our numerical results are depicted in Fig. 5. We find a similar qualitative behaviour for the other exceptional points, which we do not report here.

Comparing the rate of the approach for different values of λ we conclude that $\mathcal{H}(N, \zeta, \lambda = 1)$ is the best approximation to the complex Mathieu system for some finite values of N.

If one is exclusively interested in the computation of the exceptional point it is most efficient to carry out the double scaling limit already for the three-term relation (10) and (12) as explained in [3, 24].

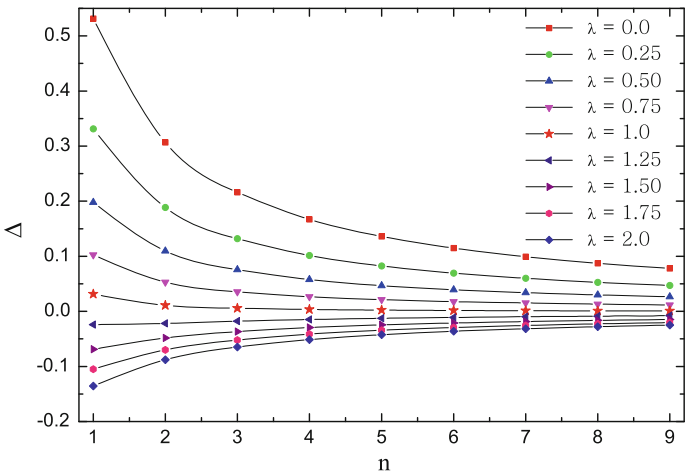

Fig. 5 Double scaling limit of $\lim_{N\to\infty,\zeta\to 0} \mathcal{H}(N, \zeta, \lambda) = \mathcal{H}_{\text{Mat}}$ to the smallest exceptional point at $\zeta_M = 1.46877$ with $\Delta(n) = \zeta_0 N(n) - \zeta_M$, $N(n) = (n + 1) + n\lambda$ for $n = 1, 2, 3, \ldots$

4 Weakly Orthogonal Polynomials

It is well known from Favard's theorem [35, 36] that polynomials $\Phi_n(E)$ constructed from three-term relations in the way mentioned above possess a norm N_n^Φ

$$\mathcal{L}(\Phi_n \Phi_m) = N_n^\Phi \delta_{nm}. \tag{25}$$

defined by the action of a linear functional $\mathcal{L}$ acting on arbitrary polynomials p in E as

$$\mathcal{L}(p) = \int_{-\infty}^{\infty} p(E)\omega(E)dE, \qquad \mathcal{L}(1) = 1. \tag{26}$$

This norm may be computed in two alternative ways. The simplest way is to multiply the three-term relation by Φ_{n-1} and act subsequently on the resulting equation with $\mathcal{L}$. Using the property $N_n^\Phi = \mathcal{L}(\Phi_n^2) = \mathcal{L}(E\Phi_{n-1}\Phi_n)$ together with (25) then simply yields $N_n^\Phi = \prod_{k=1}^n b_k$, where the b_k are the negative coefficients in front of Φ_{n-1}. Whereas the first method simply assumes that the functional exist the second method goes further and actually provides an explicit expressions for the measure. As argued in [37] the concrete formulae for $\omega(E)$ may be computed from

$$\omega(E) = \sum_{k=1}^{\ell} \omega_k \delta(E - E_k), \tag{27}$$

where the energies E_k are the ℓ roots of the polynomial $\Phi(E)$. The ℓ constants ω_k can be determined by the ℓ equations

$$\sum_{k=1}^{\ell} \omega_k \Phi_n(E_k) = \delta_{n0}, \qquad \text{for } n \in \mathbb{N}_0. \tag{28}$$

In our case the integer ℓ are determined from $N = \ell + (\ell - 1)\lambda$ and $N = (\ell + 1) + \ell\lambda$ for the $P_\ell(E)$ and $Q_{\ell+1}(E)$, respectively.

Using the first method we obtain

$$N_n^P = 2\zeta^{2n}(1+\lambda)^{2n} \left(\frac{1-N}{1+\lambda}\right)_n \left(\frac{\lambda+N}{1+\lambda}\right)_n, \qquad n = 1, 2, 3, ... \tag{29}$$

$$N_n^Q = \frac{1}{2(N+\lambda)(1-N)} N_n^P, \qquad n = 2, 3, 4, ... \tag{30}$$

with $N_0^P = N_1^Q = 1$. Due to the non-Hermitian nature of the Hamiltonian this norm is in general not positive definite. For instance for $N = 4 + 3\lambda$ we have

$$N_0^P = 1, \quad N_1^P = -24\zeta^2(1+\lambda)^2, \quad N_2^P = 240\zeta^4(1+\lambda)^4, \quad N_3^P = -1440\zeta^6(1+\lambda)^6. \tag{31}$$

The exception is the class of models where the Hamiltonian becomes Hermitian, i.e. when $\lambda = 1 - 2N$ holds. For this value of λ the expressions in (29) and (30) become positive definite

$$N_n^P = 2^{1+2n}\zeta^{2n}(N-1)^{2n}\left(\frac{1}{2}\right)_n^2 = 2\zeta^2(N-1)^2 N_n^Q. \tag{32}$$

Let us now consider the second method and compute explicitly the measure for a few examples. For $N = 2 + \lambda$ and $N = 3 + 2\lambda$ we solve (28) for the even and odd solutions, respectively, to

$$\omega_\pm^c = \frac{1}{2} \pm \frac{1}{2\sqrt{1-(1+\lambda)^2\zeta^2}}, \quad \text{and} \quad \omega_\pm^s = \frac{1}{2} \pm \frac{3}{2\sqrt{9-(1+\lambda)^2\zeta^2}}. \tag{33}$$

Computing now (25) with (26) agrees with (29) and (30)

$$N_0^P = \mathcal{L}(P_0^2) = \omega_+^c + \omega_-^c = 1 \tag{34}$$

$$N_1^P = \mathcal{L}(P_1^2) = \omega_+^c \left(E_2^{c,+} - \lambda\zeta^2\right)^2 + \omega_-^c \left(E_2^{c,-} - \lambda\zeta^2\right)^2 = -4\hat{\zeta}^2, \tag{35}$$

$$N_2^Q = \mathcal{L}(Q_2^2) = \omega_+^s \left(E_3^{s,+} - 4 - \lambda\zeta^2\right)^2 + \omega_-^s \left(E_3^{s,-} - 4 - \lambda\zeta^2\right)^2 = -4\hat{\zeta}^2. \tag{36}$$

Similarly we compute for $N = 3 + 2\lambda$

$$\omega_1^c = \frac{1}{3} - \frac{\left(260 - 60\hat{\zeta}^2\right)\Omega + \left(3\hat{\zeta}^2 + 4\right)\Omega^2 + 20\Omega^3}{12\left[\left(13 - 3\hat{\zeta}^2\right)^2 + \left(13 - 3\hat{\zeta}^2\right)\Omega^2 + \Omega^4\right]}, \qquad \omega_2^c = \chi_{-2}, \qquad \omega_3^c = \chi_2, \tag{37}$$

$$\chi_\ell = \frac{1}{3} + \frac{\left(3\hat{\zeta}^2 - 20\Omega + 4\right)\left(1 + 2e^{\frac{i\pi\ell}{3}}\right)}{36(3\hat{\zeta}^2 + \Omega^2 - 13)} + \frac{4 + 3\hat{\zeta}^2 - 20e^{\frac{i\pi\ell}{3}}\Omega}{12\left(1 + 2e^{\frac{i\pi\ell}{3}}\right)\left(3\hat{\zeta}^2 - 13\right) + \left(1 - e^{\frac{i\pi\ell}{3}}\right)\Omega^2}$$

and confirm that

$$\begin{aligned} N_0^P &= \mathcal{L}(P_0^2) = \omega_1^c + \omega_2^c + \omega_3^c = 1, \\ N_1^P &= \mathcal{L}(P_1^2) = \omega_1^c P_1^2(E_3^{c,0}) + \omega_2^c P_1^2(E_3^{c,-2}) + \omega_3^c P_1^2(E_3^{c,2}) = -12\hat{\zeta}^2, \\ N_2^P &= \mathcal{L}(P_2^2) = \omega_1^c P_2^2(E_3^{c,0}) + \omega_2^c P_2^2(E_3^{c,-2}) + \omega_3^c P_2^2(E_3^{c,2}) = 48\hat{\zeta}^4 \\ \mathcal{L}(P_1 P_2) &= \omega_1^c P_1(E_3^{c,0}) P_2(E_3^{c,0}) + \omega_2^c P_1(E_3^{c,-2}) P_2(E_3^{c,-2}) + \omega_3^c P_1(E_3^{c,2}) P_2(E_3^{c,2}) = 0. \end{aligned} \tag{38}$$

Note that the last relation in (38) does not follow from the first method.

As the final quantity we also compute the moment functionals defined in [35, 36] as

$$\mu_n := \mathcal{L}(E^n) = \sum_{k=1}^{\ell} \omega_k E_k^n = \sum_{k=0}^{n-1} \nu_k^{(n)} \mu_k, \tag{39}$$

Once again also these quantities can be obtained in two alternative ways, that is either from the computation of the integrals or directly from the original polynomials P_n and Q_n without the knowledge of the constants ω_k. In the last equation the coefficients $\nu_k^{(n)}$ are defined through the expansion $P_n(E) = 2^{n-1}E^n - \sum_{k=0}^{n-1} \nu_k^{(n)} E^k$ and $Q_n(E) = 2^{n-1}E^{n-1} - \sum_{k=0}^{n-2} \nu_k^{(n)} E^k$ for our even and odd solutions, respectively. For the even solutions with $N = 2 + \lambda$ we obtain

$$\mu_0^P = 1, \tag{40}$$
$$\mu_1^P = \lambda\zeta^2, \tag{41}$$
$$\mu_2^P = \lambda^2\zeta^4 - 4\hat{\zeta}^2, \tag{42}$$
$$\mu_3^P = \lambda^3\zeta^6 - 12\lambda\zeta^2\hat{\zeta}^2 - 16\hat{\zeta}^2, \tag{43}$$
$$\mu_4^P = \lambda^4\zeta^8 - 24\lambda^2\zeta^4\hat{\zeta}^2 + 16\left(\zeta^2 - 1\right)^2\zeta^4 - 64\hat{\zeta}^2, \tag{44}$$

and similarly for the odd solutions with $N = 3 + 2\lambda$ we compute for instance

$$\mu_0^Q = 1, \tag{45}$$
$$\mu_1^Q = 4 + \lambda\zeta^2, \tag{46}$$
$$\mu_2^Q = 16 - 4\hat{\zeta}^2 + \lambda^2\zeta^4, \tag{47}$$
$$\mu_3^Q = \lambda^3\zeta^6 - 12\left(\lambda^3 + \lambda^2 + \lambda\right)\zeta^4 - 48(2\lambda^2 + 3\lambda + 2)\zeta^2 + 64. \tag{48}$$

Thus $\mathcal{H}(N, \zeta, \lambda)$ possesses indeed all the standard features of a quasi-exactly solvable model of E_2-type.

5 Conclusions

Following the principles outlined in [3] we have constructed a new three-parameter quasi-exactly solvable model of E_2-type. One of the parameters can be employed to interpolate between two previously constructed models. With regard to one of the original motivations that triggered the investigation of these models, that is the double scaling limit towards the complex Mathieu equation, we found that for $\lambda = 1$, i.e. $\mathcal{H}_{E_2}^{(1)}$, finite values for N best approximate the complex Mathieu system and mimic its qualitative behaviour. We provided a detailed discussion of the determination of the exceptional points and the energy branch cut structure responsible for the

intricate energy loop structure stretching over several Riemann sheets. The coefficient functions are shown to possess the standard properties of weakly orthogonal polynomials.

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Sublattice Signatures of Transitions in a $\mathscr{P}\mathscr{T}$-Symmetric Dimer Lattice

Andrew K. Harter and Yogesh N. Joglekar

Abstract Lattice models with non-hermitian, parity and time-reversal ($\mathscr{P}\mathscr{T}$) symmetric Hamiltonians, realized most readily in coupled optical systems, have been intensely studied in the past few years. A $\mathscr{P}\mathscr{T}$-symmetric dimer lattice consists of dimers with intra-dimer coupling v, inter-dimer coupling v', and balanced gain and loss potentials $\pm i\gamma$ within each dimer. This model undergoes two independent transitions, namely a $\mathscr{P}\mathscr{T}$-breaking transition and a topological transition. We numerically and analytically investigate the signatures of these transitions in the time-evolution of states that are initially localized on the gain-site or the loss-site.

1 Introduction

Finite, discrete systems have always been an important testing ground in that they are often amenable to straightforward numerical approach, while retaining the complex and interesting features of their infinite or continuum counterparts. Lattice models, where a quantum particle occupies discrete locations and only tunnels between adjacent sites, successfully describe physical properties of a number of crystalline, condensed matter systems [1, 2] as well as light propagation in arrays of coupled optical waveguides [3] in the paraxial approximation [4]. A dimer model, where the tunneling strength alternates between two values, was first explored by Su, Schrieffer, and Heeger (SSH) in the context of solitons in polyacetylene [5, 6]. Since then, the one-dimensional SSH model has been extensively studied because it exhibits topologically non-trivial edge states [7] and its generalizations lead to band structures with nonzero Chern numbers [8, 9].

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Realizations of an SSH model in coupled optical waveguides instead of the nature-given long acetylene chains are advantageous [10]. In the former, the ratio of tunneling strengths, and the size and parity of the dimer chain can be varied over a wide range, and the entire bandwidth of the SSH band structure is accessible; and one can model non-hermitian, gain and loss potentials because the absorption and amplification of electromagnetic waves are both easily implemented [11]. Experimental realizations of non-uniform waveguide lattices have been demonstrated with lattice sites $N \sim 10 - 100$ [12], single-site or wide-beam input [13], and single-photon source inputs [14]; in particular, edge states and their adiabatic transfer in quasi-periodic waveguide lattices have been experimentally investigated [15].

The past 5 years have seen a surge of interest, driven primarily by experiments on optical systems [16–26], in open systems that are faithfully described by an effective, non-hermitian Hamiltonian that is invariant under combined parity and time-reversal ($\mathscr{P}\mathscr{T}$) operations [27, 28]. Typically, a $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian H is comprised of a hermitian, kinetic energy term H_0 and a non-hermitian, $\mathscr{P}\mathscr{T}$-symmetric potential term $V = \mathscr{P}\mathscr{T} V \mathscr{P}\mathscr{T} \neq V^\dagger$ that represents balanced, spatially separated gain and loss. Although H is not hermitian, its spectrum is purely real when the strength of the non-hermitian potential is small, and changes into complex-conjugate pairs when it exceeds a threshold called the $\mathscr{P}\mathscr{T}$-breaking threshold [28]. In contrast with the traditional hermitian case, the non-hermitian, $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian is defective at the $\mathscr{P}\mathscr{T}$-breaking threshold [29, 30]. A $\mathscr{P}\mathscr{T}$-symmetric SSH model, or equivalently a dimer model, has gain and loss of equal strengths on alternate sites [31], and is mathematically equivalent to a dimer model which has only a loss term on every other site. This purely lossy dimer model shows a quantized mean displacement that, under certain constraints, has a topological origin. This transition is driven by the ratio of inter-dimer and intra-dimer tunneling amplitudes, and befitting a topological transition, is independent of the strength of the loss potential and robust over a broad range of model parameters [32].

In this paper, we discuss the properties of the $\mathscr{P}\mathscr{T}$-symmetric dimer model over a wide range of parameters, such that it undergoes *both the $\mathscr{P}\mathscr{T}$-breaking transition and the topological transition.* The $\mathscr{P}\mathscr{T}$-breaking transition in a $\mathscr{P}\mathscr{T}$-dimer model was studied by Zheng et al. [31], and the topological transition in a purely lossy dimer model was predicted by Rudner and Levitor [32]. Neither, however, investigated the interplay between these two transitions.

The plan of the paper is as follows. In Sect. 2 we present the key properties of a $\mathscr{P}\mathscr{T}$-symmetric dimer model, as they relate to the two transitions it undergoes. In Sect. 3 we present numerical results for the time evolution of a wave packet that is initially localized on a gain site or a loss site. Since the intensities on the gain sites are orders of magnitude higher than those on the loss sites, particularly in the $\mathscr{P}\mathscr{T}$-broken phase, we separately consider the intensity distributions on the gain-sublattice and the loss-sublattice. We show that these distributions undergo a qualitative change across the topological transition. In Sect. 4, we obtain approximate, analytical expressions for the two sublattice intensity distributions. We conclude the paper with a brief discussion in Sect. 5. Our results show that the

signatures of the topological transition imprint themselves on the sublattice intensity distributions in the broken $\mathscr{P}\mathscr{T}$-symmetric phase.

2 The $\mathscr{P}\mathscr{T}$-Symmetric Dimer Model

In this section, we establish the notation and recall results for the $\mathscr{P}\mathscr{T}$-breaking transition in a dimer lattice [31], and the topological transition in a purely lossy dimer lattice [32]. Let us consider a $\mathscr{P}\mathscr{T}$-symmetric dimer lattice, where each dimer consists of a gain site (G) with potential $+i\gamma$ and a loss site (L) with potential $-i\gamma$. The dimer is labeled by the index m where $-M \leq m \leq M$ denotes a finite lattice with $N = 2M + 1$ dimers, v denotes the tunneling within a dimer, and v' denotes the tunneling between two adjacent dimers. In this case, the parity operator $\mathscr{P}$ exchanges the gain and the loss sites *within each dimer* whereas the time-reversal operator $\mathscr{T}$ corresponds to complex conjugation, thus interchanging the gain with the loss. Figure 1 shows a schematic of such a lattice.

The non-hermitian, $\mathscr{P}\mathscr{T}$-symmetric Hamiltonian $H = H_0 + V$ for the lattice is given by

$$H_0 = -\sum_{m=-M}^{M-1} \left(v|mG\rangle\langle mL| + v'|mL\rangle\langle m+1G| + \text{h.c.} \right), \tag{1}$$

$$V = +i\gamma \sum_{m=-M}^{M} \left(|mG\rangle\langle mG| - |mL\rangle\langle mL| \right), \tag{2}$$

where $|mG\rangle$ and $|mL\rangle$ denote single-particle states localized on the gain and loss sites of dimer m, h.c. denotes the hermitian conjugate, and we have considered a lattice with open boundary conditions. In the Fourier space, this Hamiltonian is block-diagonalized into 2×2 sectors given by

$$H_{k_n} = \begin{bmatrix} i\gamma & -v^*_{k_n} \\ -v_{k_n} & -i\gamma \end{bmatrix} = i\gamma\sigma_z - (v + v'\cos k_n)\sigma_x - v'\sin k_n \sigma_y. \tag{3}$$

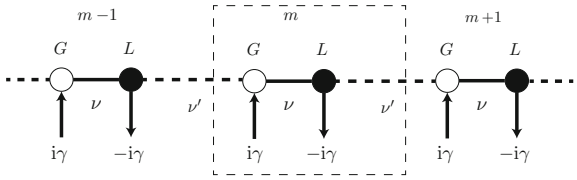

Fig. 1 Schematic of a $\mathscr{P}\mathscr{T}$-symmetric dimer lattice. The gain-sites G, shown by *open circles*, have a gain potential $+i\gamma$ while the loss sites L, shown by *black solid circles*, have the decay potential $-i\gamma$. The *dashed rectangular box* indicates the central, $m = 0$, dimer. The tunneling within a dimer is given by v and the inter-dimer tunneling is v'

Here σ_i are the Pauli matrices, $\nu_{k_n} = \nu + \nu' \exp(ik_n)$, * denotes complex conjugation, and $k_n = n\pi/(N+1)$ $(1 \leq n \leq N)$ are the eigenmomenta consistent with open boundary conditions. For periodic boundary conditions, the corresponding eigenmomenta are given by $k_n = 2\pi n/N$ with $|n| \leq (N/2)$. The spectrum of the Hamiltonian H_k is given by $\pm\epsilon_k = \pm\sqrt{|\nu_k|^2 - \gamma^2}$; therefore, the $\mathscr{P}\mathscr{T}$-breaking threshold for the dimer lattice is given by $\gamma_{PT} = \min_k(|\nu_k|)$ and becomes, in the infinite-lattice limit [31], $\gamma_{PT} = |\nu_k|_{k=\pi} = |\nu - \nu'|$.

In the $\mathscr{P}\mathscr{T}$-symmetric phase, the eigenvalues ϵ_k are real for all k, the non-unitary time evolution generated by the Hamiltonian is periodic, and the total intensity $I(t) = \langle\psi(t)|\psi(t)\rangle$ of an initially normalized wave packet $|\psi(t)\rangle$ remains bounded as a function of time. When the gain-loss strength exceeds γ_{PT} but is smaller than $\max_k |\nu_k| = \nu + \nu'$, some Fourier components of the initial state grow exponentially while others remain bounded, leading to a total intensity $I(t)$ that oscillates with an amplitude that increases exponentially with time. For $\gamma > |\nu_k|_{k=0} = \nu + \nu'$, all Fourier components grow exponentially and so does the net intensity. Figure 2 shows the intensities for the gain sublattice $I_G(m,t) = |\langle mG|\psi(t)\rangle|^2$ and the lossy sublattice $I_L(m,t) = |\langle mL|\psi(t)\rangle|^2$, for a 41-site dimer lattice with $\nu'/\nu = 1$, gain-loss strength $\gamma/\nu = 0.5$, and an initial state localized on the gain site of the central dimer, $|\psi(0)\rangle = \delta_{m0}|mG\rangle$. We remind the reader that since the Hamiltonian $H = H_0 + V$ is not hermitian, the time-evolved state $|\psi(t)\rangle = \exp(-iHt)|\psi(0)\rangle$ does not have a constant norm. (We use $\hbar = 1$.) We see that the intensities on the two sublattices differ by orders of magnitude; therefore it is useful to consider the two intensity distributions separately.

Next, we recall the results for the topological transition in a purely lossy dimer lattice [32], and present its generalization to a $\mathscr{P}\mathscr{T}$-symmetric dimer lattice. For a lossy lattice, each dimer has one neutral site (N) and one lossy site (L). The Hamiltonian for the lossy lattice with open boundary conditions is given by

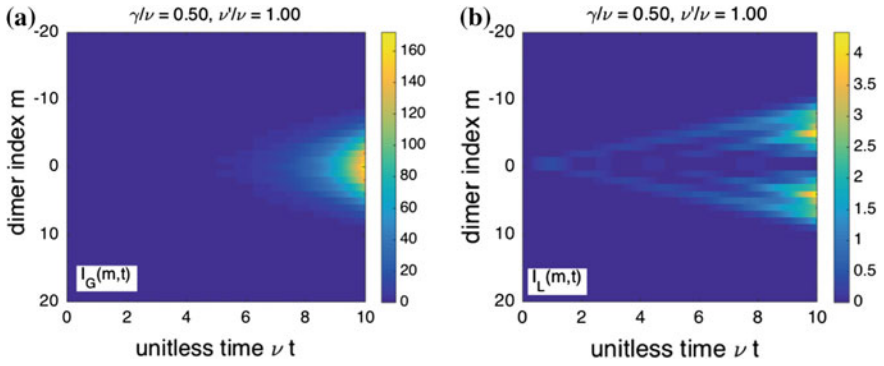

Fig. 2 The gain (**a**) and loss (**b**) sublattice intensities for an $N = 41$ dimer lattice with $\nu'/\nu = 1$ and gain-loss strength $\gamma/\nu = 0.5$. The *vertical axis* shows the dimer index m with $-20 \leq m \leq 20$, and the *horizontal axis* denotes normalized time νt. Note the order of magnitude difference between intensities on the gain sublattice and the loss sublattice

$H^L(\nu, \nu', \gamma) = H_0 + V^L(\gamma)$ where

$$V^L(\gamma) = -2i\gamma \sum_{m=-M}^{M} |mL\rangle\langle mL|. \tag{4}$$

The eigenvalues of the non-hermitian, non-$\mathscr{P}\mathscr{T}$-symmetric Hamiltonian H_k^L have a purely decaying part for all eigenmomenta k, and therefore any typical initial state is eventually completely absorbed. The mean displacement of the wave packet before it is absorbed is determined solely by the intensities on the loss sublattice,

$$\Delta m(\nu, \nu', \gamma) = \sum_m m \int_0^\infty dt\, 4\gamma I_L(m, t). \tag{5}$$

Prima facie, (5) represents a complicated global measure of the intensity distribution on the loss sublattice; it depends on the initial state, the decay rate γ, and the two tunneling amplitudes ν, ν' that characterize the dimer lattice. For an initial state localized on the neutral site in the central dimer, $m = 0$, however, it can be shown—through some non-trivial algebra [32]—that the mean displacement Δm is equal to the winding number of the k-space tunneling amplitude $\nu_k^* = \nu + \nu' \exp(-ik)$ [32]. Since the winding number is a topological quantity that changes discontinuously and is robust against small disorder perturbations, it follows that the mean displacement, defined by (5), is quantized and robust. It changes sharply from 0 to -1 as the inter-dimer tunneling strength ν' exceeds the intra-dimer tunneling strength ν, and is independent of the decay rate $\gamma > 0$.

Physically, this result can be understood as follows: when the inter-dimer coupling ν' is small, the wave packet is primarily absorbed on the loss site within the initial dimer; on the other hand, when the inter-dimer coupling ν' becomes large, the loss-site corresponding to absorption is in the dimer to the left, with index $m = -1$. Although the mean-time to absorption depends on the decay rate γ, since (5) integrates over all possible times, the final result is independent of the decay rate. Being topological in its origin, the analytical result for Δm is independent of the loss strength and small disorder, but is valid only for the specific initial state in an infinite lattice [32]. Experimentally, the transition is substantially softened and broadened due to the finite size and disorder effects [33]. It follows from Fig. 1 that a dimer lattice with $\nu' > \nu$ after time reversal and shift by half-a-cell is equivalent to a dimer lattice with $\nu < \nu'$.

These two lattices—a $\mathscr{P}\mathscr{T}$-symmetric dimer lattice [31] and the purely lossy dimer lattice á la Rudner and Levitov [32]—are equivalent to each other because their respective Hamiltonians differ only by a non-hermitian shift proportional to the identity, $H(\nu, \nu', \gamma) = i\gamma \cdot \mathbf{1} + H^L(\nu, \nu', \gamma)$. Therefore, we can define a scaled mean-displacement by considering the intensities on the lossy sublattice [34],

$$\Delta m_{PT}(\nu, \nu', \gamma) = \sum_m m \int_0^\infty dt\, 4\gamma e^{-2\gamma t} I_L(m, t). \tag{6}$$

It follows that the scaled mean displacement Δm_{PT} undergoes a topological transition at $\nu' = \nu$ which corresponds to a vanishing $\mathscr{PT}$-breaking threshold, $\gamma_{PT} = |\nu - \nu'| = 0$. Therefore, in a $\mathscr{PT}$-symmetric dimer, the topological transition in Δm_{PT} always occurs in the $\mathscr{PT}$-broken phase. Note that for a general initial state, the intensities $I_G(m, t)$ and $I_L(m, t)$ on both sub-lattices increase exponentially with time in the $\mathscr{PT}$-symmetry broken phase. However, the integral in (6) converges. In the following section, we numerically investigate the signatures of this transition in the site- and time-dependent intensities $I_G(m, t)$ and $I_L(m, t)$ on the gain and loss sublattices respectively.

3 Numerical Results

The two independent transitions in the $\mathscr{PT}$-symmetric dimer lattice are driven by two dimensionless parameters, namely the tunneling ratio ν'/ν which governs the topological transition, and the gain-loss strength γ/ν which determines the $\mathscr{PT}$-breaking phase boundary. Figures 3 and 4 show the gain and loss sublattice intensities for $\nu'/\nu = \{0, 0.5, 1, 1.5, 2\}$ and $\gamma/\nu = \{0, 0.5, 1\}$. In each frame, the vertical axis denotes the dimer index m ranging from -20 to 20, and the horizontal axis denotes normalized time νt ranging from 0 to 10. Note that when $\nu'/\nu = 0$ (top row in all panels), the system consists of uncoupled, $\mathscr{PT}$-symmetric dimers, and therefore the wave packet remains confined to the central dimer alone; as ν'/ν increases, the lateral spread of the wave packet across the lattice also increases.

First, let us consider the time evolution of a wave packet initially localized on the gain site of the central dimer, $|\psi(0)\rangle = \delta_{m0}|mG\rangle$. Panel (a) in Fig. 3 shows the gain-sublattice intensity $I_G(m, t)$ and panel (b) shows the corresponding loss-sublattice intensity $I_L(m, t)$. Note that the topological transition occurs across the central row, $\nu' = \nu$, whereas the $\mathscr{PT}$-breaking transition occurs across the two dot-dashed grey lines, given by $\gamma/\nu = |1 - \nu'/\nu|$. Therefore, in both panels, we see that the sublattice intensities are bounded and oscillatory in the $\mathscr{PT}$-symmetric phase (PT-S). In the $\mathscr{PT}$-broken phase (PT-B), the gain-sublattice distribution $I_G(m, t)$ shows a single Gaussian whose intensity is maximum at $\nu' = \nu$ because it corresponds to a vanishing $\mathscr{PT}$-breaking threshold. The loss-sublattice distribution $I_L(m, t)$ also shows a single Gaussian, except at $\nu' = \nu$, when the intensity shows a symmetric, bimodal distribution, marked by the white oval in panel (b).

The time-evolution of a state initially localized on the loss-site of the central dimer, $|\psi(0)\rangle = \delta_{m0}|mL\rangle$ is shown in Fig. 4. Note that in this case, the mean displacement Δm_{PT} does not undergo any change as ν'/ν is varied; it remains zero, meaning the particle is primarily absorbed on the loss-site it is initially located on [33]. The dash-dotted gray lines in both panels denote the $\mathscr{PT}$-symmetry breaking threshold $\gamma/\nu = |1 - \nu'/\nu|$. Both panels show that in the $\mathscr{PT}$-symmetric phase (PT-S), the time-evolution is oscillatory and the net intensities on the gain and the loss sublattices are comparable to each other.

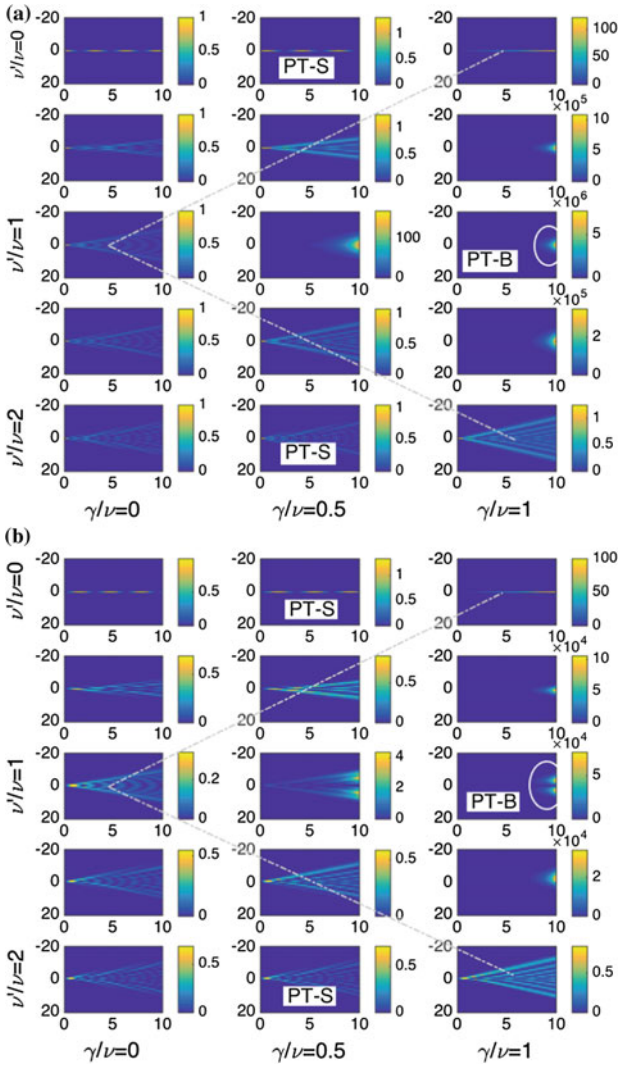

Fig. 3 Evolution of gain-sublattice (**a**) and loss-sublattice (**b**) intensities for $0 \leq \nu'/\nu \leq 2$ and $0 \leq \gamma/\nu \leq 1$, and an initial state on the gain-site of the central dimer, $|\psi(0)\rangle = \delta_{m0}|mG\rangle$. The *vertical axis* in each frame denotes the dimer index m and the *horizontal axis* denotes normalized time νt. The *dot-dashed gray lines* denote the $\mathscr{P}\mathscr{T}$-symmetric phase boundary $\gamma_{PT}/\nu = |1 - \nu'/\nu|$. In the $\mathscr{P}\mathscr{T}$-symmetric phase (*PT-S*), the intensities are bounded and oscillatory. In the $\mathscr{P}\mathscr{T}$-broken phase (*PT-B*), they are Gaussian except for the loss-sublattice distribution $I_L(m, t)$ at the topological transition $\nu = \nu'$, denoted by a white oval in (**b**)

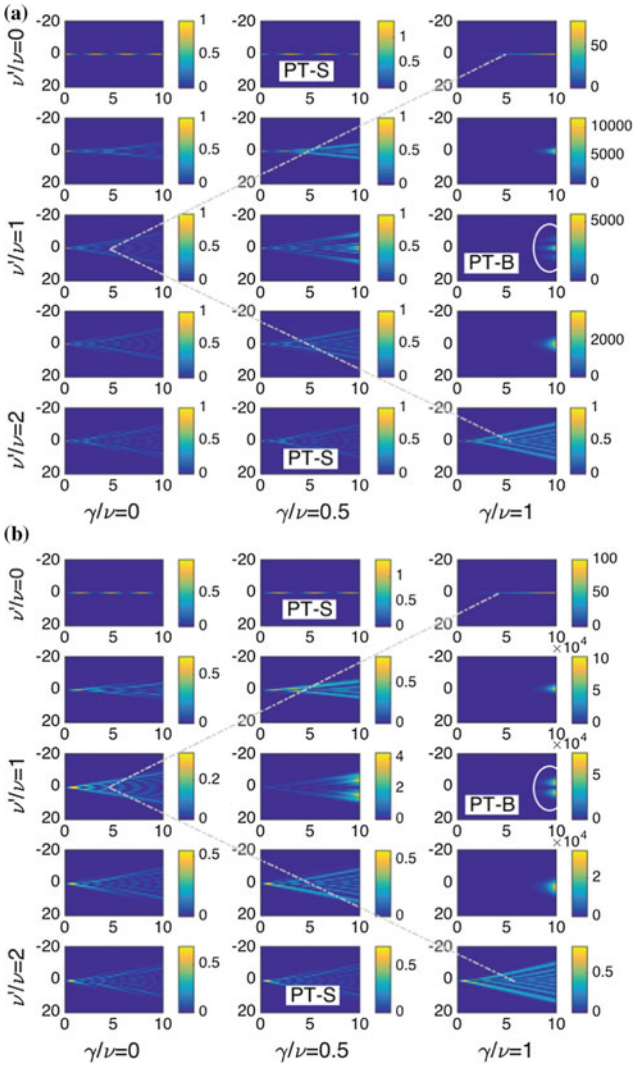

Fig. 4 Loss-sublattice (**a**) and gain-sublattice (**b**) intensities for an initial state localized on the loss site, $|\psi(0)\rangle = \delta_{m0}|mL\rangle$. The *vertical axis* in each frame denotes the dimer index m and the *horizontal axis* denotes normalized time νt. The *dot-dashed gray lines* denote the $\mathscr{P}\mathscr{T}$-symmetric phase boundary $\gamma_{PT}/\nu = |1 - \nu'/\nu|$. Both intensities $I_L(m,t)$ and $I_G(m,t)$ show Gaussian behavior except at $\nu' = \nu$, marked by *white ovals* in both panels

Panel (a) shows that in the $\mathscr{P}\mathscr{T}$-broken phase (PT-B), the loss-sublattice intensity profile $I_L(m,t)$ has a *symmetric, trimodal distribution*, marked by a white oval in (a) when $\nu'/\nu = 1$. This is in sharp contrast to the results for $\nu'/\nu \neq 1$, when the distribution consists of a single Gaussian. Panel (b) shows that in the $\mathscr{P}\mathscr{T}$-broken

phase, the average gain-site intensity is orders of magnitude higher than the average loss-site intensity. The gain intensity $I_G(m,t)$ shows a symmetric, bimodal distribution exactly at $v'/v = 1$ whereas for $v'/v \neq 1$, the intensity distribution has a single Gaussian peak.

Thus, the key numerical observations can be summarized as follows. At $v'/v = 1$, when the winding number of $v_k = v + v' \exp(ik)$ changes from 0 to 1, for an initial state on the gain sublattice, the gain intensity $I_G(m,t)$ shows a single Gaussian peak, whereas the loss intensity $I_L(m,t)$ shows a two-peak structure. When the initial state is localized on the loss sublattice, the gain intensity $I_G(m,t)$ shows a two-peak structure whereas the loss intensity $I_L(m,t)$ shows a structure with three peaks. When $v'/v \neq 1$, both gain and loss intensities show a single Gaussian peak at long times in the $\mathscr{P}\mathscr{T}$-broken region. In the next section, we will analytically investigate this behavior.

4 Analytical Approximations in the $\mathscr{P}\mathscr{T}$-Broken Region

In this section, we will develop approximate analytical expressions for the real-space, time-dependent wave functions for the two sublattices in the $\mathscr{P}\mathscr{T}$-broken region. As discussed in Sect. 2, the $\mathscr{P}\mathscr{T}$-symmetric dimer Hamiltonian is most easily diagonalized in the Fourier space, and the first emergence of complex-conjugate eigenvalues occurs at $k = \pi$. In the $\mathscr{P}\mathscr{T}$-broken phase, the 2×2 time evolution operator is given by [10]

$$G_k(t) = \exp(-i H_k t) = \cosh(\Gamma_k t)\mathbf{1} - i \frac{H_k}{\Gamma_k} \sinh(\Gamma_k t), \tag{7}$$

where $\Gamma_k = \sqrt{\gamma^2 - |v_k|^2} > 0$ is the effective amplification rate. At long times $\Gamma_k t \gg 1$, the Fourier-space time-evolution operator becomes $G_k(t) = \exp(\Gamma_k t)(\mathbf{1} - i H_k/\Gamma_k)/2$. Therefore, equivalently, the real space propagator is given by

$$G_{mn}(t) = \frac{1}{4\pi} \int_0^{2\pi} dk\, e^{i(m-n)k + \Gamma_k t} \left(\mathbf{1} - i \frac{H_k}{\Gamma_k} \right). \tag{8}$$

Note that (8) is valid in the $\mathscr{P}\mathscr{T}$-broken phase even if the eigenvalues of H_k are real for momenta away from $k = \pi$. These momenta, with real eigenvalues ϵ_k, lead to a time evolution operator $G_k(t)$ with bounded norm, and therefore their contribution to (8) is vanishingly small at long times $\Gamma_k t \gg 1$. Since the largest contribution to the integral arises from a vanishingly small neighborhood of $k = \pi + p$, the integrand in (8) is estimated by approximating $\Gamma_{\pi+p} \approx \Gamma - Dp^2/2$ with $\Gamma^2 = \gamma^2 - \gamma_{PT}^2$ and $D = vv'/\Gamma$, leading to

$$G_{m0}(t) = \frac{(-1)^m e^{\Gamma t}}{4\pi} \int_{-\infty}^{\infty} dp\, e^{ipm - Dtp^2/2} \begin{bmatrix} 1+\frac{\gamma}{\Gamma} & -\frac{i}{\Gamma}(\nu - \nu' e^{+ip}) \\ -\frac{i}{\Gamma}(\nu - \nu' e^{-ip}) & 1 - \frac{\gamma}{\Gamma - Dp^2/2} \end{bmatrix}. \tag{9}$$

Here, without loss of generality, we have chosen $n = 0$ as the location of the initial wave packet, and extended the integration range for p to the entire real line because in the long-time limit, $Dt \gg 1$, the integrand contains a Gaussian sharply peaked at $p = 0$. We have retained the p^2 dependence in the denominator of one of the matrix elements because the matrix element otherwise vanishes at the topological transition boundary $\nu = \nu'$. It is now straightforward to carry out the Gaussian integrals and obtain explicit expressions for the time-dependent wave function at long times in the $\mathscr{P}\mathscr{T}$-broken phase.

For an initial state localized on the gain-sublattice, $|\psi(0)\rangle = \delta_{n0}|nG\rangle$ (Fig. 3), we obtain the following expressions for the gain and loss sublattice wave functions,

$$\psi_G(m,t) \sim \frac{(-1)^m e^{\Gamma t}}{\sqrt{8\pi Dt}} \left(1 + \frac{\gamma}{\Gamma}\right) \exp\left[-\frac{m^2}{2Dt}\right], \tag{10}$$

$$\psi_L(m,t) \sim \frac{i(-1)^m e^{\Gamma t}}{\Gamma\sqrt{8\pi Dt}} \left\{ \nu \exp\left[-\frac{m^2}{2Dt}\right] - \nu' \exp\left[-\frac{(m+1)^2}{2Dt}\right] \right\}. \tag{11}$$

Note that both wave functions grow exponentially with the amplification rate $\Gamma \leq \gamma$. It follows from (10) that the wave function $\psi_G(m,t)$ describes a classical, diffusing particle with diffusion constant $D = \nu\nu'/\Gamma$. This result is expected because, in the $\mathscr{P}\mathscr{T}$-broken phase, where the wave packet intensity increases exponentially with time, we should recover the classical behavior [35]. For the loss sublattice, we find that $\psi_L(m,t)$ is the difference of two diffusing Gaussians with centers at $m = 0$ and $m = -1$ respectively, weighted by the intra-dimer and inter-dimer tunneling strengths. In particular when the topological transition takes place, $\nu = \nu'$, the loss sublattice wave function $\psi_L(m,t)$ shows a symmetric, two-peak structure.

For an initial state localized on the loss-sublattice, $|\psi(0)\rangle = \delta_{n0}|nL\rangle$ (Fig. 4), the wave functions are given by

$$\psi_G(m,t) \sim \frac{i(-1)^m e^{\Gamma t}}{\Gamma\sqrt{8\pi Dt}} \left\{ \nu \exp\left[-\frac{m^2}{2Dt}\right] - \nu' \exp\left[-\frac{(m-1)^2}{2Dt}\right] \right\}, \tag{12}$$

$$\psi_L(m,t) \sim \frac{(-1)^m e^{\Gamma t}}{\sqrt{8\pi Dt}} e^{-m^2/2Dt} \left[1 - \frac{\gamma}{\Gamma}\left(1 + \frac{1}{2\Gamma t} - \frac{m^2}{2\nu\nu' t^2}\right)\right]. \tag{13}$$

It follows from (12) that the gain-sublattice intensity distribution is the difference of two diffusing Gaussians centered at $m = 0$ and $m = +1$, weighted by the tunneling strengths. In particular, when $\nu = \nu'$, we obtain the symmetric, bimodal distribution seen in panel (b) of Fig. 4. Equation (13) implies that the loss-sites wave function $\psi_L(m,t)$ is a diffusing Gaussian centered at $m = 0$. However, *only at* $\nu = \nu'$, *the leading order term in the square bracket vanishes*. It generates a multiplicative factor

$(1 - m^2/Dt)$ that accompanies the diffusive Gaussian. This implies that the loss-sublattice intensity vanishes at $m^* = \pm\sqrt{Dt} = \pm\sqrt{v^2 t/\gamma}$, and gives rise to the three-peak structure seen in panel (a) of Fig. 4.

These results can be easily generalized to an arbitrary state on the central dimer, $|\psi(0)\rangle = \delta_{n0}(\cos\theta|nG\rangle + \sin\theta e^{i\phi}|nL\rangle)$. When the initial state has a transverse momentum, $\phi \neq 0 \mod \pi$, the system does not undergo a topological transition [34], whereas when $\phi = 0 \mod \pi$, it has a quantized scaled mean displacement.

5 Conclusion

In this paper, we have investigated the interplay between two transitions that are predicted to take place in a $\mathscr{P}\mathscr{T}$-symmetric dimer (or SSH) model. The $\mathscr{P}\mathscr{T}$-symmetry breaking transition is governed by the gain-loss strength γ relative to the tunneling modulation strength $|v - v'|$, whereas the topological transition in the scaled mean displacement Δm_{PT} is governed by the ratio of the inter-dimer to intra-dimer tunneling v'/v.

We have shown that the gain and loss sublattice intensity profiles, $I_G(m, t)$ and $I_L(m, t)$ respectively, show distinct features at the intersection of the topological transition $v = v'$ and the $\mathscr{P}\mathscr{T}$-symmetry breaking transition $\gamma_{PT} = |v - v'|$. These features can be understood through the long-time behavior of the gain-site and loss-site wave functions, which also capture the classical, diffusive behavior that is expected in the $\mathscr{P}\mathscr{T}$-broken phase. Although experimental realization of an active SSH model, where half the waveguides have a constant amplification, is challenging, it is feasible with the current sample fabrication technology; therefore, we expect that all of its attendant properties, including symmetric, edge-localized states will be observable in it.

