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Unfolding a diabolic point: a generalized crossing scenario

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Abstract

The typical avoided crossings for Hermitian quantum systems depending on parameters, the diabolic crossing scenario, are generalized to the non-Hermitian case, e.g. for resonances. Two types of crossings appear: for type I, the real parts show an avoided and the imaginary parts a true crossing of the eigenenergies, and for type II the opposite is found. A simple symmetric non-Hermitian two-state matrix Hamiltonian is analysed in detail. The diabolic point bifurcates into two exceptional ones on exceptional lines where the matrices are defective. The adiabatic transport of eigenvectors and eigenstates in parameter space is discussed in this generalized diabolic crossing scenario, in particular the geometric Berry phases for a cyclic variation of system parameters, depending on the topology of the closed curves with respect to the exceptional lines.

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1. Introduction

In quantum mechanics, many dynamical processes are described by (avoided) level crossings. Typically they appear in the form of a (Hermitian) matrix Hamiltonian, where the matrix elements depend on parameters, $\mathbf{c} = (c_1, c_2, \ldots)$, e.g. on the internuclear distance for electronic transitions in atom–atom interactions, which can be considered as slowly varying in time. The instantaneous eigenvalues show the familiar avoided level crossings when a single parameter is varied. True crossings require the variation of more parameters, two in the case of 2×2 matrices, which constitutes the celebrated diabolic crossing scenario of the levels $\mathcal{E}_\pm$ analysed in the following.

Recently, avoided crossing phenomena of quantum eigenvalues and eigenstates well known from Hermitian Hamiltonians have been extended to the non-Hermitian case. Here, novel effects have been found, which attracted considerable theoretical [1–5] and (very recently) also experimental interest [6, 7]. Such non-Hermitian systems appear quite naturally in different situations, in particular for resonance states in open quantum systems.

(i) It has been shown—mainly in a semiclassical context—that the transitions induced between the states can be described by an analytic continuation into the complex parameter space. For a complex value of a single parameter, the levels can actually cross, $\mathcal{E}_+(c_\mathrm{x}) = \mathcal{E}_-(c_\mathrm{x})$, at critical values $c_\mathrm{x} \in \mathbb{C}$, the so-called Kohn branch points [8]. Such critical crossing points will appear as *exceptional points* in the following and play an important role in the dynamics. The semiclassical approach treats the transition in terms of complex-valued paths encircling the complex crossing points ending up on the excited level, i.e. the upper Riemann sheet of the complex eigenvalue surface (see, e.g., [9–11] and references therein) and the transition amplitudes can be described by the integral

$$\oint \mathcal{E}(c)\,\mathrm{d}c \tag{1}$$

for a closed integration path encircling the branch points.

(ii) In the case of an open system, the (coupled) states can be expressed in a basis of resonance states. In this case the levels are complex from the onset, i.e. $\mathcal{E}_j = E_j - \mathrm{i}\Gamma_j/2$ where the Γ_j are the decay rates. In most applications, the Hamiltonian matrix can be chosen in a symmetric representation.

(iii) Non-Hermitian matrices arise also from resonance boundary conditions, e.g. purely outgoing or incoming asymptotics. The same is true for the case of complex scaling techniques for resonance calculations [12], where the coordinates or parameters are rotated into the complex plane. Also in such applications, one chooses a complex symmetric matrix representation [13]. In this context it has been shown that the Hamiltonian $H = V + \eta T$, where V and T are non-commuting symmetric matrices, is defective for a parameter $\eta \in \mathbb{C}$ [14] (see also [5]; a recent application to resonances in molecules can be found in [15]).

Not surprisingly, the crossing scenario for non-Hermitian matrices is richer than diabolic avoided crossings for the Hermitian case. In particular, a different crossing type, a *type II* crossing, arises, which complements the *type I* crossings already familiar from the Hermitian case. A discussion of type II crossings of resonance eigenvalues can be found in a theoretical analysis of Wannier–Stark systems [16, 17] (see also [18] for more recent references) and can also be detected in the very different studies of resonances, such as for example in biased multiple quantum wells [19] or predissociation of HNO molecules [20]. It turns out, that the global crossing scenario is determined by the positions of the exceptional points in parameter space. In addition to the different behaviour of the energy levels, also the eigenvectors show novel effects related to the geometry of the paths traced out by the system parameters in relation to the exceptional points [3–7]. Recently, the phenomena related to the behaviour of the resonance eigenstates have been observed experimentally for microcavity modes [6, 7]. Because of its generality, it can be expected to appear in many other systems.

