Quantum Resonances: Theory and Models

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Abstract. Along this paper, we give a short review of some interesting aspects of a formulation of quantum resonances. In particular how and why to characterize quantum resonances through Gamow state vectors as functionals of spaces constructed using Hardy functions on a half-plane. In addition, we give a couple of quite distinct interesting examples of resonance models. Here, we limit ourselves to the non-relativistic case.

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1. Introduction

This article contains a brief review in some interesting aspects of quantum resonances and their relation with some lines of research in modern quantum theory like time asymmetric quantum mechanics (TAQM) [1]. In the present summary, our discussion will be preferentially focused on non relativistic resonances. Explicit examples of resonance models will be also discussed.

It is reasonable to begin our discussion with a presentation of the different definitions of quantum resonances. Although, they are not equivalent in all cases, there exists an account in the literature of some sufficient conditions among them. This account is far to be complete and a research on this direction is probably worthy to carry out. For this purpose, we address the interested reader to the standard literature on the subject [2–8].

There are some techniques to obtain the parameters of resonances in given models. Rigorous mathematical methods like complex scaling and the use of Krein formula are of order here. Nevertheless, in the case of the very illustrative onedimensional models, these methods are usually too sophisticated. Instead, the use of the so-called purely outgoing boundary conditions gives resonances in onedimensional models, as solutions of a transcendental algebraic equation. This can

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usually be solved numerically, to give the parameters of a finite number of resonances, with a reasonable level of accuracy. We can also study the behavior of a limited number of resonances as well as bound and antibound states with the variation of some given parameters, using this method. An example of such a procedure will be given in the last section.

Resonances in quantum mechanics describe unstable quantum states. When considered as pure quantum states, they are described by a vector state. Resonance vector states split into a sum of two contributions, one that decays exponentially with time and other that produces deviations of this exponential decay for very short and very long values of time. The range of observation usually covers this exponential decay being the other modes not easily observable. This characteristic and the fact that the vector state for the exponentially decay mode can be often constructed explicitly, permits the identification of it with the resonance state. This vector state is usually called the Gamow vector. It has, however, a basic difficulty as it cannot be given by a normalizable vector in the usual Hilbert space. Then, the use of extensions of the Hilbert space to rigged Hilbert spaces (RHS) is necessary for this description of quantum resonances. In this context, Gamow vectors are realized as objects in a space of functionals that admit the Hilbert space as a subspace.

It is often convenient to describe resonances as produced in resonance scattering. By an appropriate choice of the RHS based on the use of Hardy functions on a half-plane, we can split this scattering into a preparation and a registration processes. This is used as a basis for the formulation of a Time Asymmetric Quantum Mechanics, which requires a simple refinement of the concept of pure state [1].

In the study of resonances, textbooks often propose an identification between the width of a bump in the cross section, which is characteristic of resonance phenomena and the inverse of the mean life. However, this identification suffers some structural problems like measuring difficulties [9]. This identification can be better understood in the context of our formalism based in RHS of Hardy functions.

The Friedrichs model and its refinements and generalizations [10] give a good laboratory to investigate basic properties of resonances, Gamow vectors, etc, having applications to a wide set of realistic physical systems. Also, one-dimensional models can be proposed for the study of resonance as well as bound and antibound states behavior, which can be somehow unexpected.

Finally, we are summarizing here a formalism of non-relativistic resonance and have included two models that we consider as interesting. The extension of this formalism to relativistic resonances as well as unstable interaction of quantum fields has been discussed elsewhere. See [11] and references therein.

2. Definitions and characterizations of quantum resonances

A quantum resonance may be caused by the action of an interaction on an otherwise free particle. As the interaction is usually produced by a potential, it is customary to consider two Hamiltonians in the production of resonance phenomena, a so-called "free" Hamiltonian H_0 under which the particle is supposed to move freely and a total or interaction Hamiltonian $H = H_0 + V$, where V is the potential. The physical effect of V is the creation of a metastable state in which V retains the studied particle in a bounded region a time which is much larger than the time the particle would stay in this region should the interaction not exist. Then, for resonances to be produced, we need a Hamiltonian pair $\{H_0, H\}$.

This situation can be better understood in the context of resonance scattering, which is a scattering process that produces resonances. Let us assume that the potential V is of compact support just to give a better intuitive image of the process. In the remote past, a state ψ^{in} is prepared in a preparation apparatus and evolves under the action of the free Hamiltonian H_0 . This state is captured inside the interacting region (the support of the potential) and stays for a long delay time, i.e., it forms a resonance. In the far future it becomes ψ^{out} and again its time evolution is governed by H_0 . Both "in" and "out" state vectors are related through the S-matrix, $\psi^{\text{out}} = S\psi^{\text{in}}$.

The definitions of quantum resonances resonances most popular in the standard literature are discussed below.

2.1. Definitions of resonances from the mathematical point of view

Assume that both H_0 and H are defined on a separable infinite-dimensional Hilbert space \mathcal{H} and have an absolutely continuous spectrum $\mathbb{R}^+ := [0, \infty)$, which is the same for both operators. This is a very common situation. Then, the first definition of a resonance produced by the Hamiltonian pair $\{H_0, H\}$ is the following [7]:

Definition 1. Assume that there is a dense set of vectors \mathcal{D} in \mathcal{H} such that for $\psi \in \mathcal{D}$, both

$$R_{0\psi}(\lambda) = \langle \psi | (H_0 - \lambda)^{-1} \psi \rangle, \quad R_{\psi}(\lambda) = \langle \psi | (H - \lambda)^{-1} \psi \rangle \tag{1}$$

have analytic continuation through the positive real axis. Assume that $R_{0\psi}(\lambda)$ is analytic at $z_R = E_R - i\Gamma/2$ for any ψ , but there exists a $\psi \in \mathcal{D}$ for which $R_{\psi}(\lambda)$ shows a pole. Then, we say that z_R is a resonance of the Hamiltonian pair $\{H_0, H\}$.

We should stress that both $R_{0\psi}(\lambda)$ and $R_{\psi}(\lambda)$ are analytic functions on the complex plane of λ with a branch cut on the positive semiaxis \mathbb{R}^+ . Their possible isolated singularities lie on their analytic continuations through the cut. In the language of Riemann surfaces, these poles appear on the second sheet. Resonance poles may not be unique and in fact, in most realistic models they appear in an infinite number. Also resonance poles appear in complex conjugate pairs of the same multiplicity, each pair of resonance poles represent the same resonance.