In this work, we have not considered the effects of nonlinearity [36]. In the $\mathscr{P}\mathscr{T}$-broken phase, the nonlinearity manifests itself in two ways. First, it introduces a state-dependent potential $V_G(m) \propto |\psi_G(m, t)|^2$ on each gain site and a corresponding potential $V_L(m)$ on each loss site; physically, this potential represents the intensity-dependent change in the local index of refraction [37–39]. Second, as the site-dependent intensity increases, the model with *constant, local-intensity independent* gain and loss coefficients becomes less reliable [40]. Thus, our findings are valid in a range of parameters where the effects of nonlinearity are mitigated. They suggest that the interplay between the $\mathscr{P}\mathscr{T}$-symmetry breaking transition, and the topological transitions in one or two dimensional $\mathscr{P}\mathscr{T}$-symmetric models leads to interesting results.

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Physical Aspect of Exceptional Point in the Liouvillian Dynamics for a Quantum Lorentz Gas

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Abstract Physical aspect of the exceptional point in the spectrum of the Liouville-von Neumann operator (Liouvillian) is discussed. The example we study in this paper is the weakly-coupled one-dimensional quantum perfect Lorentz gas. The effective Liouvillian for the system derived by applying the Brillouin-Wigner-Feshbach formalism takes non-Hermitian form due to resonance singularity, thus its spectra take complex values. We find that the complex spectra has two second order exceptional points in the wavenumber space. As a physical effect of the exceptional points, we show that the time evolution of the Wigner distribution function is described by the telegraph equation. The time evolution described by the telegraph equation shows a shifting motion in space. We also show that mechanism of the shifting motion completely changes at the exceptional points.

1 Introduction

In modern physics, the importance of non-Hermitian operator as a generator of motion has been recognized in many area of physics, both on an applied level and on a fundamental level. A typical example of the appearance of non-Hermitian operator is in a situation where we discuss irreversible processes. For example, in decaying processes in unstable systems, the effective Hamiltonian takes a non-Hermitian form

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[1–3]. Non-Hermitian operator also plays a central role in PT (parity-time) symmetric systems [4–7].

In statistical mechanics, the Liouville-von Neumann operator (Liouvillian) generates time evolution of the distribution function, or of the density matrix [8]. As in the case of the effective Hamiltonian in open quantum systems, the effective Liouvillian takes a non-Hermitian form for thermodynamic systems where the intensive variables and the extensive variables exist in the thermodynamic limit [9].

Among many characteristic properties of the non-Hermitian operator, the appearance of the exceptional points in parameter space is especially interesting and it has been studied in many contexts in recent years [10–13]. The exceptional point is a singular point in the parameter space at which both eigenvalues and eigenvectors coalesce [10]. As a result, the non-Hermitian operator cannot be diagonalized at the point. Instead, the operator can be reduced to the Jordan block form. In the time evolution of the wave function in the Hamiltonian dynamics, the Jordan block leads to a linear time dependence besides the usual exponential time behavior as $t \exp[-\gamma t]$ [11]. Such time behavior at the exceptional point has been studied recently, for example, in [12] for an optical microcavity and in [13] for Rabi oscillation.

In our recent study, we have found that the exceptional point also appears in the spectrum of the Liouvillian for variety of physical systems both in quantum and classical mechanics. Such systems include the one-dimensional (1D) quantum perfect Lorentz gas [14], the two-dimensional classical perfect Lorentz gas [15] and the one-dimensional polaron system [16]. Although the physics of the exceptional point in Hamiltonian dynamics has been studied extensively, the study of the exceptional point in the Liouvillian dynamics is still in a poor level, as far as the authors knowledge.

The main purpose of this paper is to report our recent results on the physical effects of the exceptional points in the Liouvillian dynamics. The example we discuss in this paper is the weakly-coupled 1D quantum perfect Lorentz gas [14, 15]. The Lorentz gas is one of the simplest system that have the exceptional point in the spectrum of the Liouvillian.

In this paper, we shall show that the spectrum of the Liouvillian for the system has the second order exceptional points in the wavenumber space. We shall discuss physical effect of the exceptional points by analyzing time evolution of the Wigner distribution function. We shall show that the second order exceptional point leads to the telegraph equation in its spatial time evolution. There we shall also show that the time evolution of the distribution function in space shows a shifting motion, but its mechanism completely changes at the exceptional points; one is due to asymmetry of the momentum distribution function, while the other is due to wave propagation associated to the real part of the complex spectrum.

The structure of the paper is as follows: In Sect. 2, we introduce the model. In Sect. 3, we summarize essential formulae in the Liouville space description. In Sect. 4, we briefly summarize the complex spectral representation of the Liouvillian. In Sect. 5, we derive the effective Liouvillian for the system. In Sect. 6, we show a solution of the eigenvalue problem of the effective Liouvillian. In Sect. 7, we discuss the relation between the time evolution of the system and the exceptional points. In Sect. 8, we give a summary and a concluding remark.

2 System

We consider a weakly-coupled one-dimensional (1D) quantum Lorentz gas. The Lorentz gas consists of one light-mass particle (the test particle) with mass m and N heavy particles with mass M. We suppose that the system is enclosed in a large 1D box of volume L with the periodic boundary condition. The Hamiltonian of the system is given by

$$H = H_0 + gV = \frac{p^2}{2m} + \sum_{j=1}^{N} \frac{p_j^2}{2M} + g \sum_{j=1}^{N} \frac{1}{\Omega} \sum_{n} V_{q_n} e^{iq_n(x-x_j)}, \tag{1}$$

where g is a dimensionless coupling constant, $\Omega \equiv L/2\pi$ and $q_n \equiv n\Delta q$ with $\Delta q \equiv 1/\Omega$ and $n = 0, \pm 1, \pm 2, \ldots$. The interaction is given by the Fourier expansion of $V(|x - x_j|)$ with $V_{q_n} = V_{|q_n|}$, which is assumed to be a short-range repulsive potential. We assume V_{q_n} is a continuous function at $q_n = 0$ in the continuous limit $\Delta q \to 0$, and satisfies the condition $O(|q_n|^{3/2}) < \left|V_{q_n}\right| < O(|q_n|^{1/2})$ for $q_n \to 0$, in order to avoid a singular transport process characteristic in 1D system. We also consider the weak-coupling situation ($g \ll 1$). In the following analysis, we restrict our attention to the limit $m/M \to 0$ in which the system is called the *perfect Lorentz gas* [17].

In this paper, we shall consider the thermodynamic limit,

$$L \to \infty, \quad N \to \infty, \quad c \equiv \frac{N}{L} = \text{finite}, \tag{2}$$

where c is the concentration of heavy particles. In this limit, we have $\Delta q \to 0$ and the wavenumber and the momentum become continuous variables. At an appropriate stage, we shall replace a summation with an integration and a Kronecker delta δ^{Kr} with a Dirac δ-function as

$$\frac{1}{\Omega} \sum_{q} \to \int dq, \quad \Omega_\hbar \delta^{Kr}(P - P') \to \delta(P - P'), \tag{3}$$

with $\Omega_\hbar \equiv \Omega/\hbar$ (Hereafter we use a conventional notation $\sum_q$ for $\sum_n$ and drop the index n in q_n).

In this paper we investigate the time evolution of the reduced density matrix for the test particle, which is defined as

$$f(t) \equiv \mathrm{Tr}_{\mathrm{hev}}[\rho(t)], \tag{4}$$

where $\rho(t)$ is the density matrix for the whole system and $\mathrm{Tr}_{\mathrm{hev}}$ denotes a partial trace over all heavy particles. We assume that the initial condition of the system is given by

$$\rho(0) = f(0) \otimes \rho_{\mathrm{hev}}^{eq}, \tag{5}$$

where $\rho_{\rm hev}^{eq}$ is the Maxwell distribution of the heavy particles with temperature T,

$$\rho_{\rm hev}^{eq} = \prod_{j=1}^{N} \frac{\exp(-p_j^2/2Mk_BT)}{\mathrm{Tr}[\exp(-p_j^2/2Mk_BT)]}, \tag{6}$$

where k_B is the Boltzmann constant. In the thermodynamic limit the time evolution of the density matrix associated with the heavy particles is negligible since its deviation from $\rho_{\rm hev}^{eq}$ is proportional to $1/L$ in this limit, as can be easily shown.

3 The Liouville Space Description

The time evolution of the system is governed by the Liouville-von Neumann equation for the density matrix $\rho(t)$,

$$i\frac{\partial}{\partial t}\rho(t) = L_H\rho(t). \tag{7}$$

Here L_H is the Liouville-von Neumann operator (Liouvillan in short) which is defined by $L_H\rho \equiv [H, \rho]/\hbar$.

To discuss the space and momentum dependence of the distribution of the particles in parallel with classical mechanics, it is convenient to introduce the Wigner distribution function:

$$\rho^W(X, \{X_j\}, P, \{P_j\}, t) \equiv \frac{1}{L^{N+1}} \sum_{k,\{k_j\}} \rho_{k,\{k_j\}}(P, \{P_j\}, t) e^{i(kX+k_1X_1+\cdots+k_NX_N)}, \tag{8}$$

which is a quantum analog of the phase space distribution function [9]. Here the notation $\{X_j\}$ represents a set of variables for the N heavy particles and

$$\begin{aligned}\rho_{k,\{k_j\}}(P, \{P_j\}, t) &\equiv \left\langle P + \frac{\hbar}{2}k, \left\{P_j + \frac{\hbar}{2}k_j\right\}\middle|\rho(t)\middle|P - \frac{\hbar}{2}k, \left\{P_j - \frac{\hbar}{2}k_j\right\}\right\rangle \\ &\equiv \langle\langle k, \{k_j\}; P, \{P_i\}|\rho(t)\rangle\rangle,\end{aligned} \tag{9}$$

where the single bra-ket vectors stand for vectors in the wave function space and the double bra-ket vectors stand for vectors in the Liouville space [9]. Here the "wavenumbers" and the "momenta" in the Wigner representation are defined as

$$k \equiv \frac{p - p'}{\hbar}, \quad P \equiv \frac{p + p'}{2}, \tag{10}$$

and the Wigner basis is defined by a dyad of two eigenstates of H_0 as

$$|k, \{k_j\}; P, \{P_j\}\rangle\rangle \equiv |p, \{p_j\}\rangle\langle p', \{p_j'\}|. \tag{11}$$

We represent a linear operator A in the wave function space as a ket-vector $|A\rangle\rangle$ in the Liouville space. The inner product of the bra- and ket-vectors is then defined by $\langle\langle B|A\rangle\rangle = \mathrm{Tr}[B^\dagger A]$, where $B^\dagger$ is the Hermitian conjugate of a liner operator B. As a result, it is easy to show that the Wigner basis vectors are normalized with respect to the box normalization condition

$$\begin{aligned}&\langle\langle k,\{k_j\};P,\{P_j\}|k',\{k'_j\};P',\{P'_j\}\rangle\rangle \\ &= \delta^{Kr}(k-k')\delta^{Kr}(P-P')\prod_{j=1}^{N}\delta^{Kr}(k_j-k'_j)\delta^{Kr}(P_j-P'_j). \end{aligned} \tag{12}$$

4 The Complex Spectral Representation of the Liouvillian

The eigenvalue problem of the Liouvillian is given by

$$L_H|F_\alpha^{(\nu)}\rangle\rangle = Z_\alpha^{(\nu)}|F_\alpha^{(\nu)}\rangle\rangle, \quad \langle\langle\tilde{F}_\alpha^{(\nu)}|L_H = \langle\langle\tilde{F}_\alpha^{(\nu)}|Z_\alpha^{(\nu)}, \tag{13}$$

where the indices α and ν specify an eigenstate (especially ν denotes the spatial correlation subspace (see [9])), and $|F_\alpha^{(\nu)}\rangle\rangle$ and $\langle\langle\tilde{F}_\alpha^{(\nu)}|$ are right- and left-eigenstates of the Liouvillian, respectively. We solve the eigenvalue problem of the Liouvillian by using the well-known Brillouin-Wigner-Feshbach formalism with projection operators $P^{(\nu)}$ and $Q^{(\nu)}$ satisfying the following relations,

$$P^{(\nu)}L_0 = L_0P^{(\nu)},\ P^{(\nu)}P^{(\mu)} = \delta_{\nu,\mu},\ \sum_\nu P^{(\nu)} = \hat{I}_{N+1},\quad P^{(\nu)}+Q^{(\nu)} = \hat{I}_{N+1}, \tag{14}$$

where $\hat{I}_{N+1}$ is the unit operator for the $N+1$ particle system. By applying these projection operators on the first equation in (13), we have

$$\Psi^{(\nu)}(Z_\alpha^{(\nu)})P^{(\nu)}|F_\alpha^{(\nu)}\rangle\rangle = Z_\alpha^{(\nu)}P^{(\nu)}|F_\alpha^{(\nu)}\rangle\rangle, \tag{15}$$

where

$$\Psi^{(\nu)}(z) \equiv P^{(\nu)}L_HP^{(\nu)} + P^{(\nu)}L_HQ^{(\nu)}\frac{1}{z-Q^{(\nu)}L_HQ^{(\nu)}}Q^{(\nu)}L_HP^{(\nu)}, \tag{16}$$

is the *effective Liouvillian*. Its second term is the self-frequency part that corresponds to the self-energy part of an effective Hamiltonian in the case of the Hamiltonian operator in the wave function space. The effective Liouvillian is also called the *collision operator* which is a central object in the kinetic theory in non-equilibrium statistical mechanics [8, 9]. One can see from its eigenvalue equation (15) that the collision operator shares the eigenvalues with the Liouvillian. The eigenvalue

equation of the effective Liouvillian (15) is *non-linear*, i.e. the effective Liouvillian itself depends on the eigenvalue.

In terms of the right- and left-eigenstates of the effective Liouvillian $\Psi^{(\nu)}(z)$, the right- and the left-eigenvectors of the original Liouvillian L_H are given by

$$|F_\alpha^{(\nu)}\rangle\!\rangle = \left[P^{(\nu)} + \mathscr{C}^{(\nu)}(Z_\alpha^{(\nu)})\right]P^{(\nu)}|F_\alpha^{(\nu)}\rangle\!\rangle, \quad \langle\!\langle \tilde{F}_\alpha^{(\nu)}| = \langle\!\langle \tilde{F}_\alpha^{(\nu)}|P^{(\nu)}\left[P^{(\nu)} + \mathscr{D}^{(\nu)}(Z_\alpha^{(\nu)})\right], \tag{17}$$

where

$$\mathscr{C}^{(\nu)}(z) = \frac{1}{z - Q^{(\nu)}L_H Q^{(\nu)}} Q^{(\nu)} L_H P^{(\nu)}, \quad \mathscr{D}^{(\nu)}(z) = P^{(\nu)} L_H Q^{(\nu)} \frac{1}{z - Q^{(\nu)}L_H Q^{(\nu)}} \tag{18}$$

are the *creation-of-correlation operator* and the *destruction-of-correlation operator*, respectively, which are off-diagonal transitions between the $Q^{(\nu)}$ subspace and the $P^{(\nu)}$ subspace [9].

It is well-known for an unstable quantum system with a continuous spectrum that the effective Hamiltonian becomes a non-Hermitian operator due to the resonance singularity in the self-energy part [1]. Similarly, the effective Liouvillian becomes a non-Hermitian operator in the Liouville space in the thermodynamic limit. As a result, the effective Liouvillian has eigenstates with complex eigenvalues that are called *resonance states*. The imaginary part of the complex eigenvalue of the Liouvillian gives a transport coefficient of the system [18].

5 Effective Liouvillian for the System

We apply the general formalism presented above to the weakly-coupled 1D quantum perfect Lorentz gas. In the weak-coupling situation, the effective Liouvillian can be approximated up to the second order in g as

$$\Psi_2^{(k)}(z) = P^{(k)} L_0 P^{(k)} + g^2 P^{(k)} L_V Q^{(k)} \frac{1}{z - L_0} Q^{(k)} L_V P^{(k)}. \tag{19}$$

Here we define the projection operators as

$$P^{(k)} \equiv \frac{1}{\Omega_\hbar^{N+1}} \sum_{P,\{P_j\}} |k, \{0_j\}; P, \{P_j\}\rangle\!\rangle\langle\!\langle k, \{0_j\}; P, \{P_j\}|, \tag{20}$$

and $Q^{(k)} \equiv 1 - P^{(k)}$, where we have used the notation $\{0_j\}$ to indicate that all wavenumbers associated to the heavy particle are zero. For the projection operator $P^{(k)}$, we have

$$P^{(k)}L_0P^{(k)}|k,\{0_j\};P,\{P_j\}\rangle\!\rangle = \frac{kP}{m}|k,\{0_j\};P,\{P_j\}\rangle\!\rangle, \tag{21}$$

and

$$P^{(k)}gL_VP^{(k)} = 0, \tag{22}$$

because of the condition $V_0 = 0$.

We focus our attention on the test particle, then we trace out the variables for the heavy particles. We also take the limit $m/M \to 0$ to obtain the perfect Lorentz gas. Thus we define the reduced effective Liouvillian for the 1D quantum perfect Lorentz gas as

$$\psi^{(k)}(z) \equiv \lim_{m/M\to 0} \mathrm{Tr}_{\mathrm{hev}}[\Psi_2^{(k)}(z)\rho_{\mathrm{hev}}^{eq}]. \tag{23}$$

Expression of a matrix element of the reduced effective Liouvillian in the Wigner representation is given by

$$\langle\!\langle k;P|\psi^{(k)}(z)|k;P'\rangle\!\rangle = \left[\frac{kP}{m} - \frac{2\pi g^2 c}{\hbar^2}\frac{1}{\Omega}\sum_{q\neq 0}|V_q|^2\partial_P^{\hbar q/2}\frac{1}{z-(k-q)P/m}\partial_P^{\hbar q/2}\right] \times\delta_{\Omega_\hbar}(P-P'), \tag{24}$$

where we have dropped the variables for the heavy particles on the Wigner basis, and $\partial_P^{\hbar q/2} \equiv \hat{\eta}_P^{\hbar q/2} - \hat{\eta}_P^{-\hbar q/2}$ with $\hat{\eta}_P^{\hbar q/2} f(P) = f(P+\hbar q/2)$. Note that the expression (24) does not depend on the temperature of the heavy particles T. This is due to the limit of the perfect Lorentz gas $m/M \to 0$ where there is no energy exchange between the test particle and the heavy particles.

For the reduced effective Liouvillian, we write the eigenvalue problem as

$$\psi^{(k)}(z_\alpha^{(k)})|u_\alpha^{(k)}\rangle\!\rangle = z_\alpha^{(k)}|u_\alpha^{(k)}\rangle\!\rangle, \quad \langle\!\langle\tilde{v}_\alpha^{(k)}|\psi^{(k)}(z_\alpha^{(k)}) = z_\alpha^{(k)}\langle\!\langle\tilde{v}_\alpha^{(k)}|, \tag{25}$$

We note that $z_\alpha^{(k)} = Z_\alpha^{(k)}$ for our Lorentz gas, because the heavy particles are in an eigenstate with zero eigenvalue, i.e. they remain in thermal equilibrium. The effective Liouvillian in (25) depends on its eigenvalue. In this sense, the eigenvalue equation is non-linear. Assuming bicompleteness in the subspace

$$\hat{p}^{(k)} \equiv \frac{1}{\Omega_\hbar}\sum_P |k;P\rangle\!\rangle\langle\!\langle k;P|, \tag{26}$$

we can always construct sets of eigenstates $\{\langle\!\langle\tilde{u}_\alpha^{(k)}|\}$, which is biorthogonal to $\{|u_\alpha^{(k)}\rangle\!\rangle\}$, and $\{|v_\alpha^{(k)}\rangle\!\rangle\}$, which is orthogonal to $\{\langle\!\langle\tilde{v}_\alpha^{(k)}|\}$, with $\langle\!\langle\tilde{u}_\alpha^{(k)}| \neq \langle\!\langle\tilde{v}_\alpha^{(k)}|$ and $|v_\alpha^{(k)}\rangle\!\rangle \neq |u_\alpha^{(k)}\rangle\!\rangle$ [9].

6 Solution of the Eigenvalue Problem

6.1 The Boltzmann Approximation

In order to solve the eigenvalue problem (25), here we study a situation where the wavenumber k satisfies

$$|k| \ll d^{-1}, \tag{27}$$

where d is the interaction range between particles. In this situation in addition to the weak-coupling, we shall show that the eigenvalue dependence of the effective Liouvillian (24) is negligible and the non-linear eigenvalue problem (25) is linearized. There the effective Liouvillian is reduced to the phenomenological Boltzmann collision operator.

For a spatial inhomogeneity satisfying the condition (27), a typical value of q appearing in V_q is much larger than k in (24), i.e., $|k| \ll |q|$. Then we can neglect k in the denominator in the second term in (24). On the other hand, we may expect that the imaginary part of the eigenvalue z in (25) is proportional to g^2 for $g \ll 1$ because of the factor g^2 in front of the collision term in (24). If this is the case, we can evaluate z in (24) at $z = 0$. Then we have $\psi^{(k)}(z_\alpha^{(k)}) = \psi^{(k)}(+i0) + O(g^4)$. Here $+i0$ means that the collision operator $\psi^{(k)}(z)$ is evaluated on the real axis approaching from the upper half-plane of z to ensure the time evolution is oriented to the future $t > 0$ [9]. Combining these arguments, we can approximate $\psi^{(k)}(z_\alpha^{(k)})$ by the new operator given by

$$\langle\langle k;\, P|\psi_B^{(k)}|k;\, P'\rangle\rangle \equiv \left[\frac{kP}{m} - \frac{2\pi g^2 c}{\hbar^2} \lim_{\epsilon\to+0} \int_{-\infty}^{\infty} dq |V_q|^2 \partial_P^{\hbar q/2} \frac{1}{+i\epsilon + qP/m} \partial_P^{\hbar q/2}\right] \times \delta(P - P'), \tag{28}$$

where we have taken the thermodynamic limit (2). This is identical with the phenomenological Boltzmann collision operator for the 1D quantum perfect Lorentz gas [15, 19], for which the first term in the square bracket in (28) is called the flow term, and the second term is called Boltzmann's collision term.

By performing the q integration in (28), one can see that the Boltzmann collision operator has non-vanishing matrix elements only between the states $|k;\, P\rangle\rangle$ and $|k;\, -P\rangle\rangle$ [14]. Physically, this is because there are only forward and backward scattering in the 1D quantum system. Hence, in terms of these basis, the Boltzmann collision operator is represented by a 2×2 non-Hermitian matrix,

$$\psi_B^{(k)} = \begin{pmatrix} kP/m - ig^2\gamma_P/2 & ig^2\gamma_P/2 \\ ig^2\gamma_P/2 & -kP/m - ig^2\gamma_P/2 \end{pmatrix}, \tag{29}$$

with

$$g^2\gamma_P \equiv g^2\frac{8\pi^2 mc}{\hbar^2|P|}\left|V_{\frac{2P}{\hbar}}\right|^2, \tag{30}$$

where $\gamma_P \to 0$ for $P \to 0$ due to the condition $V_0 = 0$.

In terms of the Boltzmann collision operator, the time evolution equation of the reduced density matrix is given by

$$i\frac{\partial}{\partial t}\hat{p}^{(k)}|f(t)\rangle\!\rangle = \psi_B^{(k)}\hat{p}^{(k)}|f(t)\rangle\!\rangle, \tag{31}$$

which is the Boltzmann equation for the system.

6.2 Eigenstates of the Boltzmann Collision Operator

Let us denote the right- and left-eigenstates of the collision operator (29) as $|\phi_\alpha^{(k)}\rangle\!\rangle$ and $\langle\!\langle\tilde{\phi}_\alpha^{(k)}|$, respectively, i.e.,

$$\psi_B^{(k)}|\phi_\alpha^{(k)}\rangle\!\rangle = z_\alpha^{(k)}|\phi_\alpha^{(k)}\rangle\!\rangle, \quad \langle\!\langle\tilde{\phi}_\alpha^{(k)}|\psi_B^{(k)} = z_\alpha^{(k)}\langle\!\langle\tilde{\phi}_\alpha^{(k)}|. \tag{32}$$

Here we present the solution of the eigenvalue problem and show that the solution has exceptional points in the wavenumber k space.

The characteristic equation for (29) is given by

$$\det[\psi_B^{(k)} - z\hat{I}_2] = \left(z + i\frac{g^2\gamma_P}{2}\right)^2 - \left(\frac{kP}{m}\right)^2 + \left(\frac{g^2\gamma_P}{2}\right)^2 = 0, \tag{33}$$

where $\hat{I}_2$ is the unit matrix of size 2. Hence, the eigenvalues are

$$z_{\pm;P}^{(k)} = -i\frac{g^2\gamma_P}{2} \pm \frac{|P|}{m}(k^2 - k_P^2)^{1/2}, \tag{34}$$

where

$$k_P \equiv \frac{g^2\gamma_P}{2|P|/m} = \frac{1}{l_P}, \tag{35}$$

is a wavenumber that is equal to the inverse of the mean-free-length of the test particle with momentum P denoted by l_P.

In Fig. 1, we show a k-dependence of the real part and the imaginary part of the eigenvalues for $P \neq 0$. In the figures, the dashed lines and the dot-dashed lines represent the eigenvalues $z_{+;P}^{(k)B}$ and $z_{-;P}^{(k)B}$, respectively. The solid lines represent that these two lines overlap.

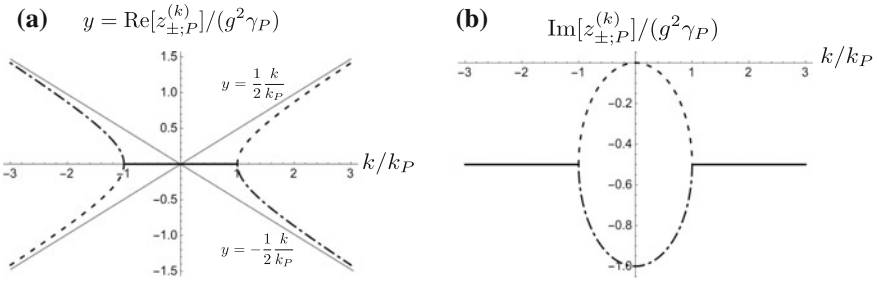

Fig. 1 Eigenvalues of the Boltzmann collision operator (34) are drawn as functions of k. **a** is the real part and **b** is imaginary part. In each figure, the *dashed lines* represent eigenvalue with $\alpha = +$ and the *dot-dashed* lines represent eigenvalue with $\alpha = -$. The *solid lines* represent that these two lines are overlapping. The *gray lines* in **a** represents eigenvalues of the Liouvillian for a free light-mass particle $y = \pm(1/2)(k/k_P)$

Corresponding right- and left-eigenvectors are

$$|\chi^{(k)}_{\pm;P}\rangle\rangle = \left[1 \pm \frac{(k^2 - k_P^2)^{1/2}_+}{k}\right]^{1/2} |k;|P|\rangle\rangle + i\frac{|k|}{k}\left[1 \mp \frac{(k^2 - k_P^2)^{1/2}}{k}\right]^{1/2} |k;-|P|\rangle\rangle, \tag{36a}$$

$$\langle\langle\tilde{\chi}^{(k)}_{\pm;P}| = \frac{|k|}{k}\left[1 \pm \frac{(k^2 - k_P^2)^{1/2}}{k}\right]^{1/2} \langle\langle k;|P|| + i\left[1 \mp \frac{(k^2 - k_P^2)^{1/2}}{k}\right]^{1/2} \langle\langle k;-|P||. \tag{36b}$$

Here we have not yet normalized the eigenvectors by taking account of the fact that we have a diverging normalization constant at $k = \pm k_P$ (see (39)). The inner products of these right- and left-eigenstates are given by

$$\langle\langle\tilde{\chi}^{(k)}_{\pm;P}|\chi^{(k)}_{\pm;P'}\rangle\rangle = \pm\frac{2(k^2 - k_P^2)^{1/2}}{|k|}\left[\delta(P - P') + \delta(P + P')\right]. \tag{37}$$

Then, normalized eigenstates for $k \neq \pm k_P$ are given by

$$|\phi^{(k)}_{\pm;P}\rangle\rangle \equiv \sqrt{N^{(k)}_{\pm;P}}|\chi^{(k)}_{\pm;P}\rangle\rangle, \quad \langle\langle\tilde{\phi}^{(k)}_{\pm;P}| \equiv \sqrt{N^{(k)}_{\pm;P}}\langle\langle\tilde{\chi}^{(k)}_{\pm;P}|, \tag{38}$$

where the normalization constants are

$$N^{(k)}_{\pm;P} \equiv \pm\frac{|k|}{2(k^2 - k_P^2)^{1/2}}. \tag{39}$$

For $k \neq \pm k_P$, they satisfy the following bi-orthonormal and bi-completeness relations,

$$\langle\langle \tilde{\phi}^{(k)}_{\alpha;P} | \phi^{(k)}_{\alpha';P'} \rangle\rangle = \delta_{\alpha,\alpha'} \left[\delta(P - P') + \delta(P + P') \right], \quad \sum_{\alpha=\pm} \int_0^\infty dP |\phi^{(k)}_{\alpha;P}\rangle\rangle\langle\langle \tilde{\phi}^{(k)}_{\alpha;P}| = \hat{p}^{(k)}. \tag{40}$$

As a function of the wavenumber k, the eigenvalues (34) have the following two exceptional points on the real k axis,

$$k = \pm k_P. \tag{41}$$

At these points, both eigenvalues and eigenvectors coalesce. Since there is only one linearly independent eigenvector at these points, the Boltzmann collision operator (29) can not be diagonalized. Instead, the collision operator has the Jordan block structure at these points (see [3, 14]). This coalescence of eigenvectors does not take place at the usual degeneracy point of the eigenvalues of a Hermitian operator for which a degenerate eigenvalue is shared by two distinct eigenstates. In this sense, the exceptional point is often referred as the non-Hermitian degeneracy [20] In the previous paper [14], we have introduced a divergence free representation at exceptional points by continuously extending the Jordan block representation away from exceptional points.

7 A Physical Aspect of the Spectrum of the Liouvillian with the Exceptional Point

7.1 EP2 and the Telegraph Equation

In this subsection, we show that the second order exceptional point (EP2) in the spectrum of the Liouvillian leads to the telegraph equation, which has a hybrid nature of the diffusion equation and the wave equation. Let us first introduce the Wigner distribution function for the test particle,

$$f^W(X, P, t) \equiv \int_{-\infty}^{\infty} dk \; f_k(P, t) \equiv \int_{-\infty}^{\infty} dk \; \langle\langle k; P | f(t) \rangle\rangle. \tag{42}$$

We rewrite the characteristic equation of the collision operator (33) as

$$z^2 - ig^2\gamma_P z - |v|^2 k^2 = 0, \tag{43}$$

where $v \equiv P/m$. Its inverse Fourier transformation on the variables z and k leads to the telegraph equation

$$\frac{\partial^2}{\partial t^2} f^W(X, P, t) + g^2 \gamma_P \frac{\partial}{\partial t} f^W(X, P, t) = |v|^2 \frac{\partial^2}{\partial X^2} f^W(X, P, t). \tag{44}$$

In other words, the characteristic equation of the Boltzmann collision operator (43) is the same as the characteristic equation of the telegraph equation with regard to the X- and t-dependence as $\exp[i(kX - zt)]$. Hence our Boltzmann equation (31) is equivalent to the telegraph equation with regard to the dependence os the Wigner function on X and t. One can see that the telegraph equation reduces to the diffusion equation in long-time behavior in $t \gg (g^2\gamma_P)^{-1}$ (see (50) as well as [14]).

The equivalence of the Boltzmann equation and the telegraph equation in their time development in X space is remarkable, since the telegraph equation represents a prototypical time behavior of the system with the EP2 in the spectrum of the Liouvillian with respect to the wavenumber. This is because, when the spectrum of the Liouvillian has the EP2 in the wavenumber space, the essential properties of the EP2 can be effectively described by a 2×2 matrix [21, 22], and the characteristic equation for the matrix always takes the quadratic form (43).

7.2 Time Evolution of the Wigner Distribution Function

As a demonstration of the time development of the system described by the telegraph equation, here we report a shifting motion of the Wigner distribution function localized in moderately small spatial scale less than the mean-free-length, but yet with a large enough width as compared with the microscopic scale given by the interaction range. We found shifting motion of the peak of the distribution function in space in addition to spreading as a result of a diffusion type process. However, the mechanism of the shifting motion completely changes at the exceptional points $k = \pm k_P$ as the following manner:

1. For $|k| \leq k_P$, the shifting motion comes from asymmetry in the momentum distribution before the momentum relaxation is complete.
2. For $|k| > k_P$, the shifting motion comes from the real part of the eigenvalue that leads to a wave propagation with the initial velocity P/m.

In order to see the above results, we consider the following situation as an initial condition,

$$f_k(P, 0) = \chi_{k_b}(k) h(P), \tag{45}$$

where $\chi_{k_b}(k)$ is a step function which is defined with a given value of k_b by $\chi_{k_b}(k) = 1$ for $|k| \leq k_b$ or $\chi_{k_b}(k) = 0$ for $|k| > k_b$, and $h(P)$ is a momentum distribution function that is normalized as

$$\int_{-\infty}^{\infty} dP\, h(P) = 1. \tag{46}$$

To extract the essence of the mechanism of the shifting motion, we here assume $h(P) = 0$ for $P < 0$, i.e., initial distribution is composed of particles with positive momentum.

The time evolution described by the telegraph equation (44) is also described by the Boltzmann equation (31). The formal solution of the Boltzmann equation is

$$\hat{p}^{(k)}|f(t)\rangle\!\rangle = e^{-i\psi_B^{(k)}t}\hat{p}^{(k)}|f(0)\rangle\!\rangle. \tag{47}$$

By multiplying $\langle\!\langle k;\, P|$ and using the completeness relation in (40), we have a special solution for the initial condition (45),

$$f_k(P,t) = \frac{1}{2}\left(e^{-iz_{+;P}^{(k)}t} + e^{-iz_{-;P}^{(k)}t}\right)f_k(P,0) + \frac{kP}{m}\left(\frac{e^{-iz_{+;P}^{(k)}t} - e^{-iz_{-;P}^{(k)}t}}{z_{+;P}^{(k)} - z_{-;P}^{(k)}}\right)f_k(P,0). \tag{48}$$

We use the units in which $l_P = 1/k_P = 1$ and $\tau_P = 1/(g^2\gamma_P) = 1$, when we present results of numerical calculations (see e.g. Fig. 2). With these units, the eigenvalues and the eigenvectors are independent of the value of P [23].

7.2.1 Time Evolution with the Spectrum in $|k| \leq K_P$

Let us first consider the situation where the initial distribution is composed of the Fourier components with k in the region $|k| \leq k_P$. Hence, we take $k_b \leq k_P$. In this case, the time evolution of the Wigner distribution function for $P > 0$ is expressed by

$$f^W(X,P,t) = \int_{-k_b}^{k_b} dk \frac{k_P}{2\sqrt{k_P^2 - k^2}}\left[e^{-iz_{+;P}^{(k)}t}\cos(kX - \varphi_{k,P}) + e^{-iz_{-;P}^{(k)}t}\cos(kX + \varphi_{k,P})\right] \times f_k(P,0), \tag{49}$$

with $\varphi_{k,P} \equiv \arctan[k/\sqrt{k_P^2 - k^2}]$.

In Fig. 2, we present the time evolution of (49) in X space with a specific value of momentum $P > 0$, which is implicitly given as a function of l_P and τ_P. In the figure, the solid line is the initial distribution, and the dashed lines are the distribution of later times. As shown in the figure, the peak of the distribution function shifts toward $X = l_P$ in the first stage of its time evolution. Afterwards, it stops the shifting motion with spreading its width with damping centering on the position of the peak, where the time evolution is described by the diffusion equation. This can be seen by the fact that (49) can be approximated after the above mentioned first stage as,

$$f^W(X,P,t) \simeq \int_{-\infty}^{\infty} dk \frac{1}{2} e^{-D_P k^2 t}\cos[k(X - l_P)]f_k(P,0), \tag{50}$$

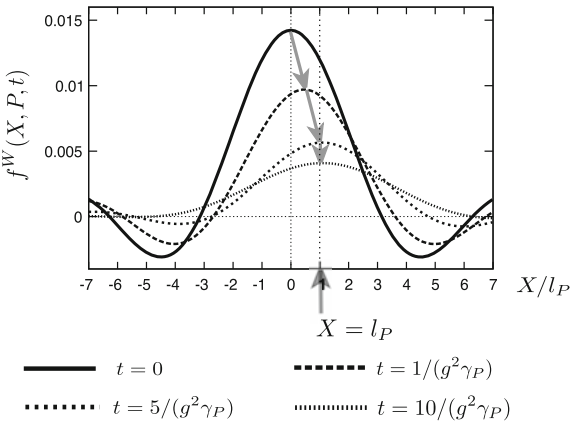

Fig. 2 Time evolution of the Wigner distribution function for $P > 0$. The *solid line* represents the initial distribution. The initial distribution is given by (45) with $k_b = k_P$. The initial distribution evolves to the distributions represented by the *dotted lines* as represented by the *arrows*

with

$$D_P \equiv \frac{g^2\gamma_P}{4k_P^2} = \frac{(P/m)^2}{g^2\gamma_P}, \tag{51}$$

which is a solution of the diffusion equation with a diffusion coefficient D_P [23].

We note that, for $t \to \infty$, the momentum distribution function is stationary as $f_0(P,t) = f_0(-P,t) = f_0(P,0)/2$. This implies that the momentum relaxation has been completed, and this is the reason that the peak of the distribution no longer moves.

7.2.2 Time Evolution with the Spectrum in $|k| > k_P$

The eigenvalues (34) take complex values for $|k| > k_P$ and their real part approach to the eigenvalues of a free particle $\pm kP/m$ for $|k| \gg k_P$. Here we discuss how the structure of the spectrum affects to the time evolution of the system. For this purpose, we analyze time evolution with an initial condition (45) with $k_b > k_P$. For this initial condition, the time evolution of the Wigner distribution function for $P > 0$ can be divided into two parts; (i) $f_{\rm d}^W$ with pure imaginary eigenvalues and (ii) $f_{\rm p}^W$ with complex eigenvalues as

$$f^W(X,P,t) \equiv \int_{-\infty}^{\infty} dk f_k(P,t) e^{ikX} = f_{\rm d}^W(X,P,t) + f_{\rm p}^W(X,P,t), \tag{52}$$

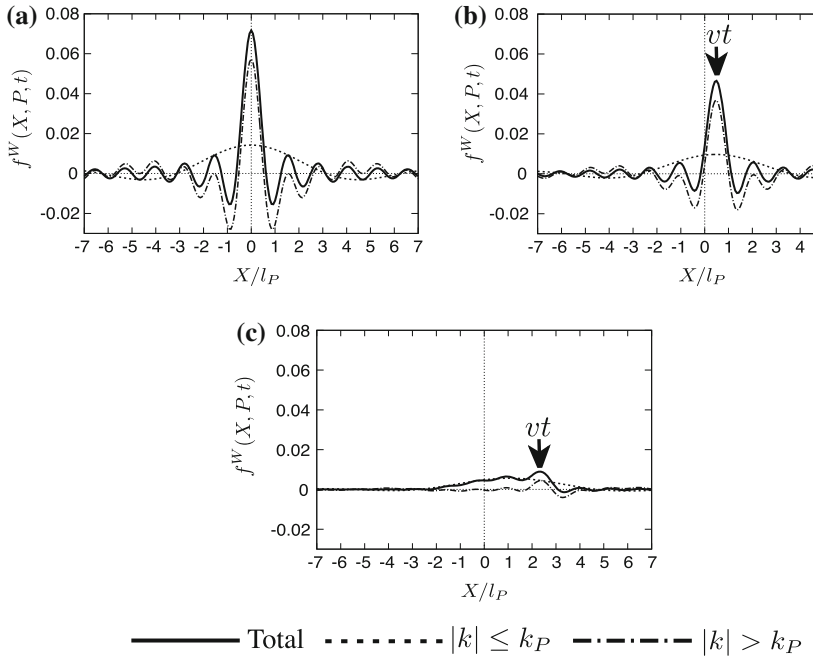

Fig. 3 Time evolution of the Wigner distribution function for $P > 0$. The initial distribution **a** is given by (45) with $k_b = 5.0k_P$. The distribution functions are shown for **a** $t = 0$, **b** $t = 1/(g^2\gamma_P)$ and **c** $t = 5/(g^2\gamma_P)$. In each figure, the *solid line* represents total value of the function f^W, the *dashed line* and the *dot-dashed line* represents $f_{\rm d}^W$ and $f_{\rm p}^W$, respectively

with

$$f_{\rm d}^W(X,P,t) \equiv \int_{-k_P}^{k_P} dk f_k(P,t)e^{ikX}, \quad f_{\rm p}^W(X,P,t) \equiv \left(\int_{-k_b}^{-k_P} + \int_{k_P}^{k_b}\right) dk f_k(P,t)e^{ikX}. \tag{53}$$

In Fig. 3, we show the time evolution of $f_{\rm d}^W$ and $f_{\rm p}^W$ as well as the total distribution function f^W with a specific value of momentum $P > 0$. In each figure, the solid line represents the total distribution f^W, the dashed line represents $f_{\rm d}^W$ and the dot-dashed line represents $f_{\rm p}^W$.

The time evolution of $f_{\rm d}^W$ has the same character as the time evolution of (49) discussed in the above subsection A, namely the distribution $f_{\rm d}^W(X,P,t)$ firstly shifts toward $X = l_P$, within the time interval $0 \le t \lesssim 1/(g^2\gamma_P)$. Afterwards, the distribution no longer shift and spreads its width by the diffusion process with its center fixed at l_P. On the other hand, the distribution $f_{\rm p}^W(X,P,t)$ propagates as a wave packet with a velocity nearly equal to the initially given velocity P/m and decays in time. The wave propagation is due to the real part of the eigenvalues of the Liouvillian in the region $|k| > k_P$.

8 Summary and a Concluding Remark

In this paper, we have discussed physical significance of the exceptional point in the Liouvillian dynamics. The example we have studied is the weakly-coupled 1D quantum perfect Lorentz gas. We have solved the complex eigenvalue problem of the Liouvillian with a linear approximation where we approximate the effective Liouvillian by the Boltzmann collision operator. There we have shown that the spectrum has the second order exceptional points in the wavenumber space.

We have discussed the physical aspects of the exceptional points by studying the time evolution of the Wigner distribution function. There we have shown that when the Liouvillian of the system has the second order exceptional points in the wavenumber space, the time evolution obeys the telegraph equation. We have also shown that the time evolution described by the telegraph equation shows a shifting motion in space. There we have found two completely different mechanisms of the shifting motion; one is due to the asymmetry of the momentum distribution function, while the other is due to the wave propagation associated to the real part in the eigenvalue.

Among many properties of the exceptional point, the geometrical phase around it is especially interesting. Indeed, one can find many theoretical [2, 11, 20, 22, 24–32] and experimental papers [7, 13, 33–35] on this subject. However, all of these previous studies in this subject have been performed on the Hamiltonian level, and there is no study performed on the Liouvillian level. We hope to discuss this subject elsewhere.

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Some Features of Exceptional Points

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Abstract A short resumé of the essentials of exceptional points of second order is given. We then concentrate on a discussion of specific features of exceptional points of third order. While general properties of these singularities have been expounded extensively in the literature, we here concentrate on some specific aspects, that is the occurrence of 'hidden' or 'concealed' third order exceptional points. They occur under specific circumstances when an apparent second order exceptional point is accompanied by a third eigenvalue being equal to the other two at the singularity.

1 Introduction

When physical phenomena are described in terms of mathematical functions it is usually the singularities of such functions that point to particular physical phenomena. For instance, in scattering theory it is the pole terms in the complex energy plane of the scattering function that describe resonance phenomena observable at real energies. During the past two decades a different type of singularities has given rise to much attention. The Exceptional Points (EPs), so named by Kato [1], are spectral singularities giving rise to a great variety of physical phenomena. They occur generically in eigenvalue problems when eigenvalues and eigenfunctions depend on parameters and are thus potentially encountered in almost any problem of physical interest. As such they occur in classical as well as in quantum mechanical problems. In fact, the classical damped harmonic oscillator provides for a prime example being presented below. While there are numerous classical phenomena, in the literature most applications and effects seem to relate to quantum mechanical problems. Some of the more important ones, in our opinion, are briefly described in the following section.

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In the subsequent section we present a rehash of the basic properties of EPs followed by a short discussion of some major phenomena associated with EPs. This part is aimed at the general reader and not at the experts. In Sect. 3 we present a few special facts and examples in connection with EPs of higher order with an emphasis on 'hidden' third order EPs.

2 Exceptional Points of Second Order

2.1 Formal Properties

Consider one of the simplest problem in classical mechanics: the damped classical oscillator. In suitable units it is described by the differential equation

$$\ddot{x} + 2k\dot{x} + \omega^2 x = 0 \tag{1}$$

with the two linearly independent solutions

$$x_{1,2}(t) = \exp(\mathrm{i}\,\tilde{\omega}_{1,2}t) \quad \text{where} \quad \tilde{\omega}_{1,2} = \mathrm{i}k \pm \sqrt{\omega^2 - k^2}. \tag{2}$$

Obviously, for $k = \omega$ the two solutions coalesce and here we encounter an EP in its simplest form. It is well known that in this case the additional independent solution bears the factor t being multiplied to the exponential function $\exp(-kt)$. In this context see also [2–5].