The occurrence of crossings in the energy levels is connected to the topic of geometrical phases. The notion of a geometrical phase was first introduced by Berry [21] in the context of adiabatic evolution of a system described by a parameter-dependent Hermitian Hamiltonian. Varying the parameters along a closed curve, the propagated state acquires in addition to the dynamical phase a geometrical one, which depends only on the topological properties of the parameter curve, which is nowadays denoted as the Berry phase.

Berry phases have also been considered for non-adiabatic time evolution [22, 23]. The assumption of a Hermitian system has also been dropped [1, 2]. Geometrical decay rates have been discussed in [24, 25]. A generalization to non-cyclic evolution of the initial state can be found in [26]. A first discussion of Berry phases of symmetric matrices is given in [3–5].

The structure of the paper is as follows. We start with an introduction to cyclic evolution in non-Hermitian systems (section 2). Afterwards, we discuss the different crossing scenarios observed in these systems and their influence on the adiabatic evolution of eigenstates (section 3). Furthermore, the behaviour of the eigenvalues is considered. We conclude with section 4.

2. Non-Hermitian cyclic evolution

In this paper, we consider a setup described in almost all works on Berry phases, emphasizing the points essential for the non-Hermitian case. The discussion in this section is based on a previous work by Mondragón and Hernández [2], where more details can be found.

We consider a quantum system described by the parameter-dependent Hamiltonian $H(\mathbf{c}(t))$. The parameters $\mathbf{c}(t) = (c_1(t), \ldots, c_p(t))$ are functions of the time t, which leads to an implicit time dependence of $H(\mathbf{c}(t))$. We consider the behaviour of the solutions of the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H(\mathbf{c}(t))|\psi(t)\rangle \tag{2}$$

for an adiabatic variation of the parameters. In the present case the Hamiltonian is not necessarily Hermitian; we assume, however, that the spectrum is discrete and, in order to avoid complications unnecessary for the present purpose, we will assume that the system Hamiltonian is already given by a finite matrix representation in a basis which takes care of the boundary conditions leading to a non-Hermitian matrix. As an example, one may consider resonance (Siegert) boundary conditions.

It is convenient to base the analysis on the instantaneous eigenstates $|\varphi_n(\mathbf{c})\rangle$ of the Hamiltonian,

$$H(\mathbf{c})|\varphi_n(\mathbf{c})\rangle = E_n(\mathbf{c})|\varphi_n(\mathbf{c})\rangle \tag{3}$$

together with the eigenstates $|\chi_n(\mathbf{c})\rangle$ of the adjoint operator $H^\dagger(\mathbf{c})$,

$$H^\dagger(\mathbf{c})|\chi_n(\mathbf{c})\rangle = E_n^*(\mathbf{c})|\chi_n(\mathbf{c})\rangle. \tag{4}$$

Because of

$$\langle\chi_n(\mathbf{c})|H(\mathbf{c}) = \langle\chi_n(\mathbf{c})|E_n(\mathbf{c}) \tag{5}$$

the two sets of states are often denoted as right and left eigenstates of H. Note that, in general, both types of states define a non-orthogonal basis. However, the two sets are orthogonal to each other,

$$\langle\chi_n(\mathbf{c})|\varphi_m(\mathbf{c})\rangle = 0 \qquad \text{for} \quad E_n \neq E_m \tag{6}$$

i.e. they form a bi-orthogonal basis [27]. The convenient normalization

$$\langle\chi_m(\mathbf{c})|\varphi_n(\mathbf{c})\rangle = \delta_{mn} \tag{7}$$

used in the following requires $\langle\chi_n(\mathbf{c})|\varphi_n(\mathbf{c})\rangle \neq 0$, which can actually be violated with serious consequences for the global behaviour of the states on parameter space. We will return to this later in this paper.

Two special cases are often encountered in applications:

(a) For a *Hermitian* Hamiltonian, $H = H^\dagger$, the eigenvalues E_n are real, the eigenstates $|\chi_n\rangle$ and $|\varphi_n\rangle$ coincide and (7) agrees with the well-known orthonormality relation.

(b) For a *symmetric* Hamiltonian, $H = H^{\mathrm{t}}$, we have $H^{\dagger} = H^{*}$ with the consequence that the complex conjugate of an eigenstate $|\varphi_n\rangle$ of H is an eigenstate of $H^{\dagger}$, i.e. the left eigenstates can be chosen as

$$|\chi_n(\mathbf{c})\rangle = |\varphi_n^*(\mathbf{c})\rangle \tag{8}$$

which reduces to the common choice of real eigenstates if the Hamiltonian is also Hermitian (i.e. real).