A second definition of quantum resonance is the celebrated *pair of complex* conjugate poles of the analytic continuation of the S-matrix:

Definition 2. Let S(k) and S(E) the S-matrix in the momentum and energy representations, respectively $(E = \hbar^2 k^2/2m)$. Assume that S(k) can be analytically continued to a meromorphic function on the whole complex plane \mathbb{C} . Then, a resonance is defined as one of these equivalent forms:

- i) Pairs of poles of the analytic continuation of S(k) located symmetrically with respect to the negative imaginary axis;
- ii) Pairs of complex conjugate poles of the analytic continuation of S(E) across the positive real axis.

In the language of Riemann surfaces, these poles lie on the second sheet of the Riemann surface corresponding to the transformation $k = \sqrt{E}$. These pairs are located at: $z_R = E_R - i\Gamma/2$ and $z_R^* = E_R + i\Gamma/2$, E_R , $\Gamma > 0$. Each of these pairs of resonance poles may have a multiplicity bigger than one, which is the same for each member of the pair. This multiplicity is preserved when we change from the momentum representation S(k) to the energy representation S(E) and vice-versa.

The existence of these analytic continuations is usually related to the verification of certain *causality conditions* [3].

2.2. Definition of resonances from the physicists point of view

We here mention a few definitions that come from the resonance scattering. From this point of view, we can define resonances by one of these usually equivalent choices [3, 5]:

- i) Large delay times. This is the difference of times that an incident particle would stay in the interacting region with or without interaction. Delay times are measurable [5].
- ii) Sudden bump in the cross section around a given energy E_R and with width Γ . The bump's width is associated to the mean life $\tau = 1/\Gamma$.
- iii) Sudden change of the phase shift $\delta_{\ell}(E)$, around E_R , in the energy representation.
- iv) The scattering amplitude $\psi(E)$ for the decaying state has a Lorentzian shape:

$$|\psi(E)|^2 \approx N \frac{\Gamma}{(E - E_R)^2 + \Gamma^2/4} \,. \tag{2}$$

Physics determines the meaning of the constants E_R and Γ , respectively, the real and imaginary parts of the resonance poles of the definitions in the previous subsection. E_R means the energy at which the resonance is produced and Γ is the width of the bump in the cross section that detects the resonance.

Concerning the physical meaning of the imaginary part $\Gamma/2$. The usual identification between the width Γ and the inverse of the mean life τ [5] is far from being trivial. First of all, the width is often quite difficult to be measured with precision. Sometimes it is not possible to measure both for a decaying process. Thus, this identification is often ambiguous [9].

Probably the best characterization of a resonance state is that it should have a scattering amplitude (proportional to the square of the modulus of the wave function in the energy representation) of Breit–Wigner type as in (2). This unifies both meanings of Γ as the width and as the inverse of the mean life. In fact, Γ is the width of (2) and its Fourier transform, that gives the decay mode, an exact decaying exponential [12]. On the other hand, no vector in Hilbert space may have an energy distribution of Breit–Wigner type. It can be the case of a Gamow vector constructed, as explained below, with the help of spaces of Hardy functions.

2.3. On the decay of a quantum state

Let us consider a vector state ϕ in the absolutely continuous Hilbert space for the total Hamiltonian H and consider the decay amplitude given by $|\langle \phi|e^{-itH}\phi \rangle|^2$, with t > 0. As a consequence of the Riemann–Lebesgue lemma for integrable functions, one has that $\lim_{t\to\infty} |\langle \phi|e^{-itH}\phi \rangle| = 0$. The state ϕ can be considered as a vector state describing a resonance if for a large range of values of time, neither close to zero nor very large, the function $|\langle \phi|e^{-itH}\phi \rangle|^2$ is approximately proportional to $e^{-\Gamma t}$ with $\Gamma > 0$, i.e., ϕ decays exponentially for this time range. However, as a consequence of the semiboundedness of the Hamiltonian H, no vector state may decay exponentially for all positive values of time [6]. In fact, due to the properties of the Fourier transform, the amplitude of such a state in the energy representation must be proportional to (1), which is only possible if the spectrum of H is the whole real line. Deviations of the exponential law decay are attributed to the interaction of the resonance with the external media (background) or other effects like re-scattering [6].

A possible cure is the split of the decaying state into a term that decays exponentially for all values of time t > 0, plus another term that justifies the deviations (background term), $\phi = \psi^D + \psi^B$. But then, neither ψ^D nor ψ^B can be Hilbert space normalizable vector states. However, such a cure is possible and it is quite reasonable, as we shall discuss in the sequel.

2.4. Determination of resonances

The purpose of this paragraph is to present a very brief review on the most usual methods for the determination of the resonances.

These methods are based in different definitions of resonances. The complex scaling method and the use of the Krein formula start from the definition of resonances as singularities of the analytic extensions of the resolvent. The Krein formula relates different self-adjoint extensions of symmetric operators with finite equal deficiency indices.

The second type of methods comes from the consideration of resonances as poles of the analytic continuation of the S-matrix. In general, it is not easy to find the explicit form of the S-matrix, and therefore, we have to resort to indirect methods. This is quite feasible for one-dimensional systems as we shall discuss later.

Also, resonances poles are often looked as generalized complex eigenvalues of the total Hamiltonian $H\psi^D = z_R\psi^D$, with $z_R = E_R - i\Gamma/2$. The self-adjointness of H shows that the corresponding eigenvector ψ^D cannot belong to the Hilbert space \mathcal{H} of the states of the system, but instead it is a functional which belongs to an extension of \mathcal{H} , as shall discussed later. The problem here is that in these extensions, the discrete spectrum of H may be even a whole complex half-plane. The point is how to isolate the eigenvalues of H, which are resonance poles. This problem has been solved by H. Baumgärtel [13]. The vector ψ^D is then the decaying Gamow vector. Along $H\psi^D = z_R\psi^D$, we also have the solution to the eigenvalue problem $H\psi^G = z_R^*\psi^G$ and ψ^G is called the growing Gamow vector, which is nothing else that the time reversal of ψ^D .

2.4.1. The Complex Scaling Method and the Krein formula. Here, we include a few comments on the methods that derive from the consideration of resonances as poles of the analytic continuation of the resolvent.