We next confine our discussion to the eigenvalues of a two-dimensional matrix where the direct connection of an EP and the phenomenon of level repulsion is easily demonstrated. Consider the problem

$$\begin{aligned} H(\lambda) &= H_0 + \lambda V \\ &= \begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{pmatrix} + \lambda \begin{pmatrix} \omega_1 & \delta \\ \delta & \omega_2 \end{pmatrix} \end{aligned} \tag{3}$$

where the parameters ϵ_k and ω_k determine the non-interacting resonance energies $E_k = \epsilon_k + \lambda\omega_k$, $k = 1, 2$ being two crossing lines as a function of λ. We may choose all parameters complex and we require $[H_0, V] \neq 0$ to avoid the problem from being trivial. Owing to the interaction invoked by the matrix elements δ the two levels do not cross but repel each other. However, the two levels *coalesce* at specific values of λ in the vicinity of the level repulsion, that is at the two EPs

$$\lambda_{1,2} = \frac{(\epsilon_1 - \epsilon_2)}{(\omega_2 - \omega_1) \pm 2i\delta}. \tag{4}$$

For $\delta \neq 0$ the energy levels have a square root singularity as a function of λ and read

$$E_{1,2}(\lambda) = \frac{1}{2}\left(\epsilon_1 + \epsilon_2 + \lambda(\omega_1 + \omega_2) \pm \sqrt{(\omega_1 - \omega_2)^2 + 4\delta^2}\sqrt{(\lambda - \lambda_1)(\lambda - \lambda_2)}\right). \tag{5}$$

We use the term *coalesce* as the pattern is distinctly different from a degeneracy usually encountered for Hermitian operators. Note that $H(\lambda)$ is Hermitian if all parameters in (3) are real. However, in this case, λ_1 and λ_2 are complex, in other words, at the EP the Hamiltonian is non-Hermitian. In fact, an EP cannot occur for a Hermitian matrix or any Hamiltonian. This becomes obvious when looking at the eigenfunctions. At $\lambda = \lambda_1$ there is only one eigenvector which reads (up to a factor)

$$|\phi_1\rangle = \begin{pmatrix} +i \\ 1 \end{pmatrix} \tag{6}$$

and similar at $\lambda = \lambda_2$

$$|\phi_2\rangle = \begin{pmatrix} -i \\ 1 \end{pmatrix}. \tag{7}$$

Since H is non-Hermitian at the EPs, we have to use the bi-orthogonal basis. The corresponding left hand eigenvector of H are at λ_1 and λ_2

$$\langle\tilde{\phi}_{1,2}| = (\pm i, 1), \tag{8}$$

respectively. Note that the norm—that is the scalar product $\langle\tilde{\phi}_k|\phi_k\rangle$, $k = 1, 2$—vanishes which is often referred to as self-orthogonality [6]. Note that, for a (complex) symmetric Hamiltonian as in (3), the eigenvector at the EP is independent of parameters occurring in (3).

At the EP the difference between a degeneracy and a coalescence is clearly manifested by the occurrence of only *one* eigenvector instead of the familiar two in the case of a genuine twofold degeneracy. Note, however, that a non-Hermitian operator can also have a genuine degeneracy which is, of course, not an EP. The important point is the converse: a Hermitian operator can never have an EP.

The existence of only one eigenvector with vanishing norm is related to the fact that for $\lambda = \lambda_1$ or $\lambda = \lambda_2$ the matrix $H(\lambda)$ cannot be diagonalised [1]. At these points the Jordan decomposition reads

$$H(\lambda_1) = S\begin{pmatrix} E(\lambda_1) & 1 \\ 0 & E(\lambda_1) \end{pmatrix} S^{-1} \tag{9}$$

with

$$S = \begin{pmatrix} i & \frac{2i\delta - \omega_1 + \omega_2}{(\epsilon_1 - \epsilon_2)\delta} \\ 1 & 0 \end{pmatrix} \tag{10}$$

and $E(\lambda_1)$ being the eigenvalue at the EP. Similar expressions hold at $\lambda = \lambda_2$. We mention that the second column of S is often referred to as an associate vector obeying $(H(\lambda_1) - E(\lambda_1))|\psi_{assoc}\rangle = |\phi_1\rangle$.

The consideration of a two dimensional problem covers all aspect of an EP, since the vanishing of the norm of the eigenvectors allows to reduce a high dimensional problem approximately to two dimensions in close vicinity of an EP (see for instance [7]).

2.2 Physical Effects

To the best of our knowledge, the first direct experimental verification of the analytic properties of an EP has been achieved by the Darmstadt group some fifteen years ago. In two papers [8] an encircling of the square root branch point was performed using a microwave cavity. The expected behaviour, i.e. the interchange of the energies as well as the interchange of the corresponding eigenfunctions including their global phase change has been verified experimentally. Moreover, the phase difference $\pi/2$ between the two components of the eigenstate at the EP (see (6)) has been established experimentally. There are many more physical effects related to EPs as discussed in the literature (see a survey e.g. in [9]), the list is still continuously expanding. They cover classical as well as quantum mechanical problems.

Three more general aspects deserve to be mentioned. The idea of $\mathcal{PT}$-symmetric Hamiltonians suggested in [10] has given rise to a host of literature during the past few years. The point of $\mathcal{PT}$-symmetry breaking under parameter variation is an EP. In other words, the specific non-Hermitian Hamiltonians being symmetric under the combined action of parity and time reversal can have a real spectrum. In this case the eigenfunctions are also symmetric under $\mathcal{PT}$. At a particular point of some suitable parameter the symmetry gets broken, the eigenvalue becomes complex and the eigenfunction ceases to be $\mathcal{PT}$-symmetric. Usually two real eigenvalues coalesce and move into the complex plane when such parameter sweeps over the symmetry breaking point. This point has all characteristics of an EP. Note that owing to the non-hermiticity from the outset of the Hamiltonian such parameters and in particular the energy is real at the EP being impossible, as we recall, for a Hermitian Hamiltonian.

The second aspect refers to the combined effect of many EPs in many body problems. As has been points out many years ago [11] quantum phase transitions are related to singularities of the partition function. This has been elaborated in detail using the Lipkin model [12] where the role of EPs and their accumulation in the thermodynamic limit is demonstrated. Moreover, when such models are perturbed the onset of chaos, especially in the transitional region, can be understood by the irregular trajectories of the EPs under a perturbation. The connection between chaos and EPs in many body problems has been pointed out earlier in [13].

The third aspect, being more of theoretical interest, is the role of EPs in approximation schemes. The Random Phase Approximation, often used in the past to calculate excited states in a mean field approach [14], yields an approximate Hamiltonian that

is non-Hermitian. The instability point which occurs when the particle-hole interaction is increased is in fact an EP, where two energies coalesce and then move into the complex plane. Yet, in some cases, this point can be interpreted as the onset of a phase transition of the many body system. Being singularities the EPs also affect the convergence radius of power expansions in, say, a strength parameter. A typical case in point are the "intruder" states introduced in [15] in a shell model approach of an effective interaction.

3 Exceptional Points of Third Order

Exceptional points of higher order are possible if sufficient parameters are at one's disposal. For the special case of (complex) symmetric matrices the occurrence of an EPN (Nth order EP) requires $(N^2 + N - 2)/2$ parameters for the N-dimensional matrix, and even more parameters for a more general N-dimensional matrix. As an implementation in the laboratory would require a very special experimental effort for $N > 3$ we restrict ourselves to EP3s. Some general properties have been discussed in [16, 17] where the latter paper also gives special examples of particular simple matrices giving rise to an EP3. Here we focus upon the study of some special cases which we like to denote as *concealed* EP3: the spectrum has three *equal* eigenvalues at some parameter value that seem to appear as an EP2 in addition to an incidentally coinciding third eigenvalue, whereas for some specific perturbation the three eigenvalues turn out to be an EP3. A situation of this nature occurred in the study of a Bose system by the Pitaevski equation being a non-linear problem [18].

It is obvious that the spectrum alone of three equal eigenvalues cannot give any indication as to whether we encounter a degeneracy or an EP of second or third order. Recall that it is the eigenfunctions that distinguish between a coalescence and a degeneracy. Related to this is the Jordan form J of the full original matrix problem involving the interaction between the levels: if J is diagonal the three equal eigenvalues constitute a true degeneracy, if one element of the (upper) side diagonal is unity we expect an EP2 and an EP3 if both elements of the side diagonal are unity.

As an example consider the y-dependent eigenvalue problem of the matrix

$$H = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ y & -2-y & 3 \end{pmatrix}. \tag{11}$$

Its Jordan-decomposition $H = SJS^{-1}$ yields

$$J = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\sqrt{1-y} & 0 \\ 0 & 0 & 1+\sqrt{1-y} \end{pmatrix} \tag{12}$$

with

$$S = \begin{pmatrix} 1 & 1-\sqrt{1-y} & 1+\sqrt{1-y} \\ 1 & (1-\sqrt{1-y})^2 & (1+\sqrt{1-y})^2 \\ 1 & (1-\sqrt{1-y})^3 & (1+\sqrt{1-y})^3 \end{pmatrix}. \tag{13}$$

At first superficial glance this might appear to be an EP2 as by going around the branch point at $y = 1$ the eigenvalues and eigenfunctions simply interchange. An indication for the richer structure is the rank drop of S at $y = 1$: the rank drop is 2 while for a genuine EP2 it should be only 1. In fact, when y is put equal to unity from the outset in H, the Jordan form turns out to be

$$J_{H(y=1)} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix} \tag{14}$$

clearly suggesting an EP3. The actual patterns become clear when we perturb H and consider instead

$$H_\epsilon = \begin{pmatrix} \epsilon & 1 & 0 \\ 0 & 0 & 1 \\ y & -2-y & 3 \end{pmatrix}. \tag{15}$$

We expand the eigenvalues of H_ϵ in powers of ϵ and obtain

$$E_1 = 1 + \frac{y}{1-y}\,\epsilon + O(\epsilon^2) \tag{16}$$

$$E_2 = 1 - \sqrt{1-y} + \frac{1-y-\sqrt{(1-y)^3}}{2(1-y)^2}\,\epsilon + O(\epsilon^2) \tag{17}$$

$$E_3 = 1 + \sqrt{1-y} + \frac{1-y+\sqrt{(1-y)^3}}{2(1-y)^2}\,\epsilon + O(\epsilon^2) \tag{18}$$

again confirming our finding from above as long as $y \neq 1$; for $y = 1$ the expansion fails. If, however, y is set equal to unity from the outset in H_ϵ we this time obtain the expansions

$$E_1 = 1 + \epsilon^{1/3} + O\left(\epsilon^{2/3}\right) \tag{19}$$

$$E_2 = 1 + \exp\left(\frac{2\pi i}{3}\right)\epsilon^{1/3} + O\left(\epsilon^{2/3}\right) \tag{20}$$

$$E_3 = 1 + \exp\left(\frac{4\pi i}{3}\right)\epsilon^{1/3} + O\left(\epsilon^{2/3}\right) \tag{21}$$

clearly indicating the sprouting out of the three solutions from the EP3 at $y = 1$. Any perturbation of a similar kind yields the same qualitative result, while the coefficients of the powers of ϵ may be different.

There are, however, specific non-generic perturbations of H that do not give rise to an EP3. If we replace H by $H + \epsilon Ptb$ where each row of the perturbing matrix Ptb contains the same number of the same element (say unity) irrespective of their position while the other elements are zero, then the perturbed matrix $H + \epsilon Ptb$ cannot have an EP3. To show this analytically consider the transformed matrix

$$S^{-1}(H + \epsilon Ptb)S = D + \epsilon\, S^{-1} Ptb\, S$$

with D the diagonal form of H and keeping in mind that $\det[H + \epsilon Ptb] = \det[S^{-1}(H + \epsilon Ptb)S]$. The first column of S can always be arranged to contain only unities, hence the first column of the product $Ptb\, S$ contains likewise the same element under the condition made for Ptb. As a consequence, the first column of $S^{-1} Ptb\, S$ has the form $\{c, 0, 0\}^T$ with c a non-zero number. Thus, also $D + \epsilon\, S^{-1} Ptb\, S$ has this form of the first column (with different first element $\tilde{c} = 1 + \epsilon c$). The eigenvalues are obtained from the characteristic polynomial in E, i.e. from $\det(D + \epsilon\, S^{-1} Ptb\, S - E\, I) = 0$ which factors into $(\tilde{c} - E) \times Q_2(E)$, with $Q_2(E)$ being a second order polynomial yielding an EP2 and making an EP3 impossible.

It may be of interest to contrast the matrix in (11) with the slightly modified form

$$h = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ -1 + y & -y & 2 \end{pmatrix} \tag{22}$$

which has the same spectrum (diagonal form) as H but the corresponding similarity transformation is now

$$s = \begin{pmatrix} 1 & 0 & 0 \\ 1 & (1 - \sqrt{1 - y}) & (1 + \sqrt{1 - y}) \\ 1 & (1 - \sqrt{1 - y})^2 & (1 + \sqrt{1 - y})^2 \end{pmatrix}. \tag{23}$$

The rank drop of s at $y = 1$ is now 1, it implies that h has no 'hidden' EP3 at the singularity which is just an EP2. In fact, the Jordan form of h at $y = 1$ is

$$J_{h(y=1)} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{24}$$

Of course, the similarity transformation to obtain this form cannot be identified with s in (23) by setting $y = 1$ as s^{-1} does not exist; as usually in such case s contains an associate vector.

To summarise: whether or not three equal eigenvalues correspond to a threefold degeneracy or to a coalescence of two or even three eigenvalues can only been decided by looking at the full problem, that is the type of interaction between the three states. A singularity like the square root behaviour of levels as a function of an external

parameters must also occur in the eigenfunctions to ensure the characteristics of an EP. An important criterion is the rank of the matrix listing the three eigenvectors. If it keeps its full rank when approaching the apparent singularity there is no EP but a genuine degeneracy, if the rank drop is 1 or 2 there is an EP2 or an EP3, respectively. This principle can be spun further to higher dimensions implying of course a rapidly increasing number of different possibilities. While the Jordan decomposition at the singularity yields all information at the singularity, the physically interesting aspect is the analytic behaviour when by variation of an external parameter the particular singularity is approached. Note that such limit is not uniform for the eigenvectors. In fact, owing to the rank drop of the matrix listing the eigenvectors at the singularity, its inverse does not exist. It is here where the associate vectors come into play for the Jordan decomposition.

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Spontaneous Breakdown of a PT-Symmetry in the Liouvillian Dynamics at a Non-Hermitian Degeneracy Point

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Abstract We consider the prevalent phenomenon that a pair of eigenvalues of the Liouville-von Neumann operator (Liouvillian) changes from pure imaginary to complex values with a common imaginary part for resonance states in an extended function space outside the Hilbert space. Such a transition point is an exceptional point, where non-Hermitian degeneracy occurs and both the pairs of eigenvalues and of eigenvectors coalesce. The transition can be attributed to a spontaneous breakdown of a parity and time-reversal (PT)-symmetry. This PT-symmetry in the Liouvillian dynamics results from the microscopic dynamics based on the fundamental physical laws. The kinetic equation of the Boltzmann type for a particle weakly coupled with a bath consists of the collision term, which is similar to a Hermitian operator and has even parity, and the flow term, which is anti-Hermitian and has odd parity. As a result of the competition between the two terms, a pair of PT-symmetric eigenstates of the effective Liouvillian converts to a PT-symmetry related pair as the flow term becomes more dominant than the collision term beyond an exceptional point.

1 Introduction

Physics related to non-Hermitian time evolution operators has attracted much interest [1–4]. One of the remarkable properties of non-Hermitian operators is that they cannot always be diagonalized. A point in the parameter space where a non-Hermitian

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operator is non-diagonalizable is called an exceptional point. At an exceptional point a non-Hermitian degeneracy occurs, meaning that not only the eigenvalues but also the eigenvectors coalesce [5–7]. Emergence of a non-Hermitian degeneracy is generic for non-Hermitian operators in the sense of the following theorem [8, 9]: *If* S_0 *and* S_1 *are Hermitian and do not commute, then there exists at least one complex value of* λ *for which* $S = S_0 + \lambda S_1$ *is not diagonalizable.*

We found that it often happens that a pair of eigenvalues of the Liouville-von Neumann operator (Liouvillian) changes from pure imaginary to complex values with a common imaginary part for resonance states in an extended function space outside the Hilbert space. Such a transition point is an exceptional point, where non-Hermitian degeneracy occurs. We show that the transition can be attributed to a spontaneous breakdown of a PT-symmetry, which occurs at a branch point where a non-Hermitian parameter reaches the radius of convergence of the perturbation expansion. In our case of a PT-symmetry breaking in the Liouvillian dynamics, the PT-symmetry means that the collision operator, defined to be the effective Liouvillian multiplied by $(-i)$, commutes with an anti-linear operator $\mathscr{P}\mathscr{T}$, where $\mathscr{P}$ is a linear operator representing a symmetry corresponding to parity and $\mathscr{T}$ is the complex conjugation. This PT-symmetry is intrinsic in the Liouvillian dynamics based on the fundamental physical laws, in contrast to the case of "PT-symmetric quantum mechanics" [10, 11], where PT-symmetry often appears as a result of phenomenological assumptions, such as a complex valued potential energy or balancing gain and loss.

The kinetic equation for a particle weakly coupled with a bath has the form of the Boltzmann equation in situations with moderately strong spatial inhomogeneity [12]. The collision operator in the kinetic equation is comprised of the collision term, which is similar to a Hermitian operator and has even parity, and the flow term, which is anti-Hermitian and has odd parity. As a result of the competition between the two terms, in general there occurs a phase transition between a PT-symmetric phase and a PT-symmetry broken phase as spatial inhomogeneity increases. In this paper we demonstrate this result in the perfect Lorentz gas, as well as a one-dimensional (1D) quantum polaron model in which both cases of presence and absence of PT-symmetry are realized depending on a parameter.

This paper is organized as follows: In Sect. 2 we review the concept of PT-symmetry and its breakdown. In Sect. 3 we briefly summarize the theory of the complex spectral representation of the Liouvillian. In Sect. 4 we introduce the Boltzmann type kinetic equation for a particle coupled with a bath, and discuss that the kinetic equation has a PT-symmetry. In Sect. 5 we treat perfect Lorentz gas models, in which PT-symmetry breaking occurs in the kinetic equation. In Sect. 6 we introduce a 1D polaron model. In Sect. 7 we give concluding remarks.

2 PT-Symmetry and Its Breakdown

In this section we review discussions [13–15] on the mechanism for PT-symmetry breakdown. That a time evolution operator (effective Hamiltonian or effective Liouvillian) K has a PT-symmetry means that K commutes with an antilinear operator $\mathscr{P}\mathscr{T}$, $[K, \mathscr{P}\mathscr{T}] = 0$, where $\mathscr{P}$ and $\mathscr{T}$ are the parity and time-reversal operators[1] with $\mathscr{P}^2 = \mathscr{T}^2 = 1$ and $[\mathscr{P}, \mathscr{T}] = 0$. If $|\psi_j\rangle$ is an eigenstate of an PT-symmetric operator K with an eigenvalue ζ_j,

$$K|\psi_j\rangle = \zeta_j|\psi_j\rangle, \tag{1}$$

then

$$K\left[\mathscr{P}\mathscr{T}|\psi_j\rangle\right] = \zeta_j^*\left[\mathscr{P}\mathscr{T}|\psi_j\rangle\right]. \tag{2}$$

Hence eigenvalues of an PT-symmetric operator either are real or appear in complex conjugate pairs. If an eigenstate $|\psi_j\rangle$ has a real eigenvalue, it is PT-symmetric, i.e. it is an eigenstate of $\mathscr{P}\mathscr{T}$, $\mathscr{P}\mathscr{T}|\psi_j\rangle = \pm|\psi_j\rangle$. On the other hand, if $|\psi_j\rangle$, $|\psi_{j+1}\rangle$ are eigenstates which have a complex conjugate pair of eigenstates, i.e. $\zeta_j, \zeta_{j+1} = \zeta_j^*$, $\mathscr{P}\mathscr{T}$ transforms one eigenstate into the other, $\mathscr{P}\mathscr{T}|\psi_j\rangle = |\psi_{j+1}\rangle$.

A left eigenstate $\langle\tilde{\psi}_j|$, satisfying $\langle\tilde{\psi}_j|K = \zeta_j\langle\tilde{\psi}_j|$, is not in general the Hermitian conjugate of the right eigenstate $|\psi_j\rangle$ with the same eigenvalue ζ_j. The left- and right-eigenstates satisfies the biorthogonality and bicompleteness relations,

$$\langle\tilde{\psi}_j|\psi_l\rangle = \delta_{j,l}, \tag{3}$$

$$\sum_j |\psi_j\rangle\langle\tilde{\psi}_j| = 1, \tag{4}$$

except at exceptional points. At an exceptional point two eigenstates collapse into one, and the norm of the coalesced eigenstate vanishes, $\langle\tilde{\psi}_j|\psi_j\rangle = 0$. Thus at this point the eigenstates are deficient to satisfy the completeness relation, and it is needed to introduce pseudoeigenstates to represent the operator resulting in a Jordan block [5, 17].

Following [13, 14], we assume for the operator K the form,[2]

$$K(i\lambda) = K_0 + i\lambda K_1, \tag{5}$$

[1] PT-symmetry is a case of pseudo-Hermiticity [11, 14, 16], which is equivalent to an antilinear symmetry.

[2] Every finite-dimensional matrix can be similarly transformed into this form, because every finite-dimensional matrix is similar to a complex symmetric matrix [18].

where λ is a real parameter, K_0 and K_1 are real symmetric. In order for the operator $K(i\lambda)$ to be PT-symmetric, K_0 and K_1 must be even and odd, respectively, i.e. $\mathscr{P}K_0\mathscr{P}^{-1} = K_0$ and $\mathscr{P}K_1\mathscr{P}^{-1} = -K_1$. Consider the eigenvalue equation,

$$K(i\lambda)|\Psi_j(i\lambda)\rangle = \zeta_j(i\lambda)|\Psi_j(i\lambda)\rangle, \tag{6}$$

The Rayleigh-Schrödinger perturbation expansion [13, 19] of the jth eigenvector and eigenvalue is expressed as

$$|\Psi_j(i\lambda)\rangle = \sum_{n=0}^{\infty}(i\lambda)^n|\psi_j^{(n)}\rangle, \tag{7}$$

$$\zeta_j(i\lambda) = \sum_{n=0}^{\infty}(i\lambda)^n\zeta_j^{(n)}. \tag{8}$$

If we impose the normalization condition $\langle\psi_j^{(0)}|\Psi_j(i\lambda)\rangle = 1$, where $|\psi_j^{(0)}\rangle$ are the normalized eigenvectors of K_0, the corrections for the eigenvalues $\zeta_j^{(n)}$ for $n \geq 1$ are given by

$$\zeta_j^{(n)} = \langle\psi_j^{(0)}|K_1|\psi_j^{(n-1)}\rangle, \tag{9}$$

and the corrections for the eigenvectors $|\psi_j^{(n)}\rangle$ are given recursively by,

$$|\psi_j^{(1)}\rangle = \sum_{l(\neq j)}|\psi_l^{(0)}\rangle\frac{\langle\psi_l^{(0)}|K_1|\psi_j^{(0)}\rangle}{\zeta_j^{(0)} - \zeta_l^{(0)}}, \tag{10}$$

and

$$|\psi_j^{(n)}\rangle = \sum_{l(\neq j)}|\psi_l^{(0)}\rangle\left(\frac{\langle\psi_l^{(0)}|K_1|\psi_j^{(n-1)}\rangle}{\zeta_j^{(0)} - \zeta_l^{(0)}} - \sum_{m=1}^{n-1}\frac{\zeta_j^{(m)}}{\zeta_j^{(0)} - \zeta_l^{(0)}}\langle\psi_l^{(0)}|\psi_j^{(n-m)}\rangle\right), \tag{11}$$

for $n \geq 2$. Here the unperturbed eigenvalue $\zeta_j^{(0)}$ is assumed to be non-degenerate, and hence each $|\psi_j^{(0)}\rangle$ has a definite parity, i.e. $\mathscr{P}|\psi_j^{(0)}\rangle = \sigma_j|\psi_j^{(0)}\rangle$ with $\sigma_j = 1$ or -1. Note also that all the components of a vector $|\psi_j^{(0)}\rangle$ can be chosen to be real numbers.

It can be shown by inductive reasoning with (9–11) that $\mathscr{P}|\psi_j^{(n)}\rangle = (-1)^n\sigma_j|\psi_j^{(n)}\rangle$, $\zeta_j^{(2n+1)} = 0$, and $\zeta_j^{(2n)}$ are real. Then it follows that

$$\zeta_j(i\lambda) = \zeta_j(-i\lambda) = \sum_{n=0}^{\infty}(-1)^n\lambda^{2n}\zeta_j^{(2n)}, \tag{12}$$

$$\mathscr{P}|\Psi_j(i\lambda)\rangle = \sigma_j|\Psi_j(-i\lambda)\rangle, \tag{13}$$

and

$$\mathscr{P}\mathscr{T}|\Psi_j(i\lambda)\rangle = \mathscr{P}|\Psi_j(-i\lambda)\rangle = \sigma_j|\Psi_j(i\lambda)\rangle. \tag{14}$$

This result follows also from the relation [15],

$$[\mathscr{P}K(i\lambda)\mathscr{P}]\,\mathscr{P}|\Psi_j(i\lambda)\rangle = K(-i\lambda)\mathscr{P}|\Psi_j(i\lambda)\rangle = \zeta_j(i\lambda)\mathscr{P}|\Psi_j(i\lambda)\rangle, \tag{15}$$

which is obtained by applying $\mathscr{P}$ to (6).

We conclude that if the unperturbed eigenvalue $\zeta_j(0)$ is non-degenerate and $|\lambda| < \lambda_j^{\rm c}$, where $\lambda_j^{\rm c}$ is the radius of convergence of the perturbation expansion, the eigenvalue $\zeta_j(i\lambda)$ is real and the eigenstate $|\Psi_j(i\lambda)\rangle$ of K is an eigenstate of the $\mathscr{P}\mathscr{T}$-operator [13]. A radius of convergence $\lambda_j^{\rm c}$ is finite, as seen from the fact that in the limit $\lambda \to \infty$ the eigenvalues $\zeta_j(i\lambda)/\lambda$, which are eigenvalues of the anti-Hermitian operator iK_1, approach pure imaginary values. Furthermore, it can be shown [14] that $\lambda = \pm\lambda_j^{\rm c}$ are exceptional points, where a pair of eigenstates coalesce, and a corresponding pair of real eigenvalues for $|\lambda| < \lambda_j^{\rm c}$ become a complex conjugate pair for $|\lambda| > \lambda_j^{\rm c}$.

3 Complex Spectral Representation of the Liouvillian

In this section we briefly summarize the theory of the complex spectral representation of Liouvillian. See [20, 21] for details.

We consider a system with the Hamiltonian of the form

$$H = H_0 + gV, \tag{16}$$

where H_0 is the non-interacting part, gV is the interaction between the degrees of freedom and g is the dimensionless coupling constant. We are interested in the time evolution of the density operator $\rho(t)$ governed by the Liouville-von Neumann equation,

$$i\frac{\partial}{\partial t}\rho(t) = L_H\rho(t), \tag{17}$$

where the Liouville-von Neumann operator (Liouvillian) L_H is defined by

$$L_H\rho \equiv \frac{1}{\hbar}[H, \rho]. \tag{18}$$

According to (16) the Liouvillian is decomposed as

$$L_H = L_0 + gL_V. \tag{19}$$

The eigenvalue problem of the Liouvillian in each correlation subspace denoted by ν is given by

$$L_H|F_j^{(\nu)}\rangle = Z_j^{(\nu)}|F_j^{(\nu)}\rangle. \tag{20}$$

We reduce the eigenvalue problem of the Liouvillian to that of the effective Liouvillian in each correlation subspace by applying the Brillouin-Wigner-Feshbach method with projection operators $P^{(\nu)}$ and $Q^{(\nu)}$, which satisfies

$$P^{(\nu)}H_0 = H_0P^{(\nu)}, \tag{21}$$

and

$$P^{(\nu)} + Q^{(\nu)} = 1. \tag{22}$$

The eigenvalue problem of the effective Liouvillian is given by

$$\Psi^{(\nu)}(Z_j^{(\nu)})P^{(\nu)}|F_j^{(\nu)}\rangle\!\rangle = Z_j^{(\nu)}P^{(\nu)}|F_j^{(\nu)}\rangle\!\rangle, \tag{23}$$

where

$$\Psi^{(\nu)}(z) = P^{(\nu)}H_0P^{(\nu)} + P^{(\nu)}gL_VQ^{(\nu)}\frac{1}{z - Q^{(\nu)}L_HQ^{(\nu)}}Q^{(\nu)}gL_VP^{(\nu)} \tag{24}$$

is the effective Liouvillian. The effective Liouvillian is also known as the collision operator, which is of central importance in the kinetic theory in nonequilibrium statistical mechanics. In terms of the eigenstates of the effective Liouvillian we obtain the eigenstates of the Liouvillian as

$$|F_j^{(\nu)}\rangle\!\rangle = \left[P^{(\nu)} + \mathscr{C}^{(\nu)}(Z_j^{(\nu)})\right]P^{(\nu)}|F_j^{(\nu)}\rangle\!\rangle, \tag{25}$$

with the creation-of-correlation operator

$$\mathscr{C}^{(\nu)}(z) \equiv \frac{1}{z - Q^{(\nu)}L_HQ^{(\nu)}}Q^{(\nu)}gL_VP^{(\nu)}. \tag{26}$$

The eigenvalue equation of the effective Liouvillian (23) is nonlinear in the sense that the effective Liouvillian $\Psi^{(\nu)}(Z_j^{(\nu)})$ itself depends on the eigenvalue $Z_j^{(\nu)}$. If the spectrum of the unperturbed Liouvillian L_0 is continuous, the resonance singularity in the perturbation expansion of the resolvent in the effective Liouvillian gives rise to complex eigenvalues.

4 PT-Symmetry of the Kinetic Equation for a Dissipative Particle

4.1 Boltzmann Type Kinetic Equation

We consider systems which consists of a particle and a bath. We take the thermodynamic limit of the bath and assume it is in thermal equilibrium with a temperature T. We are interested in the time evolution of the reduced density operator of the particle defined by

$$f(t) \equiv \mathrm{Tr}_{\mathrm{bath}}\rho(t), \tag{27}$$

where $\mathrm{Tr}_{\mathrm{bath}}$ means that the trace is taken over the degrees of freedom of the bath. Let us introduce the Wigner representation of the reduced density operator,

$$f_{\mathbf{k}}(\mathbf{P}, t) \equiv \langle\langle \mathbf{k}, \mathbf{P}|f(t)\rangle\rangle = \left\langle \mathbf{P} + \frac{\hbar\mathbf{k}}{2}\right| f(t) \left|\mathbf{P} - \frac{\hbar\mathbf{k}}{2}\right\rangle, \tag{28}$$

where $|f(t)\rangle\rangle$ is a representation of the reduced density operator as a vector in the Liouville space for the particle, and $|\mathbf{k}, \mathbf{P}\rangle\rangle \equiv |\mathbf{P} + \hbar\mathbf{k}/2\rangle\langle\mathbf{P} - \hbar\mathbf{k}/2|$.[3]

The Fourier transform of $f_{\mathbf{k}}(\mathbf{P}, t)$ gives the Wigner function in "phase space"

$$f^{\mathrm{W}}(\mathbf{X}, \mathbf{P}, t) \equiv \frac{1}{(2\pi)^D}\int d\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{X}} f_{\mathbf{k}}(\mathbf{P}, t), \tag{29}$$

where D is the spatial dimension of the system. We apply the formalism introduced in the previous section with the projection operator defined by

$$P^{(\mathbf{k})}\rho(t) \equiv \int d\mathbf{P}|\mathbf{k}, \mathbf{P}\rangle\rangle\langle\langle \mathbf{k}, \mathbf{P}|\mathrm{Tr}_{\mathrm{bath}}\{\rho(t)\} \otimes \rho^{\mathrm{eq}}_{\mathrm{bath}}, \tag{30}$$

where $\rho^{\mathrm{eq}}_{\mathrm{bath}}$ denotes the density operator of the bath in thermal equilibrium.

We consider weak coupling situations, and assume that the spatial inhomogeneity is such that the wave-vector $\mathbf{k}$ of concern satisfies $|\mathbf{k}| \ll d^{-1}$, where d is the interaction range between the particles. Then the effective Liouvillian can be approximated by the Boltzmann collision operator $\psi^{(\mathbf{k})}_{\mathrm{B}}$,[4] the matrix elements of which are given by

$$\langle\langle \mathbf{k}, \mathbf{P}|\psi^{(\mathbf{k})}_{\mathrm{B}}|\mathbf{k}, \mathbf{P}'\rangle\rangle \equiv w_{\mathbf{k},\mathbf{P}}\langle\langle \mathbf{k}, \mathbf{P}|\mathbf{k}, \mathbf{P}'\rangle\rangle + \langle\langle \mathbf{0}, \mathbf{P}|\Psi^{(0)}_2(i0^+)|\mathbf{0}, \mathbf{P}'\rangle\rangle, \tag{31}$$

[3] The inner product of the linear operators A and B in the wave function space as vectors in the Liouville space is defined by $\langle\langle A|B\rangle\rangle \equiv \mathrm{Tr}\left(A^{\dagger}B\right)$.

[4] Detailed analysis on the validity of the Boltzmann approximation will be given elsewhere [22].

where $\Psi_2^{(0)}(i0^+)$ is given by (24) with L_H in the second term replaced by L_0. The first term on the right hand side of (31), which is called the flow term, comes from the unperturbed Liouvillian, and

$$w_{\mathbf{k},\mathbf{P}} = (\varepsilon_{\mathbf{P}+\hbar\mathbf{k}/2} - \varepsilon_{\mathbf{P}-\hbar\mathbf{k}/2})/\hbar, \tag{32}$$

where $\varepsilon_{\mathbf{p}}$ is the unperturbed energy of the particle with momentum $\mathbf{p}$. As a result, we obtain the kinetic equation of the following form

$$\frac{\partial}{\partial t} f_{\mathbf{k}}(\mathbf{P}, t) = \int d\mathbf{P}' K^{(\mathbf{k})}_{\mathbf{P},\mathbf{P}'} f_{\mathbf{k}}(\mathbf{P}', t), \tag{33}$$

with

$$K^{(\mathbf{k})}_{\mathbf{P},\mathbf{P}'} \equiv -i\langle\langle \mathbf{k}, \mathbf{P}|\psi_{\mathrm{B}}^{(\mathbf{k})}|\mathbf{k}, \mathbf{P}'\rangle\rangle = -i w_{\mathbf{k},\mathbf{P}}\delta(\mathbf{P} - \mathbf{P}') + \mathscr{K}_{\mathbf{P},\mathbf{P}'} \tag{34}$$

where $\mathscr{K}_{\mathbf{P},\mathbf{P}'} \equiv -i\langle\langle \mathbf{0}, \mathbf{P}|\Psi_2^{(0)}(i0^+)|\mathbf{0}, \mathbf{P}'\rangle\rangle$. In the 1D quantum systems we treat in the following sections, the resonance condition in the collision term sort out discrete states connected to a momentum state. Consequently, the kinetic equation has the form of (33) with the integral replaced by a summation.

Let $z_j^{(\mathbf{k})}$ and $\zeta_j^{(\mathbf{k})}$, respectively, denote the eigenvalues of the effective Liouvillian $\psi_{\mathrm{B}}^{(\mathbf{k})}$ and those of the collision operator $K^{(\mathbf{k})}$ whose matrix elements are $K^{(\mathbf{k})}_{\mathbf{P},\mathbf{P}'}$ given by (34). According to (34), $K^{(\mathbf{k})} = -i\psi_{\mathrm{B}}^{(\mathbf{k})}$, and hence

$$\zeta_j^{(\mathbf{k})} = -i z_j^{(\mathbf{k})}. \tag{35}$$

4.2 PT-Symmetry in the Kinetic Equation

In this subsection we show that the collision operator $K^{(\mathbf{k})}$ whose matrix elements are given by (34) has a PT-symmetry.

First, we define the $\mathscr{P}$ operator as

$$\mathscr{P} \equiv \iint d\mathbf{k} d\mathbf{P}|\mathbf{k}, -\mathbf{P}\rangle\rangle\langle\langle \mathbf{k}, \mathbf{P}|. \tag{36}$$

In terms of its matrix elements an operator A is transformed with the $\mathscr{P}$ operator as

$$\langle\langle \mathbf{k}, \mathbf{P}|(\mathscr{P}A\mathscr{P}^{-1})|\mathbf{k}, \mathbf{P}'\rangle\rangle = \langle\langle \mathbf{k}, -\mathbf{P}|A|\mathbf{k}, -\mathbf{P}'\rangle\rangle. \tag{37}$$

Next, we define the $\mathscr{T}$ operator as the complex conjugation operator associated with the Wigner representation $\{|\mathbf{k}, \mathbf{P}\rangle\rangle\}$ [23]. The definition means that the $\mathscr{T}$ operator leaves the Wigner basis vectors $|\mathbf{k}, \mathbf{P}\rangle\rangle$ invariant,

$$\mathscr{T}|\mathbf{k}, \mathbf{P}\rangle\rangle = |\mathbf{k}, \mathbf{P}\rangle\rangle, \tag{38}$$

and that the $\mathscr{T}$ operator transforms the components of vectors and the matrix elements of linear operators in the Wigner representation into their complex conjugates,

$$\langle\langle \mathbf{k}, \mathbf{P}| \left(\mathscr{T}|u\rangle\right)\rangle = \langle\langle \mathbf{k}, \mathbf{P}|u\rangle\rangle^*, \quad \left(\langle\langle v|\mathscr{T}\right)|\mathbf{k}, \mathbf{P}\rangle\rangle = \langle\langle v|\mathbf{k}, \mathbf{P}\rangle\rangle^*, \tag{39}$$

$$\langle\langle \mathbf{k}, \mathbf{P}| \left(\mathscr{T} A \mathscr{T}^{-1}\right)|\mathbf{k}, \mathbf{P}'\rangle\rangle = \langle\langle \mathbf{k}, \mathbf{P}|A|\mathbf{k}, \mathbf{P}'\rangle\rangle^*, \tag{40}$$

where $|u\rangle\rangle$ and $\langle\langle v|$ are any vectors and A is a linear operator.

We assume that the system has the space inversion symmetry and $\varepsilon_{\mathbf{p}} = \varepsilon_{-\mathbf{p}}$. Then the collision operator $K^{(\mathbf{k})}$ defined by (34) is invariant under the $\mathscr{P}\mathscr{T}$ transformation. This can be seen from the following. The collision term in the collision operator (34) is transformed with $\mathscr{P}\mathscr{T}$ as

$$\mathscr{K}_{\mathbf{P},\mathbf{P}'} \overset{\mathscr{T}}{\longmapsto} \mathscr{K}_{\mathbf{P},\mathbf{P}'} \overset{\mathscr{P}}{\longmapsto} \mathscr{K}_{-\mathbf{P},-\mathbf{P}'} = \mathscr{K}_{\mathbf{P},\mathbf{P}'}, \tag{41}$$

and the flow term is transformed as

$$-iw_{\mathbf{k},\mathbf{P}} \overset{\mathscr{T}}{\longmapsto} iw_{\mathbf{k},\mathbf{P}} \overset{\mathscr{P}}{\longmapsto} iw_{\mathbf{k},-\mathbf{P}} = -iw_{\mathbf{k},\mathbf{P}}. \tag{42}$$

In addition to the PT-symmetry, the collision operator $K^{(\mathbf{k})}$ can be transformed into a symmetric matrix with a similarity transformation. This is because the matrix elements $\mathscr{K}_{\mathbf{P},\mathbf{P}'}$ of the collision term satisfy the detailed balance condition,

$$\mathscr{K}_{\mathbf{P},\mathbf{P}'} e^{-\beta\varepsilon_{\mathbf{P}'}} = \mathscr{K}_{\mathbf{P}',\mathbf{P}} e^{-\beta\varepsilon_{\mathbf{P}}}, \tag{43}$$

where $\beta \equiv 1/(k_{\mathrm{B}}T)$ and k_{B} is the Boltzmann constant. The symmetric matrix $\bar{\mathscr{K}}$ similar to $\mathscr{K}$ is defined by

$$\bar{\mathscr{K}}_{\mathbf{P},\mathbf{P}'} \equiv e^{\beta\varepsilon_{\mathbf{P}}/2} \mathscr{K}_{\mathbf{P},\mathbf{P}'} e^{-\beta\varepsilon_{\mathbf{P}'}/2}. \tag{44}$$

Under this transformation the flow term $-iw_{\mathbf{k},\mathbf{P}}\delta(\mathbf{P}-\mathbf{P}')$ remains intact and diagonal, and the $K^{(\mathbf{k})}$ matrix is transformed into a symmetric matrix, which we denote by $\bar{K}^{(\mathbf{k})}$.

The symmetrized collision operator $\bar{K}^{(\mathbf{k})}$ has the form of (33) with the collision term $\bar{\mathscr{K}}_{\mathbf{P},\mathbf{P}'}$ corresponding to K_0 in (33) and the flow term $-iw_{\mathbf{k},\mathbf{P}}\delta(\mathbf{P}-\mathbf{P}')$ to $i\lambda K_1$. Therefore the results of Sect. 2 apply to the collision operator $K^{(\mathbf{k})}$, and we conclude that if the unperturbed eigenstates are non-degenerate and each state has a definite parity, there necessarily appear exceptional points as a parameter $\lambda(\mathbf{k})$ increases which measures the strength of the flow term relative to the collision term. At the exceptional points, the PT-symmetry breaks down and a pair of real eigenvalues $\zeta_j^{(\mathbf{k})}$ of the collision operator $K^{(\mathbf{k})}$ change into a complex conjugate pair. In terms of the eigenvalues $z^{(\mathbf{k})}$ of the Liouvillian, according to (35), a pair of pure imaginary eigenvalues convert into a pair of complex eigenvalues with a common imaginary part.

5 Perfect Lorentz Gas

The Lorentz gas consists of one light-mass particle (the test particle) with mass m and N heavy particles with mass M [12]. The Hamiltonian of the system is given by

$$H = H_0 + gV = \frac{\mathbf{p}^2}{2m} + \sum_{j=1}^{N} \frac{\mathbf{p}_j^2}{2M} + g \sum_{j=1}^{N} V(|\mathbf{x} - \mathbf{x}_j|), \tag{45}$$

where g is a dimensionless coupling constant and the interaction V is assumed to be a short-range repulsive potential. We consider the system in the thermodynamic limit: $\Omega \to \infty$, $N \to \infty$ and $n_{\mathrm{h}} \equiv N/\Omega$ remaining finite, where Ω is the volume of the system. The heavy particles are assumed to be in thermal equilibrium.

The resonance singularity of the effective Liouvillian gives rise to off-diagonal matrix elements of the Boltzmann collision operator (31) with $\mathbf{P}, \mathbf{P}'$ only if the following resonance condition is satisfied with some $\mathbf{P}_j$,

$$\frac{\mathbf{P}^2}{2m} + \frac{\mathbf{P}_j^2}{2M} - \frac{\mathbf{P}'^2}{2m} - \frac{(\mathbf{P} + \mathbf{P}_j - \mathbf{P}')^2}{2M} = 0. \tag{46}$$

In the limit of the perfect Lorentz gas, $m/M \to 0$, this resonance condition reduces to

$$\mathbf{P}^2 - \mathbf{P}'^2 = 0. \tag{47}$$

5.1 1D Perfect Quantum Lorentz Gas

In 1D the resonance condition (47) gives $P = \pm P'$, which implies that the test particle with a momentum P is scattered either forward to P or backward to $-P$. Thus the collision operator is block-diagonalized with blocks of size 2×2. Each of the blocks has the form

$$\begin{pmatrix} \mathscr{K}_{P,P} & \mathscr{K}_{P,-P} \\ \mathscr{K}_{-P,P} & \mathscr{K}_{-P,-P} \end{pmatrix} = \begin{pmatrix} -ikv_P - g^2\gamma_P/2 & g^2\gamma_P/2 \\ g^2\gamma_P/2 & ikv_P - g^2\gamma_P/2 \end{pmatrix}, \tag{48}$$

where $v_P \equiv P/m$ and $g^2\gamma_P$ is the momentum relaxation rate of the particle with momentum $\pm P$. The eigenvalues of this 2×2 matrix is given by

$$\zeta_{P;\pm} = \frac{g^2\gamma_P}{2} \left\{ -1 \pm \left(1 - \frac{k^2}{k_P^2} \right)^{1/2} \right\}, \tag{49}$$

where $k_P \equiv g^2\gamma_P/(2|v_P|)$. Thus, as expected from the argument in the previous section, we obtain exceptional points at $k/k_P = \pm 1$. For details on the behavior of the system, see [17, 24].

5.2 2D Perfect Classical Lorentz Gas

In the classical limit $\hbar \to 0$ the momentum displacement operator in the effective Liouvillian coming from L_V is replaced by a differential operator as

$$\frac{1}{\hbar}\left[\exp\left(\frac{1}{2}\hbar\mathbf{q}\cdot\frac{\partial}{\partial\mathbf{P}}\right) - \exp\left(-\frac{1}{2}\hbar\mathbf{q}\cdot\frac{\partial}{\partial\mathbf{P}}\right)\right] \to \mathbf{q}\cdot\frac{\partial}{\partial\mathbf{P}}. \tag{50}$$

It follows that in 1D the collision term vanishes, because the differential cannot give rise to a finite shift of the momentum from P to $-P$. In more than one dimension the collision term exists in the classical limit, because a momentum vector can rotate continuously.

The kinetic equation in 2D for the test particle is written as [12, 25]

$$\frac{\partial}{\partial t} f_{\mathbf{k}}(\mathbf{P}, t) = K_{\mathbf{P}}^{(\mathbf{k})} f_{\mathbf{k}}(\mathbf{P}, t), \tag{51}$$

with

$$K_{\mathbf{P}}^{(\mathbf{k})} = g^2 A v_P^{-3} \frac{\partial^2}{\partial\theta^2} - ikv_P\cos\theta, \tag{52}$$

where the polar coordinate for the momentum is introduced as $P_x = P\cos\theta$, $P_y = P\sin\theta$ with θ measured with respect to the direction of the vector $\mathbf{k}$, $v_P = P/m$, and $A \equiv 2\pi n_{\mathrm{h}} \int_0^\infty dq q^2 |V_q|^2$, V_q being the Fourier component of the interaction potential. Note that in the polar coordinate the parity operator $\mathscr{P}$ acts as $\theta \mapsto \theta + \pi$.

