

Green's Functions at Exceptional Points

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Abstract The Green's function is an essential tool for the description of scattering. Spectral singularities such as exceptional points have a very specific effect upon the structure of Green's functions. It is well known that the coalescence of two eigenvalues gives rise to a pole of second order in addition to the usual first order pole. The present paper describes the general patterns of Green's functions at exceptional points of arbitrary order. The higher orders of the pole terms as well as their respective coefficients - being matrices - are presented in terms of the underlying Hamiltonian. For the coalescence of three eigenvalues this appears to be of immediate physical interest while the coalescence of four or more levels is still awaiting experimental realisation in the laboratory.

Keywords Spectral singularities · Green's function

1 Introduction

Spectral singularities associated with a Hamilton operator H are expected to have specific effects upon the Green's function. It is defined by

$$G(E) = (E I - H)^{-1}$$

with I being the identity. The well known singularities of $G(E)$ are of course first order poles which correspond to solutions of the Schrödinger equation with the boundary conditions of purely outgoing waves. In the present context we will not touch upon the continuous spectrum of H and branch points of $G(E)$ associated with it. Physically, the poles correspond to bound states (usually, or rather conventionally, at negative energies) and to resonances when they occur in the second Riemann sheet in the lower complex energy

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plane. While these are well established facts from scattering theory [1] (see also [2]) there are spectral singularities of a different nature that have distinctly different effects upon the singularity structure of the Green's function. As a consequence, there can be dramatic physical effects in a great variety of phenomena. It is the *exceptional points* (EPs) that give rise to special physical effects associated with particular singularities of the Green's function (see for instance [3]).

For reader's convenience we present a short resumé about EPs in the following section. Here we mention that it is well known [4] that the Green's function has a pole of second order in addition to the usual first order pole at the simplest EP where two levels coalesce. When a cross section is obtained from the square of the modulus of the scattering function $T(E) = V + VG(E)V$ the interference of the first and second order pole term can invoke specific effects; this has been used in a recent paper [5] to explain resonance shape asymmetries familiar from Fano-Feshbach resonances in atomic and nuclear physics.

In the present paper we derive a general expression for the Green's function at an EP of arbitrary finite order. The occurrence of an EP3 (three coalescing levels) seems to be of topical interest: it has been encountered in specific non-linear problems [6] and also suggested for three coupled wave guides [7]. With increasing sophistication of experimental techniques higher order EPs may become within reach in the laboratory.

So far we did not specify a particular Hamiltonian to which the Green's function is referring. In fact, at an EP the particular physical problem has always the same mathematical structure depending only on the order of the EP. Moreover, while a Green's function, like the Hamiltonian, appears usually as an infinite dimensional matrix or, for $G(E)$, as an integral operator, at an EP it can be reduced to a finite dimensional matrix with the dimension given by the order of the EP. This is clarified in the following section.

The derivation presented here is aimed at physicists. Similar results have been reported in recent mathematical textbooks about linear operators and treating in particular resolvents of non-hermitian operators (see for instance [8, 9]).¹ An even older treatise [10] gives an explicit expression resembling our result. However, it is felt that our derivation has a special appeal to physicists as it does not follow the strictly formal pattern used in the Mathematics literature but rather uses the parallel between energy and time domain of propagators (Green's functions).

2 Exceptional Points

Whenever an eigenvalue problem depends on a parameter λ there are generically specific parameter values, usually complex, where two eigenvalues coalesce. In contrast to a degeneracy of eigenvalues being associated to a higher dimensional eigenspace, a coalescence is characterised by a simultaneous coalescence of the corresponding eigenvectors. Moreover, the norm of the one eigenvector vanishes which is sometimes referred to as 'self-orthogonality' [11]. At these specific points a matrix eigenvalue problem yields a matrix that cannot be diagonalised. They have been dubbed *exceptional points* in a textbook by Kato [12]. These singularities can occur only for non-hermitian operators; note, however, that genuine degeneracies can also occur for non-hermitian operators.

¹I am indebted to Dr Uwe Guenther who pointed out to me these references

At the EPs the coalescing eigenvalues have an algebraic singularity: it is a square root branch point as a function of the parameter λ under consideration. Formally there is the expansion

$$E_{1,2}(\lambda) = E_{EP} \pm \text{const.}\sqrt{\lambda - \lambda_{EP}} + \dots$$

As stated above, the Green’s function acquires an additional pole of second order at the EP [3, 4]. Here we mention that the square root singularity, that is the Riemann sheet structure, has been shown experimentally to be a physical reality [13, 14], and more recently in an experiment including time reversal symmetry breaking [15] (see also [16]).