The Complex Scaling Method [7, 14] requires potentials belonging to the so-called class of dilation analytic potentials (DAP) [7, 14]. One starts with the transformation $U(\theta)\psi(\mathbf{x}) = e^{3\theta/2}\psi(e^{\theta}\mathbf{x})$. When $V(\mathbf{x})$ is a DAP, then, $H(\theta) :=$ $U(\theta)[H_0 + V]U^{-1}(\theta) = e^{-2\theta}H_0 + V(\theta)$ admits an analytic continuation for complex values of θ in a strip of the complex plane. The spectrum $\sigma(H(\theta))$ of $H(\theta)$, only depends on the imaginary part of θ and has two components: i.) a complex continuous spectrum, which is the semiaxis $e^{-2\theta}\lambda$, with $\lambda \in [0, \infty)$ and ii.) a discrete spectrum of complex eigenvalues having zero as the only possible limit point. These eigenvalues are the resonance poles (in the sense of the above definition making use of the resolvents) [7, 14] and do not depend on θ (although the number eigenvectors of $H(\theta)$ does depend on θ). Each of the resonances, say z_n , satisfies an eigenvalue equation of the type $H(\theta)\psi_n(\theta) = z_n\psi(\theta)$.

This method is quite suggesting. In fact is like a curtain with a rail (the continuous spectrum for $H(\theta)$) with the origin as a fixed point were being moved downwards with angle θ , disclosing the resonance poles. In addition the eigenvectors $\psi_n(\theta)$ are normalizable, i.e., vectors in the Hilbert space \mathcal{H} . However, they depend on the value of θ and therefore cannot be used as Gamow vectors, i.e., vector states for resonances.

The Krein formula as stated before, gives us the relations between the resolvents of two different self-adjoint extensions of a symmetric operator [15]. This can be useful to obtain resonances produced by point potentials, since these potentials are often defined by this type of self-adjoint extensions, as is the case of a delta type perturbation. In such a case, H_0 and $H = H_0 + V$ may be two different self-adjoint extensions of the same symmetric operators and therefore their resolvents be easily comparable through the Krein formula. This formula is easily computable when the deficiency indices are (1, 1), becomes computationally more involved when they are (2, 2) and difficult or even intractable in most cases for higher deficiency indices.

2.4.2. One-dimensional resonance scattering. The one-dimensional resonance scattering is a laboratory friendly to user for the study of resonance behavior. A particularly common situation arises when both H_0 (usually $H_0 = \mathbf{p}^2/(2m)$) and $V(\mathbf{x})$

are spherically symmetric. When $\ell = 0$, where ℓ is the orbital angular momentum, the Schrödinger equation is an ordinary differential equation in the radial variable $r \geq 0$. Let us denote by $\chi(r; E)$ an arbitrary solution with eenergy E > 0. The asymptotic form of $\chi(r; E)$ far from the region in which the potential acts has the following form [2]:

$$\chi(r; E) = \mathcal{F}_1(k) e^{ikr} + \mathcal{F}_2(k) e^{-ikr}, \quad k = \sqrt{2mE/\hbar^2}.$$
 (3)

Observe that e^{-ikr} denotes a free incoming wave and e^{ikr} a free outgoing wave, so that the S-matrix has the form

$$S(k) = -\frac{\mathcal{F}_1(k)}{\mathcal{F}_2(k)}.$$
(4)

Thus, the search for resonances as poles of the S-matrix is equivalent to the search of complex zeros of $\mathcal{F}_2(k)$. This gives in general a transcendental function that should be solved numerically. Resonances exist for many known models and its number is often infinite. If for a complex value k_R , we have that $\mathcal{F}_2(k_R) = 0$, write $z_R := k_R^2 \hbar^2/(2m)$, then, for large values of r, the wave function has the form:

$$\chi(r; z_R) \approx \mathcal{F}_1(k_R) \, e^{ik_R r} \,. \tag{5}$$

We see that there is only an outgoing wave function without incoming wave function. This situation is a consequence of imposing the condition $\mathcal{F}_2(k) = 0$, the purely outgoing boundary condition. Since $\chi(r; E)$ is a solution of the Schrödinger equation $H\chi(r; E) = E\chi(r; E)$, we must have $H\chi(r; z_R) = z_R\chi(r; z_R)$, i.e., $\chi(r; z_R)$ is the decaying Gamow vector (or Gamow function). Since the imaginary part of k_R is negative [3], the decaying Gamow function grows exponentially for large values of r. Note that this Gamow vector (or Gamow function) should fulfill the boundary condition $\chi(0; z_R) = 0$.

However, the interesting range of one-dimensional models covers more situations in which resonances play an interesting role. Examples are the finite square well potential and the semi oscillator with or without point potentials. This model has resonances with sometimes unexpected behavior and we shall describe it briefly later. In such case, resonances are found by imposing again purely outgoing boundary conditions, as we shall do in the proposed example.

2.5. Resonance scattering

Here, we are considering a resonance scattering situation as described in the beginning of Section 2, with the Hamiltonian pair $\{H_0, H\}$. Assume that the incoming free state is ψ^{in} and the outgoing free state is ψ^{out} . However, after the scattering we cannot detect the whole state ψ^{out} but instead its projection into the region occupied by a *registration apparatus*. The projection of ψ^{out} into this region is a state vector here denoted as ϕ^{out} . The main object in our formalism is the *transition amplitude* between the scattered state and the registered state.

$$\langle \phi^{\text{out}} | \psi^{\text{out}} \rangle = \langle \phi^{\text{out}} | S \psi^{\text{in}} \rangle = \int_0^\infty [\phi^{\text{out}}(E)]^* S(E) \, \psi^{\text{in}}(E) \, dE \,. \tag{6}$$

For simplicity, we are assuming that H_0 has a simple absolutely continuous spectrum which is $\mathbb{R}^+ = [0, \infty)$. Then, it is unitarily equivalent to the multiplication operator by E on $L^2(\mathbb{R}^+)$. This variable E is the energy. On the other hand, since the S-matrix commutes with H_0 , on $L^2(\mathbb{R}^+)$ is represented by a function S(E) of the energy. We have already seen that S(E) is often analytically continuable and its analytic continuation admits as support the Riemann surface associated the square root. If we choose $[\phi^{\text{out}}(E)]^*$ and $\psi^{\text{in}}(E)$ to be analytically continuable functions from above to below on the lower half-plane, we can find an interesting decomposition for the integral in (6):

$$\int_{\gamma} [\phi^{\text{out}}(z^*)]^* S_{II}(z) \psi^{\text{in}}(z) dz - 2\pi i \sum \text{Residues} [[\phi^{\text{out}}(z^*)]^* S_{II}(z) \psi^{\text{in}}(z)].$$
(7)