If the bi-orthogonal states are chosen as (8) and normalized as (7), then each pair of the basis states is fixed by these conditions up to a common sign and not a phase factor as usual. In addition, it should be pointed out that in the symmetric case with the choice (8) of the left eigenstates the normalization (7) appears as

$$\langle\varphi_m^*(\mathbf{c})|\varphi_n(\mathbf{c})\rangle = \delta_{mn}. \tag{9}$$

This should not, however, be misinterpreted as a special scalar product as, e.g., the c-product [12, 28, 29], and we stress that here we use the familiar scalar product of quantum mechanics throughout.

In the next section, we will confine ourselves to a detailed discussion of the symmetric case. Here, however, the Hamiltonian can still be general. Expanding the state into the instantaneous (right) eigenstates

$$|\psi(t)\rangle = \sum_n a_n(t)|\varphi_n(\mathbf{c}(t))\rangle \tag{10}$$

and projecting onto the left eigenstate $|\chi_m\rangle$ yields

$$\frac{\mathrm{d}}{\mathrm{d}t}a_m(t) + \sum_n \langle\chi_m|\nabla_{\mathbf{c}}\varphi_n\rangle \cdot \frac{\mathrm{d}\mathbf{c}(t)}{\mathrm{d}t}a_n(t) = -\frac{\mathrm{i}}{\hbar}E_m(t)a_m(t) \tag{11}$$

where the normalization (7) has been used and the instantaneous eigenstates are assumed to be differentiable with respect to the parameters $\mathbf{c}$.

Following the adiabatic approximation scheme (for a recent discussion of the non-Hermitian case see [30]), the non-diagonal terms are neglected and the decoupled differential equations have the solution

$$a_n(t) = \exp\left\{-\frac{\mathrm{i}}{\hbar}\int_0^t E_n(t')\mathrm{d}t' + \mathrm{i}\gamma_n(t)\right\} a_n(0) \tag{12}$$

where the exponential contains a dynamical part $\int_0^t E_n(t')\,\mathrm{d}t'$, and

$$\gamma_n(t) = \mathrm{i}\int \langle\chi_n|\nabla_{\mathbf{c}}\varphi_n\rangle \cdot \frac{\mathrm{d}\mathbf{c}(t)}{\mathrm{d}t}\,\mathrm{d}t = \mathrm{i}\int_{\mathbf{c}}\langle\chi_n|\nabla_{\mathbf{c}}\varphi_n\rangle \cdot \mathrm{d}\mathbf{c} \tag{13}$$

is a geometric phase. If the system is initially in an eigenstate

$$|\psi(0)\rangle = |\varphi_n(\mathbf{c}(0))\rangle \tag{14}$$

the adiabatic time evolution is then given by

$$|\psi(t)\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_0^t E_n(t')\mathrm{d}t'}\mathrm{e}^{\mathrm{i}\gamma_n(t)}|\varphi_n(\mathbf{c}(t))\rangle. \tag{15}$$

Let us consider a cyclic state evolution, i.e. an adiabatic transport of an eigenstate $|\psi(0)\rangle = |\varphi_n(\mathbf{c}(0))\rangle$ along a closed curve. Assuming that the state returns to its initial state after a time T up to a prefactor, it can be written as [21]

$$|\psi(T)\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_0^T E_n(t')\mathrm{d}t'}\mathrm{e}^{\mathrm{i}\gamma_n^B}|\varphi_n(\mathbf{c}(0))\rangle. \tag{16}$$

Here, γ_n^B is the geometric Berry phase, which is, however, complex valued in the non-Hermitian case considered here. Comparing with (15) we have

$$\gamma_n^B = \gamma_n(T) + \lambda_n(T) \tag{17}$$

with

$$\mathrm{e}^{\mathrm{i}\lambda_n(T)} = \langle \chi_n(\mathbf{c}(0))|\varphi_n(\mathbf{c}(T))\rangle. \tag{18}$$

Note that after the time T, the transported basis need not necessarily reproduce itself (compare for example equation (19)) which leads to a non-vanishing $\lambda_n(T)$.

It is instructive to check explicitly that the phase term γ_n^B is well defined, i.e. independent of the scale factor of the chosen basis states. In a scaled basis

$$|\tilde{\varphi}_n(t)\rangle = \theta_n(\mathbf{c}(t))|\varphi_n(t)\rangle \qquad \langle\tilde{\chi}_n(t)| = \frac{1}{\theta_n(\mathbf{c}(t))}\langle\chi_n(t)| \tag{19}$$

which conserves the normalization (7), the time-evolved state reads

$$|\psi(T)\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_0^T E_n(t')\mathrm{d}t'}\mathrm{e}^{\mathrm{i}\tilde{\gamma}_n(T)}|\tilde{\varphi}_n(\mathbf{c}(T))\rangle \tag{20}$$

with

$$\tilde{\gamma}_n(T) = \mathrm{i}\int_0^T \langle\tilde{\chi}(\mathbf{c}(t))|\nabla_{\mathbf{c}}\tilde{\varphi}_n(\mathbf{c}(t))\rangle \cdot \frac{\mathrm{d}\mathbf{c}(t)}{\mathrm{d}t}\,\mathrm{d}t. \tag{21}$$