The eigenvalue equation can be expressed in the form of the complex Mathieu equation [26],

$$-\frac{\partial^2}{\partial\theta^2}\psi_{P;j}^{(k)}(\theta) + i\lambda_P^{(k)}\cos\theta\,\psi_{P;j}^{(k)}(\theta) = \bar{\zeta}_{P;j}^{(k)}\psi_{P;j}^{(k)}(\theta), \tag{53}$$

where $\lambda_P^{(k)} \equiv kv_P^4/(g^2A)$ and $\bar{\zeta}_{P;j}^{(k)} = -[v_P^3/(g^2A)]\zeta_{P;j}^{(k)}$, $\zeta_{P;j}^{(k)}$ being the eigenvalues of $K_{\mathbf{P}}^{(\mathbf{k})}$ given by (52). Exactly the same equation has been studied as the Schödinger equation with a PT-symmetric non-Hermitian Hamiltonian containing a complex-valued potential [27].

The unperturbed eigenfunctions for $\lambda_P^{(k)} = 0$ are $\cos(n\theta)(n = 0, 1, 2, \ldots)$ and $\sin(n\theta)(n = 1, 2, 3, \ldots)$. Although each non-zero eigenvalue is doubly degenerate, as both $\cos(n\theta)$ and $\sin(n\theta)$ have the same unperturbed eigenvalue n^2, the perturbation proportional to $\cos\theta$ does not couple the subspace of cos-functions with that of

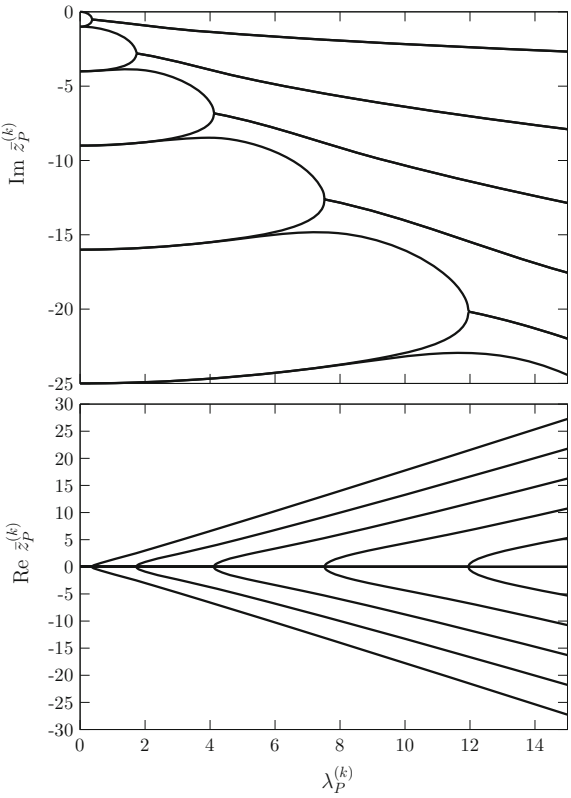

Fig. 1 Spectra of the Liouvillian for the 2D perfect classical Lorentz gas. The *vertical axis* is for $\bar{z}_{P;j}^{(k)} \equiv -i\bar{\zeta}_{P;j}^{(k)}$, and *horizontal axis* is for $\lambda_P^{(k)} \propto k$

sin-functions, and in each subspace the unperturbed eigenvalues are nondegenerate. Therefore the results of Sect. 2 apply to this case, and there appear exceptional points as the parameter $\lambda_P^{(k)}$ increases, as shown in Fig. 1.

6 1D Polaron—Presence and Absence of PT-Symmetry

In this section we consider a 1D polaron system [21, 28–31] in which a particle on a 1D lattice is coupled with an acoustic phonon field, described by the Hamiltonian (16) with

$$H_0 = \sum_p \varepsilon_p |p\rangle\langle p| + \sum_q \hbar\omega_q b_q^\dagger b_q, \tag{54}$$

$$V = \sqrt{\frac{2\pi}{L}} \sum_{p,q} g_q |p + \hbar q\rangle\langle p|(b_q + b_{-q}^\dagger), \tag{55}$$

where $|p\rangle$ denotes a state of the particle with momentum p, b_q is an annihilation operator of the phonon with wave number q, and L is the system size. We assume the following dispersion relation for the energy of the particle and the frequency of the phonon,

$$\varepsilon_p = E_0 - 2J\cos\left(\frac{pa}{\hbar}\right), \tag{56}$$

$$\omega_q = \frac{2c}{a}\left|\sin\left(\frac{qa}{2}\right)\right|, \tag{57}$$

where a is the lattice constant, and c is the sound velocity of the acoustic phonon in the long wavelength limit.

The resonance singularity of the effective Liouvillian gives rise to off-diagonal matrix elements of the Boltzmann collision operator (31) with P, P' only if the following resonance condition is satisfied,

$$\varepsilon_P - \varepsilon_{P'} \pm \hbar\omega_{(P-P')/\hbar} = 0. \tag{58}$$

From (58) it follows that [32]

$$P' = -P \pm 2\pi R(\hbar/a), \tag{59}$$

where $R \equiv (\sin^{-1} B)/\pi$ with $B = \hbar c/(2aJ)$ being the ratio of the phonon bandwidth to the particle bandwidth. By using the relation (59) recursively, we can enumerate the sequence of the momenta which are successively related to an initial one P_0 as

$$P_n = (-1)^n(P_0 - 2\pi n R(\hbar/a)), \qquad (n = 0, \pm1, \pm2, \ldots) \tag{60}$$

which we call the P_0-subset of momenta, and the subspace associated with a P_0-subset will be called the P_0-subspace. The action of the collision operator is closed in each P_0-subspace, i.e. there are no matrix elements which connect a P_0-subspace to another and the collision operator is block-diagonalized.

Because of the spatial periodicity of the system, two momenta that differ by a multiple of $2\pi\hbar/a$ are equivalent. As a result, in the eigenvalue problem of the collision operator, there are two different situations depending on R being a rational number or an irrational number. While for an irrational R all the momenta in the sequence (60) are different from each other, for a rational R the sequence (60) comes back to the original P_0 and repeats itself. Thus, if R is a rational number, each block of the collision operator for a P_0-subspace is a finite-dimensional matrix, the eigenvalue problem of which can be solved numerically.

Specifically, let us denote a rational number by $R = l/m$, where l and m are relatively prime integers. The case of an odd m and that of an even m differs with regard to the PT-symmetry.

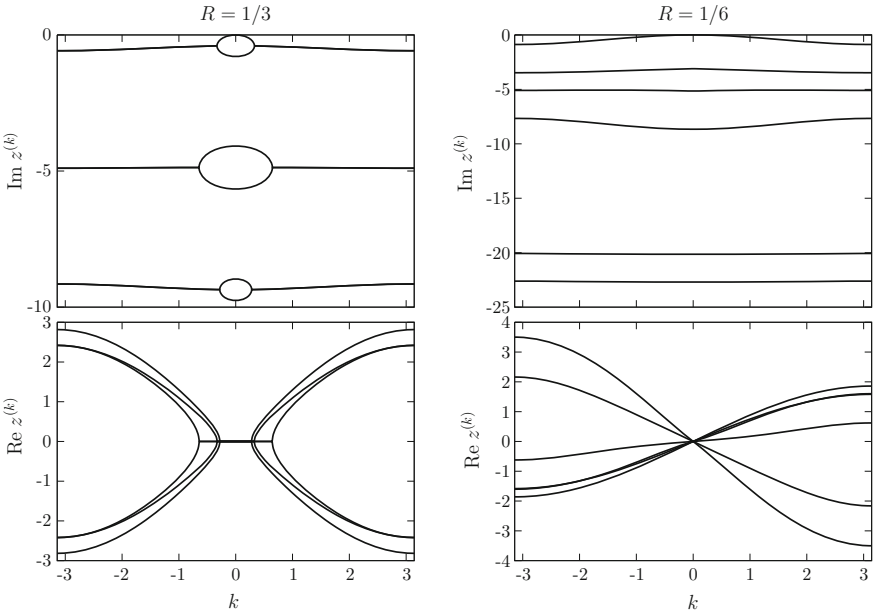

Fig. 2 Spectra of the Liouvillian for the 1D polaron system with $R = 1/3$ (*left*) and $R = 1/6$ (*right*). Each spectrum is obtained by numerically diagonalizing a 6×6 matrix

6.1 PT-Symmetry for R with an Odd Denominator

Let us assume m is odd. Then $P_{n+m} \equiv -P_n$ and $P_{n+2m} \equiv P_n$, where the equivalence $\equiv$ means that the left-hand-side and the right-hand-side of an $\equiv$ differs by an integer multiple of $2\pi\hbar/a$. Thus a P_0-subset consists of $N = 2m$ momenta, and if a P is in a subset, then $-P$ is also in the same subset. Hence, the collision operator has a PT-symmetry in each P_0-subspace. It follows from the conclusion of Sect. 4.2 that as the magnitude of the flow term relative to the collision term increases, an eigenstate of the collision operator merges with another at an exceptional point, if at $k = 0$ the eigenvalue of that eigenstate is nondegenerate[5] and thus the eigenstate has a definite parity. As an example, the spectrum of the collision operator for $R = 1/3$ is shown in Fig. 2.

[5]Nondegeneracy of zero eigenvalue of the collision term follows from Perron-Frobenius theorem [33], if the matrix elements of the collision operator are non-vanishing between any two adjacent momenta along the chain (60).

6.2 *Absence of PT-Symmetry for R with an Even Denominator*

Let us assume m is even. Then $P_{n+m} \equiv P_n$. Thus a P_0-subset consists of $N = m$ momenta. In contrast to the other case, except for $P_0 = 0$, if the P_0-subset has a P, the subset does not contain $-P$. Hence, there is no PT-symmetry in a P_0-subspace ($P_0 \neq 0$), because the $\mathscr{P}$-operation (36) itself does not exist. Consequently, there is no exceptional point in the spectrum of the collision operator.

We can give another reasoning as follows. The collision operator has a PT-symmetry in a combined space of a P_0-subspace and its counterpart, i.e. the $(-P_0)$-subspace ($P_0 \neq 0$). In this space each eigenvalue of the collision term is doubly degenerate, because each eigenstate of the collision operator in the P_0-subspace is transformed into an eigenstate in the $(-P_0)$-subspace with the $\mathscr{P}$ operator, both the eigenstates sharing an eigenvalue. This double degeneracy is lifted immediately by the flow term.

As an example, the spectrum of the collision operator for $R = 1/6$ is shown in Fig. 2.

7 Concluding Remarks

We have discussed PT-symmetry and its breakdown in the Liouvillian dynamics with the Boltzmann type kinetic equation as an example. A spontaneous breakdown of a PT-symmetry occurs at a branch point where a non-Hermitian parameter in the collision operator reaches the radius of convergence of the perturbation expansion, and a pair of eigenvalues of the Liouvillian for resonance states changes from pure imaginary to complex values with a common imaginary part.

In the kinetic equation, PT-symmetric eigenmodes with purely imaginary eigenvalues of the Liouvillian correspond to diffusion processes and eigenmodes with non-vanishing real part of the eigenvalues in a PT-symmetry broken phase lead to translational motion with damping [17, 24]. In 1D the time evolution is described by telegrapher's equation [17, 25] in a time region where only the two eigenmodes with the smallest decay rates has survived. The telegrapher's equation reduces to the diffusion equation in the hydrodynamic regime. On the other hand in the case without PT-symmetry, the first order term of the perturbation expansion with respect to the flow term of the eigenvalue of the hydrodynamic mode does not vanish and gives a hydrodynamic sound wave mode [30].

There are other types of time evolution equations of the density matrix which has exceptional points [34–37]. For example the Markov master equation has the collision operator whose matrix elements are transition probabilities. Such a real matrix has the same property as the PT-symmetric complex matrix in that its eigenvalues either are real or appear in complex conjugate pairs. Indeed, it is possible to similarly transform

a real matrix into a complex PT-symmetric matrix [38]. Moreover, we expect that conditions for emergence of exceptional points can be clarified by transforming the collision operator into the form of (5).

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Pseudo-Hermitian β-Ensembles with Complex Eigenvalues

Gabriel Marinello and Mauricio Porto Pato

Abstract Pseudo-Hermitian and PT-symmetric matrices have been a topic of interest since the first papers on the subject in the late 90s. In this paper we utilize properties of tridiagonal random matrices described in the framework of generalized β ensembles to explore variations of that ensemble, which cause the eigenvalues to move from the real line into the complex plane in conjugate pairs, while still maintaining the pseudo-Hermitian property.

1 Introduction

Soon after Mostafazadeh's early papers on pseudo-Hermiticity [1–3] appeared the interest in investigating random pseudo-Hermitian matrices. In this context, ensembles for 2×2 matrices were worked on in the early 2000s [4, 5] and the topic is still the focus of recent efforts not only in the 2×2 case [6], but also more general approaches [7, 8]. And even more recently, ensembles of $N \times N$ Gaussian split-complex and split-quaternion Hermitian matrices have been introduced in [9], where the level densities and spacings were also obtained for the real eigenvalues of 2×2 matrices.

PT symmetric systems are characterized by the invariance of their Hamiltonian under the combined parity (P) and time-reversal (T) transformations [10, 11]. *PT*-symmetric Hamiltonians have been associated in the literature to a class of non-Hermitian operators connected to their adjoints by a similarity transformation

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Springer Proceedings in Physics 184, DOI 10.1007/978-3-319-31356-6_20

$$H^{\dagger} = \eta H \eta^{-1}. \tag{1}$$

This relation defines a pseudo-Hermitian operator and means that the operator shares with its adjoint the same set of eigenvalues [1–3] implying that the eigenvalues are real or come in complex conjugate pairs.

Symmetries play an important role in random matrix theory (RMT). Since the early works of Wigner [12, 13] the symmetries of the discrete portion spectrum of a Hamiltonian system played a key role in the study of its statistical properties. In the context of the Gaussian ensembles of RMT, time reversal symmetry and rotational symmetry distinguish the three classical Wigner ensembles [14]. This justifies the interest in finding ensembles of random matrices which verify (1), as pseudo-Hermiticity is closely connected to PT-symmetry [15, 16].

It has been shown that the Gaussian matrices of RMT may be reduced to a family of tridiagonal matrices parametrized by the Dyson index β [17], which generalize the classical Gaussian ensembles such that this index can assume any real positive value. This generalized tridiagonal family constitutes the β-ensemble and in the case of the generalization of the Wigner-type matrices, the ensemble is typically refereed to as β-Hermite [18], whereas Wishart-type matrices are typically referred to as β-Laguerre [19]. It is worthy of note that sparse tridiagonal matrices have special properties which made them suitable tools to study problems in different areas [20, 21], and have been previously been used in a model of non-Hermitian tridiagonal matrices by Hatano and Nelson to unveil the presence of a transition to delocalization [22]. Related tight-binding models in lattices have also been proposed to study unidirectional invisibility [23].

It has then been shown [24] that by explicitly allowing the subdiagonals of the β-ensemble matrices to be sorted independently, an ensemble of non-Hermitian tridiagonal matrices in which all the eigenvalues are real is obtained. This non-Hermitian ensemble was constructed as an effort to provide an ensemble whose matrices could, in principle, model aspects of *PT* symmetric systems. More recently [25], it was shown that although matrices belonging to this non-Hermitian ensemble are pseudo-Hermitian, they also fit into the more restrictive category of quasi-Hermitian matrices such that no transition into the complex plane may be expected. Also in [25], a new ensemble was constructed, isospectral to the β-ensemble, whose eigenvalues transition into the complex plane under the effect of small perturbations.

The article is organized as follows. In Sect. 2, the results of [24] regarding Hermitian and Quasi-Hermitian β-ensembles are reviewed. In the following Sect. 3, the results of the isospectral matrices of [25] are reviewed and extended. Then in Sect. 4, we present a new ensemble of matrices derived from the β-ensemble, for which the transition into the complex plane is undergone through a different mechanism than the previously cited cases. Finally, in Sect. 5, we present our concluding remarks.

2 The Hermitian and the Quasi-Hermitian β-Hermite Ensembles

The characteristic polynomial of a $N \times N$ real square tridiagonal matrix

$$M = \begin{pmatrix} a_1 & b_1 & 0 & \dots & 0 & 0 \\ c_1 & a_2 & b_2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & a_{N-1} & b_{N-1} \\ 0 & 0 & 0 & \dots & c_{N-1} & a_N \end{pmatrix} \tag{2}$$

may be written in terms of the recurrence relation

$$Q_k(x) = (x - a_k)Q_{k-1}(x) - b_k c_k Q_{k-2}(x) \tag{3}$$

which is obtained straightforwardly by expanding the determinant equation for the characteristic polynomial in terms of the first row.

The β-ensemble, generalization of the Gaussian classical ensembles, consists of $N \times N$ symmetric tridiagonal matrices [17] in which the diagonal elements are independently and normally distributed random variables with null mean and unit variance, denoted by $N(0, 1)$, and the off-diagonal are random variables independently distributed according to the χ-distribution with parameter $\nu = \beta(N - k)$, where k is the row index of the upper subdiagonal element and column index of the lower subdiagonal element. The classical Gaussian ensembles were described by their Dyson β index, which took the values $\beta = 1, 2, 4$ for matrices of real, complex and quaternion elements, respectively. The generalized β ensemble, on the other hand, extends the results of the classical Gaussian ensembles to positive real β.

We denote a matrix of this ensemble as

$$H_\beta = \frac{1}{\sqrt{2}} \begin{pmatrix} N(0,2) & \chi_{\beta(N-1)} & 0 & \dots & 0 & 0 \\ \chi_{\beta(N-1)} & N(0,2) & \chi_{\beta(N-2)} & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & N(0,2) & \chi_\beta \\ 0 & 0 & 0 & \dots & \chi_\beta & N(0,2) \end{pmatrix} \tag{4}$$

where the identity $N(0, 1) \equiv N(0, 2)/\sqrt{2}$ was used, and both subdiagonals are equal.

The joint density distribution of the eigenvalues is then given by [17]

$$P(x_1, x_2, ..., x_N) = C_N \exp\left(-\frac{1}{2}\sum_{k=1}^{N} x_k^2\right) \prod_{j>i} |x_j - x_i|^\beta, \tag{5}$$

and for large matrices the eigenvalue density is the Wigner semi-circle law [14].

$$\rho(\lambda) = \frac{1}{\pi\beta}\sqrt{2N\beta - \lambda^2}. \tag{6}$$

The average characteristic polynomials satisfy for $1 \leq k \leq N$ the recurrence relation [24]

$$\langle P_k \rangle = -x \langle P_{k-1} \rangle - \frac{k-1}{2}\beta \langle P_{k-2} \rangle. \tag{7}$$

by means of which the identification

$$\langle P_N \rangle = \left(\frac{\beta}{4}\right)^{N/2} H_N\left(-\frac{x}{\sqrt{\beta}}\right) \tag{8}$$

follows, where H_N is the Hermite polynomial of order N.

The semi-circle, (6), naturally appears as the density distribution of the roots of the above Hermite polynomials. This result means that the eigenvalues of the β-ensemble fluctuate around the zeros of the Hermite polynomials.

In [24] these matrices were made non-Hermitian by filling the two off-diagonals with different values taken from the same distribution. We denote the new matrices by

$$\hat{H}_\beta = \frac{1}{\sqrt{2}}\begin{pmatrix} N(0,2) & \chi'_{\beta(N-1)} & 0 & \dots & 0 & 0 \\ \chi_{\beta(N-1)} & N(0,2) & \chi'_{\beta(N-2)} & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & N(0,2) & \chi'_\beta \\ 0 & 0 & 0 & \dots & \chi_\beta & N(0,2) \end{pmatrix} \tag{9}$$

where the primed elements are independently sorted from the same distribution as their unprimed counterpart.

It was then shown that the non-Hermitian matrices thus constructed are pseudo-Hermitian with real eigenvalues since the matrices η and $\eta^{1/2}$ can be defined such that (1) is satisfied. Utilizing the notation of (2) to write

$$\eta = \mathrm{diag}\left(1, \frac{b_1}{c_1}, \frac{b_1}{c_1}\frac{b_2}{c_2}, \dots, \prod_{k=1}^{N-1}\frac{b_k}{c_k}\right). \tag{10}$$

Provided that the matrices, as in the case presently discussed, are real, the construction of the matrix $\eta^{1/2}$ follows immediately.

The real eigenvalues of these non-Hermitian matrices also occupy the same compact support of H_β with the same semi-circle law density, although the spacing distribution between neighboring eigenvalues has a logarithmic repulsion.

It is also noteworthy that the matrix η given in reference [24] which verifies (1) fluctuates around finite values for all its elements [25]. In particular, when $N \to \infty$, the average goes as $\langle \eta_{NN} \rangle \to 1$ and the variance goes as $\sigma^2_{\eta_{NN}} \to 0$. A quasi-hermitian operator [26, 27] A is one for which there exists a hermitian linear

operator T such that its domain is the Hilbert space being considered, T is positive definite and bounded and, also, $TA = A^{\dagger}T$. The last condition is equivalent to (1), but quasi-Hermiticity imposes greater restraints in the operator by requiring positive-definiteness and boundedness. In the case studied in [24], the fact that each pair b_j/c_j fluctuates around unity implies that even as we consider the $N \to \infty$ limit, the quasi-Hermitian operator corresponding to this η matrix will remain bounded, implying that no transition into the complex plane may be expected.

3 Pseudo-Hermitian β-Hermite Ensemble with Unbounded Metric

In the authors' previous work, the construction of a pseudo-Hermitian ensemble whose matrices are isospectral with those of the β-ensemble was presented [25]. This was done by assuming real tridiagonal non-Hermitian matrices with diagonal composed of random Gaussian variables of mean zero and variance one, lower subdiagonal equal to unity and kth element of the upper subdiagonal following the $\chi^2_{\nu(k)}$ distribution

$$F_{\nu}(x) = \frac{1}{\Gamma[\nu/2]} x^{\frac{\nu}{2}-1} \exp(-x) \tag{11}$$

where $\nu(k) = \beta(N-k)$. The resulting family of matrices constitutes a pseudo-Hermitian ensemble with the same real eigenvalues of the β-Hermite ensemble.

Let us now consider the real non-Hermitian random matrix

$$H_{\beta,\alpha} = \begin{pmatrix} a_N & b_{N-1}^{1+\alpha} & & & \\ b_{N-1}^{1-\alpha} & a_{N-1} & b_{N-2}^{1+\alpha} & & \\ & \ddots & \ddots & \ddots & \\ & & b_2^{1-\alpha} & a_2 & b_1^{1+\alpha} \\ & & & b_1^{1-\alpha} & a_1 \end{pmatrix}, \tag{12}$$

where the diagonal elements $\{a_k\}$ and subdiagonal elements $\{b_k\}$ are those of (4) and α is a real parameter, such that the characteristic polynomial satisfies the recurrence relation

$$P_N(x) = (a_N - x)P_{N-1}(x) - b_{N-1}^2 P_{N-2}(x). \tag{13}$$

Immediately we find that this matrix belongs to a family of isospectral matrices parametrized by the value of α. This parameter α, which may assume any real value, is symmetrical with respect to zero. That is, since the matrix is real, the matrix obtained for $-\alpha$ is exactly the transpose of the matrix obtained for α and $\alpha = 0$ gives the original matrix. Besides, this is a family of pseudo-Hermitian matrices with respect to the diagonal metric with elements

$$\mu = \mathrm{diag}\left[1, b_{N-1}^{2\alpha}, (b_{N-1}b_{N-2})^{2\alpha}, ..., (b_{N-1}b_{N-2}...b_1)^{2\alpha}\right]. \tag{14}$$

If the distributions of the b's are such that they are localized and their averages increase with N then the metric is asymptotically singular in the large N limit. In the case of the family isospectral with the β ensemble discussed above, both locality and increasing average conditions are satisfied as the b_k elements follow a χ_ν distribution with parameter $\nu = \beta(N-k)$. This implies that the inverse of the metric operator vanishes, which is associated with potentially interesting phenomena [28]. As a consequence, we should expect that the matrices become increasingly affected to small perturbations as N becomes larger. Under this circumstance, we are dealing with a family of non-normal matrices.

We introduce a perturbation by a matrix whose only non-zero element has a small value ε located at the positions i, j and j, i:

$$g_{mn} = \varepsilon\left(\delta_{mi}\delta_{nj} + \delta_{ni}\delta_{mj}\right). \tag{15}$$

In Fig. 1 we present the results of varying the α parameter for a set of values of the perturbations ε in the positions $N, 1$ and $1, N$. The progression from the smallest perturbation, Fig. 1a, into the largest, Fig. 1d, shows that the effect of increasing the perturbation and of increasing the exponent α is similar. The results presented describe the behavior of the average matrix of the ensemble, that is, the matrix whose entries are obtained from averaging the matrix from definition (12).

To investigate this behavior under perturbations let us consider the case with parameter $\alpha = 1$ from [25], that is

$$G_\beta = \begin{pmatrix} a_N & b_{N-1}^2 & & & \\ 1 & a_{N-1} & b_{N-2}^2 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & a_2 & b_1^2 \\ & & & 1 & a_1 \end{pmatrix}, \tag{16}$$

which is then perturbed by the same g of (15). In this case, the characteristic polynomial may be expressed as

$$P_N(\lambda, \varepsilon) = P_N(\lambda, 0) - \varepsilon\left(1 + \prod_{k=N-j}^{N-i} b_k\right) Q_i(\lambda, 0) P_{n-j}(\lambda, 0) \tag{17}$$

up to first order in ε, where Q_i is the characteristic polynomial of the $i \times i$ upper left square block of the original matrix H. This follows from straightforward algebraic manipulation of Laplace's formula for the determinant of $\lambda I - H - g_{ij}$.

In Fig. 2 we present the calculated behavior of the eigenvalues of matrices of the ensemble with $\alpha = 1$, as the position of a perturbation $\varepsilon = 10^{-20}$ is changed. It is

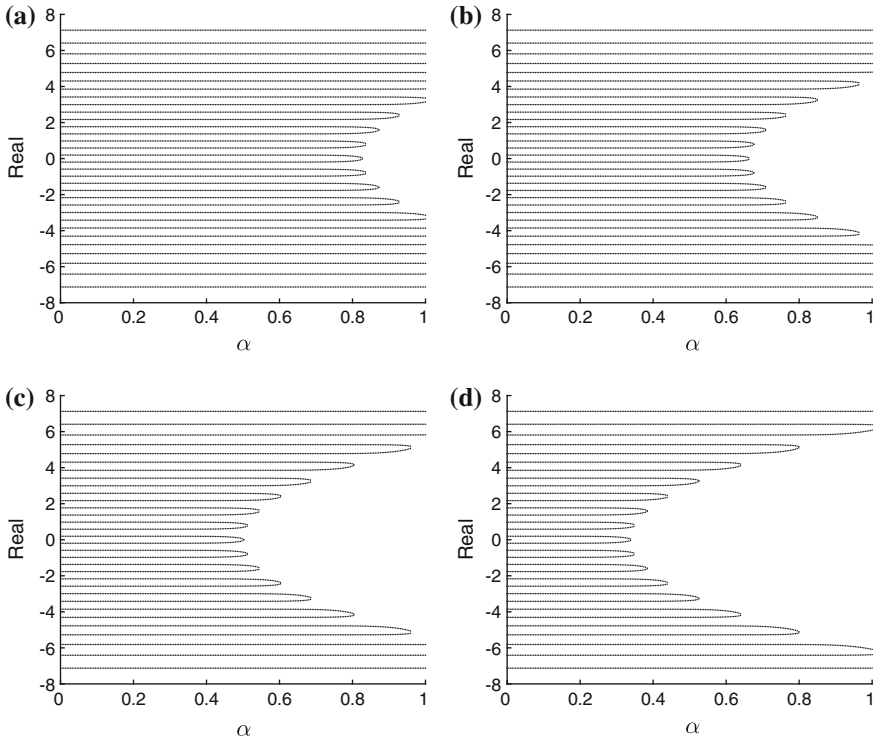


Fig. 1 Eigenvalue behavior in a sample of the average matrix of the variable α-exponent matrices for size $n = 32$ matrices for ε **a** 10^{-10}, **b** 10^{-8}, **c** 10^{-6} and **d** 10^{-4}

worthy of note that as the perturbation moves closer to the diagonal, its effect is diminished.

Figs. 1 and 2 show that the eigenvalues move into the complex plane. To understand these results, let us consider the matrix

$$\eta_G(G_\beta + g)\eta_G^{-1} = \begin{pmatrix} a_N & 1 & & & \frac{\varepsilon}{\prod b_{N-i}^2} \\ b_{N-1}^2 & a_{N-1} & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & & b_2^2 & a_2 & 1 \\ \varepsilon \prod b_{N-i}^2 & & & & b_1^2 & a_1 \end{pmatrix} \tag{18}$$

related to the perturbed matrix by a similarity transform, where η_G is obtained from (10) and (16).

If we consider a perturbation in the $(N, 1)$ and $(1, N)$ elements, (17) allows us to write, up to first order in ε,

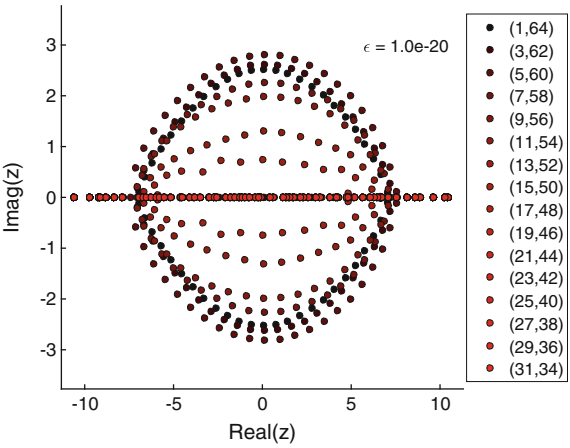


Fig. 2 Sample spectrum for an order $N = 64$ matrix of the pseudo-Hermitian $\beta = 1$ ensemble, disturbed with $\varepsilon = 10^{-20}$. The pairs listed in the panel in the left denote the row and column, respectively, of the perturbation

$$P_N(\lambda, \varepsilon) = P_N(\lambda, 0) - (-1)^N (b_{N-1}^2 b_{N-2}^2 \dots b_1^2 + 1)\varepsilon, \tag{19}$$

In the limit of large N, the term $(-1)^{N+1}\varepsilon$ is negligible such that the eigenvalues are then obtained by solving the equation

$$P_N(\lambda) = (-1)^N \varepsilon b_{N-1}^2 b_{N-2}^2 ... b_1^2. \tag{20}$$

In this regime of large matrices, a better insight is obtained by averaging this equation. In this case, the averaged characteristic polynomial is the Hermite polynomial and equation (20) becomes

$$\langle P_N(\lambda) \rangle = \left(\frac{\beta}{4}\right)^{N/2} H_N\left(-\frac{\lambda}{\sqrt{\beta}}\right) = (-1)^N \varepsilon \left(\frac{\beta}{2}\right)^{N-1} \Gamma(N), \tag{21}$$

where the rhs was averaged with the Gamma distribution. The Hermite polynomial oscillates inside the interval containing the roots and outside it, it diverges. The amplitude of the oscillations is smaller at the region around the center and monotonically increases as one moves to the edge. If the constant term in the rhs is smaller than the minimum amplitude at the center all eigenvalues are real, otherwise pairs of conjugated complex eigenvalues appear at the center. With a fixed g, the size of the rhs is controlled by the size N of the matrix, therefore by increasing N there will necessarily be some value of $N = N_0$ at which the constant term gets larger than the minimum amplitude, no matter how small ε is. From this value on, the eigenvalues progressively move to a line in the complex plane. Vice versa, with a fixed matrix size N, starting with a very small value by increasing ε, from some value ε_0 on, pairs of conjugate eigenvalues will pop up.

The oval shape with wings shown in Fig. 2 can be analytically reproduced by considering the uniform asymptotic expansion [29]

$$\exp\left(-\frac{x^2}{2}\right) H_n(x) = \frac{2^{\frac{n}{2}+\frac{1}{4}}}{(n\pi)^{\frac{1}{4}}} \sqrt{\frac{n!}{\sin\theta}} \sin\left[\left(\frac{n}{2}+\frac{1}{4}\right)(\sin 2\theta - 2\theta) + \frac{3\pi}{4}\right] \quad (22)$$

of the Hermite polynomials where $x = \sqrt{2n+1}\cos\theta$. This expression can successfully be extended to the complex plane by allowing θ in (22) to be complex, yielding [18, 30]

$$H_n(z) = \frac{2^{n/2-1} n! e^{n+z^2-z(z^2-2n-1)^{1/2}/2}}{\pi^{1/2} n^{(n+1)/2} \left(\frac{z^2}{2n+1}-1\right)}. \quad (23)$$

Calculations done in this asymptotic formalism are compared with eigenvalues obtained numerically in Fig. 3. In Fig. 3a, the comparison is done with just one random matrix for increasing values of ε. It is clear that the asymptotic expressions work well.

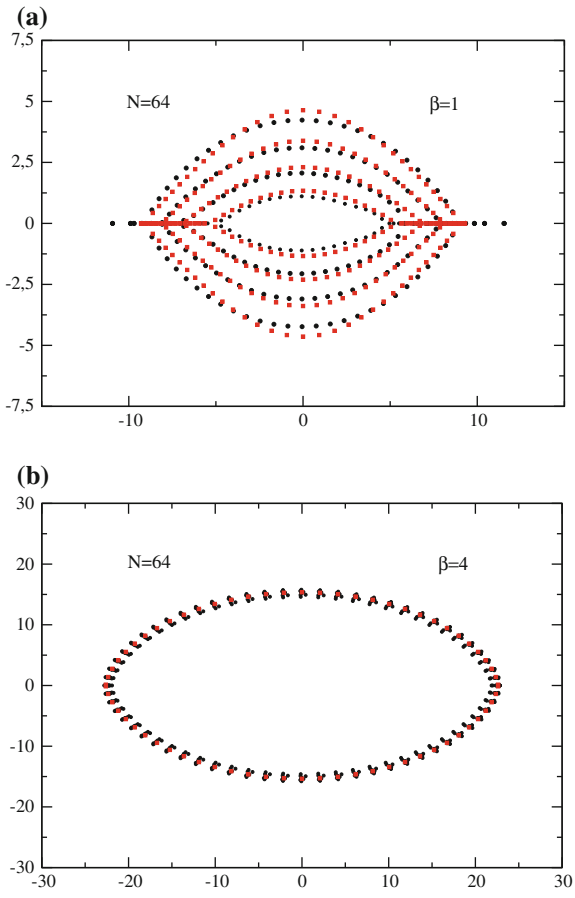


Fig. 3 Spectrum (*black*) and asymptotic calculation (*red*) for $n = 64$ and **a** $\beta = 1$, **b** $\beta = 4$

This is made even clearer in Fig. 3b, when the comparison is made with a sample of 10 random matrices in which all but the two edge eigenvalues are complex.

4 The Non-positive-definite Pseudo-Hermitian β-Hermite Ensemble

Here we are interested in the construction of an ensemble whose matrices have their Hermiticity progressively broken by changing the signs of the matrix's subdiagonal elements. For a given matrix $H_{\beta,\alpha}$ as written in (12) with $\alpha = 0$, we construct a matrix with m changed signs denoted by

$$S_{\beta,\alpha,m} = \begin{pmatrix} a_N & -b_{N-1}^{1+\alpha} & 0 & \dots & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ b_{N-1}^{1-\alpha} & a_{N-1} & -b_{N-2}^{1+\alpha} & \dots & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & b_{N-2}^{1-\alpha} & a_{N-2} & \dots & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & a_{N-m+1} & -b_{N-(m-1)}^{1+\alpha} & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & b_{N-(m-1)}^{1-\alpha} & a_{N-m} & b_{N-m}^{1+\alpha} & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & \dots & a_3 & b_2^{1+\alpha} & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & \dots & b_2^{1-\alpha} & a_2 & b_1^{1+\alpha} \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & \dots & 0 & b_1^{1-\alpha} & a_1 \end{pmatrix}. \tag{24}$$

As in the case of the pseudo-Hermitian ensemble described in [24], the respective matrix η may be written following (10) for arbitrary α,

$$\eta_m = \mathrm{diag}\left(1, -b_{N-1}^{2\alpha}, b_{N-1}^{2\alpha} b_{N-2}^{2\alpha}, \dots, (-1)^{m-1} \prod_{k=1}^{m-1} b_{N-k}^{2\alpha}, (-1)^m \prod_{k=1}^{m} b_{N-k}^{2\alpha}, \right. \\ \left. \dots, (-1)^m \prod_{k=1}^{N-2} b_{N-k}^{2\alpha}, (-1)^m \prod_{k=1}^{N-1} b_{N-k}^{2\alpha}\right), \tag{25}$$

which is clearly a non positive-definite operator for any integer m and positive $\{b_k\}$. In the present work, we shall focus on the special case of $\alpha = 0$, for which

$$\eta_m = \mathrm{diag}\left(1, -1, 1, \dots, (-1)^{m-1}, (-1)^m, \dots, (-1)^m, (-1)^m\right), \tag{26}$$

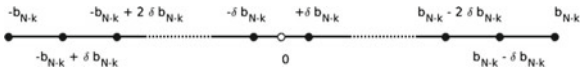
which corresponds to the Hermitian H_β of [17] for $m = 0$.

This procedure may be generalized by introducing, instead of a sign change, a smooth transition along the real line for each element b_k in the upper subdiagonal. For the kth element of the subdiagonal, the subdiagonal element would become

$$\hat{S}_{\beta,\alpha,f}(\tau) = \begin{pmatrix} \ddots & & & & \\ & a_{N-(k-1)+1} & b_{N-(k-1)}^{1+\alpha} & 0 & 0 \\ & b_{N-(k-1)}^{1-\alpha} & a_{N-k+1} & f(\tau) & 0 \\ & 0 & b_{N-k}^{1-\alpha} & a_{N-(k+1)+1} & b_{N-(k+1)}^{1+\alpha} \\ & & & & \ddots \end{pmatrix} \tag{27}$$

where $\tau \in [0, 1]$ and $f : [0, 1] \to [-b_{N-k}^{1+\alpha}, 0) \cup (0, +b_{N-k}^{1+\alpha}] \equiv I$ such that $f(0) = +b_{N-k}^{1+\alpha}$ and $f(1) = -b_{N-k}^{1+\alpha}$. By means of this parametrization, we may perform a smooth change while ensuring that a matrix η of the kind written in (10) is still definable. We restrict ourselves to the case of $\alpha = 0$ is this case as well.

In order to perform numerical studies of this transformation, we partition the interval I in q discrete segments



(28)

and choose the discrete function f_τ such that $f_\tau = b_{N-k} - \tau\delta b_{N-k}$, $\tau = 0, 1/q$, $2/q$..., 1 and $\delta b_{N-k} = 2b_{N-k}$.

We shift the kth subdiagonal into each of the f_τ and study the effect on the eigenvalues. Beginning with $\tau = 0$, once the case $\tau = 1$ is reached, we perform the same procedure in the next element. In this case, if there are m fully changed signs and the kth subdiagonal is transformed to f_τ, the $\eta_{m,j}$ matrix becomes

$$\eta_{m,\tau} = \text{diag}\left(1, -1, 1 \ldots, (-1)^{m-1}, (-1)^m, (-1)^m \frac{z_j}{b_{N-k}}, \ldots, (-1)^m \frac{z_j}{b_{N-k}}\right) \tag{29}$$

which is again non-positive definite.

In Fig. 4 we present the results for the real and complex eigenvalues for a matrix of size $N = 64$ for which the upper subdiagonal elements were shifted progressively toward their negative. Figure 4a, c present the eigenvalues that lie on the real axis for a sample matrix and the average matrix, respectively. Figure 4b, d present the remaining eigenvalues which have moved onto the complex plane for a sample matrix and the average matrix, respectively.

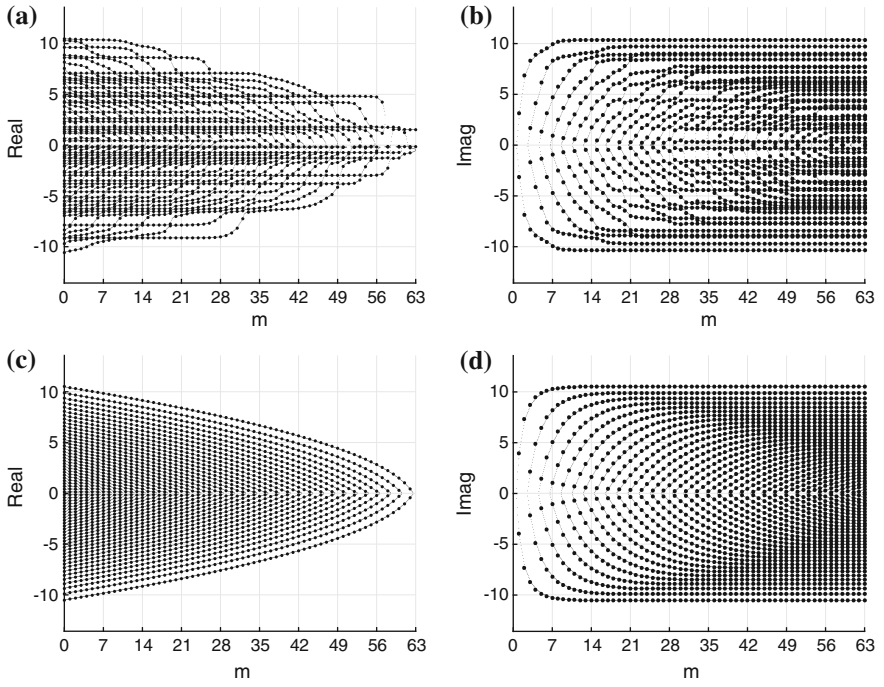


Fig. 4 Eigenvalue behavior in a sample of the sign changed matrices for a size $n = 8$ matrix. The larger circles denote the points in which a sign is fully changed as well as the initial eigenvalues for $m = 0$. **a** Shows the real eigenvalues a sampled matrix, whereas **b** shows the imaginary part of the complex eigenvalues. **c** and **d** present those same results for the average matrix

5 Conclusion

Based in the work on the previous ensemble of reference [24], in which a pseudo-Hermitian β-ensemble with real eigenvalues was proposed, and benefiting from properties of tridiagonal matrices we have extended the results of [25] and ensembles based on the β-ensemble were analyzed. One of those, dealt with perturbations outside of the edges of the matrix and allowing for the parametrization of the relationship between the two subdiagonals, presents a diverging metric operator in the asymptotic limit of large matrices. The second one loses positive-definiteness as the subdiagonals are successively shifted toward their negatives. In both cases the behavior of the eigenvalues presented similar qualitative behavior, as they shift into the complex plane in complex conjugate pairs. The precise behavior of each of these ensembles is not identical, however. In the first ensemble presented in Fig. 1, the eigenvalues begin to move to the complex plane from the eigenvalues with the smallest real part, whereas in the second ensemble presented in Fig. 4, those with the largest real part move first. and those differences illustrate possible ways by means of which random systems described by β ensembles may have levels shifting into the complex plane.

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Green's Function of a General PT-Symmetric Non-Hermitian Non-central Potential

Brijesh Kumar Mourya and Bhabani Prasad Mandal

Abstract We study the path integral solution of a system of particle moving in certain class of PT symmetric non-Hermitian and non-central potential. The Hamiltonian of the system is converted to a separable Hamiltonian of Liouville type in parabolic coordinates and is further mapped into a Hamiltonian corresponding to two 2-dimensional simple harmonic oscillators (SHOs). Thus the explicit Green's functions for a general non-central PT symmetric non hermitian potential are calculated in terms of that of 2d SHOs. The entire spectrum for this three dimensional system is shown to be always real leading to the fact that the system remains in unbroken PT phase all the time.

1 Introduction

Feynman's path integral (PI) approach to quantum mechanical systems is an elegant formalism and powerful in semi-classical calculations [1]. PI formalism which is generally tied to the Lagrangian formalism of mechanics is an extremely powerful technique in quantum mechanics. In a class of problems it provides the Green's function with tremendous ease and also provides valuable insight into the relation between classical and quantum mechanics. Green's functions which in mathematics are to solve non-homogeneous boundary value problems are the backbone of any calculations of physical quantities in quantum field theory [2]. Thus it is extremely important for any physical theory that the Green's functions are well defined. The purpose of the present work is to discuss the PI formulation of a general non-central, combined parity (P) and time reversal (T) symmetric non-Hermitian system in 3d by calculating the explicit Green's functions for such a system. Consistent quantum theory with real energy eigenvalues, unitary time evolution and probabilistic interpretation for PT symmetric non-Hermitian theories in a different Hilbert space

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equipped with positive definite inner product has been the subject of intrinsic research in frontier physics over the last one and half decades [3]. Such non-Hermitian PT symmetric systems generally exhibit PT phase transition or more specifically a PT breaking transition [4] which has been realised experimentally [5]. In-spite of huge success and wide applicability [6–11] of this field the study of non-Hermitian quantum mechanics is mostly restricted to one dimensional or central potentials in higher dimension potential problems. In this article we consider a general and very important non-central PT symmetric non-Hermitian system in the PI formulation. First we show that how the Hamiltonian corresponding to this potential is reduced to a separable Hamiltonian of Liouville type [12, 13] in a different coordinate system. This further enables us to map the system into two non-interacting 2d harmonic oscillators with the appropriate choice of coordinates. We then calculate the Green's functions of the system in terms of the Green's functions of 2d harmonic oscillators. Further we write the Hamiltonian in terms of appropriate creation and annihilation operators to calculate the energy eigenvalues of this non-central non-Hermitian system. We find that the energy eigenvalues are always real as long as the parameters in the potential are real. This indicates that system is always in unbroken PT phase.