Here, $S_{II}(z)$ is the analytic continuation of S(E) beyond its cut $\mathbb{R}^+ = [0, \infty)$, supported on the second sheet of the Riemann surface. The functions $[\phi^{\text{out}}(E)]^*$ and $\psi^{\text{in}}(E)$ should be defined on the upper rim of the cut, so that the analytic continuation is supported on the lower half-plane in the second sheet. The contour γ lies on this half-plane, although under some conditions it can be moved to the negative semiaxis of the second sheet [16]. This integral is the *background integral*.

When sufficient conditions for the existence and asymptotic completeness of the Møller wave operators are fulfilled [27, 28, 30], the *S*-matrix can be written as the product $S = \Omega^{\dagger}_{OUT}\Omega_{IN}$, where Ω_{IN} and Ω_{OUT} are these Møller wave operators. Let us write $\phi^+ := \Omega_{OUT}\phi^{out}$ and $\psi^- := \Omega_{IN}\psi^{in}$. From (6)–(7), one finds that $\langle \phi^{out} | S\psi^{in} \rangle$ is equal to

$$\langle \phi^+ | \psi^- \rangle = \text{background} - 2\pi i \sum \text{Residues} \left[[\phi^{\text{out}}(z^*)]^* S_{II}(z) \psi^{\text{in}}(z) \right].$$
 (8)

The vectors ϕ^+ , ψ^- belong to the locally convex spaces Φ^+ and Φ^- , respectively, to be defined in the next section. Now, for arbitrary vectors $\phi^+ \in \Phi^+$ and $\psi^- \in \Phi^-$, let us define the following maps:

$$\phi^+ \longrightarrow [\phi^{\text{out}}(z_R^*)]^* = \langle \phi^+ | \psi^D \rangle \quad \text{and} \quad \psi^- \longrightarrow [\psi^{\text{in}}(z_R^*)]^* = \langle \psi^- | \psi^G \rangle.$$
(9)

These maps define functionals $|\psi^D\rangle$ and $|\psi^G\rangle$ on the spaces Φ^+ and Φ^- , respectively (we use the notations ψ^D and the Dirac version $|\psi^D\rangle$ indistinctly). These maps are anti-linear and continuous [12] and therefore, elements of the respective duals of these spaces. Then, for the case of having one unique resonance, or include one unique resonance between the contour γ and the positive semi-axis, (9) becomes

$$\langle \phi^+ | \psi^- \rangle = \text{background} - 2\pi i \langle \phi^+ | \psi^D \rangle s_1 \langle \psi^G | \psi^- \rangle.$$
 (10)

We can write the background term in the form $\langle \phi^+ | \text{bgk} \rangle$, where $| \text{bgk} \rangle$ is a continuous antilinear functional on Φ^+ [12]. The extension of this formula to more resonance poles is straightforward. Then, if we omit the arbitrary $\phi^+ \in \Phi^+$, we have:

$$\psi^{-} = |\mathrm{bgk}\rangle - 2\pi i |\psi^{D}\rangle s_{1} \langle \psi^{G} |\psi^{-}\rangle = |\mathrm{bgk}\rangle + c |\psi^{D}\rangle.$$
(11)

This equation is an identity in the dual space of Φ^+ . Now assume that the resonance pole is at $z_R = E_R - i\Gamma/2$. Then the functional $|\psi^D\rangle$ has the following properties:

$$H|\psi^D\rangle = z_R|\psi^D\rangle, \quad e^{-itH}|\psi^D\rangle = e^{-iz_R t}|\psi^D\rangle = e^{-iE_R t} e^{\Gamma t/2} |\psi^D\rangle.$$
(12)

According to the previous definitions and discussion on the Gamow vectors, $|\psi^D\rangle$ is the decaying Gamow vector. The formalism thus far summarized manages to separate the exponential decay of an unstable quantum state from the background, supposedly responsible of the deviations of the exponential decay and their consequences [12, 16].

3. Mathematical interlude

Gamow vectors are generalized eigenvectors of the total Hamiltonian with given complex eigenvalues. Since the Hamiltonian is self adjoint, no solution of this eigenvalue equation is given by a Hilbert space. To give meaning to them, we need to extend the action of the Hamiltonian beyond the Hilbert space vector, for which we need rigged Hilbert spaces (RHS). As is well known, a RHS is a triplet of spaces

$$\Phi \subset \mathcal{H} \subset \Phi^{\times} \,, \tag{13}$$

where: i.) \mathcal{H} is an infinite-dimensional separable Hilbert space that contains all the pure states of a given physical system. In the case of a scattering process with two Hamiltonians $\{H_0, H\}$, both must be defined and be self adjoint on \mathcal{H} ; ii.) Φ is a subspace dense in \mathcal{H} endowed with a locally convex topology finer that the topology on \mathcal{H} . Although not strictly necessary, Φ is often chosen to be a nuclear space [17]. Finally, iii.) Φ^{\times} is the antidual space of Φ , the space of continuous antilinear functionals on Φ . It is endowed with any topology compatible with the dual pair (Φ, Φ^{\times}) [18].

We need to find a RHS such that H can be extended into an operator to Φ^{\times} . One possible form is to choose Φ such that for any $\varphi \in \Phi$, $H\varphi \in \Phi$, so that Φ is stable under the action of H. If H is self adjoint, we can always find Φ with this property and also being continuous on Φ [19–22]. In this case, we can extend uniquely H to Φ^{\times} using the so-called duality formula. If the action of $F \in \Phi^{\times}$ on $\varphi \in \Phi$ is represented by $\langle \varphi | F \rangle$, then, the extension is defined with the property:

$$\langle H\varphi|F\rangle = \langle \varphi|HF\rangle, \qquad (14)$$

where the extension is also denoted by the same letter H. If H is continuous on Φ , with its local convex topology, then its extension is continuous on Φ^{\times} endowed with the weak topology of the dual pair (Φ, Φ^{\times}) .