Consequently, we have

$$\begin{aligned}\mathrm{e}^{\mathrm{i}\lambda_n(T)} &= \langle\chi_n(\mathbf{c}(0))|\varphi_n(\mathbf{c}(T))\rangle \\ &= \frac{\theta_n(\mathbf{c}(0))}{\theta_n(\mathbf{c}(T))}\langle\tilde{\chi}_n(\mathbf{c}(0))|\tilde{\varphi}_n(\mathbf{c}(T))\rangle = \frac{\theta_n(\mathbf{c}(0))}{\theta_n(\mathbf{c}(T))}\,\mathrm{e}^{\mathrm{i}\tilde{\lambda}_n(T)}\end{aligned} \tag{22}$$

and the Berry phase is

$$\begin{aligned}\gamma_n^B &= \tilde{\gamma}_n(T) + \tilde{\lambda}_n(T) \\ &= \mathrm{i}\int_0^T \langle\tilde{\chi}_n(\mathbf{c}(t))|\nabla_{\mathbf{c}}\tilde{\varphi}_n(\mathbf{c}(t))\rangle \cdot \frac{\mathrm{d}\mathbf{c}(t)}{\mathrm{d}t}\,\mathrm{d}t + \tilde{\lambda}_n(T) \\ &= \mathrm{i}\int_0^T \frac{1}{\theta_n(\mathbf{c}(t))}\langle\chi_n(\mathbf{c}(t))|\nabla_{\mathbf{c}}\left[\theta_n(\mathbf{c}(t))\varphi_n(\mathbf{c}(t))\right]\rangle \cdot \frac{\mathrm{d}\mathbf{c}(t)}{\mathrm{d}t}\,\mathrm{d}t + \tilde{\lambda}_n(T) \\ &= \mathrm{i}\int_0^T \langle\chi_n(\mathbf{c}(t))|\nabla_{\mathbf{c}}\varphi_n(\mathbf{c}(t))\rangle \cdot \frac{\mathrm{d}\mathbf{c}(t)}{\mathrm{d}t}\mathrm{d}t + \mathrm{i}\int_0^T \frac{\nabla_{\mathbf{c}}\theta_n(\mathbf{c}(t))}{\theta_n(\mathbf{c}(t))} \cdot \frac{\mathrm{d}\mathbf{c}(t)}{\mathrm{d}t}\,\mathrm{d}t \\ &\quad + \lambda_n(T) - \mathrm{i}\ln\left(\frac{\theta_n(c(T))}{\theta_n(c(0))}\right) = \gamma_n(T) + \lambda_n(T)\end{aligned} \tag{23}$$

which shows that γ_n^B is indeed independent of the scaling.

Choosing an appropriate scaling of the instantaneous basis, it is now possible to express the Berry phase by the geometrical phase $\left(\gamma_n^B = \gamma_n(T)\right)$ or by the phase change $\left(\gamma_n^B = \lambda_n(T)\right)$ of the instantaneous basis state alone. In both cases, the states are required to be differentiable along the circuit in parameter space up to a set of measure zero. If we additionally have $|\varphi_n(\mathbf{c}(T))\rangle = |\varphi_n(\mathbf{c}(0))\rangle$, i.e. if the phase term $\lambda_n(T)$ vanishes, then the Berry phase is given by the term $\gamma_n(T)$ alone. In most applications, however, this is not at all easily realized. Such an explicit assignment of the phase can be circumvented if the integral (13) can be rewritten as a surface integral by means of Stokes theorem [21]. As we will see more clearly in the

following section, this can be difficult or even impossible for non-Hermitian Hamiltonians when certain critical lines are encircled by the integration path [2]. In the case of a symmetric non-Hermitian Hamiltonian, however, the bi-orthogonal instantaneous eigenstates provide a simple requisite for a different phase assignment, using (8) and (9). Differentiation of the orthogonalization relation (9) yields

$$0 = \langle \nabla_{\mathbf{c}} \varphi_n^*(\mathbf{c}) | \varphi_n(\mathbf{c}(t)) \rangle + \langle \varphi_n^*(\mathbf{c}) | \nabla_{\mathbf{c}} \varphi_n(\mathbf{c}) \rangle = 2 \langle \nabla_{\mathbf{c}} \varphi_n^*(\mathbf{c}) | \varphi_n(\mathbf{c}) \rangle \tag{24}$$

i.e. $\gamma_n(T) = 0$, and the Berry phase is solely determined by the phase change of the instantaneous basis state:

$$\gamma_n^B = \lambda_n(T). \tag{25}$$

3. Curve crossings in a two-state system

In many cases of interest, the dynamics is predominantly determined by two states, and the dynamics can be well described by a two-state system. We will therefore study a simple however quite typical two-state model in detail. The matrix representation of the Hamiltonian is given by

$$H = \begin{pmatrix} \epsilon & V \\ V & -\epsilon \end{pmatrix} \tag{26}$$

where V denotes the coupling. The zero point of the energy scale has been chosen in the middle of the uncoupled states. For $\epsilon, V \in \mathbb{R}$ the eigenvalues

$$\mathcal{E}_\pm(\epsilon, \gamma, V) = \pm\sqrt{\epsilon^2 + V^2} \tag{27}$$

of the Hamiltonian are real valued and show a double cone in the space $(\epsilon, V, \mathcal{E}_\pm)$ with a degeneracy at the *diabolic point* $\epsilon = V = 0$. Varying the parameter ϵ for $V \neq 0$, the eigenvalues show the well-known avoided crossing behaviour with a minimum distance $2|V|$ at $\epsilon = 0$. The corresponding eigenstates $\mathbf{u}_\pm$ are orthogonal, because H is Hermitian. Berry [31] analysed a Hermitian extension of this Hamiltonian in detail, i.e. the three-parameter Hamiltonian for the case of a complex-valued coupling $V = x + \mathrm{i}y$,

$$H = \begin{pmatrix} \epsilon & x + \mathrm{i}y \\ x - \mathrm{i}y & -\epsilon \end{pmatrix} \tag{28}$$

where the diabolic crossing scenario survives. Here we will consider a non-Hermitian, symmetric extension of the Hamiltonian (26) modelling a decaying system by allowing the energies on the diagonal to be complex valued. (Note that any matrix can be transformed to the complex symmetric form by a similarity transformation [32].) In most applications the lower state is much more stable than the upper one. Here we assume for simplicity that only the upper state possesses a decay width,

$$H = \begin{pmatrix} \epsilon - 2\mathrm{i}\gamma & V \\ V & -\epsilon \end{pmatrix} \tag{29}$$

with $\epsilon, V, \gamma \in \mathbb{R}$ and $\gamma \geqslant 0$. One can easily show that this models also the general case in which both states can decay.

3.1. Resonance eigenvalues

The eigenvalues

$$\mathcal{E}_\pm(\epsilon, \gamma, V) = -\mathrm{i}\gamma \pm \sqrt{(\epsilon - \mathrm{i}\gamma)^2 + V^2} = E_\pm - \mathrm{i}\Gamma_\pm/2. \tag{30}$$

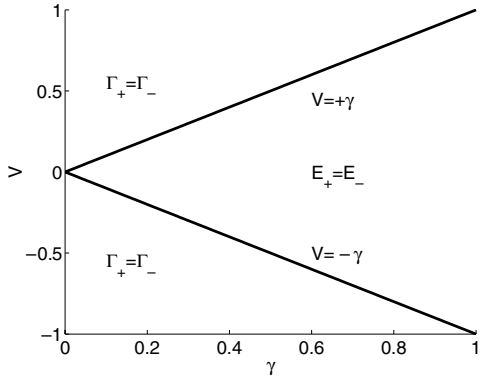

Figure 1. The exceptional lines $V = \pm\gamma$ separate the critical plane $\epsilon = 0$ into regions of type I ($\Gamma_+ = \Gamma_-$) and type II ($E_+ = E_-$) crossings.

of the Hamiltonian (29) are degenerate for real values of the parameters if the conditions

$$\epsilon = 0 \qquad \text{and} \qquad V = \pm\gamma \tag{31}$$

are satisfied. Figure 1 shows the critical plane $\epsilon = 0$ in the three-dimensional parameter space ϵ, V, γ. The critical or *exceptional* lines [3] $V = \pm\gamma$ separate the critical plane into different regions:

(a) For $|V| > \gamma$ the imaginary parts of the eigenvalues coincide, $\Gamma_+ = \Gamma_- = 2\gamma$. The real parts differ by $E_+ - E_- = 2\sqrt{V^2 - \gamma^2}$. We will denote this case as a *type I crossing*.
(b) For $|V| < \gamma$ the real parts of the eigenvalues coincide, $E_+ = E_- = 0$, and the imaginary parts differ, $\Gamma_+ - \Gamma_- = 4\sqrt{\gamma^2 - V^2}$. This case will be denoted as a *type II crossing*.
(c) Along the critical lines $V = \pm\gamma$ we have a full degeneracy, $\mathcal{E}_+ = \mathcal{E}_-$.