Now we present the plan of the paper. In Sect. 2 we calculate the Green's function for the system in terms of SHO Green's functions. The reality of the spectrum is shown in Sect. 3. Section 4 is kept for concluding remarks.

2 Green's Functions for the PT-Symmetric Non-central Potential

We consider a system described by a general non-central non-Hermitian potential in 3-dimension in spherical polar coordinates as

$$H = \frac{P_r^2}{2m} + \frac{P_\theta^2}{2mr^2} + \frac{P_\phi^2}{2mr^2 sin^2\theta} + V(r,\theta) \tag{1}$$

where the non-Hermitian potential is

$$V(r,\theta) = -\frac{\alpha}{r} + \frac{B\hbar^2}{2mr^2\sin^2\theta} + \frac{iC\hbar^2\cos\theta}{2mr^2\sin^2\theta}. \tag{2}$$

α, B and C are real constants. It is straight forward to check that this non-Hermitian system is PT symmetric, where in 3-d in spherical polar coordinates the parity transformation is defined as, $r \to r;\ \theta \to \pi - \theta,\ \phi \to \phi + 2\pi$. This particular potential is very important as the Coulomb and the ring-shaped potentials are particular cases of this potential. For $C = 0$ this potential becomes Hartman's ring shaped potential which was originally proposed to model Benzene molecule [14]. To proceed with this Hamiltonian we first consider the most general Hamiltonian of Liouville type written as

$$H = \frac{1}{V_1(q_1) + V_2(q_2)} \left\{ \frac{1}{2mW_1(q_1)} p_1^2 + \frac{1}{2mW_2(q_2)} p_2^2 + U_1(q_1) + U_2(q_2) \right\} \quad (3)$$

This is reduced to a simpler form by using some canonical transformation and redefining U's and V's as [12]

$$H = \frac{1}{V_1(q_1) + V_2(q_2)} \left\{ \frac{1}{2m} p_1^2 + \frac{1}{2m} p_2^2 + U_1(q_1) + U_2(q_2) \right\} \quad (4)$$

The time independent Schrodinger equation corresponding to this Hamiltonian is then written as

$$\hat{H}_T \psi = 0$$

with a total Hamiltonian is defined as

$$\hat{H}_T = \frac{1}{2m} p_1^2 + \frac{1}{2m} p_2^2 + U_1(q_1) + U_2(q_2) - E(V_1(q_1) + V_2(q_2)) \quad (5)$$

Now, to obtain the path integral for this Hamiltonian $\hat{H}_T$, let us consider the evaluation of this operator for a arbitrary parameter τ:

$$\left\langle q_{1b},\, q_{2b} \left| \exp\left\{ -i \frac{\hat{H}_T \tau}{\hbar} \right\} \right| q_{1a},\, q_{2a} \right\rangle = \left\langle q_{1b} \left| \exp\left\{ -(\frac{i}{\hbar}) \left[\frac{1}{2m} \hat{p}_1^2 + U_1(q_1) - EV_1(q_1) \right] \tau \right\} \right| q_{1a} \right\rangle \times \left\langle q_{2b} \left| \exp\left\{ -(\frac{i}{\hbar}) \left[\frac{1}{2m} \hat{p}_2^2 + U_2(q_2) - EV_2(q_2) \right] \tau \right\} \right| q_{2a} \right\rangle \quad (6)$$

The RHS of (6) is written in terms of path integral [12].

$$\left\langle q_{1b},\, q_{2b} \left| \exp\left\{ -i \frac{\hat{H}_T \tau}{\hbar} \right\} \right| q_{1a},\, q_{2a} \right\rangle = \int \mathcal{D}q_1 \mathcal{D}p_1 \exp\left\{ (\frac{i}{\hbar} \int_0^\tau \left[p_1 \dot{q}_1 - \left(\frac{\hat{p}_1^2}{2m} + U_1(q_1) - EV_1(q_1) \right) \right] d\tau \right\} \times \int \mathcal{D}q_2 \mathcal{D}p_2 \exp\left\{ (\frac{i}{\hbar} \int_0^\tau \left[p_2 \dot{q}_2 - \left(\frac{\hat{p}_2^2}{2m} + U_2(q_2) - EV_2(q_2) \right) \right] d\tau \right\} \quad (7)$$

The parameter τ is arbitrary and one can obtain physically meaningful quantity out of (6) by integrating over τ from 0 to ∞.

$$\left\langle q_{1b},\, q_{2b} \left| \frac{\hbar}{\hat{H}_T} \right| q_{1a},\, q_{2a} \right\rangle_{\text{Semi-classical}} = \int_0^\infty d\tau \left\langle q_{1b} \left| \exp\left\{ -(\frac{i}{\hbar}) \left[\frac{1}{2m} \hat{p}_1^2 + U_1(q_1) - EV_1(q_1) \right] \tau \right\} \right| q_{1a} \right\rangle \times \left\langle q_{2b} \left| \exp\left\{ -(\frac{i}{\hbar}) \left[\frac{1}{2m} \hat{p}_2^2 + U_2(q_2) - EV_2(q_2) \right] \tau \right\} \right| q_{2a} \right\rangle \quad (8)$$

The meaning of RHS of (8) has been explained in [12]. And the LHS of it is written as,

$$\left\langle q_{1b},\, q_{2b} \left| \frac{\hbar}{\hat{H}_T} \right| q_{1a},\, q_{2a} \right\rangle = \left\langle q_{1b},\, q_{2b} \left| \frac{\hbar}{\hat{H} - E} \right| q_{1a},\, q_{2a} \right\rangle \frac{1}{V_1(q_{1a}) + V_2(q_{2a})} \tag{9}$$

with the completeness relation

$$\int |q_1\, q_2\rangle \frac{dV}{V_1(q_1) + V_2(q_2)} \langle q_1\, q_2| = 1 \tag{10}$$

Now we show that the Hamiltonian of a particle in a non-central potential is reduced to a separable Hamiltonian of the above kind. Let us start with the non-central system written in (2)

$$H = \frac{P_r^2}{2m} + \frac{P_\theta^2}{2mr^2} + \frac{P_\phi^2}{2mr^2 \sin^2\theta} - \frac{\alpha}{r} + \frac{\beta}{r^2 \sin^2\theta} + \frac{i\gamma \cos\theta}{r^2 \sin^2\theta} \tag{11}$$

where $\beta = \frac{B\hbar^2}{2m}$; $\gamma = \frac{C\hbar^2}{2m}$. This system will be reduced to separable system of Liouville type in parabolic coordinate system. To express the Hamiltonian in parabolic coordinates (ξ, η, ϕ), it is useful to first express this potential $V(r, \theta)$ in cylindrical coordinates (ρ, ϕ, z). In cylindrical coordinate the potential looks like,

$$V(\rho, z) = -\frac{\alpha}{\sqrt{\rho^2 + z^2}} + \frac{\beta}{\rho^2} + \frac{i\gamma z}{\rho^2\sqrt{\rho^2 + z^2}}; \qquad \rho^2 = x^2 + y^2 \tag{12}$$

The parabolic coordinates are expressed in terms of cylindrical coordinates as

$$\begin{aligned} \xi &= \frac{1}{2}\left(\sqrt{\rho^2 + z^2} - z\right); \\ \eta &= \frac{1}{2}\left(\sqrt{\rho^2 + z^2} + z\right); \quad \phi = \phi. \end{aligned} \tag{13}$$

Now the potential in (12) in terms of these parabolic coordinates, is

$$V(\xi, \eta) = -\frac{\alpha}{\xi + \eta} + \frac{\beta}{4\xi\eta} + \frac{i\gamma(\eta - \xi)}{4\eta\xi(\eta + \xi)} \tag{14}$$

and the Hamiltonian in parabolic coordinate is written as

$$H(\xi, \eta, \phi) = \frac{1}{2m(\xi + \eta)}\left[\xi \hat{p}_\xi^2 + \eta \hat{p}_\eta^2\right] + \frac{1}{8m\eta\xi}\hat{p}_\phi^2 + V(\xi, \eta) \tag{15}$$

We define variables u, v

$$\xi = \frac{1}{4}u^2; \quad 0 \leq u \langle \infty$$
$$\eta = \frac{1}{4}v^2; \quad 0 \leq v \langle \infty \tag{16}$$

and perform a canonical transformation

$$\sqrt{\xi}\,\hat{p}_\xi = \hat{p}_u; \ \sqrt{\eta}\,\hat{p}_\eta = \hat{p}_v \tag{17}$$

to simplify the kinetic term in H in (15) as

$$H(u, v, \phi) = \frac{4}{u+v}\left\{\frac{1}{2m}\left[\hat{p}_u^2 + \hat{p}_v^2 + \left(\frac{1}{u^2} + \frac{1}{v^2}\right)\hat{p}_\phi^2\right] - \alpha + \frac{\beta + i\gamma}{u^2} + \frac{\beta - i\gamma}{v^2}\right\} \tag{18}$$

This is further written compactly as

$$H(u, v, \phi) = \frac{4}{u^2+v^2}\left\{\frac{1}{2m}\left[\hat{p}_u^2 + \hat{p}_v^2 + \frac{1}{u^2}\hat{p}_{\phi_1}^2 + \frac{1}{v^2}\hat{p}_{\phi_2}^2\right] - \alpha\right\} \tag{19}$$

where

$$\hat{p}_{\phi_1}^2 = \hat{p}_\phi^2 + 2m(\beta + i\gamma); \quad \hat{p}_{\phi_2}^2 = \hat{p}_\phi^2 + 2m(\beta - i\gamma) \tag{20}$$

Note $\hat{p}_{\phi_1}$ and $\hat{p}_{\phi_2}$ are not Hermitian but complex conjugate to each other. This Hamiltonian is still not a separable one of Liouville type. We further consider the total Hamiltonian $H_T (= H - E)$ with $E = -2m\omega^2$ for the bound state case ($E \langle 0$),

$$\hat{H}_T = \frac{1}{2m}\left[\hat{p}_u^2 + \hat{p}_v^2 + \frac{1}{u^2}\hat{p}_{\phi_1}^2 + \frac{1}{v^2}\hat{p}_{\phi_2}^2\right] - \alpha + \frac{1}{2}m\omega^2(u^2 + v^2) \tag{21}$$

Now we introduce the components of 2-dimensional vectors **u** and **v** as

$$\mathbf{u} = (u_1, u_2) = (u\cos\phi_1, u\sin\phi_1)$$
$$\mathbf{v} = (v_1, v_2) = (v\cos\phi_2, v\sin\phi_2) \tag{22}$$

to have

$$\mathbf{p}_u^2 = \hat{p}_u^2 + \frac{1}{u^2}\hat{p}_{\phi_1}^2; \qquad \mathbf{p}_v^2 = \hat{p}_v^2 + \frac{1}{v^2}\hat{p}_{\phi_2}^2; \tag{23}$$

Putting all these in (21) we obtain

$$\hat{H}_T = \frac{1}{2m}\mathbf{p}_u^2 + \frac{m\omega^2}{2}\mathbf{u}^2 + \frac{1}{2m}\mathbf{p}_v^2 + \frac{m\omega^2}{2}\mathbf{v}^2 - \alpha \tag{24}$$

This is the Hamiltonian which is separable of Liouville type. Thus, the Hamiltonian for the non-central potential has been reduced to that of two 2-dimensional oscillators (apart from some constant shift in ground state energy).

Now by using (6) for this separable Hamiltonian, we find the path integral for the non-Hermitian non-central potential exactly as

$$\left\langle \mathbf{u}_b,\ \mathbf{v}_b \left| \exp\left[-i\frac{\hat{H}_T\tau}{\hbar}\right] \right| \mathbf{u}_a,\ \mathbf{v}_a \right\rangle = e^{\frac{i\alpha\tau}{\hbar}} \left\langle \mathbf{u}_b \left| \exp\left[-(\frac{i}{\hbar})\left(\frac{\mathbf{p}_u^2}{2m}+\frac{m\omega^2}{2}\mathbf{u}^2\right)\tau\right] \right| \mathbf{u}_a \right\rangle$$
$$\times \left\langle \mathbf{v}_b \left| \exp\left[-(\frac{i}{\hbar})\left(\frac{\mathbf{p}_v^2}{2m}+\frac{m\omega^2}{2}\mathbf{v}^2\right)\tau\right] \right| \mathbf{u}_a \right\rangle = e^{(\frac{i\alpha\tau}{\hbar})}\left(\frac{im\omega}{2\pi i\hbar\sin\omega\tau}\right)^{\frac{4}{2}}$$
$$\exp\left\{\frac{im\omega}{2\hbar\sin\omega\tau}\left[\left(\mathbf{u}_b^2+\mathbf{v}_b^2+\mathbf{u}_a^2+\mathbf{v}_a^2\right)\cos\omega\tau - 2\mathbf{u}_b\cdot\mathbf{u}_a - 2\mathbf{v}_b\cdot\mathbf{v}_a\right]\right\} \tag{25}$$

where the exact result for one dimensional simple harmonic oscillator has been used [1].

$$\left\langle q_b \left| \exp\left[-\frac{i}{\hbar}\left(\frac{\hat{p}^2}{2m}+\frac{m\omega^2q^2}{2}\right)\tau\right] \right| q_a \right\rangle = \left(\frac{m\omega}{2\pi i\hbar\sin\omega\tau}\right)^{\frac{1}{2}}$$
$$\exp\left\{\frac{im\omega}{2\hbar\sin\omega\tau}\left[(q_a^2+q_b^2)\cos\omega\tau - 2q_aq_b\right]\right\} \tag{26}$$

The (25) contains the arbitrary parameter τ and has to be eliminated to obtain physically meaningful quantity. This can be done by integrating over τ from 0 to ∞ in both side of the (25). When we integrate over τ in the LHS of the (25), it is nothing but the Green's functions of the operator $\frac{1}{\hat{H}-E}$ as discussed at beginning of this section. And the integration in the RHS can be done in a straightforward manner [12]. Thus we obtain the explicit Green's functions for the system of non central non-Hermitian potential.

3 Reality of the Spectrum

Since this system with non-Hermitian, non-central potential is equivalent to two 2d SHOs, conjugate to each other we define the creation and annihilation operators for this theory as

$$a_k = \frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}u_k + \frac{i}{\sqrt{m\omega\hbar}}\hat{p}_{u_k}\right]$$
$$\tilde{a}_k = \frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}v_k + \frac{i}{\sqrt{m\omega\hbar}}\hat{p}_{v_k}\right] \tag{27}$$

where $k = 1, 2$ to obtain the energy levels for this system of non-central potential in a simple algebraic way. The total Hamiltonian in (24) is written in terms of these creation and annihilation operators as follows:

$$\hat{H}_T = \hbar\omega\left[\sum_{k=1}^{2}\left(a_k^\dagger a_k + \tilde{a}_k^\dagger \tilde{a}_k\right) + 2\right] - \alpha \tag{28}$$

and the conjugate momentum variables are written as

$$\begin{aligned}\hat{p}_{\phi_1} &= i\hbar\left[a_1^\dagger a_2 - a_2^\dagger a_1\right] \\ \hat{p}_{\phi_2} &= i\hbar\left[\tilde{a}_1^\dagger \tilde{a}_2 - \tilde{a}_2^\dagger \tilde{a}_1\right]\end{aligned} \tag{29}$$

We further perform an unitary transformation of the following type,

$$\begin{aligned}a_1 &= \frac{1}{\sqrt{2}}\left(b_1 - ib_2\right) \\ a_2 &= \frac{1}{\sqrt{2}}\left(-ib_1 + b_2\right)\end{aligned} \tag{30}$$

and similar transformations for $\tilde{a}_1, \tilde{a}_2$ also in (28) and (29) to get,

$$\hat{H}_T = \hbar\omega\left[\sum_{k=1}^{2}\left(b_k^\dagger b_k + \tilde{b}_k^\dagger \tilde{b}_k\right) + 2\right] - \alpha \tag{31}$$

and

$$\begin{aligned}\hat{p}_{\phi_1} &= \hbar\left[b_1^\dagger b_1 - b_2^\dagger b_2\right] \\ \hat{p}_{\phi_2} &= \hbar\left[\tilde{b}_1^\dagger \tilde{b}_1 - \tilde{b}_2^\dagger \tilde{b}_2\right]\end{aligned} \tag{32}$$

The number operators, $n_k = b_k^\dagger b_k$, $\tilde{n}_k = \tilde{b}_k^\dagger \tilde{b}_k$ are defined for this system. In terms of number operators the total Hamiltonian in (31) is now written as

$$\begin{aligned}\hat{H}_T &= \hbar\omega\left[n_1 + n_2 + \tilde{n}_1 + \tilde{n}_2 + 2\right] - \alpha \\ &= 2\hbar\omega\left[n_2 + \tilde{n}_2 + 1 + \frac{\hat{p}_{\phi_1} + \hat{p}_{\phi_2}}{\hbar}\right] - \alpha\end{aligned} \tag{33}$$

Now considering $\left[\hat{p}_{\phi_1} + \hat{p}_{\phi_2}\right]\phi_{phy} \equiv \lambda\phi_{phy}$, the physical state condition is [12],

$$\left[2(n_2 + \tilde{n}_2 + 1)\hbar\omega + \omega\lambda - \alpha\right]\phi_{phy} = 0 \tag{34}$$

Hence the energy level can be written in terms of λ as,

$$E_{n_2,\tilde{n}_2,\lambda} \equiv -2m\omega^2 = -\frac{2m\alpha^2}{\left[2(n_2+\tilde{n}_2+1)\hbar+\lambda\right]^2}. \tag{35}$$

λ can be calculated easily using $\left[\hat{p}_{\phi_1}+\hat{p}_{\phi_2}\right]\phi_{phy} \equiv \lambda\phi_{phy}$ and (20) as

$$\begin{aligned}\lambda &= \hbar\left[\left(\nu^2+B+iC\right)^{\frac{1}{2}}+\left(\nu^2+B-iC\right)^{\frac{1}{2}}\right] \\ &= \left[\left(\nu^2\hbar^2+2m(\beta+i\gamma)\right)^{\frac{1}{2}}+\left(\nu^2\hbar^2+2m(\beta-i\gamma)\right)^{\frac{1}{2}}\right]\end{aligned} \tag{36}$$

where ν is non-negative integer and λ is real as $\lambda = \lambda^*$. Therefore, the complete real bound state spectrum for the problem is

$$\begin{aligned}E_{n_2,\tilde{n}_2,\nu} &= \frac{-m\alpha^2}{2\hbar^2\left[n_2+\tilde{n}_2+1+\frac{\sqrt{\nu^2+B+iC}+\sqrt{\nu^2+B-iC}}{2}\right]^2} \\ &= \frac{-m\alpha^2}{2\left[(n_2+\tilde{n}_2+1)\hbar+\frac{\sqrt{\nu^2\hbar^2+2m(\beta+i\gamma)}+\sqrt{\nu^2\hbar^2+2m(\beta-i\gamma)}}{2}\right]^2}\end{aligned} \tag{37}$$

The corresponding result for the real potential agrees with that of in [15, 16] where energy spectrum has been calculated by solving Schroedinger equation using complicated KS transformation [17, 18].

4 Conclusion

The Hamiltonian corresponding to the PT symmetric non-Hermitian non-central potential in (2) has been mapped into a Hamiltonian of two 2d harmonic oscillators by choosing appropriate coordinate system and using a suitable canonical transformation. Next we have calculated the Green's functions for the system using path integral method for this separable Hamiltonian of Liouville type. The exact spectrum are calculated by writing this Hamiltonian in terms of creation and annihilation operators of 2d SHO. The entire spectrum is real for any real values of the parameters α, β and γ indicating that system is always in unbroken phase.

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Non-Hermitian Quantum Annealing and Superradiance

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Abstract We consider the non-Hermitian quantum annealing (NQA) for a one-dimensional Ising spin chain, and for a large number of qubits. We show that the annealing time is significantly reduced for the non-Hermitian quantum algorithm in comparison with the Hermitian one. We optimize a performance of the NQA, and demonstrate the relation of the NQA with the superradiance transition in this system.

1 Introduction

It is generally recognized that quantum annealing (QA) algorithms can be useful for solving many hard problems related to optimization of complex networks, finding the global minimum of multi-valued functions, and cost minimization [1–7]. Opposite to classical annealing algorithm, the QA operates at zero temperature. Then, one can reformulate the optimization problem in terms of finding the ground state of the N-qubits system governed by the effective quantum Hamiltonian. (No classical sub-systems are involved.)

The idea of the QA algorithm can be formulated as follows. (The approach used below, is based on [8], where many details can be found.) Consider the time-dependent quantum Hamiltonian, $\mathscr{H}(t) = \mathscr{H}_0 + \Gamma(t)\mathscr{H}_1$. Here $\mathscr{H}_0$ is the quantum Ising-type Hamiltonian to be optimized, $\mathscr{H}_1$ is an auxiliary ("initial") quantum

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Hamiltonian, and it is assumed that $[\mathscr{H}_0, \mathscr{H}_1] \neq 0$. During the quantum annealing, the external time-dependent field, $\Gamma(t)$, decreases from a large enough value to zero. Then, the ground state of $\mathscr{H}_1$ at $t = 0$ (which is assumed to be known and relatively simple), can be considered as the initial (ground) state for the whole quantum system. If $\Gamma(t)$ decreases sufficiently slowly, the adiabatic theorem guarantees finding the ground state of the main Hamiltonian, $\mathscr{H}_0$, with rather high probability (see the text), at the end of annealing. Sure, when the time of QA is finite, the finite probability of formation of defects is expected. (See numerical simulations below.)

One of the main challenges is to accelerate the speed of QA algorithms, so that the annealing time grows not exponentially, but polynomially with the size of the problem [9–14]. In [15], we proposed the non-Hermitian quantum annealing (NQA) algorithm, which leads to a significant reduction of the annealing time. In NQA it is assumed that the part of the auxiliary non-Hermitian Hamiltonian vanishes (together with the auxiliary Hermitian part) at the end of the time-evolution. So, after the annealing is finished, the system is governed by the Hermitian Hamiltonian of the system whose ground state is supposed to be found.

Recently, we have applied the NQA algorithm to Grover's problem of finding a marked item in an unsorted database, and to study the transition to the ground state in a 1-dimensional ferromagnetic (and anti-ferromagnetic) Ising chain [8, 16, 17]. Analytical and numerical results demonstrate that, even for a moderate value of the decay parameter, the NQA has a complexity of order $\ln N$, where N is the number of qubits in the quantum register. The main reason for this is the following. In the NQA regime the minimal gap in the energy spectrum shifts in the region of short wavelengths, which are not significantly excited in the dynamical process of the NQA. This encouraging result could be important, for example, in using classical computers in combination with quantum algorithms for fast solutions of hard optimization problems.

One of the open problems in the NQA is a dependence of annealing time on the value of the decay parameter. The answer is not obvious due to the interplay of the dynamical process of NQA and the decay of discrete states of the quantum register to continuum. As will be discussed below, the later could be associated with the superradiance transition (ST), which occurs in the process of NQA. Usually, the ST is associated with a significant enhancement of the spontaneous radiation due to quantum coherent effects, as it first was shown by Dicke in 1954 [18]. Later it was demonstrated that the ST occurs in many quantum optical systems, nuclear systems (heavy nuclei decay), nano- and bio-systems [19–27]. In these systems, the ST occurs when the discrete energy states of the system (associated with the quantum register) interact with the continuum spectra (associated with the sinks). In our case, the discrete energy states of the Hermitian Hamiltonian, $\mathscr{H}_0$, interact with the continuum energy spectrum provided by the non-Hermitian part, $\mathscr{H}_1$, of the whole Hamiltonian. An adequate approach for describing the dynamics of such systems can be based on an effective non-Hermitian Hamiltonian [19–24].

In this paper, we describe in details the NQA for finding the ground state of the ferromagnetic 1D chain of 1/2 spins (qubits), and establish the relation of this problem with the ST in this system. The paper is organized as follows. In Sec II,

we describe the model and the conditions of the applicability of the NQA. In Sec. III, we describe the dynamics of the NQA and present the results of the numerical simulations. In Sec IV, we discuss the relation between the NQA and the ST. In Conclusion, we discuss our results.

2 Non-Hermitian Quantum Annealing

The generic adiabatic quantum optimization problem, based on the QA algorithm, can be formulated as follows [15]. Let $\mathscr{H}_0$ be the Hermitian quantum Hamiltonian whose ground state is to be found. Consider the non-Hermitian time-dependent quantum Hamiltonian:

$$\tilde{\mathscr{H}_\tau}(t) = \mathscr{H}_0 + \tilde{\mathscr{H}_1}(t/\tau), \tag{1}$$

where τ is the time of QA, and $[\mathscr{H}_0, \tilde{\mathscr{H}_1}] \neq 0$. The evolution of the system is described by the Schrödinger equation ($\hbar = 1$):

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = \tilde{\mathscr{H}_\tau}(t)|\psi(t)\rangle. \tag{2}$$

The initial conditions are imposed as follows: $|\psi(0)\rangle = |\psi_g\rangle$, where $|\psi_g\rangle$ is the ground state of the auxiliary non-Hermitian quantum Hamiltonian: $\tilde{\mathscr{H}_1}(0)|\psi_g\rangle = E_g|\psi_g\rangle$. At the end of the evolution, the total Hamiltonian, $\tilde{\mathscr{H}_\tau}(\tau) = \mathscr{H}_0$, and the adiabatic theorem guarantees that the final state will be the ground state of $\mathscr{H}_0$, if the evolution was slow enough. As was already mentioned, the finite time of QA results in a finite number of defects, which is a well-known result. (See also below.)

We denote by $|\psi_n(t)\rangle$ and $\langle\tilde{\psi}_n(t)|$ the right and the left instantaneous eigenvectors of the total Hamiltonian: $\tilde{\mathscr{H}_\tau}(t)|\psi_n(t)\rangle = E_n(t)|\psi_n\rangle$, $\langle\tilde{\psi}_n(t)|\tilde{\mathscr{H}_\tau}(t) = \langle\tilde{\psi}_n(t)|E_n(t)$. We assume that these eigenvectors form a bi-orthonormal basis, $\langle\tilde{\psi}_m|\psi_n\rangle = \delta_{mn}$ [28]. For the non-Hermitian quantum optimization problem, governed by the Hamiltonian (1), the validity of the adiabatic approximation requires [8, 29–31],

$$\tau \gg \frac{\max|\langle\tilde{\psi}_e(t)|\dot{\tilde{\mathscr{H}}}_\tau(t)|\psi_g(t)\rangle|}{\min|E_e(t) - E_g(t)|^2}, \tag{3}$$

where "dot" denotes the derivative with respect to the dimensionless time, $s = t/\tau$, and E_e is the energy of the first excited state, $|\psi_e\rangle$. This restriction is violated near the ground state degeneracy, where complex energy levels cross. The degeneracy is known as the exceptional point (EP), and it is characterized by a coalescence of eigenvalues and their corresponding eigenvectors, as well [32–39]. Thus, if the gap, $\Delta E = \min|E_e - E_g|$, is small enough, the time required to pass from the initial state to the final state becomes very large, and the NQA loses its advantage over the thermal annealing.

2.1 Description of the Model

We consider the time-dependent quantum non-Hermitian Hamiltonian, $\tilde{\mathscr{H}}_\tau(t) = \mathscr{H}_0 + \tilde{\mathscr{H}}_1(t)$, where

$$\mathscr{H}_0 = -J \sum_k (\cos\varphi_k \mathbf{I} - \sin\varphi_k \sigma_x + \cos\varphi_k \sigma_z) \tag{4}$$

and

$$\tilde{\mathscr{H}}_1(t) = J \sum_k (-i\delta(1 - t/\tau)\mathbf{I} + \tilde{g}(t)\sigma_z). \tag{5}$$

We denote $\varphi_k = \pi(2k-1)/N$, where $k = \pm 1, 2, \ldots, \pm N/2$, with $N/2$ being an even integer. We assume linear dependence of the function $\tilde{g}(t)$ on time:

$$\tilde{g}(t) = \begin{cases} (g + i\delta)(1 - t/\tau), & 0 \le t \le \tau, \\ 0, & t > \tau, \end{cases} \tag{6}$$

where g and δ are real parameters.

The total Hamiltonian, $\tilde{\mathscr{H}}_\tau(t)$, can be rewritten as follows: $\tilde{\mathscr{H}}_\tau(t) = \sum_k \tilde{\mathscr{H}}_k(t)$, where

$$\tilde{\mathscr{H}}_k(t) = -\varepsilon_{0k}(t)\mathbf{I} + J \begin{pmatrix} \tilde{g}(t) - \cos\varphi_k & \sin\varphi_k \\ \sin\varphi_k & -\tilde{g}(t) + \cos\varphi_k \end{pmatrix}, \tag{7}$$

$\varepsilon_{0k}(t) = J\cos\varphi_k + iJ\delta(1 - t/\tau)$. The Hamiltonian, $\tilde{\mathscr{H}}_\tau(t)$, describes the NQA in the momentum representation for the 1D Ising model in a transverse magnetic field [8]. The external magnetic field is associated with the parameter, g, and the rate of decay into continuum (sink) is described by the parameter, δ.

Let $g \gg 1$, then the initial ground state of the total Hamiltonian is determined by the ground state of the auxiliary Hamiltonian, $\tilde{\mathscr{H}}_1(0) = J\sum_k(-i\delta + (g + i\delta)\sigma_z)$. At the end of the NQA, one obtains, $\tilde{\mathscr{H}}_\tau(\tau) = \mathscr{H}_0$. If the quench is slow enough, the adiabatic theorem guarantees the approach of the ground state of the main Hamiltonian, $\mathscr{H}_0$, at the end of the annealing.

Resolving the eigenvalue problem for the Hamiltonian, $\mathscr{H}_k(t)$, we obtain

$$|u_+(k,t)\rangle = \begin{pmatrix} \cos\frac{\theta_k(t)}{2} \\ \sin\frac{\theta_k(t)}{2} \end{pmatrix}, \ \langle \widetilde{u}_+(k)| = \big(\cos\frac{\theta_k(t)}{2}, \sin\frac{\theta_k(t)}{2}\big), \tag{8}$$

$$|u_-(k,t)\rangle = \begin{pmatrix} -\sin\frac{\theta_k(t)}{2} \\ \cos\frac{\theta_k(t)}{2} \end{pmatrix}, \ \langle \widetilde{u}_-(k,t)| = \big(-\sin\frac{\theta_k(t)}{2}, \cos\frac{\theta_k(t)}{2}\big), \tag{9}$$

where

$$\cos\theta_k(t) = \frac{\tilde{g}(t) - \cos\varphi_k}{\sqrt{\tilde{g}^2(t) - 2\tilde{g}(t)\cos\varphi_k + 1}}, \tag{10}$$

$$\sin\theta_k(t) = \frac{\sin\varphi_k}{\sqrt{\tilde{g}^2(t) - 2\tilde{g}(t)\cos\varphi_k + 1}}, \tag{11}$$

θ_k being a complex angle. We denote by $|u_\pm(k,t)\rangle$ ($\langle\widetilde{u}_\pm(k,t)|$) the right (left) instantaneous eigenvectors of the Hamiltonian $\mathscr{H}_k(t)$, and by $\varepsilon_\pm(k,t) = -\varepsilon_{0k}(t) \pm \varepsilon_k(t)$ the corresponding (complex) eigenenergies,

$$\varepsilon_{0k}(t) = J\cos\varphi_k + iJ\delta(1 - t/\tau), \tag{12}$$

$$\varepsilon_k(t) = J\sqrt{\tilde{g}^2(t) - 2\tilde{g}(t)\cos\varphi_k + 1}. \tag{13}$$

For a given value of k, the complex energy levels of the effective non-Hermitian Hamiltonian, $\mathscr{H}_k(t)$, cross at the EP, defined by the condition: $\tilde{g}(t_c) = e^{\pm i\varphi_k}$. As a result, the energy gap vanishes at the EP. The computation yields $\varphi_{k_c} = \tan^{-1}(\delta/g)$. The system reaches the EP at the moment of time

$$\frac{t_c}{\tau} = 1 - \frac{1}{\sqrt{g^2 + \delta^2}}. \tag{14}$$

Note, that the difference between the Hermitian QA ($\delta = 0$) and non-Hermitian QA is that, while in the first case the minimal gap occurs for long wavelength modes ($k \sim 1$), in the second case the minimal gap shifts to short wavelength modes ($k \sim (N/2\pi)\tan^{-1}(\delta/g)$). In particular, for $\delta \gg g$ we obtain $k \sim N/4$.

The requirement of the adiabatic theorem (3) can be rewritten in the equivalent form as,

$$\max\left|\frac{d\theta_k}{dt}\right| \ll \min 2|\varepsilon_k|. \tag{15}$$

We find

$$\max\left|\frac{d\theta_k}{dt}\right| = \frac{g\cos\alpha|\sin\varphi_k|}{\tau|\sin(\alpha - \varphi_k)\sin(\alpha + \varphi_k)|}, \tag{16}$$

$$\min|\varepsilon_k| = \frac{J}{\cos\alpha}\sqrt{|\sin(\alpha - \varphi_k)\sin(\alpha + \varphi_k)|}, \tag{17}$$

where $\alpha = \tan^{-1}(\delta/g)$. Employing these results, one can recast (15) as,

$$\eta_k = \frac{g\cos^2\alpha|\sin\varphi_k|}{2J\tau(|\sin(\alpha - \varphi_k)\sin(\alpha + \varphi_k)|)^{3/2}} \ll 1. \tag{18}$$

Thus, for a given value of k, the condition of the adiabaticity can be written as $\eta_k \ll 1$. This condition is violated in the vicinity of the EP, defined by the equation, $\alpha = \varphi_k$. In particular, for the Hermitian QA ($\alpha = 0$), we obtain

$$\eta_k = \frac{g}{2J\tau \sin^2 \varphi_k} \ll 1. \tag{19}$$

Since, $\eta_k \leq \eta_1$, we find that the adiabatic approximation is valid for all modes, if

$$\frac{g}{2J\tau \sin^2(\pi/N)} \ll 1. \tag{20}$$

For $N \gg 1$, we obtain the following estimate of the annealing time,

$$\tau \gg \frac{gN^2}{2J\pi^2}. \tag{21}$$

In the thermodynamic limit ($N \gg 1$), one can consider the variable φ_k as a continuous variable, φ. In Fig. 1, the adiabatic parameter, η, as a function of the angle, φ and the parameter, δ, is presented. One can see the regions of the adiabatic conditions, when $\eta \ll 1$.

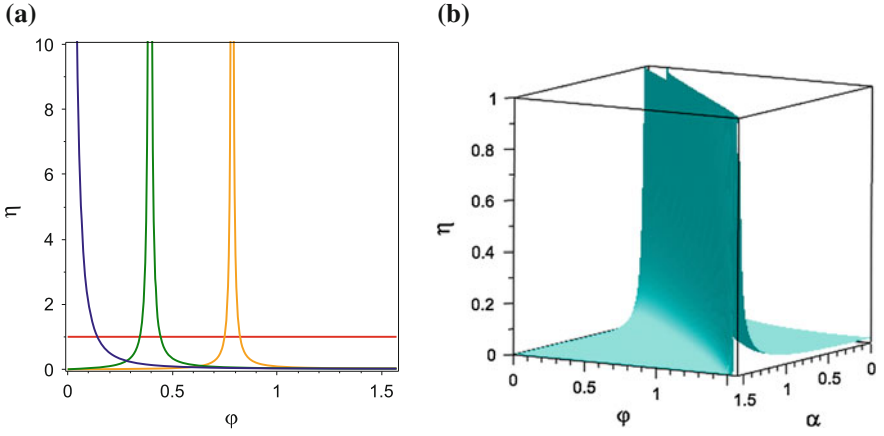

Fig. 1 **a** The dependence of the function η on φ: $\alpha = 0$ (*blue*), $\alpha = \pi/8$ (*green*), $\alpha = \pi/4$ (*orange*). *Red line* corresponds to $\eta = 1$. **b** The dependence of the function η on α and φ. Parameters: $J = 0.5$, $g = 10$, $\tau = 500$

3 Quench Dynamics

Since the Hamiltonian of the system is presented by the sum of the independent terms, the total wave functions, $|\psi\rangle$ and $\langle\tilde{\psi}|$, can be written as the product: $|\psi\rangle = \prod_k |\psi_k\rangle$ and $\langle\tilde{\psi}| = \prod_k \langle\tilde{\psi}_k|$. The wave functions, $|\psi_k\rangle$ and $\langle\tilde{\psi}_k|$, satisfy the Schrödinger equation and its adjoint equation:

$$i\frac{\partial}{\partial t}|\psi_k\rangle = \tilde{\mathscr{H}_k}(t)|\psi_k\rangle, \quad -i\frac{\partial}{\partial t}\langle\tilde{\psi}_k| = \langle\tilde{\psi}_k|\tilde{\mathscr{H}_k}(t). \tag{22}$$

Presenting $|\psi_k(t)\rangle$ as,

$$|\psi_k(t)\rangle = (u_k(t)|0\rangle + v_k(t)|1\rangle)e^{i\int \varepsilon_0(t)dt}, \tag{23}$$

and inserting expression (23) into (22), we obtain

$$i\dot{u}_k = J\big(-(\tilde{g} - \cos\varphi_k)\, u_k + \sin\varphi_k\, v_k\big), \tag{24}$$

$$i\dot{v}_k = J\big(\sin\varphi_k\, u_k + (\tilde{g} - \cos\varphi_k)\, v_k\big). \tag{25}$$

The solution can be written in terms of the parabolic cylinder functions, $D_{-iv_k}(\pm z)$. (For details see [8].)

In the adiabatic basis formed by the instantaneous eigenvectors of the Hamiltonian $\mathscr{H}_k(t)$, the wave function, $|\psi_k(t)\rangle$, can be written as,

$$|\psi_k(t)\rangle = (\alpha_k(t)|u_-(k,t)\rangle + \beta_k(t)|u_+(k,t)\rangle)e^{i\int \varepsilon_{0k}(t)dt}. \tag{26}$$

From (8) and (23) it follows

$$\alpha_k(t) = u_k(t)\cos\frac{\theta_k(t)}{2} - v_k(t)\sin\frac{\theta_k(t)}{2}, \tag{27}$$

$$\beta_k(t) = v_k(t)\cos\frac{\theta_k(t)}{2} + u_k(t)\sin\frac{\theta_k(t)}{2}. \tag{28}$$

Then one can show that,

$$|\Psi_k(t)\rangle = \begin{pmatrix}\beta_k(t)\\ \alpha_k(t)\end{pmatrix}, \tag{29}$$

satisfies the Schrödinger equation,

$$i\frac{\partial}{\partial t}|\Psi_k\rangle = \mathscr{H}_k(t)|\Psi_k\rangle, \tag{30}$$

with the new Hamiltonian,

$$\mathscr{H}_k(t) = \begin{pmatrix} \varepsilon_k & i\dot{\theta}_k/2 \\ -i\dot{\theta}_k/2 & -\varepsilon_k \end{pmatrix}. \tag{31}$$

Using the relation, $\tan\theta_k = \sin\varphi_k/(\tilde{g}(t)\cos\varphi_k)$, we obtain

$$\frac{d\theta_k}{dt} = -\frac{\dot{\tilde{g}}(t)\sin^2\theta_k(t)}{\sin\varphi_k}. \tag{32}$$

Assume that the evolution begins from the ground state. This implies $\alpha_k(0) = 1$ and $\beta_k(0) = 0$. Then, the solution of (30) can be written as [8],

$$\alpha_k(t) = C_k\left(D_{-i\nu_k}(z_k(t))\sin\frac{\varphi_k}{2} + \sqrt{i\nu_k}D_{-i\nu_k-1}(z_k(t))\cos\frac{\varphi_k}{2}\right), \tag{33}$$

$$\beta_k(t) = C_k\left(D_{-i\nu_k}(z_k(t))\cos\frac{\varphi_k}{2} - \sqrt{i\nu_k}D_{-i\nu_k-1}(z_k(t))\sin\frac{\varphi_k}{2}\right), \tag{34}$$

where

$$z_k(t) = e^{i\pi/4}\sqrt{\frac{2\tau J}{g+i\delta}}\big((g+i\delta)(1-t/\tau) - \cos\varphi_k\big), \tag{35}$$

$$\nu_k = \frac{\tau J\sin^2\varphi_k}{2(g+i\delta)}. \tag{36}$$

At the end of evolution at $t = \tau$, when $\tilde{g}(\tau) = 0$, we obtain

$$|\psi_k(\tau)\rangle = \alpha_k(\tau)|u_-(k,\tau)\rangle + \beta_k(\tau)|u_+(k,\tau)\rangle, \tag{37}$$

where

$$|u_+(k,\tau)\rangle = \begin{pmatrix} \sin\frac{\varphi_k}{2} \\ \cos\frac{\varphi_k}{2} \end{pmatrix}, \quad |u_-(k,\tau)\rangle = \begin{pmatrix} -\cos\frac{\varphi_k}{2} \\ \sin\frac{\varphi_k}{2} \end{pmatrix}. \tag{38}$$

Since for the non-Hermitian systems the norm of the wave function is not conserved, we define the partial survival probability of the quantum register as [8, 17],

$$P_k^{gs}(t) = \frac{|\alpha_k(t)|^2}{|\alpha_k(t)|^2 + |\beta_k(t)|^2}. \tag{39}$$

The probability of the whole system to stay in the ground state at the end of the evolution is the product:

$$P_{gs} = \prod_{k>0} P_k^{gs}(\tau). \tag{40}$$

For long wavelength modes with $|\varphi_k| \ll \pi/4$, using the asymptotic formulas for the Weber functions with the large value of its argument, one has [8, 17]

$$P_k(\tau) \approx \frac{1}{1 + \dfrac{|\Gamma(1+i\nu_k)|^2}{2\pi|\nu_k|}\, e^{-\pi\Re\nu_k - \Re z_k^2(\tau)}}. \tag{41}$$

In the long wavelength approximation, one can take into account only the first mode, $\varphi_1 = \pi/N$, and estimate P_{gs} as,

$$P_{gs} \approx \frac{1}{1 + \dfrac{\tau|\Gamma(i\nu)|^2}{2\pi\tau_0}\, e^{-\pi\kappa}}, \tag{42}$$

where $\tau_0 = 2gN^2/(\pi^2 J)$, $\nu = \cos\alpha e^{-i\alpha}\tau/\tau_0$ and $\kappa = (\tau/\tau_0)\cos^2\alpha + (\tau J/\pi g)\sin(2\alpha)$. For the Hermitian QA this yields the Landau-Zener formula [40, 41]

$$P_{gs} = 1 - e^{-2\pi\tau/\tau_0}. \tag{43}$$

For $\tau \gtrsim \tau_0$ we obtain $P_{gs} \approx 1$. Thus, the computational time for the Hermitian QA should be of order N^2.

When $\tau \ll \tau_0$, one can approximate the Gamma function as, $|\Gamma(i\nu)| \approx 1/|\nu|$, and rewrite (42) as,

$$P_{gs} = \frac{1}{1 + \dfrac{\tau_0}{2\pi\tau}\, e^{-\pi\kappa_0}}. \tag{44}$$

where $\kappa_0 = (\tau J/\pi g)\sin(2\alpha)$. Assuming $e^{-\pi\kappa_0} \ll 2\pi\tau/\tau_0$, we obtain

$$P_{gs} \approx 1 - \frac{\tau_0}{2\pi\tau}\, e^{-\pi\kappa}. \tag{45}$$

If the condition,

$$\frac{\tau J}{g}\sin(2\alpha) - \ln\frac{\tau_0}{2\pi\tau} \gg 1, \tag{46}$$

is satisfied, one has $P_{gs} \approx 1$. From (46), we obtain the following rough estimate of the computational time for NQA:

$$\tau \approx \frac{2g\ln(N/\pi)}{J\sin(2\alpha)} = \frac{(g^2+\delta^2)\ln(N/\pi)}{\delta J}. \tag{47}$$

Thus, while the Hermitian QA has complexity of order N^2, the NQA has complexity of order $\ln N$, which is much better.

Optimal parameters As one can see, there exists the optimal choice of the parameter α, namely, $\alpha = \pi/4$ (or $\delta = g$), that minimizes the annealing time yielding $\tau \approx (g/J)\ln(N/\pi)$. For $\delta \ll g$ the annealing time can be estimated as, $\tau \approx (g^2/(\delta J))\ln(N/\pi)$, and for $\delta \gg g$ we obtain, $\tau \approx (\delta/J)\ln(N/\pi)$.

In Fig. 2, the results of numerical simulation are demonstrated for $N = 64$, 256, 512, 1024 qubits ($g = 10$, $\tau = 500$). As one can see, for $\delta \sim g$, the probability to stay in the ground state at the end of evolution is: $P_{gs} \approx 1$. However, for $\delta \ll g$ and $\delta \gg g$, the probability to stay in the ground state significantly decreases.

Our theoretical predictions are confirmed by the results of our numerical calculations performed for $N = 1024$ qubits, and presented in Figs. 3, 4 and 5. For the Hermitian QA, the long wave modes with $\varphi_k \ll \pi/4$ are excited (see Fig. 3). For $\delta \lesssim g$, one can observe that while short wavelength excitations are essential at the critical point, at the end of the evolution their contribution to the transition probability from the ground state to the first excited state is negligible. However, for $\delta \gg g$, the contribution of the shortwave excitations is important, and this results in violation of the adiabatic theorem.