A Hardy function \mathcal{H}^2_+ on the upper complex half-plane is a complex analytic function on $\mathbb{C}^+ := \{z \in \mathbb{C}, \text{ Im } z > 0\}$, which is square integrable along every line parallel to the real axis and such that there exists a positive constant K such that (z = x + iy)

$$\int_{-\infty}^{\infty} |f(x+iy)|^2 \, dy < K \,.$$
(15)

As a consequence the function f(x) formed by the boundary values of f(z) on the real line is well defined, i.e., it is a square integrable function. The values of f(x)on the whole real line and on the positive semiaxis $[0, \infty)$ reproduce the values of f(z) for all \mathbb{C}^+ . Similarly, we define the space of Hardy functions on the lower half-plane, \mathcal{H}^2_- . Properties of these functions are summarized in [12, 16]. For a systematic study, see [29].

Now, take the Hamiltonian pair $\{H_0, H\}$ fulfilling the following conditions: i.) Their absolutely continuous spectra are simple and given by $\mathbb{R}^+ \equiv [0, \infty)$. The condition of being simple is not necessary, but simplifies discussion and notation. ii.) The Møller wave operators Ω_{IN} and Ω_{OUT} exist and are asymptotically complete. iii.) The realization of the *S*-matrix as a function in terms of the energy, S(E), is analytic and can analytically be continued through the branch cut $[0, \infty)$. This continuation has pairs of conjugate poles that are identified with resonances.

As a consequence of i.) and the spectral theorem for self-adjoint operators [23], there exists a unitary operator $U : \mathcal{H}_{ac} \mapsto L^2(\mathbb{R}^+)$ such that for any ψ in the domain of H_0 and $\psi(E) := U\psi$, $U^{-1}H_0U\psi = E\psi(E)$, where \mathcal{H}_{ac} is the absolutely continuous subspace of H_0 [23].

Now, let $\mathcal{H}^2_+ \cap S$ and $\mathcal{H}^2_- \cap S$ be the intersections of these spaces with the Schwartz space S of infinitely differentiable functions such that they and their derivatives go to zero at the infinity faster than the inverse of any polynomial. The spaces of the restrictions of these functions to \mathbb{R}^+ are called $\Psi^+ := (\mathcal{H}^2_+ \cap S)\Big|_{\mathbb{R}^+}$

and $\Psi^- := (\mathcal{H}^2_- \cap S)\Big|_{\mathbb{R}^+}$, respectively.

A Hardy function on either the upper or the lower half-plane is uniquely determined by its boundary values on the positive semiaxis \mathbb{R}^+ [24]. Then, the mappings $j_{\pm} : \mathcal{H}^2_{\pm} \cap S \longrightarrow \Psi^{\pm}$ that associate a function in \mathcal{H}^2_{\pm} to its restriction to \mathbb{R}^+ are one to one and onto (bijection). If we consider the topology induced by the topology of the Schwartz space on $\mathcal{H}^2_{\pm} \cap S$ and then, transport it by the action of j_{\pm} , we obtain as a consequence that

$$\Psi^{\pm} \subset L^2(\mathbb{R}^+) \subset (\Psi^{\pm})^{\times} \tag{16}$$

are a new pair of RHS. If we anew define $\Phi^+ := \Omega_{\text{OUT}} U^{-1} \Psi^+$ and $\Phi^- := \Omega_{\text{IN}} U^{-1} \Psi^-$ and again endow these spaces with the topology transported by the bijections $\Omega_{\text{OUT}} U^{-1}$ and $\Omega_{\text{IN}} U^{-1}$, we have a new RHS:

$$\Phi^{\pm} \subset \mathcal{H}_{\rm ac}(H) \subset (\Phi^{\pm})^{\times} , \qquad (17)$$

where $\mathcal{H}_{ac}(H)$ is the absolutely continuous subspace of H.

By construction, $H^n \Phi^{\pm} \subset \Phi^{\pm}$, n = 1, 2, ... and H^n is continuous on Φ^{\pm} . Note that the duality formula (14) extends H into both antiduals $(\Phi^{\pm})^{\times}$:

$$\langle H\phi^{\pm}|F^{\pm}\rangle = \langle \phi^{\pm}|HF^{\pm}\rangle, \quad \forall \phi^{\pm} \in \Phi^{\pm}, \quad \forall F^{\pm} \in (\Phi^{\pm})^{\times}.$$
 (18)

This formula (18) permits the definition of Gamow vectors. The above spaces and their relations can be summarized in the following diagram:

Here, *i* denotes canonical injection. Note that *i* is continuous in each case. There is an analogous diagram for Φ^- , etc and $\Omega_{\rm IN}$ [12]. From the previous diagram, one concludes that $[j_+^{-1} U \Omega_{\rm OUT}^{-1}] \Phi^+ = \mathcal{H}^2_+ \cap S$. Therefore, the mapping $j_+^{-1} U \Omega_{\rm OUT}^{-1}$ transforms $\phi^+ \in \Phi$ into an analytic function $\phi^+(E)$ on the upper half-plane. For any *z* in the open lower half-plane, the mapping

$$\phi^+ \longrightarrow [\phi^+(z^*)]^* \tag{19}$$

defines a continuous antilinear functional on Φ^- that we shall denote as $|z\rangle$. Note that the complex conjugate of a function in \mathcal{H}^2_{\pm} is a function in \mathcal{H}^2_{\pm} .

If we have a resonance pole located at the point $z_R = E_R - i\Gamma/2$, its corresponding decaying Gamow vector is given by

$$\phi^+ \longrightarrow [\phi^-(z_R^*)]^* = \langle \Phi^+ | \psi^D \rangle , \qquad (20)$$

with the following properties:

$$H|\psi^D\rangle = z_R|\psi^D\rangle, \qquad e^{-itH}|\psi^D\rangle = e^{-itE_R} e^{-\Gamma t/2} |\psi^D\rangle.$$
(21)

Along the decaying Gamow vector, we also have the growing Gamow vector: Let $\phi^-(E) := [j_-^{-1} U \Omega_{\text{IN}}] \phi^-$ for all $\phi^- \in \Phi^-$. Then, we define the following continuous antilinear functional $|\psi^G\rangle$ on Φ^- :

$$\phi^- \longrightarrow [\phi^+(z_R^*)]^* = \langle \Phi^+ | \psi^G \rangle \,. \tag{22}$$

The growing Gamow vector $|\psi^G\rangle$ has the following properties: i.) $H|\psi^G\rangle = z_R^*|\psi^G\rangle$ and ii.) $e^{-itH}|\psi^G\rangle = e^{-E_R t}e^{\Gamma t}|\psi^G\rangle$ for t < 0 [12, 16].