In the vicinity of an EP a high (or infinite) dimensional problem can be reduced to an effective two-dimensional problem owing to the vanishing of the norm of the coalescing eigenvectors. This can be understood from the spectral representation which reads for H

$$H = \sum_n E_n \frac{|\psi_n^r\rangle\langle\psi_n^l|}{\langle\psi_n^l|\psi_n^r\rangle} \tag{1}$$

where we distinguish between left hand and right hand eigenvectors as H is not necessarily hermitian or complex symmetric.² When approaching an EP where the two levels $E_{n_{EP}}$ and $E_{n_{EP}+1}$ coalesce, the vanishing of the denominator outweighs all other terms. In other words, when the parameter for which the EP occurs, is in close vicinity of the branch point, H can be represented by an effective two-dimensional matrix. However, there is a *caveat*: if a further EP occurs in close vicinity of the EP under consideration on one of its two sheets, the simple reduction to a two-dimensional problem cannot work (see also [17]).

Actually, for the situation just described, a three dimensional matrix would be needed. In fact, if additional parameters are at one’s disposal, one can choose them such that the two EPs lying near to each other merge into the coalescence of two simple EPs that share a Riemann sheet; it is equivalent to the coalescence of three energy levels denoted by EP3 in [18]. As stated in the Introduction situations of this kind have been encountered in particular non-linear problems [6] and suggested for wave guides [7]. In principle, such generalisation can be spun further and extended to the coalescence of arbitrary order. Obviously, for an EPN (N coalescing levels) an N -dimensional matrix is needed. In fact, at the EPN the Jordan normal form of the reduced Hamiltonian has the structure of the N -dimensional matrix, *viz.*

$$H_{EPN} = S \begin{pmatrix} E_{EP} & 1 & & 0 \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ 0 & & & E_{EP} \end{pmatrix} S^{-1} \tag{2}$$

where the matrix S specifies the particular Hamiltonian considered. Note that (2) is the minimal form that a Hamiltonian can assume at an EPN.

The following section presents the form of the Green’s function for an EP of arbitrary order. To ease the derivation we first restrict ourselves to an EP4 from which the generalisation to arbitrary N becomes obvious.

²As our interest is focussed on EPs the continuous spectrum is not explicitly indicated.

3 Green’s Function

Similar to (1) there is a representation for the Green’s function which reads

$$G(E) = \sum_n \frac{1}{E - E_n} \frac{|\psi_n^r\rangle \langle \psi_n^l|}{\langle \psi_n^l | \psi_n^r \rangle}. \tag{3}$$

However, for our purpose this form turns out to be rather tedious to be handled at an EP of higher order than two. In fact, when an EPN is approached by the parameter $\lambda \rightarrow \lambda_{EPN}$ there are N vanishing denominators each with a leading term behaving as $\sim (\lambda - \lambda_{EPN})^{\frac{N-1}{N}}$ [18]. Note also that the N levels are connected a follows

$$E_{1,\dots,N} = E_{EPN} + \text{const.} \sqrt[N]{\lambda - \lambda_{EPN}} + \dots$$

with the N levels lying on the N different sheets of the N -th root. Instead of engaging in the tedious analysis of (3) when $\lambda \rightarrow \lambda_{EPN}$ – note that the N terms tending to infinity have to conspire in subtle cancellations to yield the final result – it is more transparent to use the Fourier transform $\tilde{G}(t)$ of $G(E)$ at the EP. For easy presentation we demonstrate the procedure for $N = 4$.

At the EP4 we may represent the Hamiltonian as well as its Green’s function by a four dimensional matrix. To obtain the Green’s function (propagator) in the time domain we have to solve the ordinary differential equation

$$i \frac{d}{dt} |\phi\rangle = H |\phi\rangle \tag{4}$$

where H has now the form

$$H = S J S^{-1} \tag{5}$$

with

$$J = \begin{pmatrix} E_{EP} & 1 & 0 & 0 \\ 0 & E_{EP} & 1 & 0 \\ 0 & 0 & E_{EP} & 1 \\ 0 & 0 & 0 & E_{EP} \end{pmatrix}. \tag{6}$$