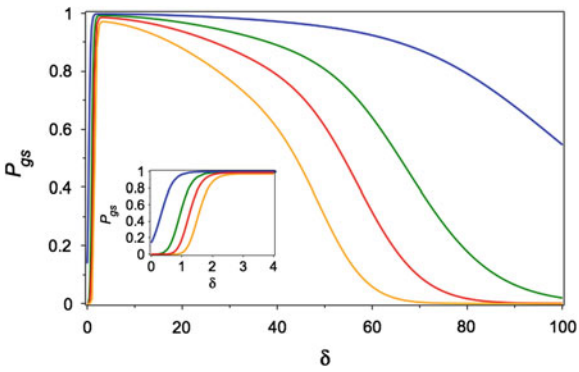

Fig. 2 The probability to stay in the ground state, P_{gs}, as a function of the decay parameter δ: $N = 64$ (*blue*), 256 (*green*), 512 (*red*), 1024 (*orange*). Parameters: $J = 0.5$, $g = 10$, $\tau = 500$

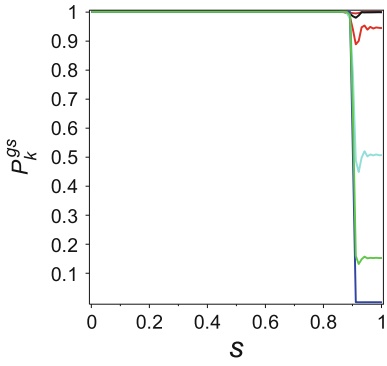

Fig. 3 The probability, P_k^{gs}, to stay in the ground state as a function of the scaled time, $s = t/\tau$, for the Hermitian QA. *Blue curve* ($k = 1$), *green curve* ($k = 8$), *cyan line* ($k = 16$), *red curve* ($k = 32$), *black curve* ($k = 48$), *orange curve* ($k = 64$). Parameters: $\delta = 0$, $J = 0.5$, $g = 10$, $\tau = 500$, $N = 1024$

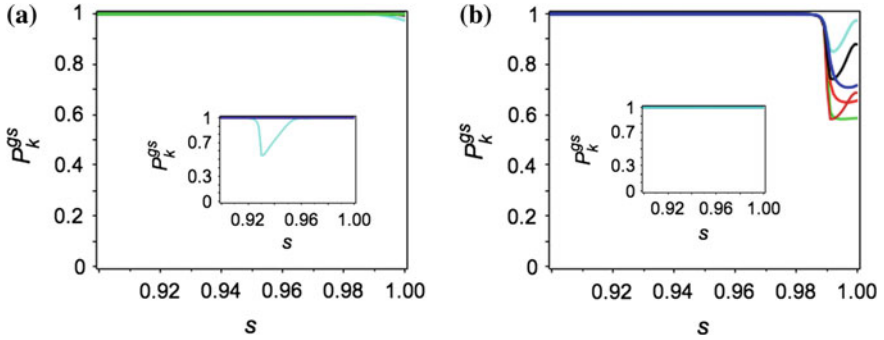

Fig. 4 NQA: the probability, P_k^{gs}, to stay in the ground state as a function of the scaled time, $s = t/\tau$. **a** *Blue curve* ($k = 1$), *red curve* ($k = 8$), *green curve* ($k = 16$), *orange curve* ($k = 32$), *black curve* ($k = 64$), *cyan line* ($k = 128$). **b** *Blue curve* ($k = 224$), *red curve* ($k = 230$), *green curve* ($k = 236$), *orange curve* ($k = 242$), *black curve* ($k = 248$), *cyan curve* ($k = 256$). Parameters: $\delta = 100$, $J = 0.5$, $g = 10$, $\tau = 500$, $N = 1024$ (inset: $\delta = 10$)

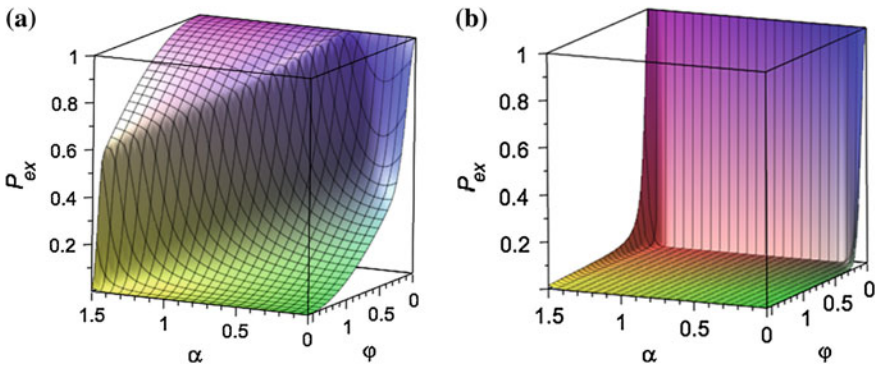

Fig. 5 The probability, P_{ex}, of excited states as a function of α and φ. **a** P_{ex} calculated at the critical point t_c. **b** P_{ex} calculated at the end of evolution, at time $t_f = \tau$. Parameters: $J = 0.5$, $g = 10$, $\tau = 500$

3.1 Defects Formation

During the QA, the system does not stay always in the ground state at all times. At the critical point, the system becomes excited, and its final state is determined by the number of defects (kinks). To evaluate the efficiency of the QA one can calculate the number of defects. Then, the computational time is the time required to achieve the number of defects below some acceptable value.

Following [42], we define the operator of the number of kinks as

$$\hat{\mathcal{N}} = \frac{1}{2}\sum_{n=1}^{N}\left(1 - \sigma_n^z \sigma_{n+1}^z\right). \tag{48}$$

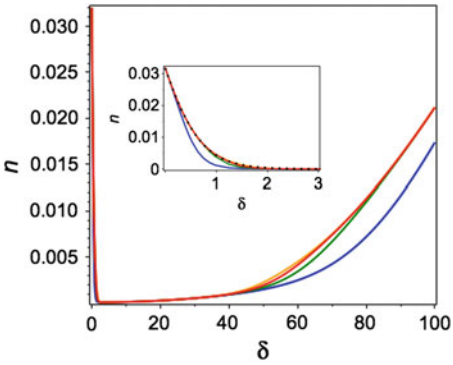

Fig. 6 Density of kinks as function of the decay parameter δ: $N = 64$ (*blue*), 256 (*green*), 512 (*red*), 1024 (*orange*). Inset: zoom of the figure (*dotted black line* presents the results of the (51)). Parameters: $J = 0.5$, $g = 10$, $\tau = 500$

As one can see, the number of kinks is equal to the number of quasiparticles excited at the end of the evolution: $\mathcal{N} = \langle \Psi_\tau | \hat{\mathcal{N}} | \Psi_\tau \rangle$. Using (37), we obtain

$$\mathcal{N} = \sum_{k>0} (1 - P_k^{gs}(\tau)), \tag{49}$$

where $P_k^{gs}(\tau)$ is given by (39).

In Fig. 6, the dependence of the density of defects on decay parameter, δ, and annealing time, τ, is presented. As one can see, even moderate dissipation essentially decreases the number of defects in the system. Our numerical results are in agreement with the previous conclusion on existing of the optimal choice of the parameter δ. Indeed, for $\delta \approx g$ the number of defects is minimal.

In the "thermodynamic" limit ($N \gg 1$) the sum in (49) can be replaced by the integral, and we obtain for the density of kinks the following expression:

$$n = \lim_{N\to\infty} \frac{\mathcal{N}}{N} = \frac{1}{\pi} \int_0^\pi dk (1 - P_k^{gs}(\tau)). \tag{50}$$

In the limit $\sqrt{2J\tau/|g + i\delta|} \gg 1$, only the long wavelength modes yield the main contribution, and one can use the Gaussian approximation to calculate the integral. By performing the integration, one obtains [8],

$$n = n_0 e^{-2\delta\tau J/g^2} \Phi\left(1 - e^{-2\delta\tau J/g^2}, \frac{1}{2}, 1\right), \tag{51}$$

where,

$$n_0 = \frac{1}{2\pi} \sqrt{\frac{g}{J\tau}}, \tag{52}$$

denotes the density of kinks for the Hermitian LZ problem [42], and $\Phi(x, a, c)$ is the Lerch transcendent [43]. The approximated formula (51) is good enough for $\delta \lesssim g$ (see the inset in Fig. 6).

4 Superradiance and NQA

The NQA is naturally related to the ST. Indeed, in this case the whole process of quantum annealing is described by the non-Hermitian Hamiltonian. Then, the discrete energy states of the Hermitian Hamiltonian, $\mathscr{H}_0$, in the qubit register of N qubits interact with the continuum spectra (sink) of the auxiliary Hamiltonian, $\mathscr{H}_1(t)$. Usually, the ST takes place in this kind of systems when the neighboring resonances, associated with complex eigenenergies, start to overlap. This means that the sum of the half-widths of the neighboring complex eigenenergies is equal or exceeds the distance between these eigenenergies (their real parts).

To describe the ST, it is convenient to express the complex eigenenergies for each mode, k, as: $\varepsilon_\alpha = \mathscr{E}_\alpha - i\Upsilon_\alpha$ ($\alpha = 1, 2$), where, $\mathscr{E}_\alpha = \Re\tilde{E}_\alpha$, and $\Upsilon_\alpha = -\Im\tilde{E}_\alpha$ is the half-width of the resonance, α. We denote: $\varepsilon_1 = \varepsilon_+(k, t)$ and $\varepsilon_2 = \varepsilon_-(k, t)$, the eigenenergies being $\varepsilon_\pm(k, t) = -\varepsilon_{0k}(t) \pm \varepsilon_k(t)$. The eigenstate with the eigenenergy, $\varepsilon_-(k, t)$, is the instantaneous ground state of the k-th mode. The eigenstate with the eigenenergy, $\varepsilon_+(k, t)$, is the instantaneous excited state of the k-th mode.

Generally, in the ST regime the segregation of the eigenstates takes place: the eigenstate with the wide width (fast decaying) is called the "superradiant" state, and the eigenstate with the narrow width (long-leaved) is called the "subradiant" state. The fast decay into a continuum is usually provided by the superradiant states. The details can be found in [19–27] (see also references therein).

The results of our numerical simulations for NQA are presented in Figs. 7 and 8. The width of the superradiant state is shown in Fig. 7 by the cyan surface, and

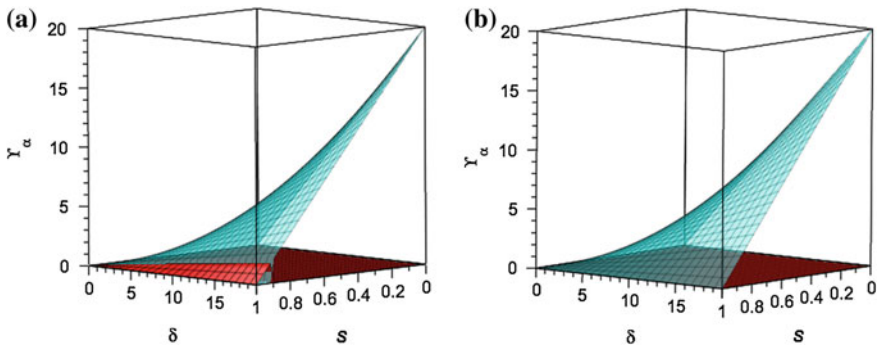

Fig. 7 Width Υ_α ($\alpha = 1, 2$) as the function of the decay rate, δ, and dimensionless time, $s = t/\tau$: Υ_1 (*red surface*) and Υ_2 (*cyan surface*). **a** $k = 1$, **b** $k = 512$. Parameters: $J = 0.5$, $g = 10$, $\tau = 500$, $N = 1024$

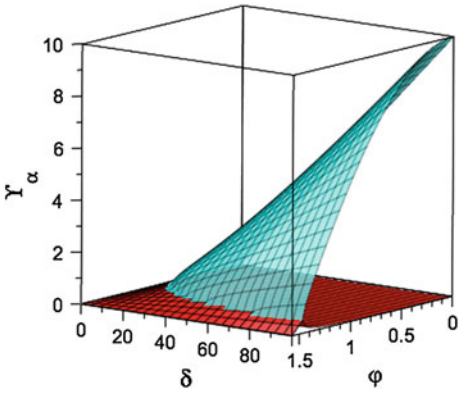

Fig. 8 Width Υ_α ($\alpha = 1, 2$) as the function of the decay rate δ and φ in the thermodynamic limit, calculated at the exceptional point: Υ_1 (*red surface*) and Υ_2 (*cyan surface*). Choice of parameters: $J = 0.5$, $g = 10$, $\tau = 500$

the width of subradiant state is shown by the red surface, for different modes. In spite of the resonances overlap from the very beginning, initially only the ground (subradiant) state of the auxiliary Hamiltonian is populated. So, the qubits do not decay significantly into continuum. As Fig. 7a, b demonstrate, this remains true up to the dynamics of NQA reaches the exceptional point. At this time, the subradiant state becomes the excited state, and it starts to decay into continuum. This is well illustrated in Fig. 7a, for long wavelength with $k = 1$. The main decay into continuum occurs at the exceptional point. When the NQA continues, the total Hamiltonian becomes "more Hermitian", the decay into continuum slows down, and at $t = \tau$ stops. The dynamical process of NQA, demonstrated in Fig. 7a, b, was performed for a large number of qubits, $N = 1024$, for different values of parameter, δ, and for long wavelength ($k = 1$) in Fig. 7a, and for short wavelength ($k = 512$) (shown in Fig. 7b). In Fig. 8, the imaginary parts of both eigenenergies are shown at the time, t_c, when the NQA crosses the exceptional point. As was already discussed, when δ increases, the small energy gap (associated with the exceptional point) is shifted in the NQA regime to the short wavelengths ($\varphi \sim 1$), which are not significantly excited. The decay of the ground state into continuum is mainly associated with the long-wave modes.

5 Conclusions

The approach presented in this paper, is related to application of NQA to the ferromagnetic Ising spin chain. We have chosen an auxiliary Hamiltonian in such a way that the total Hamiltonian is non-Hermitian. At the end of evolution the non-Hermiticity vanishes. Then, when the annealing is completed, the system is governed by the Hermitian Hamiltonian. The NQA significantly reduces the time required to find the ground state of the system, leading to the annealing time, $\tau \sim \ln N$, where N is the number of spins (qubits), which is much better than annealing time of

Hermitian QA ($\tau \sim N^2$). This effects is resulted from the fact that the small energy gap is shifted in the NQA regime in the region of short wavelengths, which are not significantly excited. We demonstrated that there exists the region of parameters which minimizes the time of NQA. We also demonstrated that the NQA is related to the ST in this system. At the beginning of the NQA, the system is populated in the ground (subradiant) state which only slowly decays into continuum. When passing the small energy gap (exceptional point), the superradiant state becomes the ground state. The decay of this state into continuum gives the main contribution to the formation of defects. At the end of NQA, the total Hamiltonian becomes a Hermitian one, and the superradiance is absent. We would like to mention that because of the time-dependence of the total non-Hermitian Hamiltonian, a more detailed analysis of the relation between the NQA and the ST is required.

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The Relationship Between Complex Quantum Hamiltonian Dynamics and Krein Space Quantization

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Abstract Negative energy states are appeared in the structure of complex Hamiltonian dynamics. These states also play the main role in Krein space quantization to achieve a naturally renormalized theory. Here, we will have an overlook on the role of negative energy states in complex mechanics and Krein space. In a previous work, we have shown that the method of complex mechanics provides us some extra wave functions within complex spacetime. We have supported our method of including negative energy states, by referring to the theory of Krein space quantization that by taking the full set of Dirac solutions is able to remove the infinities of quantum field theory (QFT), naturally. Our main proposal here is that particles and antiparticles should be treated as physical entities with positive energy instead of considering antiparticles with negative energy and the unphysical particle and antiparticle with negative energy should be introduced as the complement of the sets of solutions for Dirac equation. Therefore, we infer that the Krein space method which is supposed as a pure mathematical approach, has root on the strong foundations of Hamilton-Jacobi equations and therefore on classical dynamics and it can successfully explain the reason why the renormalization procedure in QFT works.

1 Introduction

In recent years, complex spacetime and complex mechanics has been studied by some physicists. In fact, complex spacetime originates from complex time, as first proposed by Naschie [1], according to a special case of E^{∞} theory [2–6] and then applied by Yang in a series of papers [7–16]. The complex aspects of quantum mechanics has been also dealt with by Bender (see for example [17]).The complex spacetime

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proposed by Yang is in the form $x^{\mu} = x^{\mu_R} + ix^{\mu_I}, x^{\mu_R}, x^{\mu_I} \in R; x^{\mu} = (ct, x, y, z)$, showing that quantum mechanics is nothing but an extension of classical mechanics to complex domain and relativistic quantum mechanics is an extension of special relativity to the complex domain, so that considering both relativistic and quantum effects, the Klein-Gordon equation could be derived as a special form of the Hamilton-Jacobi (H-J) equation. Also, the complex spacetime which is a natural consequence of including quantum effects in the relativistic mechanics, is a bridge connecting the causality in special relativity and the non-locality in quantum mechanics, and the entangled state causing the faster-than-light links, is a consequence of an entangled energy plus a quantum potential, i.e. $E^2 + 2m_0c^2Q$, resulting in a constant quantity [15]. Furthermore, it has been shown that negative energy states are appeared in the structure of complex Hamiltonian dynamics [15].

In a previous paper, we have shown that discussing the complex spacetime in a relativistic entangled "space-time" state leads to 12 extra wave functions than the four solutions of Dirac equation for a free particle [18], and then we have presented a new physical interpretation, realizing particles and antiparticles as physical entities with positive energy instead of considering antiparticles with negative energy [19], and introducing unphysical particle and antiparticle with negative energy, as the complement of the sets of solutions for Dirac equation, in accordance to the concept of Krein space quantization, which is a naturally renormalized theory and negative energy states play the main role in its concept [20–42]. Here, our main infer will focus on the connection between complex quantum Hamiltonian dynamics, standard quantum field theory and Krein space quantization emphasizing the point that the Krein space method which is supposed as a pure mathematical approach, has root on the strong foundations of Hamilton-Jacobi equations and therefore on classical dynamics and it can successfully explain the reason why the renormalization procedure in QFT works.

2 A Brief Review on Krein Space Quantization

Here, we have a brief review on the problem of divergence in quantum field theory and its elimination using the method of Krein space quantization. In this method, the auxiliary negative frequency states have been utilized, the modes of which do not interact with the physical states and are not affected by the physical boundary conditions. In Krein space the quantum scalar field is defined as follows [22, 25]:

$$\phi(x) = \frac{1}{\sqrt{2}}[\phi_p(x) + \phi_n(x)],$$

where

$$\phi_p(x) = \int d^3\mathbf{k}[a(\mathbf{k})u_p(k, x) + a^{\dagger}(\mathbf{k})u_p^*(k, x)],$$

$$\phi_n(x) = \int d^3\mathbf{k}[b(\mathbf{k})u_n(k,x) + b^{\dagger}(\mathbf{k})u_n^*(k,x)].$$

$a(\mathbf{k})$ and $b(\mathbf{k})$ are two independent operators and

$$u_p(k,x) = \frac{e^{i\mathbf{k}\cdot\mathbf{x}-iwt}}{\sqrt{(2\pi)^3 2w}} = \frac{e^{-ik\cdot x}}{\sqrt{(2\pi)^3 2w}}, \quad u_n(k,x) = \frac{e^{-i\mathbf{k}\cdot\mathbf{x}+iwt}}{\sqrt{(2\pi)^3 2w}} = \frac{e^{ik\cdot x}}{\sqrt{(2\pi)^3 2w}},$$

where $w(\mathbf{k}) = k^0 = (\mathbf{k}.\mathbf{k} + m^2)^{\frac{1}{2}} \geq 0$. The positive mode ϕ_p is the scalar field operator as was used in the usual QFT and ϕ_n plays the role of the regularization field. The time-ordered product is defined as:

$$iG_T(x,x') = \langle 0 \mid T\phi(x)\phi(x') \mid 0\rangle = \Re G_F(x,x'),$$

where $G_F(x,x')$ is the Feynman Green function.

As we know, the origin of divergences in standard quantum field theory lies in the singularity of the Green's function. The divergence appears in the imaginary part of the Feynman propagator, and the real part is convergent [32]:

$$G_F^P(x,x') = -\frac{1}{8\pi}\delta(\sigma_0) + \frac{m^2}{8\pi}\,\theta(\sigma_0)\left[\frac{J_1\left(\sqrt{2m^2\sigma_0}\right) - iN_1\left(\sqrt{2m^2\sigma_0}\right)}{\sqrt{2m^2\sigma_0}}\right]$$
$$-\frac{im^2}{4\pi^2}\,\theta(-\sigma_0)\frac{K_1\left(\sqrt{2m^2(-\sigma_0)}\right)}{\sqrt{2m^2(-\sigma_0)}}$$

where, J_1, N_1 and K_1 are Bessel functions:

$$J_1(z) = \frac{z}{2}\sum_{s=0}^{\infty}\frac{(-1)^s}{s!(s+1)!}\left[\frac{z}{2}\right]^{2s}, \quad \lim_{z\to 0}\frac{J_1(z)}{z} = \frac{1}{2}$$

$$N_1(z) = 2J_1(z)\log\frac{z}{2} - \frac{2}{z}, \quad \lim_{z\to 0}\frac{N_1(z)}{z} = -\frac{2}{\pi}\frac{1}{z^2}$$

$$K_1(z) = -\frac{\pi}{2}[J_1(iz) + iN_1(iz)], \quad \lim_{z\to 0}\frac{K_1(z)}{z} = \frac{1}{z^2}$$

Consideration of negative frequency states removes singularity of the Green function with exception of delta function singularity:

$$G_T(x,x') = -\frac{1}{8\pi}\delta(\sigma_0) + \frac{m^2}{8\pi}\theta(\sigma_0)\frac{J_1\left(\sqrt{2m^2\sigma_0}\right)}{\sqrt{2m^2\sigma_0}}, \quad \sigma_0 \geq 0$$

However, considering the quantum metric fluctuations removes the latter singularity:

$$\langle G_T(x,x')\rangle = -\frac{1}{8\pi}\sqrt{\frac{\pi}{2\langle\sigma_1^2\rangle}}\exp\left(-\frac{\sigma_0^2}{2\langle\sigma_1^2\rangle}\right)+\frac{m^2}{8\pi}\theta(\sigma_0)\frac{J_1\left(\sqrt{2m^2\sigma_0}\right)}{\sqrt{2m^2\sigma_0}}. \quad (1)$$

where $\langle\sigma_1^2\rangle$ is related to the density of gravitons. When $\sigma_0 = 0$, due to the metric quantum fluctuation $\langle\sigma_1^2\rangle \neq 0$, and we have

$$\langle G_T(0)\rangle = -\frac{1}{8\pi}\sqrt{\frac{\pi}{2\langle\sigma_1^2\rangle}}+\frac{m^2}{16\pi}.$$

By using the Fourier transformation, we obtain [41]

$$\langle\widetilde{G}_T(p)\rangle = \widetilde{G}_T(p) + PP\frac{m^2}{p^2(p^2-m^2)}$$

However, in the one-loop approximation, the contribution of delta function is negligible and the Green function in Krein space quantization appearing in the transition amplitude is

$$\langle\widetilde{G}_T(p)\rangle\mid_{one-loop} \equiv \widetilde{G}_T(p)\mid_{one-loop} \equiv PP\frac{m^2}{p^2(p^2-m^2)}$$

where $\tilde{G}_1(p)$ is the Fourier transformation of the first part of the Green function (1) and its explicit form is not needed for our discussion here. In a previous paper, it has proved that for the $\lambda\varphi^4$ theory in the one-loop approximation, the Green function in Krein space quantization, which appear in the s-channel contribution of transition amplitude, is the second part of (1) [25]. That means in this approximation, the contribution of the first part (i.e. quantum metric fluctuation) is negligible. It is worth mentioning that in order to improve the UV behavior in relativistic higher-derivative correction theories, the second part of (1) has been used by some authors [43, 44]. This part also appears in the super-symmetry theory [45].

The time-order product of the spinor field is:

$$\langle S_T(x-x')\rangle \equiv (i\not{\partial}+m)\langle G_T(x,x')\rangle$$

And the time-ordered product propagator in the Feynman gauge for the vector field in Krein space is given by:

$$\langle D^T_{\mu\nu}(x,x')\rangle = -\eta_{\mu\nu}\langle G_T(x,x')\rangle.$$

3 Essential Graphs of QED in Krein Space Quantization

In the standard quantum electrodynamics (QED) the divergent quantities are found in the electron self-energy, the vacuum polarization and the vertex graphs. In the standard QED, we have [46]:

$$\Sigma_{Hi}(p) = \frac{e^2}{8\pi^2}\left\{\ln\left(-\frac{\Lambda^2}{m^2}\right)\left(2m - \frac{\not{p}}{2}\right) + \left(2m - \frac{3}{4}\not{p}\right)\right.$$

$$\left. -\frac{\not{p}}{2}\left[\frac{m^4 - (p^2)^2}{(p^2)^2}\ln\left(1 - \frac{p^2}{m^2}\right)\right] + 2m\left[\frac{m^2 - p^2}{p^2}\ln\left(1 - \frac{p^2}{m^2}\right)\right]\right\}.$$

and

$$\Pi_{Hi}(k^2) = \frac{e^2}{12\pi^2}\ln\left(\frac{\Lambda^2}{m^2}\right) - \frac{e^2}{2\pi^2}\int_0^1 dx(1-x)x\ln\left(1 - x(1-x)\frac{k^2}{m^2}\right).$$

and

$$F_1^{Hi}(q^2)_{q^2\to 0} = -\frac{e^2}{16\pi^2}\ln\left(\frac{\Lambda^2}{m^2}\right) - \frac{e^2q^2}{12\pi^2m^2}\left(\ln\frac{m}{\mu} - \frac{3}{8}\right).$$

Calculating in Krein space, we get:

$$\Sigma_{kr}(p) = \frac{e^2}{8\pi^2}\left\{\ln\left(-\frac{p^2}{m^2}\right)\left(2m - \frac{\not{p}}{2}\right) - \frac{\not{p}}{2}\left(\frac{m^2}{p^2}\right)\right.$$

$$\left. -\frac{\not{p}}{2}\left[\frac{m^4 - (p^2)^2}{(p^2)^2}\ln\left(1 - \frac{p^2}{m^2}\right)\right] + 2m\left[\frac{m^2 - p^2}{p^2}\ln\left(1 - \frac{p^2}{m^2}\right)\right]\right\}.$$

and

$$\Pi_{\mu\nu}^{kr}(k^2) = (k^2 g^{\mu\nu} - k^\mu k^\nu)\Pi_{kr}(k^2),$$

where

$$\Pi_{kr}(k^2) = -\frac{e^2}{12\pi^2}\ln\left(-\frac{k^2}{m^2}\right) - \frac{e^2}{6\pi^2}\frac{k^2}{m^2} - \frac{e^2}{2\pi^2}\int_0^1 dx(1-x)x\ln\left(1 - x(1-x)\frac{k^2}{m^2}\right).$$

and

$$\Lambda^{\mu}_{kr}(p',p)=\frac{e^2}{8\pi}\int\frac{d^4k}{(2\pi)^4}\gamma^{\nu}(\not{p}'-\not{k}+m)\gamma^{\mu}(\not{p}-\not{k}+m)\gamma_{\nu}PP\frac{1}{k^2-\mu^2}$$

$$PP\left(\frac{m^2}{(p'-k)^2-m^2}\right)PP\left(\frac{m^2}{(p-k)^2-m^2}\right)=F_1^{kr}(q^2)\gamma^{\mu}+\frac{i\sigma^{\mu\nu}q_{\nu}}{2m}F_2^{kr}(q^2).$$

$F_2^{kr}(q^2)$ in the two different method is the same and $F_1^{kr}(q^2)$ in the Krein regularization is:

$$F_1^{kr}(q^2)_{q^2\to 0}=-\frac{e^2q^2}{16\pi^2m^2}+\frac{3e^2q^2}{64\pi^2m^2}-\frac{e^2q^2}{12\pi^2m^2}\left(\ln\frac{m}{\mu}-\frac{3}{8}\right),$$

where $q^2=(p-p')^2$. The singular terms of 3 standard graphs of QED are replaced with the two first terms in the resulted graphs in Krein space quantization [47, 48]. By using the value of $F_1(q^2)$ and the photon self energy in Krein space, the value of Lamb Shift is calculated to be 1018.19 MHz, whereas in standard QED it is 1052.1 MHz; and its experimental value has been given as 1057.8 MHz. The small differences may be because of neglecting the linear quantum gravitational effect and working in the one-loop approximation [39]. It should be noted that for QED, the Krein space calculations just eliminate the singularity in the theory without changing the standard physical contents i.e. in calculations of graphs, the unphysical states are eliminated in the external lines and are introduced only in the propagators and eliminate the divergence of the theory automatically.

4 Consequences of Complex Spacetime in a Relativistic Entangled "Space-Time" State

In a paper by Yang [15], it has been shown that the general form of energy can be written as two sets of positive and negative energies:

$$E(t)=\pm\sqrt{k_0^2-2m_0c^2Q(t)}=\pm\sqrt{(m_0c^2)^2+c^2p^2-2m_0c^2Q(t)}\equiv\pm E_{\pm} \qquad (2)$$

where $Q(t)$ is quantum potential and is responsible for the quantum mechanical behavior of particles. It is clear that for any time t, there are two momenta ($p>0, p<0$) and two energies ($E_+>0, E_-<0$), and in this general form of energy, the quantum potential $Q(t)$ is nonzero.

Considering $Q(t)=0$, $Q(t)\neq 0$ and discussing the complex space-time in a relativistic entangled "space-time" state, we have realized 16 wave functions i.e. 12 extra ones than the four solutions of Dirac equation for a free particle [18]:

$$\psi_1 = Ce^{\frac{i}{\hbar}(Et-p\cdot r)} \quad (E>0, p>0); \quad \psi_2 = Ce^{\frac{i}{\hbar}(Et-(-p)\cdot r)} \quad (E>0, p<0)$$

$$\psi_3 = Ce^{\frac{i}{\hbar}((-E)t-p\cdot r)} \quad (E<0, p>0); \quad \psi_4 = Ce^{\frac{i}{\hbar}((-E)t-(-p)\cdot r)} \quad (E<0, p<0)$$

$$\psi_5 = (C_0^+ e^{i(E_+/\hbar)t} + C_0^- e^{-i(E_+/\hbar)t})C^- e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}/\hbar} \quad (E_+>0, p>0)$$

$$\psi_6 = (C_0^+ e^{i(E_+/\hbar)t} + C_0^- e^{-i(E_+/\hbar)t})C^- e^{-\frac{i}{\hbar}(-\mathbf{p})\cdot\mathbf{r}/\hbar} \quad (E_+>0, p<0)$$

$$\psi_7 = (C_0^+ e^{i(E_-/\hbar)t} + C_0^- e^{-i(E_-/\hbar)t})C^- e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}/\hbar} \quad (E_-<0, p>0)$$

$$\psi_8 = (C_0^+ e^{i(E_-/\hbar)t} + C_0^- e^{-i(E_-/\hbar)t})C^- e^{-\frac{i}{\hbar}(-\mathbf{p})\cdot\mathbf{r}/\hbar} \quad (E_-<0, p<0)$$

$$\psi_9 = C_0^+ e^{i(E_+/\hbar)t}(C^+ e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}/\hbar} + C^- e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}/\hbar})(E_+>0, p>0)$$

$$\psi_{10} = C_0^+ e^{i(E_+/\hbar)t}(C^+ e^{\frac{i}{\hbar}(-\mathbf{p})\cdot\mathbf{r}/\hbar} + C^- e^{-\frac{i}{\hbar}(-\mathbf{p})\cdot\mathbf{r}/\hbar}) \quad (E_+>0, p<0)$$

$$\psi_{11} = C_0^+ e^{i(E_-/\hbar)t}(C^+ e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}/\hbar} + C^- e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}/\hbar}) \quad (E_-<0, p>0)$$

$$\psi_{12} = C_0^+ e^{i(E_-/\hbar)t}(C^+ e^{\frac{i}{\hbar}(-\mathbf{p})\cdot\mathbf{r}/\hbar} + C^- e^{-\frac{i}{\hbar}(-\mathbf{p})\cdot\mathbf{r}/\hbar}) \quad (E_-<0, p<0)$$

$$\psi_{13} = (C_0^+ e^{i(E_+/\hbar)t} + C_0^- e^{-i(E_+/\hbar)t})(C^+ e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}/\hbar} + C^- e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}/\hbar}) \quad (E_+>0, p>0)$$

$$\psi_{14} = (C_0^+ e^{i(E_+/\hbar)t} + C_0^- e^{-i(E_+/\hbar)t})(C^+ e^{\frac{i}{\hbar}(-\mathbf{p})\cdot\mathbf{r}/\hbar} + C^- e^{-\frac{i}{\hbar}(-\mathbf{p})\cdot\mathbf{r}/\hbar}) \quad (E_+>0, p<0)$$

$$\psi_{15} = (C_0^+ e^{i(E_-/\hbar)t} + C_0^- e^{-i(E_-/\hbar)t})(C^+ e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}/\hbar} + C^- e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}/\hbar}) \quad (E_-<0, p>0)$$

$$\psi_{16} = (C_0^+ e^{i(E_-/\hbar)t} + C_0^- e^{-i(E_-/\hbar)t})(C^+ e^{\frac{i}{\hbar}(-\mathbf{p})\cdot\mathbf{r}/\hbar} + C^- e^{-\frac{i}{\hbar}(-\mathbf{p})\cdot\mathbf{r}/\hbar}) \quad (E_-<0, p<0)$$

The above mentioned wave functions represent different entanglements of particles and antiparticles. In [18], we have argued that the entanglement of two particles or two antiparticles could be done only with the opposite momenta and the entanglement of particle and antiparticle could be done only with the same momenta, where the latter is in contradiction with experiments. Since empirical experiments have shown the quantum correlation at a distance of a particle-antiparticle system like kaon and antikaon system which are entwined. Therefore, introducing a parallel approach we corrected all the being results, considering the point that something was missed there. According to the theory of Dirac, antiparticles are believed to be particles of negative energy. But, due to the fact that antiparticles are detectable, so the physical antiparticles must be of positive energies. Moreover, according to (2) there are both positive and negative energy states. However, it seems that taking the negative energies as antiparticles, is not covering all the underlying physics [19]. So, we proposed that it is rational to accept that positive energy belongs to physical particles and negative energy belongs to unphysical particles. Then, we deduced that the solutions of Dirac equation describe both physical particles and antiparticles with positive energy and both unphysical particles and antiparticles with negative energy. Consequently, we modified the descriptions of wave functions $\psi_1, \psi_2, \ldots, \psi_{16}$ and as an application and verification of unphysical negative energy states, we referred to two famous paradoxes of physics, EPR and Klein [18]. In 1929, Klein [49] calculated the reflection and transmission coefficients for an incident beam of electrons of energy E, falling on a potential barrier of strength V_0. He found out that the unexpected amount of reflected electrons or transmitted electrons with a steady rate causes paradoxical results. Treating Klein's paradox with full set of Dirac solutions i.e. using the unphysical negative energy states in addition to physical positive energy states,

we have removed the Klein's paradox without the need of any further explanations or justifications like backwardly moving electrons and gain equal values for reflected and transmitted electrons and positrons [18, 19, 50]. Also, in [18], we have explained that the correct and unique solution to Einstein-Podolsky-Rosen (EPR) paradox [51], can also be verified due to the new results based on quantum Hamiltonian dynamics approach, i.e. the unique solution to the original version of EPR paradox is a particle and its antiparticle moving in opposite direction.

As an interesting result, we observe that negative energy solutions necessarily appear within the structure of the theory of complex quantum Hamiltonian dynamics and their interpretation as unphysical particles and antiparticles is vital for achieving consistence results.

5 Discussion About the Relationship Between Complex Hamiltonian Dynamics and Krein Space Quantization

In this part, we want to establish the connection between the Sects. 2, 3 and 4, in order to discuss about the relationship between complex Hamiltonian dynamics and Krein space quantization. As told before, negative energy states are appeared in the structure of complex Hamiltonian dynamics. On the other hand, negative energy states play the main role in Krein space quantization approach to achieve a naturally renormalized theory. In this method, the auxiliary negative frequency states have been utilized, the modes of which do not interact with the physical states and are not affected by the physical boundary conditions and since it is similar to Pauli-Villars regularization, so it is called the "Krein regularization", too. Considering the QED in Krein space quantization, it has been shown that the theory is automatically regularized [39]. Calculation of the three primitive divergent integrals, the vacuum polarization, electron self energy and vertex function using Krein space method leads to finite values, since the infrared and ultraviolet divergencies do not appear. Also, this method could be easily generalized to non-Abelian gauge theory and quantum gravity in the background field method, and could be used as an alternative way for solving the non-renormalizability of quantum gravity in the linear approximation. However, since Krein space quantization is a purely mathematical theory and its appearance and extension i.e. applying negative energy states is based on a historical background and not a strong theoretical foundation, so the results have been under debate by most of the physicists, up to now.

But, whereas Krein quantization is a pure mathematical approach, complex quantum Hamiltonian dynamics is based on the strong foundations of Hamilton-Jacobi equations and therefore on classical dynamics. The negative energy solutions necessarily appear within the structure of the theory of complex quantum Hamiltonian dynamics and as we referred in this paper, their interpretation as unphysical particles and antiparticles is vital for achieving consistence results. Due to the theory of Dirac, antiparticles are believed to be particles of negative energy. But, according to

the fact that antiparticles are detectable, so the physical antiparticles must be of positive energies i.e. taking the negative energies as antiparticles, is not covering all the underlying Physics [19]. Then, our main proposal in this paper is due to the results of Sect. 4, in which we deduced that particles and antiparticles should be realized as physical entities with positive energy instead of considering antiparticles with negative energy, and also unphysical particle and antiparticle with negative energy should be introduced as the complement of the sets of solutions for Dirac equation.

Now, Comparing the two approaches i.e. complex quantum Hamiltonian dynamics and Krein space quantization we can point out to the existence of a connection between quantum Hamiltonian dynamics, standard quantum field theory, and Krein space quantization. As we know, there are some gaps between the theories of classical mechanics, quantum mechanics, special relativity, Relativistic quantum mechanics, standard quantum field theory and quantum field theory in Krein space. However, the theory of complex quantum Hamiltonian dynamics has shown that quantum mechanics is nothing but the extension of classical mechanics into complex domain, so that in the viewpoint of complex H-J theory, quantum mechanics does not seem strange anymore and simplifies into an understandable theory. Also, the complex spacetime is a natural consequence of including quantum effects in the relativistic mechanics, and is a bridge connecting the causality in special relativity and the non-locality in quantum mechanics, i.e. extending special relativity to the complex domain leads to relativistic quantum mechanics. On the other hand, Krein space quantization is a parallel approach and without sufficient and strong base to quantum field theory in order to show and explain the hidden part of the theory, which is purposely omitted by physicists and then has led to infinities in QFT. In other words, in the viewpoint of Krein space quantization, the procedure of ugly mathematics of renormalization can be explained by the hidden part of theory i.e. negative energy solutions. However, it can be seen that the base of Krein space quantization i.e. appearance and applying negative energy states has root in the theory of complex quantum Hamiltonian dynamics. Hence, it seems as if complex quantum Hamiltonian dynamics can construct a connecting bridge between standard quantum field theory and Krein space quantization in order to explain the reason for the practical ugly mathematics of renormalization and provide an answer to the Feynman reply: "A Nobel prize for hiding the rushes (infinities) under the carpet"?. So, the other important result is that Krein space method is nothing but an extension of complex mechanics into the theory of quantum fields and it can successfully explain the reason why the renormalization procedure in QFT works. So that, it should not be considered as a pure mathematical approach and it is necessary to devote more efforts to include more physics in the concept of negative energy states.

It could be inferred here that investigation in complex aspects of quantum mechanics and quantum field theory may open the doors to bridge between the being theories in physics and fill their gaps, and as a result our main discussion here is that negative energies should be considered as important as positive ones, since they contribute in variety of processes and their importance has been pointed out by some famous physicists, e.g. Feynman has discussed the negative probabilities as viable concepts in quantum physics [52, 53] and Dirac has replied that Negative energies and

probabilities should not be considered as nonsense, since they are well-defined concepts mathematically like a negative sum of money, and important properties of them can still be used when they are negative [54, 55].

6 Conclusion

Negative energy states are applied in Krein space quantization approach to achieve a naturally renormalized theory. For example, this theory by taking the full set of Dirac solutions, is able to remove the propagator Green function's divergences and automatically without any normal ordering, to vanish the expected value for vacuum state energy.

On the other hand, negative energy states are also appeared in the structure of complex Hamiltonian dynamics. However, whereas Krein quantization is a pure mathematical approach, complex quantum Hamiltonian dynamics is based on strong foundations of Hamilton-Jacobi (H-J) equations and therefore on classical dynamics. Due to complex quantum Hamilton-Jacobi theory, complex spacetime is a natural consequence of including quantum effects in the relativistic mechanics. Characterizing the complex time involved in an entangled energy state and writing the general form of energy considering quantum potential, two sets of positive and negative energies could be realized that are in accordance with Krein space Quantization. Realizing new states for both positive and negative values of energy and momentum and then discussing the complex space-time in a relativistic entangled "space-time" state leading to 12 extra wave functions than the four solutions of Dirac equation for a free particle, we observed that negative energy solutions necessarily appear within the structure of the theory of complex quantum Hamiltonian dynamics and their interpretation as unphysical particles and antiparticles is vital for achieving consistence results. So, along with a previous investigation [19], we realized particles and antiparticles as physical entities with positive energy instead of considering antiparticles with negative energy. Finally, Comparing the two approaches i.e. complex quantum Hamiltonian dynamics and Krein space quantization we concluded that Krein space method is nothing but an extension of complex mechanics into the theory of quantum fields and along with the physicists desire, it can successfully explain the reason why the renormalization procedure in QFT works. Therefore, it should not be considered as a pure mathematical approach.

The main idea is that investigation in complex aspects of quantum mechanics and quantum field theory may open the doors to bridge between the being theories in physics and fill the unavoidable gaps between the theories of classical mechanics, quantum mechanics, special relativity, relativistic quantum mechanics, and quantum field theory.

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Non-Hermitian $\mathcal{PT}$-Symmetric Relativistic Quantum Theory in an Intensive Magnetic Field

V.N. Rodionov

Abstract We develop relativistic non-Hermitian quantum theory and its application to neutrino physics in a strong magnetic field. It is well known, that one of the fundamental postulates of quantum theory is the requirement of Hermiticity of physical parameters. This condition not only guarantees the reality of the eigenvalues of Hamiltonian operators, but also implies the preservation of the probabilities of the considered quantum processes. However as it was shown relatively recently (Bender and Boettcher Phys Rev Lett 80:5243, 1998), Hermiticity is a sufficient but it is not a necessary condition. It turned out that among non-Hermitian Hamiltonians it is possible to allocate a number of such which have real energy spectra and can ensure the development of systems over time with preserving unitarity. This type of Hamiltonians includes so-called parity-time ($\mathcal{PT}$) symmetric models which is already used in various fields of modern physics. The most developed in this respect are models, which used in the field of $\mathcal{PT}$-symmetric optics, where for several years produced not only theoretical but experimental studies.

1 Introduction

It is well known the Nobel Prize in Physics was awarded 2015 jointly to Takaaki Kajita and Arthur B. McDonald "for the discovery of neutrino oscillations, which shows that neutrinos have mass". This discovery has completely changed our understanding of the innermost properties of matter and showed that Standard Model (SM) cannot be the comprehensive theory of the fundamental constituents of the Universe. Obviously, that of past successes of the SM is so high that new models which is designed for modifying SM, should contain practically all basic principles lying in the basis of already existing theory. It is important to note that the generalization of the notion of Hermiticity has a strict quantum mechanical justification. Indeed it is known one

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of the fundamental postulates of quantum theory is the requirement of Hermiticity of physical parameters. This condition not only guarantees the reality of the eigenvalues of Hamilton operators, but also implies the preservation in time of the probabilities of the considered quantum processes. However, as was shown relatively recently [1], Hermiticity is a sufficient but it is not a necessary condition. It turned out that among non-Hermitian Hamiltonians it is possible to allocate a wide number having real energy spectra and providing the development of systems over time with preserving unitarity.

Now it is well-known fact, that the reality of the spectrum in models with a non-Hermitian Hamiltonian is a consequence of $\mathcal{PT}$-invariance of the theory, i.e. a combination of spatial and temporary parity of the total Hamiltonian: $[H, \mathcal{PT}]\psi = 0$. When the $\mathcal{PT}$ symmetry is unbroken, the spectrum of the quantum theory will be real. This surprising results explain the growing interest in this problem which was initiated by Bender and Boettcher's observation [1]. For the past a few years has been studied a lot of new non-Hermitian $\mathcal{PT}$-invariant systems (see, for example [2–8]).

The algebraic non-Hermitian $\mathcal{PT}$-symmetric γ_5-extension of the Dirac equation was first studied in [2] and further was developed in the works [3–5]. However in the geometrical approach to the construction of Quantum Field Theory (QFT) with fundamental mass which was developed by Kadyshevsky, equation for motion fermion with γ_5-mass extension [9] was obtained yet in seventies years of the last century (see also [10, 11]). The purpose of the present paper is the continuation of the studying examples of pseudo-Hermitian relativistic Hamiltonians, investigations of which was started by us earlier (see [3–5]). In the papers [12, 13] the energy spectra of the fermions was obtained by us as exact solutions of the modified Dirac equation in which taken into account the interaction of anomalous magnetic moment (AMM) of fermions with uniform magnetic field.