It is important to remark that, since $|\psi^{D}\rangle \in (\Phi^{+})^{\times}$, the above diagram gives [12, 16]:

$$(j_{+}^{-1})^{\times}U^{\times}(\Omega_{\text{OUT}}^{-1})^{-1}|\psi^{D}\rangle = \frac{N}{(E-E_{R})^{2} + \Gamma^{2}/4} \in (\mathcal{H}_{+}^{2} \cap S)^{\times}, \qquad (23)$$

where N is a normalization constant. In this sense, the Gamow vector $|\psi^D\rangle$ has a Breit-Wigner energy distribution [16].

4. Time asymmetric quantum mechanics

Here, we just want to call the attention to an application of the above mathematical model to a very important attempt to understand the asymmetric nature of quantum mechanics, which may have an important consequence in order to understand the existence of a time arrow at the microscopical level. It is not the objective of this section to discuss the important physical as well as philosophical implications of this asymmetry in quantum mechanics, but just give a brief notion of its existence. Then, the interested reader can go to the original sources for further information [1, 25, 26].

The notion of time asymmetric quantum mechanics (TAQM) comes from the idea according to which the process of creation of a resonance in resonance scattering is not just the time reversal of the process of decay.

According to this idea, one divides a scattering process into two parts:

1. **Preparation:** States are prepared by the preparation apparatus. Thus, in a scattering experiment a state is identified with an *incoming state* ψ^{in} . A resonance is produced.

2. **Registration:** Observables are detected in the registration apparatus, which registers and measures the result of the decay of the resonance. Detected outgoing states $|\phi^{out}(t)\rangle\langle\phi^{out}(t)|$ are indeed observables, according to this principle.

The detected outgoing state $|\phi^{\text{out}}(t)\rangle\langle\phi^{\text{out}}(t)|$ cannot be registered before the incoming state has been completely prepared (*causality principle*). If this preparation is complete at a time t_0 , this is taken as origin of times, $t_0 = 0$. The Born probability of measuring $|\phi^{\text{out}}(t)\rangle\langle\phi^{\text{out}}(t)|$ in the state $\rho(t) = |\psi^{\text{in}}(t)\rangle\langle\psi^{\text{in}}(t)|$ is given by (t > 0)

$$\mathcal{P}_{\rho(t)}(|\phi^{\text{out}}\rangle\langle\phi^{\text{out}}|) = |\langle\phi^{\text{out}}| \ \psi^{\text{in}}(t)\rangle|^{2}$$

$$= \operatorname{Tr}\{|\phi^{\text{out}}\rangle\langle\phi^{\text{out}}|[e^{-iHt}|\psi^{\text{in}}\rangle\langle\psi^{\text{in}}|e^{iHt}]$$

$$= \operatorname{Tr}\{[e^{iHt}|\phi^{\text{out}}\rangle\langle\phi^{\text{out}}|e^{-iHt}]|\psi^{\text{in}}\rangle\langle\psi^{\text{in}}|]$$

$$= |\langle\phi^{\text{out}}(t)| \ \psi^{\text{in}}\rangle| = \mathcal{P}_{\rho}(|\phi^{\text{out}}(t)\rangle\langle\phi^{\text{out}}(t)|).$$
(24)

This somehow justifies the idea of being $|\phi^{\text{out}}\rangle\langle\phi^{\text{out}}|$ an observable, since it would evolve following the Heisenberg evolution. Whenever we use the realization of wave functions in the energy representation by Hardy functions as explained before, time evolution of observables follows a semigroup law.

The fundamentals of TAQM are based on a new axiom to be added to quantum mechanics, which is relevant in the scattering processes. This new axiom refers to the choice of the relevant wave functions in the processes of preparation and registration. At this point it should be remarked that, the procedure of taking the wave functions from a dense subspace in Hilbert space is indistinguishable itself from functions in the Hilbert space, as the error in any measurement can be made arbitrarily small. This new axiom can be formulated as follows:

Preparation: For t = 0 states are prepared and given in the energy representation by functions in $\mathcal{H}^2_{-} \cap S\Big|_{\mathbb{R}^+}$. Note that $\mathcal{H}^2_{-} \cap S\Big|_{\mathbb{R}^+}$ is dense in $L^2(\mathbb{R}^+)$, so that any $\varphi(E) \in L^2(\mathbb{R}^+)$ can be approximated by a $\phi(E) \in \mathcal{H}^2_{-} \cap S\Big|_{\mathbb{R}^+}$.

Registration: Observables are $|\psi\rangle\langle\psi|$, where the ψ are approximated by functions in $\mathcal{H}^2_+ \cap S|_{\mathbb{R}^+}$.

The *time arrow* goes from the preparation apparatus to the registration apparatus [25].

5. Models of resonances

5.1. The Friedrichs model

The basic Friedrichs model has just one resonance. Nevertheless, it contains all features of resonance scattering and provides a framework for understanding resonance phenomena in realistic systems. Here, the Hamiltonian pair $\{H_0, H\}$ is given by

$$H_0 = \omega_0 |1\rangle \langle 1| + \int_0^\infty \omega |\omega\rangle \langle \omega| \, d\omega \,, \tag{25}$$

where $|1\rangle$ is an eigenvector of H_0 with eigenvalue ω_0 , $H_0|1\rangle = \omega_0|1\rangle$ and $|\omega\rangle$ are generalized eigenvectors of H with eigenvalues ω in the absolutely continuous spectrum of H_0 , which is the positive semi-axis $[0, \infty)$, $H_0|\omega\rangle = \omega|\omega\rangle$. The total Hamiltonian is $H = H_0 + \lambda V$, where λ is a real coupling constant and V is

$$V = \int_0^\infty f(\omega) \left[|\omega\rangle \langle 1| + |1\rangle \langle \omega| \right] d\omega \,. \tag{26}$$

Here $f(\omega)$ is a function, usually taken square integrable [31], called the *form factor*.