Since the matrix S is time independent (4) reduces to

$$i \frac{d}{dt} |\chi\rangle = J |\chi\rangle \quad \text{with} \quad |\phi\rangle = S |\chi\rangle \tag{7}$$

which is solved by

$$|\chi(t)\rangle = g(t) |\chi(0)\rangle \tag{8}$$

with the time dependent restricted Green’s function at the EP4

$$g(t) = \begin{pmatrix} 1 & it & -\frac{t^2}{2} & -i\frac{t^3}{6} \\ 0 & 1 & it & -\frac{t^2}{2} \\ 0 & 0 & 1 & it \\ 0 & 0 & 0 & 1 \end{pmatrix} \exp(-i E_{EP} t). \tag{9}$$

The full Green’s function is thus given by

$$\tilde{G}(t) = S g(t) S^{-1} \tag{10}$$

and the solution of (4) reads

$$|\phi(t)\rangle = \tilde{G}(t) |\phi(0)\rangle.$$

Our aim is focussed upon $G(E)$. It is now rather straightforward using (9) and (10) to perform the Fourier transform in reverse from the time to the energy domain. In fact, the matrix in (9) has the powers $(it)^k$ nicely arranged with $k = 0$ being the main diagonal, $k = 1$ being the side diagonal and so forth. Furthermore we observe the identities (denoting by I the identity matrix)

$$\begin{aligned}
 J - E_{EP} I &= \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\
 (J - E_{EP} I)^2 &= \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\
 (J - E_{EP} I)^3 &= \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.
 \end{aligned}$$

Multiplying these identities from the left by S and from the right by S^{-1} changes the matrix J into H . We read off the coefficients (matrices) of the powers $(it)^k$ for $\tilde{G}(t)$: for $k = 0$ it is the unit matrix, for $k \neq 0$ it is $(H - E_{EP} I)^k/k!$. For the Fourier transform we employ the usual rule

$$(it)^k \rightarrow \frac{d^k}{dE^k}$$

to obtain the final result

$$G(E) = \frac{I}{E - E_{EP}} + \frac{M_2}{(E - E_{EP})^2} + \frac{M_3}{(E - E_{EP})^3} + \frac{M_4}{(E - E_{EP})^4} \tag{11}$$

where $M_k = (H - E_{EP} I)^{k-1}$. Note that the matrix rank of M_k is $4 - (k - 1)$, in particular the rank of M_4 - the coefficient (matrix) of the fourth order pole - is unity. In fact, it is straightforward to show that

$$M_4 = |\psi_{EP4}^r\rangle\langle\psi_{EP4}^l|$$

being the dyadic product of the one (and only one) eigenstate of H at the EP4. Note that the scalar product $\langle\psi_{EP4}^l|\psi_{EP4}^r\rangle$ vanishes.

The generalisation is obvious. At an EPN the Green's function reads:

$$G(E) = \frac{I}{E - E_{EP}} + \frac{M_2}{(E - E_{EP})^2} + \dots + \frac{M_N}{(E - E_{EP})^N}, \tag{12}$$

where the matrix rank of $M_k = (H - E_{EP} I)^{k-1}$ is $N - (k - 1)$ and that of $M_N = |\psi_{EPN}^r\rangle\langle\psi_{EPN}^l|$ is unity.

4 Summary

It has been demonstrated that using the Green's function in the time domain is a transparent procedure to obtain the Green's function and from it its Fourier transform $G(E)$. A direct approach starting from $G(E)$ would, in contrast, be rather cumbersome. At an EPN, an

exceptional point where N levels coalesce, the Green's function $G(E)$ turns out to be a sum of pole terms of the order 1 to N with coefficients – being N -dimensional matrices – given as polynomials of the underlying Hamiltonian. The result has turned out to be of physical relevance for $N = 2$, where the result has been known before, and is expected to be of physical interest for higher orders such as $N = 3$ and $N = 4$.

We refrain from extending the result to $N \rightarrow \infty$ without further scrutiny. In fact, the convergence of (12), when the limit $N \rightarrow \infty$ is considered, is expected to depend on the particular form of H . Also, as this question does not appear to be of particular physical interest we leave this question to a more mathematically minded audience. We note, however, that a very special many body problem can give rise to an exceptional point of infinite order in the limit $N \rightarrow \infty$ but only for a specific interaction of rank unity [19]. Recently, EPs of a variety of N -dimensional matrix models have been studied with an emphasis on large values of N [20].

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