On the other hand in 1965 Markov [14] has proposed hypothesis according to which the mass spectrum of particles should be limited by the Planck mass $m_{Planck} = 10^{19}$ GeV. The particles with the limiting mass

$$m \leq m_{Planck} \tag{1}$$

were named by the author Maximons. However, condition (1) initially was purely phenomenological and until recently it has seemed that this restriction can be applied without connection with SM. And really SM is irreproachable scheme for value of mass from zero till infinity. But in the current situation, however, more and more data are accumulated that bear witness in favor of the necessity of revising some physical principles. In particular, this is confirmed by abundant evidence that "dark matter", apparently exists and absorbs a substantial part of the energy density in the Universe.

In the late 1970s, a new radical approach was offered by Kadyshevsky [9] (see also [10, 11]), in which the Markov's idea of the existence of a maximal mass used as new fundamental principle construction of QFT. This principle refutes the affirmation that mass of the elementary particle can have a value in the interval $0 \leq m < \infty$. In the geometrical theory the condition finiteness of the mass spectrum is postulated in the form

$$m \leq \mathcal{M}, \tag{2}$$

where the maximal mass parameter $\mathcal{M}$, was named by the *fundamental mass*. This physical parameter is a *new physical constant* along at the speed of light and Planck's constant. The value of $\mathcal{M}$ is considered as a curvature radius of a five dimensional hyperboloid whose surface is a realization of the curved momentum 4-space—the anti de Sitter space. Objects with a mass larger than $\mathcal{M}$ cannot be regarded as elementary particles because no local fields that correspond to them. For a free particle, condition (2) holds automatically on surface of a five dimensional hyperboloid. In the approximation $\mathcal{M} \gg m$ the anti de Sitter geometry goes over into the Minkowski geometry in the four dimensional pseudo-Euclidean space ("flat limit") [9].

Here we are producing our investigation of non-Hermitian systems with γ_5-mass contribution taking into account AMM of fermions in external magnetic field. In Sect. 2 we consider restriction of mass in pseudo-Hermitian algebraic theory. We also are studying the spectral and polarization properties of such systems (Sect. 3). The novelty of our approach is associated with predictions of new phenomena caused by a number of additional terms arising in the non-Hermitian Hamiltonians (Sect. 4). Intriguing predictions in our papers [12, 13] are connected with non-Hermitian mass extension and associated with the appearance in this the algebraic approach of any new particles. It is important that previously such particles ("exotic particles") was observed only in the framework of the geometric approach to the construction of QFT.

2 Restriction of Mass in Pseudo-Hermitian Algebraic Theory

The inequality $m_1 \geq m_2$ in this theory follows from the condition $m^2 = {m_1}^2 - {m_2}^2$, which is the basic requirement that defines unbroken symmetry of the Hamiltonian [2]. However, this inequality between m, m_1 and m_2 is not single condition, which links the parameters of γ_5-extension of mass. In particular we can write the new condition for the physical mass m, which may be more substantial. Indeed, using the simple mathematical theorem, we can obtain inequality in the form [4]

$$m \leq {m_1}^2/2m_2 = M \tag{3}$$

where the new parameter M restricts change of mass m (the details of this approach one can see at Fig. 1).

Introducing the normalized values $\nu = m/M$, $\nu_1 = m_1/M, \nu_2 = m_2/M$ and solving the system of equations $m^2 = {m_1}^2 - {m_2}^2$ and (3) we have expressions with two signs for values parameters ν_1 and ν_2:

$$\nu_1{}^{\mp} = \sqrt{2(1 \mp \sqrt{1-\nu^2})}; \quad \nu_2{}^{\mp} = (1 \mp \sqrt{1-\nu^2}). \tag{4}$$

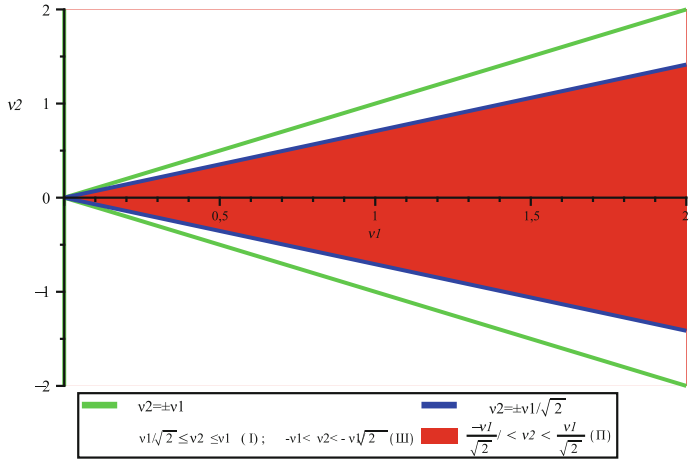

Fig. 1 The parametric domain of unbroken $\mathcal{PT}$-symmetry ${m_1}^2 \geq {m_2}^2$ for non-Hermitian Hamiltonian comprises three characteristic sub-domains: the shaded domain II corresponds to standard particles and the neighboring domains I and III correspond to the description of exotic fermions

We recall that we are investigating the issue of the existence of constraints on mass parameters in the given theory. It is shown by us that there is a constraint on the parameter m in the algebraic theory. In this case, there are reasons to believe that a direct relationship exists between M obtained by algebraic way and $\mathcal{M}$ which is consequence the *geometric approach to modified QFT with the fundamental mass* [3, 4].

Let us now consider obtaining the modified Dirac equations for free massive particles using the γ_5-factorization of the ordinary Klein-Gordon operator. It is interesting that in this case we can use simple way similar to known Dirac's procedure. As he wrote: "…get something like a square root from the equation Klein-Gordon" [15]. And really if we shall not be restricted to only Hermitian operators then we can represent the Klein-Gordon operator in the form of a product of two commuting matrix operators with γ_5-mass extension (where $\hbar = c = 1$):

$$\left({\partial_\mu}^2 + m^2\right) = \left(i\partial_\mu\gamma^\mu - m_1 - \gamma_5 m_2\right)\left(-i\partial_\mu\gamma^\mu - m_1 + \gamma_5 m_2\right), \tag{5}$$

where the physical mass of particles m is expressed through the parameters m_1 and m_2

$$m^2 = {m_1}^2 - {m_2}^2. \tag{6}$$

For the function would obey to the equations of Klein-Gordon

$$\left(\partial_\mu{}^2 + m^2\right)\widetilde{\psi}(x,t) = 0 \tag{7}$$

one can demand that it also satisfies to one of equations of the first order

$$\left(i\partial_\mu\gamma^\mu - m_1 - \gamma_5 m_2\right)\widetilde{\psi}(x,t) = 0; \quad \left(-i\partial_\mu\gamma^\mu - m_1 + \gamma_5 m_2\right)\widetilde{\psi}(x,t) = 0 \tag{8}$$

Equations (8) of course, are less common than (7), and although every solution of one of the equations (8) satisfies to (7), reverse approval has not designated.

It is also obvious that the Hamiltonians, associated with the equations (8), are non-Hermitian (pseudo-Hermitian), because in them the γ_5-dependent mass components appear ($H \neq H^+$):

$$H = \overrightarrow{\alpha}\,\mathbf{p} + \beta(m_1 + \gamma_5 m_2) = \overrightarrow{\alpha}\,\mathbf{p} + \beta m e^{\gamma_5\alpha} \tag{9}$$

and

$$H^+ = \overrightarrow{\alpha}\,\mathbf{p} + \beta(m_1 - \gamma_5 m_2) = \overrightarrow{\alpha}\,\mathbf{p} + \beta m e^{-\gamma_5\alpha}. \tag{10}$$

Here matrices $\alpha_i = \gamma_0 \cdot \gamma_i$, $\beta = \gamma_0$, $\gamma_5 = -i\gamma_0\gamma_1\gamma_2\gamma_3$ and introduced identical replacement of parameters

$$\sinh(\alpha) = m_2/m; \quad \cosh(\alpha) = m_1/m, \tag{11}$$

where parameter α varies from zero to infinity.

It is easy to see from (6) that the mass m, appearing in the equation (7) is real, when the inequality

$$m_1{}^2 \geq m_2{}^2, \tag{12}$$

is accomplished [2]. However for variable α which is identical for definitions m_1, m_2 this condition is automatically accomplished in all region of α changes.

However this area contains descriptions not only pseudo-Hermitian fermions, which in a result of transition to Hermitian limit ($m_2 \to 0$, $m_1 \to m$) coincide with the ordinary particles (see Fig. 1 and [2]). But there are the second region where fermions do not subordinate to the ordinary Dirac equations and for them the Hermitian transition is absent [3, 4]. It is easy to see that (6) can be used for new restrictions of mass parameters. Really, if we take into account inequality between arithmetic and geometrical averages of two positive numbers we have

$$m^2 + m_2{}^2 \geq 2\sqrt{m^2\, m_2{}^2}. \tag{13}$$

On the foundation of this inequality it can formulate five important Remarks.

Remark 1 The pseudo-Hermitian approach with γ_5-mass extension contains restriction of mass parameter beside (6). Indeed from (13) follows, that the sign of equality takes place when $m = m_2$. If we use parameter α then from (13)

$$1 + \sinh^2 \alpha = 2 \sinh \alpha. \tag{14}$$

From (14) we can also see that in this point $\sinh \alpha = 1$ and solving this equation we can find the value:

$$\alpha_0 = 0.881$$

Remark 2 Maximal value of mass particle $m = M$ is achieved in the point $m_2 = M$ and $m_1 = \sqrt{2}M$. The proof of this fact can be confirmed by the way defining the mass of the Maximon. Indeed, under α_0 we have the equality $m \sinh \alpha_0 = M = m_2$ and also for m_1 we have $m_1 = m \cosh \alpha_0 = \sqrt{2}M$.

Remark 3 The particle with the maximal mass (Maximon) is the pseudo-Hermitian fermion. Using Remark 2 for Maximon we can obtain expression

$$M_{Maximon} = \sqrt{2}M + \gamma_5 M. \tag{15}$$

This phenomenon may be given a very simple physical interpretation. This means that particles with the maximal mass (Maximons) $m = M$ are non-Hermitian (pseudo-Hermitian) fermions.

At the Fig. 2 we can see explicit behavior of the reduced mass distribution of $y(\alpha) = m/M$, depending on parameter α. From this picture follows that the curve, corresponding mass of the considered particles, has a maximum. This the maximal value of $y(\alpha) = m/M = 1$ corresponds to $\alpha_0 = 0.881$ that as already noted correspond to Maximon. Till to this value we are dealing with fermions, which have Hermitian limit when $M \to \infty$ (or $m_2 \to 0$). But after the value $\alpha_0 = 0.881$ is achieved

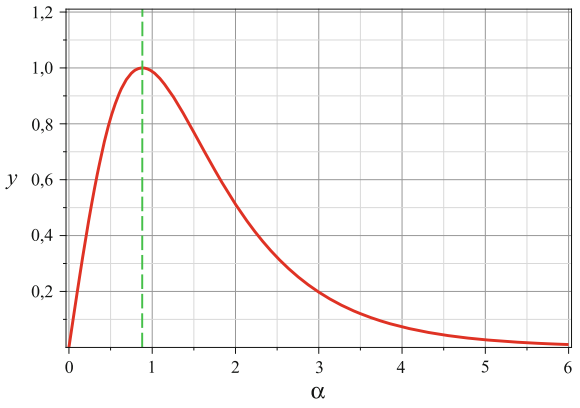

Fig. 2 Dependence of $y(\alpha) = \tilde{m} = m/M$ on the parameter α

we once more deal with decreasing mass of particles. However in this region already no the possibility with the help of the limiting transition to obtain Hermitian mass. Thus in this region particles exist, which in principal differ from the particles of the SM (exotic particles).

Remark 4 This particles (exotic particles) exist thanks to the presence of a maximal value of mass parameter, because the Hermitian limit for them is absent. If one can detect their it means that limiting mass fermions exist and our world is pseudo-Hermitian.

Remark 5 And vice versa if the restriction of mass spectrum of elementary particles does not exist then exotic particles can not arise in Nature. And it is very important because restriction of mass in SM is absent then experimental verification can be start from the most biggest values of maximal mass. In particular, it may be the Planck mass $M = 10^{19}$ GeV.

It is very interesting that the early such particles had discovered in geometrical approach to the construction of QFT with fundamental mass [9–11]. We believe

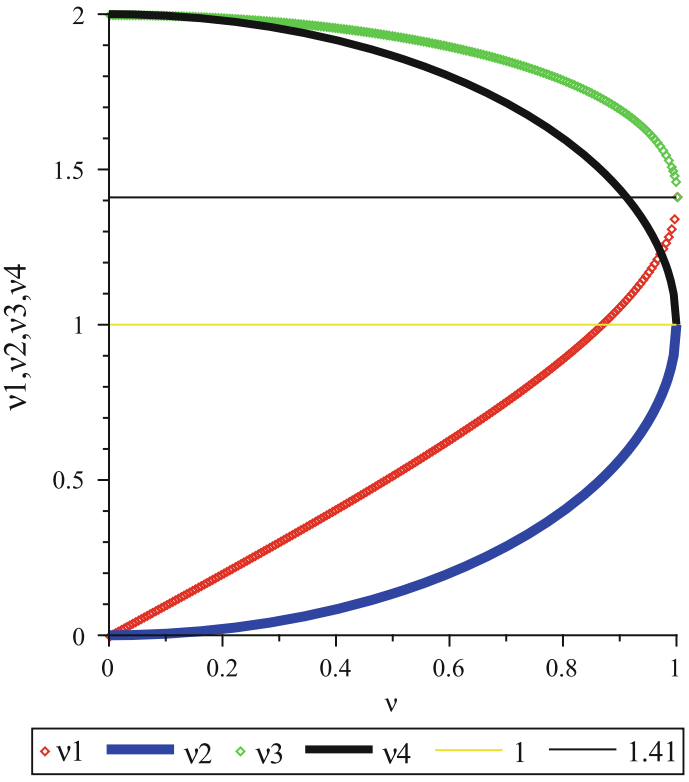

Fig. 3 Values of the parameters $\nu_1 = {m_1}^-/M, \nu_2 = {m_2}^-/M, \nu_3 = {m_1}^+/M, \nu_4 = {m_2}^+/M$ as functions of $\nu = m/M$

that exact solutions of modified Dirac-Pauli equations which were obtained by us for the pseudo-Hermitian neutrinos can let valuable information to detect the presence of "exotic particles". This is indicated also increase the effects proportionally $\sim M/m_\nu \gg 1$ associated with unusual properties of "exotic neutrinos", interacting with the magnetic fields [12, 13].

At Fig. 3 we can see values of different branches of ${\nu_1}^{\pm}$ and ${\nu_2}^{\pm}$ as a function of normalized physical parameter ν (see also (4)). The existence the domain of the $\mathcal{PT}$-symmetry is $0 \leq \nu \leq 1$. For these values of the parameters ν_1 and ν_2, the modified Dirac equation with the maximum mass describes the propagation of particles with real masses. But the lower branches ${\nu_1}^{-}$, ${\nu_2}^{-}$ correspond to ordinary particles and upper lines ${\nu_1}^{+}$, ${\nu_2}^{+}$ define the exotic partners.

3 Modified Model for the Study of Non-Hermitian Mass Parameters in Intensive Magnetic Fields

In this section, we shell want touch upon question of describing the motion of Dirac particles, if their own magnetic moment is different from the Bohr magneton. As it was shown by Schwinger [16] the equation of Dirac particles in the external electromagnetic field A^{ext} taking into account the radiative corrections may be represented in the form:

$$(\mathcal{P}\gamma - m)\,\Psi(x) - \int \mathcal{M}(x, y|A^{ext})\Psi(y)dy = 0, \tag{16}$$

where $\mathcal{M}(x, y|A^{ext})$ is the mass operator of the fermion in the external field and $\mathcal{P}_\mu = p_\mu - {A^{ext}}_\mu$. From (16) by means of expansion of the mass operator in a series of according to eA^{ext} with precision not over then linear field terms one can obtain the modified equation. This equation preserves the relativistic covariance and consistent with the phenomenological equation of Pauli obtained in his early papers (see for example [17]).

Now let us consider the model of massive fermions with γ_5-extension of mass $m \to m_1 + \gamma_5 m_2$ taking into account the interaction of their charges and AMM with the electromagnetic field $F_{\mu\nu}$:

$$\left(\gamma^\mu \mathcal{P}_\mu - m_1 - \gamma_5 m_2 - \frac{\Delta\mu}{2}\sigma^{\mu\nu}F_{\mu\nu}\right)\widetilde{\Psi}(x) = 0, \tag{17}$$

where $\Delta\mu = (\mu - \mu_0) = \mu_0(g-2)/2$. Here μ—magnetic moment of a fermion, g—fermion gyromagnetic factor, $\mu_0 = |e|/2m$—the Bohr magneton, $\sigma^{\mu\nu} = i/2(\gamma^\mu\gamma^\nu - \gamma^\nu\gamma^\mu)$. Thus phenomenological constant $\Delta\mu$, which was introduced by Pauli, is part of the equation and gets the interpretation with the point of view QFT.

The Hamiltonian form of (17) in the homogenies magnetic field is the following

$$i\frac{\partial}{\partial t}\widetilde{\Psi}(r,t) = H_{\Delta\mu}\widetilde{\Psi}(r,t), \tag{18}$$

where

$$H_{\Delta\mu} = \vec{\alpha}\vec{\mathcal{P}} + \beta(m_1 + \gamma_5 m_2) + \Delta\mu\beta(\vec{\sigma}\mathbf{H}). \tag{19}$$

For example, given the quantum electrodynamic contribution in AMM of an electron with accuracy up to e^2 order we have $\Delta\mu = \frac{\alpha}{2\pi}\mu_0$, where $\alpha = e^2 = 1/137$—the fine-structure constant and we still believe that the potential of an external field satisfies to the free Maxwell equations.

It should be noted that now the operator projection of the fermion spin at the direction of its movement $(\overrightarrow{\sigma}\,\overrightarrow{\mathcal{P}})$ is not commute with the Hamiltonian (19) and hence it is not the integral of motion. The operator μ_3 commuting with this Hamiltonian is the operator of polarization which can be represented in the form of the third component of the polarization tensor is oriented along the direction of the magnetic field [17]

$$\mu_3 = m_1\sigma_3 + \rho_2[\vec{\sigma}\vec{\mathcal{P}}]_3 \tag{20}$$

where matrices

$$\sigma_3 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}; \quad \rho_2 = \begin{pmatrix} 0 & -iI \\ iI & 0 \end{pmatrix},$$

where 0 and I are the zero and unit matrices 2×2 correspondingly.

Subjecting the wave function $\widetilde{\psi}$ to requirement to be eigenfunction of the operator polarization μ_3 and Hamilton operator (19) we can obtain:

$$\mu_3\widetilde{\psi} = \zeta k\widetilde{\psi}, \quad \mu_3 = \begin{pmatrix} m_1 & 0 & 0 & \mathcal{P}_1 - i\mathcal{P}_2 \\ 0 & -m_1 & -\mathcal{P}_1 - i\mathcal{P}_2 & 0 \\ 0 & -\mathcal{P}_1 + i\mathcal{P}_2 & m_1 & 0 \\ \mathcal{P}_1 + i\mathcal{P}_2 & 0 & 0 & -m_1 \end{pmatrix}, \tag{21}$$

where $\zeta = \pm 1$ are characterized the projection of fermion spin at the direction of the magnetic field, and

$$H_{\Delta\mu}\widetilde{\psi} = E\widetilde{\psi},$$

$$H_{\Delta\mu} = \begin{pmatrix} m_1 + H\Delta\mu & 0 & \mathcal{P}_3 - m_2 & \mathcal{P}_1 - i\mathcal{P}_2 \\ 0 & m_1 - H\Delta\mu & \mathcal{P}_1 + i\mathcal{P}_2 & -m_2 - \mathcal{P}_3 \\ m_2 + \mathcal{P}_3 & \mathcal{P}_1 - i\mathcal{P}_2 & -m_1 - H\Delta\mu & 0 \\ \mathcal{P}_1 + i\mathcal{P}_2 & m_2 - \mathcal{P}_3 & 0 & H\Delta\mu - m_1 \end{pmatrix}. \tag{22}$$

4 Exact Solutions of Dirac-Pauli Equations in the Intensive Uniform Magnetic Field

Performing calculations in many ways reminiscent of similar calculations carried out in the ordinary model in the magnetic field [17–20], in a result, for modified Dirac-Pauli equation one can find *the exact solution for energy spectrum* [12, 13]:

$$E(\zeta, p_3, 2\gamma n, H) = \sqrt{{p_3}^2 - {m_2}^2 + \left[\sqrt{{m_1}^2 + 2\gamma n} + \zeta \Delta\mu H\right]^2} \tag{23}$$

and for eigenvalues of the operator polarization μ_3 we can write in the form

$$k = \sqrt{{m_1}^2 + 2\gamma n}. \tag{24}$$

From (23) it follows that in the field where $\mathcal{PT}$ symmetry is unbroken $m \leq M$, all energy levels are real for the case of spin orientation along the magnetic field direction $\zeta = +1$ (see [12, 13]).

However, in the opposite case $\zeta = -1$ we have the imaginary part from the ground state of fermion $n = 0$ and other low energy levels, see on Fig. 4. For the cases of increasing parameter $\Delta\mu H = 0.2$ we can watch overlapping of different levels.

It is easy to see that in the case $\Delta\mu = 0$ from (23) one can obtain the ordinary expression for energy of charged particle in the magnetic field (*Landau levels*). Besides it should be emphasized that from the expression (23), in the Hermitian limit putting $m_2 = 0$ and $m_1 = m$ one can obtain:

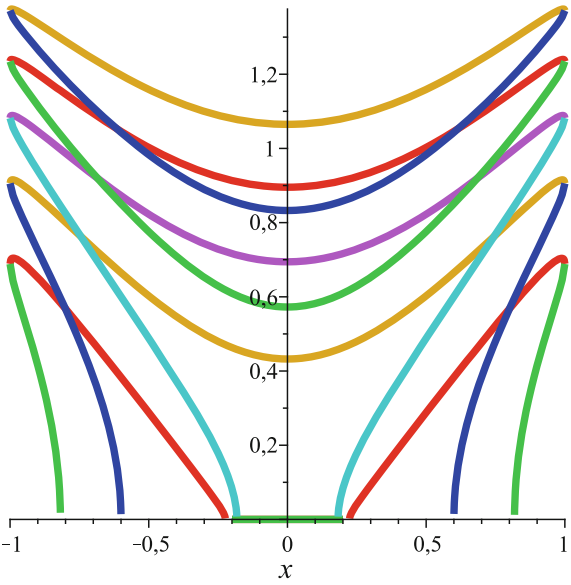

Fig. 4 Dependence of $E(-1, 0, 0.4n, 0.1)$ on the parameter $x = m/M$ for the cases $n = 0, 1, 2, 3, 4$ and $\Delta\mu H = 0.1$

$$E(\zeta, p_3, 2\gamma n, H) = \sqrt{{p_3}^2 + \left[\sqrt{m^2 + 2\gamma n} + \zeta \Delta\mu H\right]^2}. \tag{25}$$

Note that in the paper [21] was previously obtained result analogical to (25) by means of using of the Hermitian Dirac-Pauli approach. Direct comparison of formula (25) with the result [21] shows their coincidence in the Hermitian limit $M \to \infty$. It is easy to see that the expression (23) contains dependence on parameters m_1 and m_2 separately, which are not combined into *a mass of particles*, that essentially differs from the examples which were considered early [2–4].

Thus, here the calculation of interaction AMM of fermions with the magnetic field allow to put the question about the possibility of experimental studies of the non-Hermitian effects of γ_5-extensions of a fermion mass. Thus, taking into account the expressions (23) we obtain that the energetic spectrum is expressed through the fermion mass m and the value of the maximal mass M. Thus, taking into account that the interaction AMM with magnetic field removes the degeneracy on spin variable, we can obtain the energy of the ground state ($\zeta = -1$) in the form which dependence is represented at Fig. 4.

Thus, it is shown that the main progress, is obtained by us in the algebraic way of the construction of the fermion model with γ_5-mass term is consists of describing of the new energetic scale, which is defined by the parameter $M = {m_1}^2/2m_2$. This value on the scale of the masses is a point of transition from the ordinary particles $m_2 < M$ to exotic $m_2 > M$. Furthermore, description of the exotic fermions in the algebraic approach are turned out essentially the same as in the model with a maximal mass, which was investigated by Kadyshevsky with colleagues on the basis of geometrical approach [9–11].

It should be noted that the formula (23) is a valid not only for charged fermions, but and for the neutral particles possessing AMM. In this case one must simply replace the value of quantized transverse momentum of a charged particle in a magnetic field on the ordinary value $2\gamma n \to {p_1}^2 + {p_2}^2$. Thus, for the case of ultra cold polarized ($\zeta = -1$) ordinary electronic neutrino with precision not over then linear field terms we can write

$$E(-1, 0, 0, H, M \to \infty) = m_{\nu_e}\sqrt{1 - \frac{\mu_{\nu_e}}{\mu_0}\frac{H}{H_c}}, \tag{26}$$

where $Hc = m^2/e = 4.41 \cdot 10^{13}$ Gs is the quantization magnetic field for electrons.

However, in the case of exotic electronic neutrino $\tilde{m}_{\nu_e}$ we have

$$E(-1, 0, 0, H, \tilde{m}_{\nu_e}/M) = \tilde{m}_{\nu_e}\sqrt{1 - \frac{\mu_{\nu_e}}{\mu_0}\frac{2MH}{\tilde{m}_{\nu_e}H_c}}. \tag{27}$$

It is well known [22, 23] that in the minimally extended SM the one-loop radiative correction generates neutrino magnetic moment which is proportional to the neutrino mass

$$\mu_{\nu_e} = \frac{3}{8\sqrt{2}\pi^2}|e|G_F m_{\nu_e} = \left(3 \cdot 10^{-19}\right)\mu_0\left(\frac{m_{\nu_e}}{1\,\mathrm{eV}}\right), \tag{28}$$

where G_F-Fermi coupling constant and μ_0 is Bohr magneton. However note that the best laboratory upper limit on a neutrino magnetic moment, $\mu \leq 2.910^{-11}\mu_0$, has been obtained by the GEMMA collaboration [24], and the best astrophysical limit is $\mu \leq 3 \cdot 10^{-12}\mu_0$.

Existence masses of neutrino and mixing implies that neutrinos have magnetic moments. In last time one can often meet with an overviews of electromagnetic properties neutrino, (see, for example [25]). But as it was noted up in this paper "now there is no positive experimental indication in favor existence electromagnetic properties of neutrinos". With it really is hard not to agree because the interactions of ordinary neutrinos with the electromagnetic fields are extremely weak. However if one to suggest using the "exotic neutrinos" the interaction with magnetic field may be really significantly increased (see (26) and (27)) thanks to the coefficient which be equal to the ratio of maximal mass and mass of neutrinos $k = M/m_\nu \gg 1$ [12, 13]. Such experiments in our opinion may be very fruitful for creation the new physics beyond the SM. Perhaps that this effects indeed can be observed in terrestrial experiments.

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Quasi-Hermitian Lattices with Imaginary Zero-Range Interactions

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Abstract We study a general class of $\mathcal{PT}$-symmetric tridiagonal quantum Hamiltonians with purely imaginary interaction term in the quasi-Hermitian representation. This general Hamiltonian encompasses many previously studied lattice models as special cases. We provide numerical results regarding domains of observability and exceptional points, and discuss the possibility of explicit construction of general metric operators (which in turn determine all the physical Hilbert spaces). The condition of computational simplicity for the metrics motivates the introduction of certain one-parametric special cases, which consequently admit closed-form extrapolation patterns of the low-dimensional results.

1 Introduction

Quasi-Hermitian quantum Hamiltonians have received considerable attention during recent years [1–5]. The reason of their popularity may be seen in the fact, that they might express genuine quantum observables by apparently non-Hermitian (and often more computationally friendly) operators. From the mathematical viewpoint, these operators are characterized by a generalized condition of hermicity

$$H^\dagger \Theta = \Theta H \tag{1}$$

for some bounded nonsingular self-adjoint operator $\Theta > 0$, usually called the metric. Finding solutions of this equation (understood as an equation for Θ) forms an integral part of quasi-Hermitian representation of quantum mechanics. Exact solutions for quasi-Hermitian Schrödinger operators are rarely encountered, with one of the few exceptions being [6, 7]. Despite this partial success, a need for a more thorough examination of the solutions necessitates the reduction of the domain of applicability

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into finite-dimensional vector spaces, where complete solutions can be, in principle, found explicitly.

It is well known that the general solution of (1) is by far not unique. While one is often satisfied with a single solution Θ demonstrating the quasi-hermicity of the corresponding H, the unitary non-equivalence of the corresponding inner products motivates the search for general classes of metric operators for a single Hamiltonian, and in extreme cases even for a complete solution. In finite dimensions, such a solution is known to contain a definite number of free parameters, which is equal to the dimension of underlying vector space. This opens the possibility of explicit parametrization of such a metric. This approach has been pursued, among others, in [8–11], and also the recent article [12], which may be seen as a direct predecessor of the present paper.

Finite-dimensional toy models, in addition to having diverse applications in quantum and solid-state physics per se [13–16], provide also vast possibilities for the description of various physical phenomena in simplified scenarios. Indeed, finite quasi-Hermitian Hamiltonians have been succesfully used to model quantum phase transitions [17], quantum catastrophes [18] or even simplified big-bang scenarios [19]. The objects of interest in all these cases are the so-called exceptional points [20, 21], which emerge inevitably on boundaries of observability domains. These applications stand also at the origin of this article.

This paper is divided into five sections. Section 2 is devoted to general discussion of the studied Hamiltonian as well as the numerical examination of its spectral properties and observability domains. In Sect. 3, we begin with the attempt of solving (1) in full generality using brute-force methods of computer algebra. Motivated by the obtained results, we devode Sect. 4 to the possibility of having a simple complete solution for abitrary dimension n, which leads to the restriction of parameters into certain one-parametric subspaces. We examine the possibility of all but one parameters set to zero, as well as the Hamiltonian with full lattice interaction with strictly alternating interaction terms. The latter model proves exceptionally friendly in terms of pseudometric constructions, while all these models appear previously unnoticed in the literature. Finally, Sect. 5 is devoted to discussion of the discovered phenomena.

2 The Hamiltonian

Zero-range interaction Hamiltonians are without doubt the most studied and understood class of quantum-mechanical operators. In our finite-dimensional context, the zero-rangedness results in a family of tridiagonal matrices (see also [22–24]). These matrix Hamiltonians provide a discrete analogue for the differential Schrödinger operators, while at the same time having well understood spectral properties and infinite analogues acting on $\ell^2(\mathbb{N})$ [25, 26]. Our Hamiltonian is intended to have a very general nature, hence the large number of parameters. The only constraint imposed is the condition of $\mathcal{PT}$-symmetry. With this restriction in mind, the most general form of our Hamiltonian is a family of n-parametric $2n \times 2n$ matrices

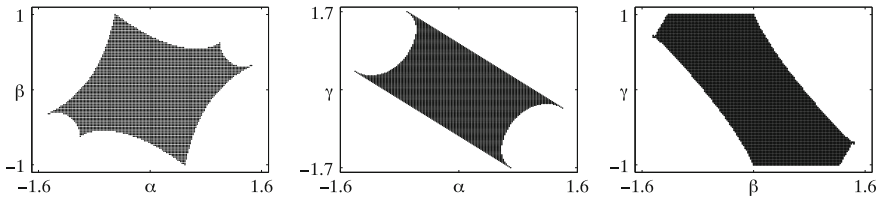

Fig. 1 Varying domains of observability for the $n = 6$ model with one parameter set to zero

Table 1 Critical values (exceptional points) for 4 different single-parametric Hamiltonians of varying dimension n

	$n = 10$	$n = 30$	$n = 50$	$n = 100$
α_{crit}	1.0000	1.0000	1.0000	1.0000
β_{crit}	0.7129	0.7089	0.7082	0.7064
γ_{crit}	0.5228	0.5085	0.5027	0.5015
δ_{crit}	0.4535	0.3936	0.3913	0.3828

$$H^{(2n)} = \begin{bmatrix} i\alpha & -1 & & & \\ -1 & i\beta & -1 & & \\ & \ddots & & & \\ & & -1 & -i\beta & -1 \\ & & & -1 & -i\alpha \end{bmatrix} \tag{2}$$

with additional parameters denoted by greek letters in alphabetical order. Although the rising number of parameters makes the model very intricate with growing dimension, the reward may be seen in the vast diversity of its spectral properties. This is demonstrated even in the next-to-trivial case $n = 6$, where three domains of observability are plotted in Fig. 1. The plots are made for a single parameter set to zero, in order to allow two-dimensional plotting (the stability of these patterns may be verified easily for higher dimensions).

The asymmetry of these plots with respect to serves also as an inspiration to undertake a deeper numerical experiment with single nonzero parameter. The results of this numerical experiment are summarized in the following table for 4 different next-to-boundary parameters. The domains of observability form a symmetric interval around zero, with the boundaries of observability domains being composed of exceptional points p_{crit}, at which the Hamiltonian ceases to be diagonalizable. The location of those exceptional points for some parameter choices are summarized in Table 1.

With exception of the parameter α, the domains are subject to a shrinking pattern for growing n. Despite this fact, the shrinking rate is deteriorating quickly and numerical experiments suggest that the limit of p_{crit} does not approach zero for

a fixed p. This opens the theoretical possibility of existence of a infinite-lattice quasi-Hermitian operator in appropriatelly defined limit $n \to \infty$ for arbitrary fixed parameter and their nontrivial combinations. For finite dimensions, this indicates the existence of nontrivial regions for any possible choice of parameters (this is one of the reasons for introducing the condition of $\mathcal{PT}$-symmetry).

3 The Pseudometrics

In this section, we address the possibility of constructing a complete solution of (1) for our general Hamiltonian. We proceed in a way common in the literature and start with the construction of the so-called pseudometrics. The pseudometrics are simply metrics with the positivity condition being relaxed. In other words, they are arbitrary bounded nonsingular self-adjoint operators satisfying the compactibility condition. In a finite-dimensional Hilbert space of dimension n, it is known that each quasi-Hermitian operator admits precisely n linearly independent pseudometrics. Consequently, we are searching for a linearly independent set $\left\{P_n^k \mid k = 1, \ldots, n\right\}$ satisfying

$$H_n^\dagger P_n^k = P_n^k H_n \tag{3}$$

We start our discussion at dimension 4. This is a compromise between the ability to demonstrate extrapolation patterns and ability to admit brute-force construction through symbolic manipulation software (in our case MAPLE). Before delving into full machinery of symbolic manipulations, we remind that the general Hamiltonian may be understood as a (sufficiently small) perturbation of the discrete Laplacian $(\Delta_n)_{ij} = -\delta_{i,i+1} + 2\delta_{i,i} - \delta_{i+1,i}$, with the diagonal terms being set to zero by appropriate energy shift. It is instructive to recall that the general pseudometric construction for such a (Hermitian) operator yields the sequence

$$P_4^1(\Delta) = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix} \quad P_4^2(\Delta) = \begin{bmatrix} 1 & & & \\ 1 & 1 & & \\ & 1 & 1 & \\ & & 1 & \end{bmatrix} \quad P_4^3(\Delta) = \begin{bmatrix} & 1 & & \\ 1 & & 1 & \\ & 1 & & 1 \\ & & 1 & \end{bmatrix} \quad P_4^4(\Delta) = \begin{bmatrix} & & & 1 \\ & & 1 & \\ & 1 & & \\ 1 & & & \end{bmatrix} \tag{4}$$

with the extrapolation pattern for $n > 4$ being clear. Since Δ is Hermitian, the identity operator belongs among admissible metrics, and we have choosen our sequence such that the identity appears there explicitly. Also, note that the identity is the only positive matrix in the sequence. On the other side of the sequence, the last pseudometric represents a discrete operator of parity. In our low-dimensional setting, we can repeat the brute-force symbolic manipulation techniques to reveal the sequence of pseudometrics

$$P_4^1(H) = \begin{bmatrix} 1 & i\alpha & -\alpha(\alpha+\beta) & -i(\alpha(\alpha^2-\beta^2)-\beta) \\ -i\alpha & 1 & i\,(\alpha+\beta) & -\alpha\,(\alpha+\beta) \\ -\alpha\;(\alpha+\beta) & -i\,(\alpha+\beta) & 1 & i\alpha \\ i(\alpha(\alpha^2-\beta^2)-\beta) & -\alpha(\alpha+\beta) & -i\alpha & 1 \end{bmatrix}$$

$$P_4^2(H) = \begin{bmatrix} & & 1 & i(\alpha+\beta) & \beta^2-\alpha^2 \\ & 1 & & 1 & i(\alpha+\beta) \\ -i(\alpha+\beta) & & 1 & & 1 \\ \beta^2-\alpha^2 & -i(\alpha+\beta) & & 1 & \end{bmatrix}$$

$$P_4^3(H) = \begin{bmatrix} & & 1 & \mathrm{i}\alpha \\ & 1 & \mathrm{i}\beta & 1 \\ 1 & -\mathrm{i}\beta & 1 & \\ -\mathrm{i}\alpha & 1 & & \end{bmatrix} \qquad P_4^4(H) = \begin{bmatrix} & & & 1 \\ & & 1 & \\ & 1 & & \\ 1 & & & \end{bmatrix} \tag{5}$$

which clearly demonstrates the preservation of structure of (4). The occurence of the last pseudometric of the sequence in an unchanged form is a direct consequence of operator $\mathcal{PT}$-symmetry. While the pseudometrics general expression for the matrix elements for individual. In all our explicit cases, we shall be constructing the pseudometrics with the same index labeling, where the kth pseudometric is a parameter-dependent perturbation of the kth pseudometric for the discrete Laplacian. This has a general character. It is expressed schematically in Fig. 2.

Although the general form of matrix elements is too complicated to be expressed explicitly with growing n, we may still employ a useful ansatz for the pseudometrics, which has a unified form for any $n \in \mathbb{N}$. The ansatz claims, that the nontrivial matrix elements occupy only a finite banded part of the matrix aligning along its antidiagonals. In the schematic drawing of Fig. 2, we express this ansatz and its trivial, real

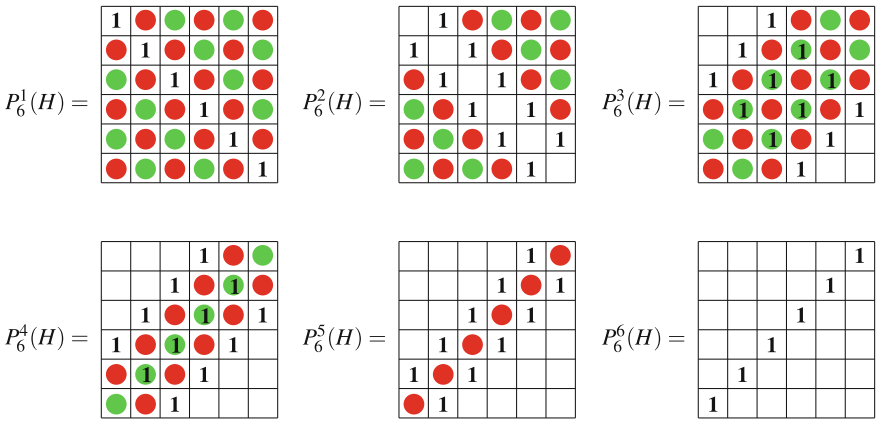

Fig. 2 Scheme of matrix elements for $n = 6$ pseudometrics (*red dots* for imaginary entries and *green dots* for real ones)

and purely complex entries for the pseudometrics with, respectively, ones, red dots and green dots (as before, the extrapolating pattern is clear enough).

4 The Special Cases

In this section, we feel motivated by the possibility of simplification of the pseudometric formulae by appropriate choice of parameters. We do not claim to exhaust all the interesting special cases, but merely point our at some interesting subclasses of (2), which have not yet received sufficient attention in the literature. Our first approach is directly inspired by [12], where, motivated by recent results in physics of condensed matter, a nicely extrapolating family of pseudometrics was constructed for

$$\alpha = \alpha \qquad \beta = \gamma = \cdots = 0 \tag{6}$$

This particular case, while not diminishing the sparsity structure of the pseudometrics in any substantial way, deserves particular attention in the uncommon elegance and expressibility of the resulting formulas. Here, in parallel with the numerical study in Table 1, we aim to extend this consideration to arbitrary single non-zero parameter. One of the motivations for such a treatment might be the discretization origin of the model of (6) in [11], which opens the possibility, that other point-interaction differential operators correspond to these generalized models. Of course, the case of the nth parameter being nonzero can be studied only the matrices of size $n \times n$ and larger. We restate the case $n = 4$ for $\alpha = 0$, which may form the basis of further development

$$P_4^1(H_\beta) = \begin{bmatrix} 1 & & & \mathrm{i}\beta \\ & 1 & i\beta & \\ & -i\beta & 1 & \\ -\mathrm{i}\beta & & & 1 \end{bmatrix} \qquad P_4^2(H_\beta) = \begin{bmatrix} & 1 & i\beta & -(i\beta)^2 \\ 1 & & 1 & i\beta \\ -i\beta & 1 & & 1 \\ -(i\beta)^2 & -\mathrm{i}\beta & 1 & \end{bmatrix}$$

$$P_4^3(H_\beta) = \begin{bmatrix} & & 1 & \\ & 1 & \mathrm{i}\beta & 1 \\ 1 & -\mathrm{i}\beta & 1 & \\ & 1 & & \end{bmatrix} \qquad P_4^4(H_\beta) = \begin{bmatrix} & & & 1 \\ & & 1 & \\ & 1 & & \\ 1 & & & \end{bmatrix} \tag{7}$$

which shows a further progression in terms of cancellation of another matrix elements. Indeed, evidence suggests that each general choice of parameter p suggests to possess a nicely extrapolating family of pseudometrics. For taste of the schemes, we provide yet the pseudometric for the parameter γ and $n = 6$. They are shown in Fig. 3.

So far, all the single-site interactions seem to admit formulas sufficiently simple, so that the complexity of the resulting matrix elements does not grow beyond the expressibility by useful closed formulas. The full treatment of this case is, however,

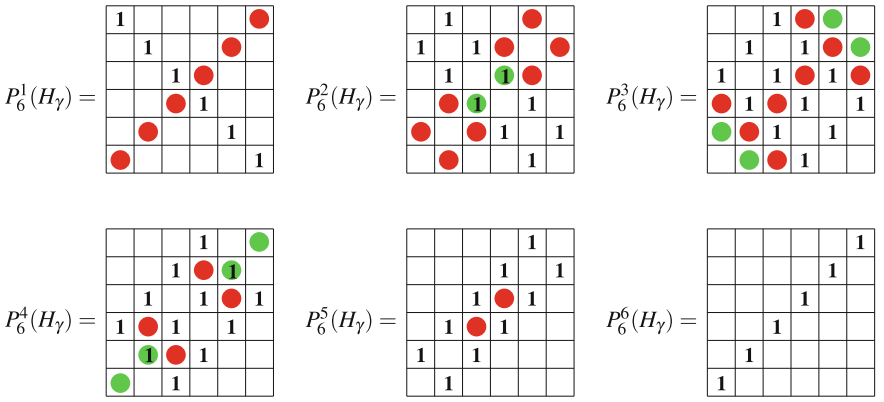

Fig. 3 Matrix entries for $n = 6$ pseudometrics for $\alpha = \beta = 0$ with *red dots* standing for $\pm i\gamma$ and *green dots* for $(i\gamma)^2$

beyond the scope of the present article, mainly because for larger parameter values one needs to begin consideration at matrices of large dimensions, which are not suitable for explicit plotting. Despite this fact, the message of this treatment is clear: the friendly form of the general pseudometrics is not restricted to the boundary interaction.

On the other side of the single-site interaction in the parametric spectrum lies the full-lattice interaction of the model (2). By the full lattice interaction, we understand the case where none of the parameters is zero at any moment. Guided by the desire for the simplification of our pseudometric patterns, and also by the explicit formulas for $n = 4$, we are tempted at the first look to choose the most friendly and matrix element eliminating interaction in an alternating form

$$\alpha = -\beta = \gamma = -\delta = \cdots \tag{8}$$

This alternating interaction Hamiltonian shall be denoted as H_a. Already the pattern for $n = 4$ indicates the extremely simple form of the resulting pseudometrics. The extreme simplicity is demonstrated in the fact, that only one type of nontrivial matrix element exists in whole family of pseudometrics, and has the form $i\alpha$. Consequently, we may drop the notation green and red dots, and denote by a red dot the element $i\alpha$ and by violet dot its complex conjugate. The results of these considerations are summarized in Fig. 4 with the extrapolation pattern again being clear for any dimension. Having succesfully constructed all the pseudometric, the final part of the task would, in principle, consist of verifying the condition of positivity of the resulting most general n-parametric linear combination. As usual in these cases, we have constructed one of the pseudometric positive for sufficiently small values of α. Using this fact, we might employ the powerful machinery of perturbation theory and write

$$\Theta_n(H_\alpha) = P_n^1(H_\alpha) + \varepsilon_2 P_n^2(H_\alpha) + \cdots + \varepsilon_n P_n^n(H_\alpha) \tag{9}$$

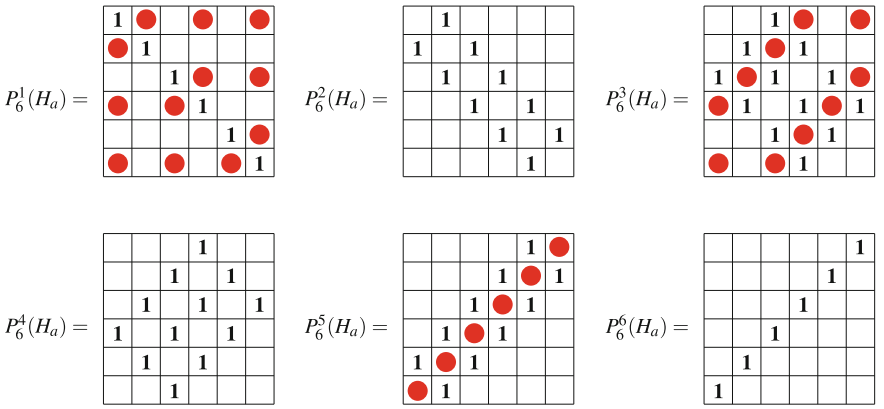

Fig. 4 Expliticit matrix entries for $n = 6$ pseudometrics for the alternating lattice interaction, *red dots* standing for $\mathrm{i}\alpha$

The exceptionally friendly character of our choice of interaction may be seen in the complete triviality of the even-numbered pseudometrics in each sequence, and also in the occurence of a single form of nontrivial matrix element. We have reached the goal we were looking for: we have succesfully constructed a complete set of pseudometrics for the special case of (5), which surpasses the previously examined toy models (e.g. [15]) both in sparsity and simplicity of the resulting pseudometric matrix elements.