Resonances are here obtained using Definition 1 in 2.1. The conclusion is that they are poles of the analytic continuation of the following function (sometimes called the reduced resolvent):

$$\frac{1}{\eta(z)} := \langle 1 | \frac{1}{H - zI} | 1 \rangle, \qquad (27)$$

with

$$\eta(z) = z - \omega_0 - \lambda^2 \int_0^\infty \frac{|f(\omega)|^2}{z - \omega} d\omega.$$
(28)

The function $\eta(z)$ is analytic on the complex plane except for a branch cut on the positive semiaxis $[0, \infty)$, with no zeroes. It admits an analytic continuation through the cut, both from above to below or from below to above, that can be supported by the two sheeted Riemann surface generated by the square root.

The analytic continuation has a pair of complex conjugate zeroes located at the following points:

$$z_R = \omega_0 + \lambda^2 \int_0^\infty \frac{|f(\omega)|^2}{z_R - \omega + i0} \, d\omega = \omega_0 + \lambda^2 \int_0^\infty \frac{|f(\omega)|^2}{\omega_0 - \omega + i0} \, d\omega + o(\lambda^4) \,, \quad (29)$$

$$z_{R}^{*} = \omega_{0} + \lambda^{2} \int_{0}^{\infty} \frac{|f(\omega)|^{2}}{z_{R} - \omega - i0} \, d\omega = \omega_{0} + \lambda^{2} \int_{0}^{\infty} \frac{|f(\omega)|^{2}}{\omega_{0} - \omega - i0} \, d\omega + o(\lambda^{4}) \,. \tag{30}$$

The meaning of $\pm i0$ in the denominator is the usual in the theory of distributions [32]. These zeroes are poles of $\eta^{-1}(z)$ and consequently show the existence of a resonance. Note on the dependence on the coupling constant λ of the resonance poles of the reduced resolvent. If $\lambda \mapsto 0$, then, both resonance poles go to ω_0 the eigenvalue of H_0 . The usual interpretation says that as the consequence of the interaction, the bound state of H_0 becomes unstable and as a result it is a resonance with resonance poles as in (29)–(30).

On the spaces Φ^+ and Φ^- as in (17), respectively, the growing and decaying Gamow vectors are functionals that can be written explicitly as

$$|\psi^D\rangle = |1\rangle + \int_0^\infty \frac{\lambda f(\omega)}{z_R - \omega + i0} |\omega\rangle d\omega, \qquad (31)$$

$$|\psi^{G}\rangle = |1\rangle + \int_{0}^{\infty} \frac{\lambda f(\omega)}{z_{R}^{*} - \omega - i0} |\omega\rangle d\omega.$$
(32)

In addition, the Hamiltonian admits respective diagonalizations as operators on $\mathcal{L}\{\Phi^-, (\Phi^+)^{\times}\}\)$ and $\mathcal{L}\{\Phi^+, (\Phi^-)^{\times}\}\)$, where $\mathcal{L}\{\Phi, \Psi\}\)$ is the space of continuous operators from the locally convex space Φ into the locally convex space Ψ , of the following form (on the duals $(\Phi^{\pm})^{\times}$ we consider the weak topology):

$$H = z_R |\psi^D\rangle \langle \psi^G | + \text{background}, \qquad (33)$$

$$H = z_R^* |\psi^G\rangle \langle \psi^D| + \text{background}.$$
(34)

The word background here denotes an integral term, which physically would correspond to the existence of the background part.

Finally, we remark that objects like Møller wave operators and the S-matrix exist for the Friedrichs model. See [31]. Poles of the S-matrix coincide with the resonance poles obtained by the method of the resolvent.

5.1.1. Double resonances. Causality conditions do not forbid the existence of resonance poles with multiplicity bigger than one. Assume for instance the existence of a resonance represented by a pair of complex conjugate poles of the analytic extension of the S-matrix S(E). In this case, the decaying state as in (11) should be written as [33]

$$\psi^{-} = |\text{bgk}\rangle + \sum_{k=0}^{N-1} c_k |\psi_k^D\rangle.$$
(35)

The first term of the sum in (35) (excluding $|bgk\rangle$) is nothing else than the previously defined Gamow vector $|\psi_0^D\rangle = |\psi^D\rangle$. Thus, the vectors in the sum in (35) are functionals on Φ^- and satisfy the condition

$$H|\psi_k^D\rangle = z_R|\psi_k^D\rangle + k|\psi_{k-1}^D\rangle, \quad k = 0, 1, \dots, N-1.$$
 (36)

Vectors $|\psi_k^D\rangle$ are the Gamow vectors for multiple pole (degenerated) resonances, also called Jordan–Gamow vectors [5]. We can project the extension to $(\Phi^-)^{\times}$ of H to the Nth-dimensional subspace of $(\Phi^-)^{\times}$ spanned by these vectors. In the basis given by the Jordan–Gamow vectors the restriction of the Hamiltonian has a typical Jordan block form:

$$H = \begin{pmatrix} z_R & 1 & 0 & \dots & 0 \\ 0 & z_R & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & 1 \\ 0 & 0 & 0 & \dots & z_R \end{pmatrix}$$
(37)

and the time evolution e^{-itH} is the corresponding exponentiation of -itH with H as in (37).

In the Friedrichs model, we can produce a resonance characterized by a pair of double poles. To do it, we need a clever choice of the form factor. This is [33]:

$$f(\omega) := \frac{\sqrt{\omega}}{P(\omega)}, \quad P(\omega) = (\omega - \alpha)(\omega - \alpha^*).$$
(38)

In this case, the Gamow–Jordan vectors are given by: $|\psi^D\rangle$ as in (31) and

$$|\psi_1^D\rangle = -\int_0^\infty \frac{f(\omega)}{(z_R - \omega + i0)^2} |\omega\rangle \, d\,\omega\,. \tag{39}$$

Other models showing a resonance with a double pole are the following: 1. The following Hamiltonian on $L^2(\mathbb{R})$ [34]:

$$H = -\frac{d^2}{dx^2} + \frac{\pi}{\alpha} \,\delta(x-a) + \frac{\pi}{\beta} \,\delta(x-b)\,. \tag{40}$$

2. The following Hamiltonian on $L^2(\mathbb{R}^+)$, i.e., the potential is infinite for $x \leq 0$ [35]:

$$H = -\frac{d^2}{dx^2} + \alpha \,\delta(x-a) + \beta \,\delta(x-b), \quad \alpha, \beta, a, b > 0.$$

$$\tag{41}$$

The double pole of the analytic continuation of S(E) can be found for some values of the constants a, b, α and β only [34, 35].