In the following, we consider the behaviour of the eigenvalues for a continuous change of the parameters. Varying the system parameters along a curve $\mathbf{c} : t \to \mathbf{c}(t) = (\epsilon(t), \gamma(t), V(t))$ extending from negative values of ϵ to positive ones, this curve will intersect the critical plane $\epsilon = 0$, and we will observe a crossing of type I or II depending on the point of intersection. As an example, figure 2 shows the eigenvalues for $-2 \leqslant \epsilon \leqslant 2, \gamma = 1$ and two values of the coupling, $V = 1.01$ and $V = 0.99$. Note that for $\gamma \neq 0$ we can measure the parameters in units of γ, i.e. we can restrict ourselves to $\gamma = 1$. In the first case, we have the familiar type I crossing, in the second, less familiar case, a type II crossing. Both types of crossings have been observed for realistic Hamiltonians. The first case is found for most curve crossing processes, e.g. in atomic collisions, and reduces to the diabolic crossing scenario in the limit $\gamma \to 0$. The second was discussed in a paper by Avron on Wannier–Stark resonance states [16] and more recently by Grecchi and Sacchetti [17] (see also [18] and references therein).

It may also be of interest to look at the *complex* crossing points of the eigenvalues (30) in the complex ϵ-plane, i.e. the Kohn branch points mentioned in the introduction. They are found at

$$\epsilon_\pm = \mathrm{i}(\gamma \pm V) \tag{32}$$

on the imaginary axis. If the parameter V is changed from $\gamma < |V|$ to $\gamma > |V|$ one of these branch points crosses the real axis for $\gamma = V$ and the crossing type changes from type I to type II (see also [17]). Here, however, we will restrict ourselves to real ϵ values.

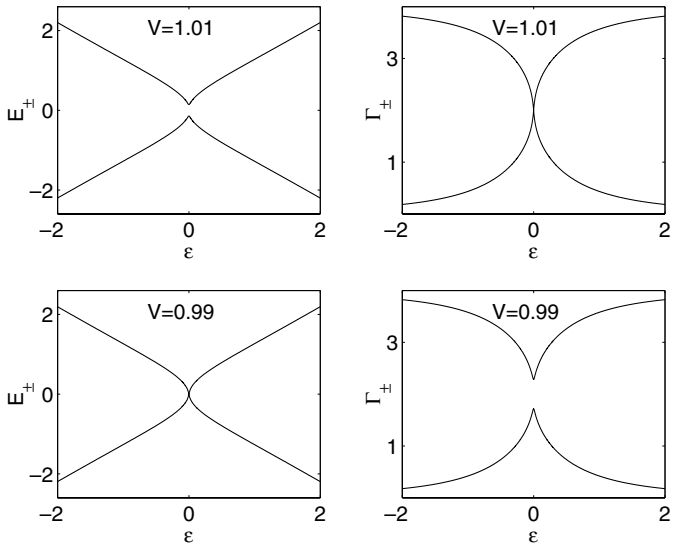

Figure 2. Real part (left) and imaginary part (right) of the eigenvalues (30) as a function of ϵ for $\gamma = 1$. In the upper figures we have a type I crossing ($V = 1.01$), in the lower figures a type II crossing ($V = 0.99$).

Let us now take a closer look at the transport of eigenvalues and eigenvectors for a *cyclic* variation of the parameters, i.e. along a closed curve in parameter space for $\gamma = 1$ and changing the other two parameters ϵ and V. The exceptional lines intersect the (ϵ, V)-plane at two points, $P_\pm = (0, 1, \pm 1)$, the exceptional points [3]. Figure 3 shows the Riemann surfaces of the energies $\mathcal{E}_\pm(\epsilon, \gamma = 1, V)$ over the (ϵ, V)-plane. On the line $\epsilon = 0$ the real parts intersect for $|V| < 1$, and for $|V| > 1$ the imaginary parts. The exceptional points $P_\pm$ are located at the boundary, i.e. at $V = \pm 1$. Note that for $\gamma \to 0$ the exceptional points move towards each other and join into a single diabolic point at $\epsilon = V = 0$. The 'double coffee filter' shaped surfaces for the real parts change into the celebrated diabolic double cone. A typical closed curve in the (ϵ, V) parameter plane does not pass through an exceptional point. In principle, we can distinguish three qualitatively different cases according to the number of exceptional points enclosed by the curve:

(a) When no exceptional point is enclosed, the resonance energies simply return to their initial values for a cyclic parameter variation.
(b) When a single exceptional point is encircled, the curve in parameter space crosses the $\epsilon = 0$ plane twice. The crossing types, however, are different. At the type I crossing, the imaginary parts move to the other sheet and interchange their character while the real parts remain on their sheets. At the type II crossing we get the opposite behaviour. After a complete cycle, both the real and the imaginary parts cross to the other sheet with the result that the eigenvalues interchange. After a second cycle they return to their original values. This characteristic behaviour of the eigenvalues can be used in applications as an indicator of the existence of an exceptional point in a region in parameter space [33].
(c) When both exceptional points are encircled, the real parts stay on their surfaces and the imaginary parts cross twice, i.e. the resonance energies return to their initial values.