5 Discussion

The directions of active research in quasi-Hermitian representation of quantum mechanics can be roughly divided into three directions, nicely summarized in a recent collection of proceedings [27]. The first direction has the goal to clarify the fundamental phenomenological foundations of such a representation, the conceptual problems with time-dependent metric operators, its time evolution or the Heisenberg representation [28, 29]. Another direction lies in giving proper mathematical foundation to quasi-Hermitian Hamiltonians with unbounded and/or singular metrics [30–33]. Finally, the third one consists of finding proper solvable quasi-Hermitian models, which are what makes quasi-Hermitian quantum mechanics a useful concept.

In this paper, we pursued the third direction with focus on finite-dimensional quantum Hamiltonians. Regarding model-building schemes for finite quasi-Hermitian Hamiltonians, different techniques may be employed to yield different useful results. The correspondence between useful models of solid state physics and lattice quasi-Hermitian operators has proved fruitful very recently [15, 16]. Also, the correspondence between (non-normalized) orthogonal polynomials [34] and

quantum-mechanical matrix models in has produces some interesting output [35, 36]. The nice feature in this case is, that the pseudometric may be constructed through a recurrent formula, which can be very often solved explicitly. The third recipe to construct finite-dimensional models has been seen to lie in discretization of infinite-dimensional models, as in [11].

The choice of our Hamiltonian stems from the attempt to provide a general treatment to various finite-dimensional operators with complex interactions scattered in the literature. Our results may be briefly summarized as follows: we addressed the general Hamiltonians for low dimensions symbolically, and found an emergent pseudometric pattern, which was then reconfirmed by further sample calculations. In order to achieve a true simplicity of the pseudometrics, we have carefully selected a number of special cases, again guided by the low-dimensional results. The simplicity of the resulting pseudometrics, in combination with the scope of the interaction not being limited to boundary terms, provides fresh scheme into the world of quasi-Hermitian matrices. It may seem encouraging that such a recipe leaves the construction non-numerical and offers unexpectedly transparent benchmark results. The full-lattice interaction may also have an interesting counterpart in the infinite-dimensional discrete limit (which can be, unlike the boundary interaction, defined with no obstacles), and finally in their appropriately-defined continuous counterparts $V(x)$. To this end, we complement the numerical experiment of Sect. 2 with its counterpart for full-lattice interactions (Table 2).

Note that the domains of observability are in orders of magnitude smaller that for single-site interactions, and have a clearly defined zero limit as $n \to \infty$. The possibilities of generalization are vast, the one which looks very promising lies in further systematic search for exactly solvable finite-dimensional models, which would admit not only closed-form representation of the eigenenergies, but also the explicit construction of the pseudometrics. The examination of full-lattice interactions not being localized at the boundaries looks particularly promising. In this direction, it may be worth studying eighter general complex interactions (instead of purely complex ones), or switching attention to finite-range interactions, which would however most likely produce a number of new obstacles to overcome. In general, the field of solvable quasi-Hermitian operators is far from being fully explored, and offers exciting new possibilities even in finite-dimensional Hilbert spaces.

Table 2 Critical values (exceptional points) for 2 different full-lattice Hamiltonians of varying dimension n

	$n = 10$	$n = 30$	$n = 50$	$n = 100$
$\alpha = -\beta = \gamma = -\delta = \cdots$	0.2934	0.1015	0.0623	0.0316
$\alpha = \beta = \gamma = \delta = \cdots$	0.1413	0.0185	0.0073	0.0018

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Quantization of Big Bang in Crypto-Hermitian Heisenberg Picture

Miloslav Znojil

Abstract A background-independent quantization of Universe near its Big Bang singularity is considered. Several conceptual issues are addressed in Heisenberg picture. (1) The observable spatial-geometry non-covariant characteristics of an empty-space expanding Universe are sampled by (quantized) distances $Q = Q(t)$ between space-attached observers. (2) In $Q(t)$ one of the Kato's exceptional-point times $t = \tau_{(EP)}$ is postulated *real-valued*. At such an instant the widely accepted "Big Bounce" regularization of the Big Bang singularity gets replaced by the full-fledged quantum degeneracy. Operators $Q(\tau_{(EP)})$ acquire a non-diagonalizable Jordan-block structure. (3) During our "Eon" (i.e., at all $t > \tau_{(EP)}$) the observability status of operators $Q(t)$ is guaranteed by their self-adjoint nature with respect to an *ad hoc* Hilbert-space metric $\Theta(t) \neq I$. (4) In adiabatic approximation the passage of the Universe through its $t = \tau_{(EP)}$ singularity is interpreted as a quantum phase transition between the preceding and the present Eon.

1 Introduction and Summary

The recent experimental success of the measurement of the cosmic microwave background [1] resulted in an amendment of the overall physical foundations of cosmology [2]. The theoretical interest moved to the study of the youngest Universe where, in the dynamical as well as kinematical regime close to Big Bang one still has to combine classical general relativity with quantum theory. Alas, the task looks quite formidable and seems far from its completion at present [3].

Fortunately, even the classical, non-quantum models suffice to describe the evolution of the Universe far from the Big Bang singularity cca 13.8 billion years ago. It is one of purposes of our present note to emphasize that near Big Bang, the recent progress in quantum theory (cf., e.g., its compact review [4]) becomes relevant and that it should be kept in mind with topmost attentiveness. We believe that the impact of certain recent updates of quantum theory upon cosmology will be nontrivial, indeed.

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In what follows our main attention will be paid to the conceptual role and increase of cosmological applicability of quantum theory using non-standard, non-Hermitian representations of the operators of observable quantities. Unfortunately, the terminology used in this direction of research did not stabilize yet. In the literature the whole innovative approach is presented under more or less equivalent names of quasi-Hermitian quantum theory [5, 6], $\mathscr{P}\mathscr{T}$-symmetric quantum theory [7, 8], pseudo-Hermitian quantum theory [9] or crypto-Hermitian quantum theory [10, 11].

We will discuss and analyze here the concept of quantum Big Bang in the recently proposed crypto-Hermitian Heisenberg-picture representation [12]. The material will be organized as follows. Firstly, in Sect. 2 we shall outline the overall cosmological framework of our considerations. Subsequently, the basic mathematical aspects of the formalism (viz., the crypto-Hermitian quantum theory in its three-Hilbert-space (THS) version of [11, 13]) will be summarized in Sects. 3 and 4 and in an Appendix. In Sect. 5 we shall finally turn attention to several aspects of the Heisenberg-picture quantization of our toy-model Universe. In the last Sect. 6 a few concluding remarks will be added.

2 Cosmological Preliminaries

There exist several imminent sources of inspiration of our present study. The oldest one is due to Mostafazadeh [14]. As early as in 2001, after my seminar talk at his University he pointed out that the non-Hermitian but $\mathscr{P}\mathscr{T}$-symmetric Schrödinger operators could find, via Wheeler-DeWitt equation, an important exemplification in cosmology. Although he abandoned the project a few years later (cf. his critical and sceptical summary of the outcome in his review paper [9]), the idea survived. The related necessary quantum-theoretical methods themselves are being actively developed (cf., e.g., [11, 12]). In what follows we intend to describe briefly both their key ideas and their potential applicability in the Big Bang setting.

2.1 Big Bang in Classical Picture

Our present methodical analysis of the Big Bang phenomenon cannot have any ambition of being realistic. In a Newtonian toy model of the evolution of an empty one-dimensional space we may visualize the history of the Universe as a circle which blows up with time (cf. Fig. 1). The hypothetical classical observers of this extremely simplified Universe are assumed co-moving with the space, detecting and confirming the Hubble's law which controls the growth of their distance $q(t)$ with time (cf. Fig. 2 or pages 5–7 in monograph [2]).

After a hypothetical return to three spatial dimensions and/or to a non-isotropic spatial geometry one will have to employ, for a similar measurement, a non-planar quadruplet of classical observers (cf. Fig. 3). They may be expected to re-confirm

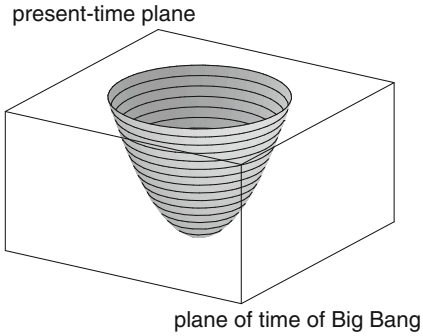


Fig. 1 Schematic picture of the classical expansion of 1D Universe after Big Bang

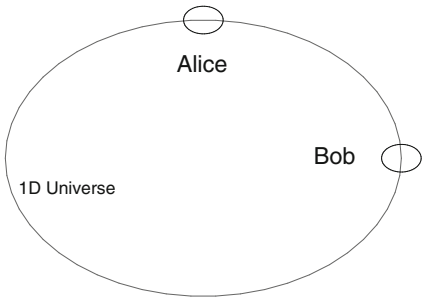


Fig. 2 Alice and Bob measure their 1D distance (non-covariant idealization)

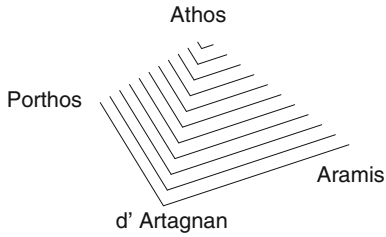


Fig. 3 Four non-planar musketeers measuring their mutual distances in 3D Universe

the Hubble's prediction of the approximate isotropy and homogeneity of the space. Thus, for our present methodical purposes we may return back to the 1D picture of Fig. 2 and consider the quantization of the single observable $q = q(t)$.

2.2 The Problem of Survival of Singularities After Quantization

One of my personal most influential discussions of the quantum Big Bang problem took place after a seminar in Paris [15] (cf. also its published version [16]) which was delivered by Wlodzimierz Piechocki from Warsaw. In his talk the speaker analyzed the quantum Friedmann-Robertson-Walker model in the setting of loop quantum

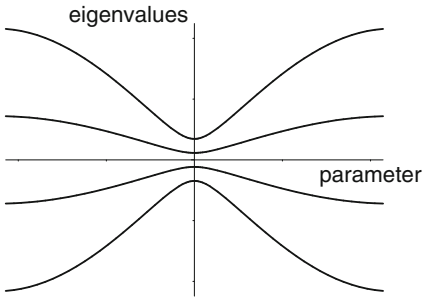


Fig. 4 Avoided crossing of eigenvalues; for Hermitian matrices the phenomenon is generic

gravity [17]. He explained why quantum theory, via Stone theorem [18], seems to lead to an inevitable regularization of the classical singularities. In the words supported by extensive literature [19], quantization was claimed to imply the necessity of replacement of the catastrophic dynamical Big Bang scenario by the mere smooth process called Big Bounce.

Besides a number of physical and thermodynamical considerations (which will not even be touched in our present text) the mathematical essence of the latter line of argumentation is comparatively easy to explain: In the absence of any symmetry (which could imply an incidental degeneracy of two eigenvalues of different symmetries) the eigenvalues of virtually any self-adjoint and parameter-dependent operator $\Lambda(\tau)$ exhibit a "repulsion" as sampled in Fig. 4.

A rigorous mathematical explanation of the phenomenon is elementary: in similar situations the coincidence of eigenvalues at a parameter $\tau_{deg.}$ may take place if and only if this value has the properties of the so called Kato's [20] exceptional point, $\tau_{deg.} = \tau_{(EP)}$. Alas, for self-adjoint operators the value of $\tau_{(EP)}$ is necessarily complex. Thus, whenever the parameter is time (i.e., a real variable), the evolution diagram has *always* the generic avoided-Big-Bang alias Big-Bounce form of Fig. 4.

3 Quantum Theory Preliminaries

One of the most straightforward methods of circumventing the above Big-Bang-avoiding paradox *must be sought in the use of the time-dependent operators of observables* $\Lambda(t)$ which possess *real* EP singularities. The problem becomes solvable via a parallel introduction of a nontrivial inner-product metric $\Theta = \Theta(t)$ *which must also be necessarily time-dependent in general* [11]. Intuitively speaking, the new degrees of freedom in $\Theta = \Theta(t)$ will suffice for an effective suppression of the repulsive tendencies of all of the eigenvalues of $\Lambda(t)$. In this manner, the currently accepted hypothesis of a mathematical necessity of the disappearance of the singularities after quantization becomes falsified.

3.1 Quantum Systems in Crypto-Hermitian Representation

A longer version of the latter statement will form the core of our present message. We shall demonstrate the non-universality of the tunneling of Fig. 4. Our main task will be the transfer of the concept of singularities from classical gravity into the crypto-Hermitian quantum theory using the language and notation of [11].

One of the quickest introductions into such a presentation of quantum theory using non-Hermitian representation of observables was provided by Scholtz et al. [6]. Within the framework of nuclear physics these authors recalled the Dyson's [5] idea that the explicit knowledge of a realistic bound-state Hamiltonian $\mathfrak{h} = \mathfrak{h}^\dagger$ may prove useless if its diagonalization (needed for the comparison of the theory with experiment) proves over-complicated.

The problem and its solution emerged during the study of the heaviest nuclei for which the self-adjoint realistic Hamiltonian $\mathfrak{h}$ operates in a textbook Hilbert space with the "curly-bra" vector elements $|\psi\succ \in \mathscr{H}^{(T)}$ (this is the notation which was introduced in Table Nr. 2 of review [11]). In the nuclear-physics literature the slow convergence of the numerical diagonalization of $\mathfrak{h}$ proved accelerated after a *non-unitary* preconditioning of wave functions,

$$|\psi\succ \quad \to \quad |\psi\rangle = \Omega^{-1}\,|\psi\succ \ \in \ \mathscr{H}^{(F)}. \tag{1}$$

The use of an appropriate, *ad hoc* "Dyson's map" Ω and of the friendlier "interacting boson" Hilbert space $\mathscr{H}^{(F)}$ was recommended. The isospectrality between self-adjoint $\mathfrak{h} = \mathfrak{h}^\dagger$ (in $\mathscr{H}^{(T)}$) and its image $H = \Omega^{-1}\mathfrak{h}\Omega \neq H^\dagger$ (which is non-Hermitian in manifestly unphysical $\mathscr{H}^{(F)}$) gets explained when one changes the inner product and when one replaces the unphysical space $\mathscr{H}^{(F)}$ by its amended alternative $\mathscr{H}^{(S)}$.

The key features of the pattern are summarized in Fig. 5. In "the second" Hilbert space $\mathscr{H}^{(S)}$ the inner product is constructed or chosen in such a way that the isospectral (but, in "the first" Hilbert space $\mathscr{H}^{(F)}$, non-unitary) image H of the Hamiltonian $\mathfrak{h}$

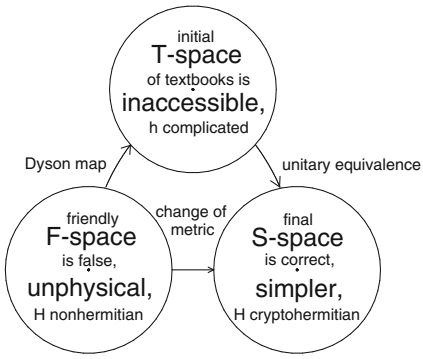


Fig. 5 The F-S-T triplet of representation spaces

(which was, by assumption, self-adjoint in "the third" Hilbert space $\mathscr{H}^{(T)}$) becomes also self-adjoint. In another formulation, Hilbert spaces $\mathscr{H}^{(S)}$ and $\mathscr{H}^{(T)}$ become unitarily equivalent and, hence, they yield the undistinguishable measurable physical predictions.

3.2 Stone Theorem Revisited

In the language of mathematics the Stone theorem about unitary evolution [18] can be given a less common formulation even in Schrödinger picture in which the evolution is controlled by Schrödinger equation

$$\mathrm{i}\,\partial_t|\psi\rangle = H\,|\psi\rangle \tag{2}$$

(here, H must have real and discrete spectrum, usually also bounded from below). The *unitary* evolution of ket vector $|\psi\rangle$ *may still be reestablished* even for $H \neq H^\dagger$ when using an *amended* inner-product metric $\Theta \neq I$. A non-equivalent Hilbert space $\mathscr{H}^{(S)}$ of the preceding paragraph is obtained in this manner.

The construction enables us to define a new operator adjoint $H^\ddagger = \Theta^{-1}H^\dagger\Theta$. Under certain natural conditions *the same* Hamiltonian H may be then declared self-adjoint in $\mathscr{H}^{(S)}$ whenever the metric is such that $H = H^\ddagger$. Some of the necessary mathematical properties of the Hamiltonian-Hermitizing metric operator were thoroughly discussed in [6]. Their rigorous study may also be found in the recent edited book [21] and, in particular, in its last chapter [22].

The sense of the whole recipe is in rendering the evolution law (2) *unitary* in $\mathscr{H}^{(S)}$, i.e., fully compatible with the first principles of quantum mechanics. In other words, a *unitary* evolution of a quantum state in $\mathscr{H}^{(S)}$ may be *misinterpreted* as non-unitary when studied in an ill-chosen Hilbert space $\mathscr{H}^{(F)}$ in which the Hamiltonian is not self-adjoint, $H \neq H^\dagger$ [9].

3.3 Unconventional Schrödinger Picture

In the the conventional Schrödinger picture (SP) the Hamiltonian $\mathfrak{h}_{(SP)}(t)$ is assumed self-adjoint in a textbook-space $\mathscr{H}^{(T)}$. It may be assumed to generate also the unitary evolution of the wave functions $|\psi(t)\succ$ of the Universe. Still, in the light of the preceding two paragraphs this generator may prove *simplified* when replaced by its isospectral, Big-Bang-passing (BBP) partner

$$H_{(BBP)}(t) = \Omega^{-1}_{(BBP)}(t)\,\mathfrak{h}_{(SP)}(t)\,\Omega_{(BBP)}(t). \tag{3}$$

One could choose here *any* (i.e., in general, non-unitary and manifestly time-dependent) invertible Dyson's operator $\Omega_{(BBP)}(t)$ which maps the initial physical

Hilbert space $\mathscr{H}^{(T)}$ on its (in general, unphysical, auxiliary) image $\mathscr{H}^{(F)}$. Subsequently, one defines the so called physical metric

$$\Theta_{(BBP)}(t) = \Omega^{\dagger}_{(BBP)}(t)\ \Omega_{(BBP)}(t). \tag{4}$$

The desired amendment of the unphysical inner product is achieved [9]. Indeed, it might look rather strange that we are now dealing with a time dependent scalar product, but an exhaustive explanation and resolution of the apparent paradox has been provided in [11]. In a way summarized in Fig. 5 one merely returns from the auxiliary Hilbert space $\mathscr{H}^{(F)}$ to its ultimate physical alternative $\mathscr{H}^{(S)}$. By construction, the latter one is "physical", i.e., unitarily equivalent to the initial one, $\mathscr{H}^{(S)} \sim \mathscr{H}^{(T)}$.

We are now prepared to make the next step and to return to the problem of the cosmological applicability of the whole representation pattern of Fig. 5 as summarized briefly also in Sect. 3.1. First of all we have to take into consideration the manifest time-dependence of our model-dependent and geometry-representing preselected observable $Q(t) = Q_{(BBP)}(t)$. This operator is defined in both $\mathscr{H}^{(F)}$ and $\mathscr{H}^{(S)}$. Via an analogue of (3) the action of this operator may be pulled back to the initial Hilbert space $\mathscr{H}^{(T)}$, yielding its self-adjoint avatar

$$\mathfrak{q}_{(SP)}(t) = \Omega_{(BBP)}(t)\, Q_{(BBP)}(t)\, \Omega^{-1}_{(BBP)}(t). \tag{5}$$

In this manner, the observability of $Q_{(BBP)}(t)$ is guaranteed if and only if

$$Q^{\dagger}_{(BBP)}(t)\Theta_{(BBP)}(t) = \Theta_{(BBP)}(t)\, Q_{(BBP)}(t). \tag{6}$$

The latter relation may be re-read as a linear operator equation for unknown $\Theta_{(BBP)}(t)$. When solved it enables us to reconstruct (and, subsequently, factorize) the metric which we need in the applied BBP context.

In the next step of the recipe of [11] our knowledge of the time-dependent operator (3) and of the Dyson's map $\Omega_{(BBP)}(t)$ enables us to introduce a new operator $G_{(BBP)}(t) = H_{(BBP)}(t) - \Sigma_{(BBP)}(t)$ where

$$\Sigma_{(BBP)}(t) = \mathrm{i}\Omega^{-1}_{(BBP)}(t)\left[\partial_t \Omega_{(BBP)}(t)\right]. \tag{7}$$

The SP evolution of wave functions in $\mathscr{H}^{(F)}$ and $\mathscr{H}^{(S)}$ will then be controlled by the pair of Schrödinger equations of [11],

$$\mathrm{i}\partial_t|\Psi^{(BBP)}(t)\rangle = G_{(BBP)}(t)\,|\Psi^{(BBP)}(t)\rangle, \quad |\psi^{(BBP)}(t)\rangle \in \mathscr{H}^{(F)}_{(BBP)}, \tag{8}$$

$$\mathrm{i}\partial_t|\Psi^{(BBP)}(t)\rangle\!\rangle = G^{\dagger}_{(BBP)}(t)\,|\Psi^{(BBP)}(t)\rangle\!\rangle, \quad |\psi^{(BBP)}(t)\rangle\!\rangle \in \mathscr{H}^{(F)}_{(BBP)}. \tag{9}$$

We may conclude that the time-dependence of mappings $\Omega_{(BBP)}(t)$ does not change the standard form of the time-evolution of wave functions too much. One only has

to keep in mind that the role of the generator of the time-evolution of the wave functions is transferred from the hiddenly Hermitian "energy" operator $H_{(BBP)}(t)$ to the "generator" operator $G_{(BBP)}(t)$ which contains, due to the time-dependence of the Dyson's map, also a Coriolis-force correction $\Sigma_{(BBP)}(t)$.

The second important warning concerns an innocent-looking but deceptive subtlety as discussed more thoroughly in [23]. Its essence is that the apparently independent F-space ket solutions of the apparently independent (9) are just the S-space physical conjugates of the usual F-space kets of (8). This means that whenever one works in $\mathscr{H}^{(F)}$, one has to evaluate the expectation values of a generic, hiddenly Hermitian observable $A_{(BBP)}(t)$ using the F-space formula

$$\langle\langle \Psi^{(BBP)}(t)|A_{(BBP)}(t)|\Psi^{(BBP)}(t)\rangle \tag{10}$$

where F-kets $|\Psi^{(BBP)}(t)\rangle$ and $|\Psi^{(BBP)}(t)\rangle\rangle = \Theta_{(BBP)}(t)|\Psi^{(BBP)}(t)\rangle$ represent just an S-ket and its Hermitian S-conjugate, i.e., just *the same* physical quantum state.

4 Evolution in Heisenberg Picture

In a Gedankenexperiment one may prepare the Universe, at some post-Big-Bang time $T > 0$, in a pure state represented by a biorthogonal pair of Hilbert-space elements $|\Psi^{(BBP)}(T)\rangle$ and $|\Psi^{(BBP)}(T)\rangle\rangle$. In such a setting we may let the time to run backwards. Then we may solve (8) and (9), in principle at least. This might enable us to reconstruct the past, i.e., we could specify the states of our Universe $|\Psi^{(BBP)}(t)\rangle$ and $|\Psi^{(BBP)}(t)\rangle\rangle$ at any $t > \tau_{(EP)} = 0$.

4.1 Heisenberg Equations

The consistent picture of the unfolding of the Universe after Big Bang cannot remain restricted to the description of the evolution of wave functions. The test of the predictive power of the theory can only be provided via a measurement, say, of the probabilistic distribution of data. Thus, the theoretical predictions are specified by the overlaps (10). By construction, the variations of wave functions as controlled by the generator $G_{(BBP)}(t)$ will interfere with the variations of the operator $A_{(BBP)}(t)$ itself.

In our cosmological considerations the "background of quantization" [24] characterizing the observable geometry of the empty Universe is represented by the "Alice-Bob distance" operator $Q(t)$ or, in general, by a set of such operators. They are assumed to be given as kinematical input, determining also the time-dependent Dyson's map via (6). For all of the other, dynamical observables in $\mathscr{H}^{(F,S)}$, with formal definition

$$A_{(BBP)}(t) = \Omega^{-1}_{(BBP)}(t)\mathfrak{a}_{(SP)}(t)\Omega_{(BBP)}(t) \tag{11}$$

a new problem emerges whenever they happen to be specified just at an "initial"/"final" time $t = T$ of the preparation/filtration of the quantum state in question. Still, the reconstruction of mean values (10) remains friendly and feasible in Heisenberg representation in which the wave functions are constant so that we must set $G(t) = 0$ and $H(t) = \Sigma(t)$ (cf. [12] for more details).

Naturally, whenever we decide to turn attention to the more general non-adiabatic options with $G(t) \neq 0$, the above most convenient assumption of our input knowledge of the map $\Omega_{(BBP)}(t)$ may prove too strong. With the purpose of weakening it we may rewrite (7) in the Cauchy-problem form

$$\mathrm{i}\partial_t \Omega_{(BBP)}(t) = \Omega_{(BBP)}(t)\Sigma_{(BBP)}(t) \tag{12}$$

to be read as a differential-equation definition of mapping $\Omega_{(BBP)}(t)$ from its suitable initial value (say, at $t = T$) and from the more natural input knowledge of the Coriolis force $\Sigma_{(BBP)}(t)$ of (7) which strongly resembles (possibly, perturbed) Hamiltonian in Heisenberg picture.

After a return to the Heisenberg-picture assumption $H(t) = \Sigma(t)$ let us now differentiate (11) with respect to time. Once we abbreviate $\partial_t \mathfrak{a}_{(SP)}(t) = \mathfrak{b}(t)$ and define

$$B_{(BBP)}(t) = \Omega^{-1}_{(BBP)}(t)\mathfrak{b}(t)\Omega_{(BBP)}(t), \quad H_{(BBP)}(t) = \Sigma_{(BBP)}(t) \tag{13}$$

this yields the first rule *alias* Heisenberg evolution equation

$$\mathrm{i}\partial_t A_{(BBP)}(t) = A_{(BBP)}(t)H_{(BBP)}(t) - H_{(BBP)}(t)A_{(BBP)}(t) + \mathrm{i}B_{(BBP)}(t) \tag{14}$$

and an accompanying, adjoint rule

$$\mathrm{i}\partial_t A^{\dagger}_{(BBP)}(t) = A^{\dagger}_{(BBP)}(t)H^{\dagger}_{(BBP)}(t) - H^{\dagger}_{(BBP)}(t)A^{\dagger}_{(BBP)}(t) + \mathrm{i}B^{\dagger}_{(BBP)}(t). \tag{15}$$

Formally, both of them resemble the Heisenberg commutation relations and contain an independent-input operator (13). Naturally, the latter operator might have been given an explicit form of an $T \to F$ transfer of the anomalous time-variability of our observable *whenever considered time-dependent* already in Schrödiger picture. Nevertheless, once we follow the classics [6] and once we treat any return $F \to T$ as prohibited (otherwise, the Dyson's non-unitary mapping would lose its *raison d'être*), "definition" (13) is inaccessible. Due to the kinematical origin of (14) or (15), our knowledge of operator $B_{(BBP)}(t)$ at all times must really be perceived as an *independent source of input information* about the dynamics.

The list of the evolution equations for a quantum system in question becomes completed. Naturally, the initial values of operators $\Theta_{(BBP)}(T)$ and $A_{(BBP)}(T)$ must be such that

$$A^{\dagger}_{(BBP)}(T)\Theta_{(BBP)}(T) = \Theta_{(BBP)}(T)A_{(BBP)}(T) \tag{16}$$

We may conclude that whenever $G(t) = 0$, the construction of any concrete toy model only requires the solution of Heisenberg evolutions (14) or (15).

4.2 The Limitations of the Heisenberg Picture of the Universe

Before recalling any examples let us re-emphasize that the Heisenberg representation *alias* Heisenberg picture (HP) of the quantum systems provides one of the most straightforward forms of hypothetical transitions between classical and quantum worlds. One should immediately add that the HP approach proves extremely tedious in the vast majority of practical calculations. It replaces the dynamics described by the SP Schrödinger equation for wave functions by its much more complicated operator, Heisenberg-equation equivalent. At the same time, once we are given our "geometry" observable $Q(t)$ in its time-dependent Heisenberg-representation form *in advance* (say, in a way motivated, somehow, by the principle of correspondence), our tasks get perceivably simplified.

In the underlying theory one assumes, therefore, that the set of the admissible (and measurable) instantaneous quantized distances $q(t) = q_n(t)$ between the two observers of Fig. 2 are eigenvalues of an operator $Q = Q(t)$ in some physical Hilbert space $\mathscr{H}^{(S)}$. This space is assumed endowed with the instantaneous physical inner product which is determined, say, by a time-independent metric $\Theta \neq \Theta(t)$ [12]. In the case of a pure-state evolution, the integer subscript $n = 1, 2, \ldots, N$ with $N \leq \infty$ may be kept fixed via a preparation or measurement over the system at a time $t = T$.

Our quantum description of the Universe shortly after Big Bang will be based, as already indicated above, on a non-Dirac, BBP amendment of the Hilbert-space metric, on its factorization (4) and on the use of preconditioning of the "clumsy" physical wave function $|\psi(t)\succ \in \mathscr{H}^{(T)}$ of the Universe,

$$|\psi(t)\succ = \Omega_{(BBP)}(t)\,|\psi(t)\rangle = \left[\Omega^{\dagger}_{(BBP)}(t)\right]^{-1}|\psi(t)\rangle\!\rangle. \tag{17}$$

(cf. (1), and note also the unfortunate typo in equation Nr. (7) of [12] where the exponent $(^{-1})$ is missing).

As long as the mapping Ω is allowed time-dependent, the standard Schrödinger equation which determined the evolution of a pure state $|\psi(t)\succ$ in space $\mathscr{H}^{(T)}$ in Schrödinger picture cannot be replaced by (2) anymore. Indeed, one must leave the standard Schrödinger picture as well as its non-Hermitian stationary amendment and implementations as described in [6, 8, 9].

Secondly, without additional assumptions one cannot employ the non-Hermitian Heisenberg picture, either. The reason is that in this framework (in which the observables are allowed to vary with time) the Hilbert space metric must still be kept constant [12]. Thus, our theoretical quantum description of the evolution of the Universe in Heisenberg picture must be accompanied by the adiabaticity assumption $\partial_t \Theta(t) =$ small.

5 What Could Have Happened Before Big Bang?

The applicability of the above-summarized crypto-Hermitian version of Heisenberg picture of [12] may be now sampled by any above-mentioned schematic toy model of the Universe in adiabatic approximation. Operator $Q(t)$ (defined as acting in a preselected Hilbert space $\mathscr{H}^{(F)}$) is assumed given (or guessed, say, on the background of correspondence principle) in advance, as a tentative input information about dynamics.

In addition, our schematic Universe living near Big Bang may be also endowed with an additional pair of observables A and B, with their mutual relation clarified by the pair of (11) and (13). In principle, in the light of (14) the former operator may be specified just at the initial time $t = T$. In this sense the models with the necessity of specification of $B(t) \neq 0$ *at all times* may be considered anomalous (cf. also the related discussion in [12]).

Naturally, even if we assume that $B(t) = 0$, the solution of Heisenberg (14) need not be easy. For this reason, we shall now display the results of a quantitative analysis of a few most elementary models. We shall employ the following simplifying assumptions: (1) In the spirit of Fig. 2, only the quantized distance between Alice and Bob (i.e., just a single geometry-representing and adiabatically variable observable $Q(t)$) will be considered. (2) For the sake of simplicity, our illustrative samples of the kinematical input information (i.e., of the operators $Q(t)$) will only be considered in a finite-dimensional, N by N matrix form, $Q(t) = Q^{(N)}(t)$.

5.1 No Tunneling and No Observable Space Before Big Bang

For illustration purposes let us first recall the N by N real matrix model of [25] with

$$Q^{(N)}(t) = Q_0^{(N)} + \sqrt{1-t} \times Q_1^{(N)} \tag{18}$$

which is composed of a diagonal matrix $Q_0^{(N)}$ with equidistant elements

$$\left[Q_0^{(N)}\right]_{nn} = \{-N+1, -N+3, \ldots, N-1\} \tag{19}$$

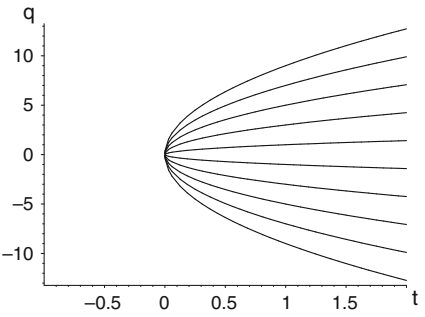


Fig. 6 Real eigenvalues of the toy-model geometry (18) in the both-sided vicinity of its Big Bang singularity at $t = 0$

and of an antisymmetric time-dependent "perturbation" with a tridiagonal-matrix coefficient $Q_1^{(N)}$ with zero diagonal and non-vanishing elements $\left[Q_0^{(N)}\right]_{n+1,n} = -\left[Q_0^{(N)}\right]_{n,n+1}$

$$= \{\sqrt{1\cdot(N-1)}, \sqrt{2\cdot(N-2)}, \sqrt{3\cdot(N-3)}, \ldots, \sqrt{(N-1)\cdot 1}, \}. \qquad (20)$$

In [25] the choice of this model was dictated by its property of having real and equidistant spectrum at all of the non-negative times $t > 0$. Another remarkable feature of this model is that while matrix (18) is real and manifestly non-Hermitian at all times $t \in (-\infty, 1)$, it becomes diagonal at $t = 1$ and complex and Hermitian at all the remaining times $t \in (1, \infty)$.

At $N = 10$ the spectrum of such a toy model is sampled in Fig. 6. Obviously, this example of a kinematical input connects, smoothly, the complete Big-Bang-type degeneracy of the eigenvalues at $t = 0$ with their unfolding at $t > 0$ which passes also through the "unperturbed", diagonal-matrix special case at $t = 1$. Needless to emphasize that in this model the spectrum is all complex and, hence, the space of the Universe remains completely unobservable *alias* non-existent before Big Bang.

5.2 Cyclic Cosmology

Not quite expectedly the spectrum gets entirely different after an apparently minor change of the time-dependence in

$$Q^{(N)}(t) = Q_0^{(N)} + \sqrt{1-t^2}\times Q_1^{(N)} \qquad (21)$$

Using $N = 8$ the resulting spectrum is displayed in Fig. 7. We see that in the new model the "geometry of the world" was the same before Big Bang so that model (21) may be perceived as reflecting a kinematics of a kind of cyclic cosmology as preferred in Hinduism or, more recently, by Roger Penrose [26].

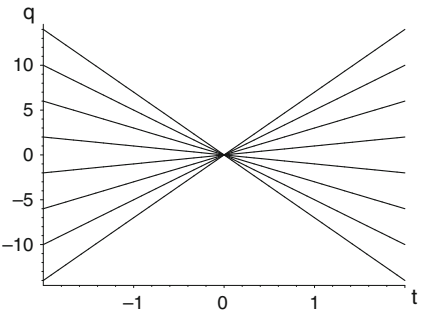


Fig. 7 Real eigenvalues of the toy-model geometry (21) in the both-sided vicinity of its Big Bang singularity at $t = 0$

5.3 *Darwinistic, Evolutionary Cosmology*

In the THS representation of the 1D Universe the "geometry" or "kinematical" operator $Q(t)$ may be assumed, in general,

- non-Hermitian (otherwise, we would lose the dynamical degrees of freedom carried by the generic metric Θ and needed and essential near the Big Bang instant),
- simple (i.e., typically, tridiagonal as above—otherwise, there would be hardly any point in our leaving the much simpler Schrödinger picture).

In the latter sense, our third class of toy models may be taken from [27, 28] and sampled by the following $N = 8$ distance operator

$$Q(t) = \begin{bmatrix} 0 & 1-t & 0 & 0 & 0 & 0 & 0 & 0 \\ t & 0 & 1-t & 0 & 0 & 0 & 0 & 0 \\ 0 & t & 0 & 1-|t| & 0 & 0 & 0 & 0 \\ 0 & 0 & |t| & 0 & 1-|t| & 0 & 0 & 0 \\ 0 & 0 & 0 & |t| & 0 & 1-|t| & 0 & 0 \\ 0 & 0 & 0 & 0 & |t| & 0 & 1-t & 0 \\ 0 & 0 & 0 & 0 & 0 & t & 0 & 1-t \\ 0 & 0 & 0 & 0 & 0 & 0 & t & 0 \end{bmatrix} \tag{22}$$

The piecewise linear time-dependence of this operator leads to the quantum phase transition between the Big Crunch collapse of the spatial grid in previous Eon and the Big Bang start of the spatial expansion of the present Eon. In the vicinity of the singularity at $t = 0$ we may characterize such a quantum cosmological toy model by the following flowchart,

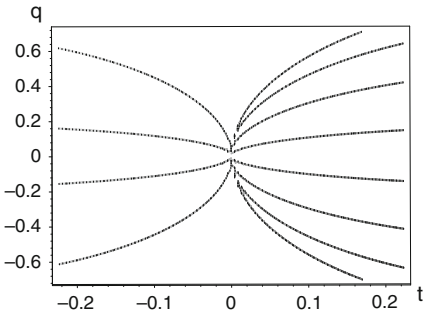
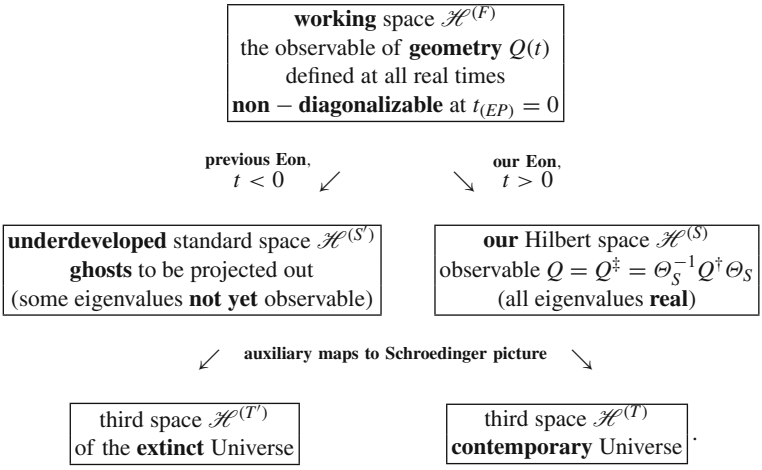


Fig. 8 Real eigenvalues of the toy-model geometry (22) in the both-sided vicinity of the Crunch-Bang singularity at $t = 0$



The evolutionary-cosmology idea of the quantum Crunch-Bang transition itself (discussed more thoroughly in [28] and illustrated also by Fig. 8) may be perceived as one of the serendipitous conceptual innovations provided by the present Heisenberg-picture background-independent [24] quantization of our schematic Universes.

6 Outlook

The results of the analysis of the solvable models of preceding section offer a nice illustration of several merits of the THS approach to the building of Big-Bang-exhibiting quantum systems.

- the Big Bang value of time $t^{(BB)} = 0$ is a point of degeneracy of all of the eigenvalues, $q_n(0) = 0$ at all $n = 1, 2, \ldots, N$;
- at $t = t^{(BB)} = 0$ all of our toy models acquire the complete, N by N Jordan-block structure so that the Big Bang time coincides with the point of confluence of *all* of the Kato's exceptional points;

- after Big Bang, i.e., at $t > t^{(BB)} = 0$ the spectra of possible (and growing) quantum distances between Alice and Bob are all real and, hence, observable, in our specific toy models at least;
- in the light of Fig. 8 our models describe also the times *before* Big Bang, $t < t^{(BB)} = 0$. In this sense the pass of our systems through the Big-Bang singularity is "causal", described by a "universal" operator $Q(t)$;
- before Big Bang (i.e., before the Big Crunch of the Penrose's [26] "previous Eon") the menu of the *real* distances $q_n(t)$ is replaced by an empty set (in Fig. 6), survives unchanged (in Fig. 7) or gets reduced to a proper subset (cf. Fig. 8);
- in the most interesting latter case the "missing", complex eigenvalues are tractable as "not yet observable". One could speak about various "evolutionary" forms of cosmology in this setting.

7 Appendix: Auxiliary Spaces and $\mathscr{P}\mathscr{T}$-Symmetries

A few years after the publication of review [6], a series of rediscoveries and an enormous growth of popularity of the pattern followed the publication of pioneering letter [29] in which Bender with his student inverted the flowchart. They choose a nice illustrative example to show that the *manifestly non-Hermitian* F-space Hamiltonian H with real spectrum may be interpreted as a hypothetical *input* information about the dynamics (cf. also review [8] for more details).

Graphically, the flowchart of $\mathscr{P}\mathscr{T}$-symmetric quantum theory is schematically depicted in Fig. 9. For completeness let us add that the Bender's and Boettcher's construction was based on the assumption of $\mathscr{P}\mathscr{T}$-symmetry $H\mathscr{P}\mathscr{T} = \mathscr{P}\mathscr{T}H$ of their dynamical-input Hamiltonians where the most common phenomenological parity $\mathscr{P}$ and time reversal $\mathscr{T}$ entered the game. Mostafazadeh (cf. his review [9]) emphasized that their theory may be generalized while working with more general $\mathscr{T}$s (typically, any antilinear operator) and $\mathscr{P}$s (basically, any indefinite, invertible operator).

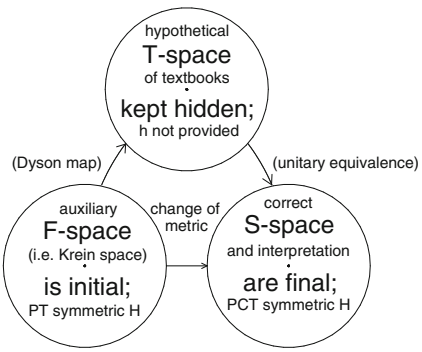
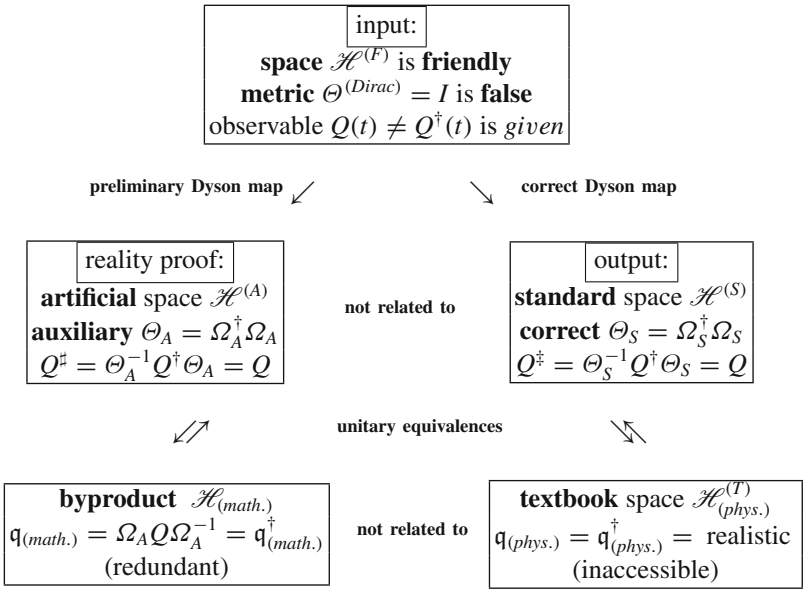


Fig. 9 THS interpretation of $\mathscr{P}\mathscr{T}$-symmetric Hamiltonians H

Several mathematical amendments of the theory were developed in the related literature, with the main purpose of making the constructions feasible. Let us only mention here that the useful heuristic role of operator $\mathscr{P}$ was successfully transferred to the Krein-space metrics η (cf. [30] for a comprehensive review). In comment [31] we explained that in principle, the role of $\mathscr{P}$ could even be transferred to some positive-definite, simplified and redundant auxiliary-Hilbert-space metrics $\tilde{\mathscr{P}} = \Theta_A \neq \Theta_S$. Such a recipe proved encouragingly efficient [32]. Its flowchart may be summarized in the following diagram:



Besides the right-side flow of mapping we see here the auxiliary, unphysical left-side flow where, typically, the non-Dirac metric Θ_A need not carry any physical contents. In some models such an auxiliary metric proved even obtainable in a trivial diagonal-matrix form [28].

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