5.2. A one-dimensional model

An interesting one-dimensional model with resonances having a great richness of features is the half oscillator with a point potential at the origin and possibly a mass jump at the same point. In principle, the interest of this model was essentially pedagogical with the presence of an infinite number of resonances that under certain limit process (the coefficient of a delta perturbation at the origin going to the infinity) become the odd bound states of the harmonic oscillator [36]. In addition, this model has well-defined *S*-matrix, scattering operators, transmission and reflections coefficients, etc. However, its particular interest lies on the

presence of some unexpected features [37], which opens the interest for the search for resonance models with unusual behavior.

The Hamiltonian for the model under consideration is the following:

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_1(x) + V_2(x)$$
(42)

with

$$V_1(x) := \begin{cases} \frac{1}{2} m\omega^2 x^2 & \text{if } x < 0\\ 0 & \text{if } x > 0 \end{cases}, \qquad V_2(x) = a\delta(x) + b\delta'(x). \tag{43}$$

In order that Hamiltonian (42) be well defined and self adjoint, we need to resort to the theory of self-adjoint extensions of symmetric operators with equal deficiency indices [15], according to which we need to construct the domain of the operator. In our case, this construction should include functions that have a jump at the origin. This mass jump cannot be arbitrary, but in any case, we should give a prescription that define the products of $\delta(x)$ and $\delta'(x)$ with functions showing a discontinuity at the origin. Let us write the solutions of the corresponding Schrödinger equation as $\psi(x) = \psi_1(x)H(-x) + \psi_2(x)H(x)$, where H(x) is the Heaviside step function. Then, this prescription for an arbitrary function $\psi(x)$ is

$$\delta(x)\psi(x) = \frac{\psi_1(0) + \psi_2(0)}{2} \,\delta(x)\,,\tag{44}$$

$$\delta'(x)\psi(x) = \frac{\psi_1(0) + \psi_2(0)}{2} \,\delta'(x) - \frac{\psi_1'(0) + \psi_2'(0)}{2} \,\delta(x) \,. \tag{45}$$

Note that these products coincide with the usual ones when both $\psi(x)$ and its derivative $\psi'(x)$ are continuous at the origin. The resulting Schrödinger equation is then an equation for distributions.

The domain of self-adjointness of the Hamiltonian (42) is the space of functions $\psi(x) = \psi_1(x)H(-x) + \psi_2(x)H(x)$ in the Sobolev space $W_2^2(\mathbb{R}\setminus\{0\})$ with the additional condition $(\hbar = 1)$

$$\begin{pmatrix} \psi_2(0) \\ \psi_2'(0) \end{pmatrix} = \begin{pmatrix} \frac{1+mb}{1-mb} & 0 \\ \frac{2ma}{1-m^2b^2} & \frac{1-mb}{1+mb} \end{pmatrix} \begin{pmatrix} \psi_1(0) \\ \psi_1'(0) \end{pmatrix}$$
(46)

Although these matching conditions do not apply in the case $b = \pm 1/m$, selfadjoint extensions can be defined for this particular case [37].

In order to obtain the resonances, we use the earlier mentioned method of the purely outgoing boundary conditions, according to which there is no incoming wave, so that it must be equal to zero. This gives a transcendental equation for which the solutions not only give the resonances, but also bound and antibound states. This transcendental equation can be numerically solved, after some algebra, with the aid of a package like Mathematica.

A thorough description of the results obtained is reported in [37]. Let us mention here some of the most relevant in order to understand the interest of the model. In absence of a mass jump at the origin:

- 1. There are a countably infinite number of resonances even in the absence of any point potential at the origin (in this case $V_2(x) \equiv 0$). When we switch on $V_2(x) = a\delta(x)$, all resonances save for one, have a smaller imaginary part (higher mean life) no matter if a is either positive or negative. For a > 0, it appears an extra resonance (which did not exist for $V_2(x) \equiv 0$) which does not follow the general pattern. When a is very small and goes to zero, its real and imaginary parts go to $+\infty$ and $-\infty$ respectively to disappear in the limit a = 0. For higher values of a, this resonance has the smaller real part and otherwise behaves like the others. Because of the unusual behavior of this resonance, we have named it as the *maverick resonance*. It does not exist for a < 0.
- 2. There exists one and only one bound state for a < 0 and below a certain threshold. Between zero and this threshold, we do not have bound states but instead one and only one antibound state.
- 3. When we switch on the term $b\delta'(x)$, we obtain analogous results except for the limit values $b = \pm 1/m$ where each resonance collapse into a bound state.

In presence of a mass jump at the origin.

- 1. Assume that the mass is m_1 if x < 0 and m_2 if x > 0. Then, the relevant parameter is $r = m_2/m_1$. The maverick resonance still exists, but its presence is only observable near r = 1, i.e., the limit of equal masses. All other features remain essentially equal except one:
- 2. There are two critical points for b, which are b = -1/r and b = -(1+r)/2. When the value of b lies on one of these two critical points, all resonances collapse into bound states. If a = 0, the energy of these bound states coincide for both critical points and is given by the even energy levels of the oscillator. If $a \neq 0$, the energy levels corresponding to both critical points are slightly different, but all them have the form A + Bn, where $n = 0, 1, 2, \ldots, B$ is always close to 2 and A depends on a and r.

In general, it is possible to plot the eigenfunctions of the Hamiltonian with complex eigenvalues which are resonance poles, i.e., Gamow vectors. One sees that for large values of x > 0, these eigenfunctions have an approximate exponential grow.

One final remark: Formula (45) shows that the contribution to the potential given by $a\delta'(x)$ behaves like the derivative of the delta. This delta prime perturbation has been given by the particular self-adjoint choice of the Hamiltonian given by the matching conditions (45). It may be surprising to say that the determination of a delta prime type perturbation is not unique. In fact, there are other possible matching conditions determining other self-adjoint determinations of the Hamiltonian that also give a delta prime term. In all cases, the operational behavior of the term $a\delta'(x)$ is the same for functions with continuous derivative at the origin, but the self-adjoint extension that determines this perturbation is different [38, 39].

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