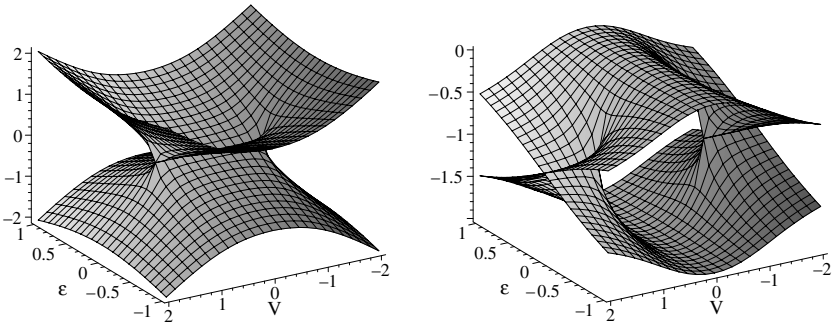

Figure 3. Real (left) and imaginary (right) parts of the eigenvalues (30) for $\gamma = 1$ as a function of ϵ and V. For $\epsilon = 0$ and $|V| > 1$ the imaginary parts cross (type I crossings), for $|V| < 1$ the imaginary parts cross (type II crossings).

3.2. Resonance eigenstates

The (right) eigenstates of the Hamiltonian (29) for the complex resonance eigenvalues $\mathcal{E}_\pm$ in equation (30) are

$$\mathbf{u}_\pm = \frac{1}{w_\pm}\begin{pmatrix} \mathcal{E}_\pm + \epsilon \\ V \end{pmatrix}. \tag{33}$$

Choosing the left eigenstates as $\mathbf{v}_\pm = \mathbf{u}_\pm^*$ and using the normalization (7) we get

$$\langle \mathbf{v}_\pm | \mathbf{u}_\pm \rangle = \langle \mathbf{u}_\pm^* | \mathbf{u}_\pm \rangle = w_\pm^{-2}((\mathcal{E}_\pm + \epsilon)^2 + V^2) \stackrel{!}{=} 1. \tag{34}$$

This determines the normalization constants up to a sign:

$$w_\pm = \sqrt{(\mathcal{E}_\pm + \epsilon)^2 + V^2}. \tag{35}$$

During a parameter variation, the sign of the square root is chosen continuously along the path in parameter space.

This normalization fails whenever the square root is zero, i.e. on the exceptional lines (31) which must be treated separately. Here the eigenvalues are degenerate, $\mathcal{E}_\pm = \mathcal{E} = -\mathrm{i}\gamma$, with an algebraic multiplicity of two, and we have two possibilities according to the dimension of the corresponding eigenspaces: only a single eigenvector exists and the Hamiltonian (29) is unitarily equivalent to a Jordan block,

$$H \sim \begin{pmatrix} \mathcal{E} & 1 \\ 0 & \mathcal{E} \end{pmatrix} \tag{36}$$

or we have two linear independent eigenvectors and

$$H \sim \begin{pmatrix} \mathcal{E} & 0 \\ 0 & \mathcal{E} \end{pmatrix}. \tag{37}$$

The first case is met on the exceptional lines $\epsilon = 0$, $V = \pm\gamma \neq 0$, and the second case at the diabolic point $\epsilon = V = \gamma = 0$. It is instructive to discuss this in more detail. On the upper ($V = +\gamma$) and lower ($V = -\gamma$) exceptional lines the (single) eigenstates $\mathbf{u}_\uparrow$ and $\mathbf{u}_\downarrow$, respectively, are

$$\mathbf{u}_\uparrow = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathrm{i} \\ 1 \end{pmatrix} \qquad \mathbf{u}_\downarrow = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathrm{i} \\ -1 \end{pmatrix}. \tag{38}$$

Both states, which are eigenstates of different Hamiltonians, are normalized as $\langle \mathbf{u}_{\uparrow\downarrow} | \mathbf{u}_{\uparrow\downarrow} \rangle = 1$, orthogonal to each other, and do not depend on the value of $\gamma = \pm V$. In the limit $\gamma = \pm V \to 0$, these two states form the two independent eigenstates at the diabolic point.

Let us now analyse the behaviour of the eigenstates in detail when the parameters V and ϵ are varied along a closed curve keeping γ constant. We recall that the eigenvectors are uniquely determined up to the choice of their signs which can be easily assigned by studying the behaviour for a simple path, a small circle of radius r around the exceptional point, chosen here as $V = +\gamma$:

$$\epsilon = -r \sin\phi \qquad V = \gamma + r\cos\phi \tag{39}$$

with $r \ll \gamma$. Representing the two eigenstates $\mathbf{u}_\pm$ in the form

$$\mathbf{u}_+ = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \qquad \mathbf{u}_- = \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix} \tag{40}$$

with

$$\theta = \arctan\left(\frac{V}{\mathcal{E}_+ + \epsilon}\right) = \arctan\left(\frac{\gamma + r\cos\phi}{-\mathrm{i}\gamma - r\sin\phi + \sqrt{r^2 + 2r\gamma\,\mathrm{e}^{\mathrm{i}\phi}}}\right) \tag{41}$$

one immediately arrives at

$$\tan\theta = \frac{V}{\mathcal{E}_+ + \epsilon} = \mathrm{i} - \sqrt{\frac{2r}{\gamma}}\,\mathrm{e}^{\mathrm{i}\frac{\phi}{2}} + O(r) \tag{42}$$

and

$$\mathrm{Re}(\theta) \approx \frac{1}{4\mathrm{i}} \ln \mathrm{e}^{\mathrm{i}\phi} = \frac{\phi}{4} \tag{43}$$

for small r. Furthermore, we get

$$\mathcal{E}_\pm(\phi) \approx -\mathrm{i}\gamma \pm \sqrt{2r\gamma}\,\mathrm{e}^{\mathrm{i}\phi/2} \tag{44}$$

which implies $\mathcal{E}_\pm(\phi = 2\pi) = \mathcal{E}_\mp(\phi = 0)$, or in an abbreviated notation

$$\mathcal{E}_\pm \xrightarrow{2\pi} \mathcal{E}_\mp \tag{45}$$

in agreement with the discussion in the preceding section. In combination with (43) this yields the desired equations for the behaviour of the eigenstates:

$$\mathbf{u}_+ \xrightarrow{2\pi} +\mathbf{u}_- \xrightarrow{2\pi} -\mathbf{u}_+ \qquad \mathbf{u}_- \xrightarrow{2\pi} -\mathbf{u}_+ \xrightarrow{2\pi} -\mathbf{u}_- \tag{46}$$

i.e. the states are interchanged in a single cycle and one of them changes its sign. After a second cycle both states are reconstructed with a phase factor $\mathrm{e}^{\mathrm{i}\pi} = -1$. After four cycles the initial eigenstates are exactly recovered again. A few remarks seem to be necessary here:

(i) The approximation $r \ll \gamma$ made in the above considerations was only used in order to extract the sign in a simple way. Because of continuity, the resulting relations are exact.

(ii) There is an apparent asymmetry in the sign changes in equation (46) which is simply due to the (arbitrary) choice of the relative phases of $\mathbf{u}_+$ and $\mathbf{u}_-$ for $\phi = 0$: For $\mathbf{u}'_+ = \mathbf{u}_+$ and $\mathbf{u}'_- = -\mathbf{u}_-$, the sequence (46) reads

$$\mathbf{u}'_+ \xrightarrow{2\pi} -\mathbf{u}'_- \xrightarrow{2\pi} -\mathbf{u}'_+ \qquad \mathbf{u}'_- \xrightarrow{2\pi} +\mathbf{u}'_+ \xrightarrow{2\pi} -\mathbf{u}'_-. \tag{47}$$

(iii) The states $\mathbf{u}_+$ and $\mathbf{u}_-$ form a (non-orthogonal) basis. Therefore, we have

$$\mathbf{x} \xrightarrow{4\pi} -\mathbf{x} \tag{48}$$

for an arbitrary linear combination. For a single cycle of 2π, however, a state generally changes. Only the special linear combinations

$$\mathbf{y}_\pm = \alpha(\mathbf{u}_+ \pm \mathrm{i}\mathbf{u}_-) \tag{49}$$

are reproduced up to a phase factor:

$$\mathbf{y}_\pm \xrightarrow{2\pi} \pm\mathrm{i}\mathbf{y}_\pm. \tag{50}$$

(iv) The behaviour of the eigenstates is the same for the other exceptional point at $V = -\gamma$.

(v) It is straightforward to show that for a closed curve encircling both exceptional points, both the eigenstates accumulate a phase factor of $\mathrm{e}^{\mathrm{i}\pi} = -1$ in a single circuit,

$$\mathbf{u}_\pm \xrightarrow{2\pi} -\mathbf{u}_\pm \tag{51}$$

(and therefore any linear combination) exactly as the eigenstates of a symmetric Hermitian Hamiltonian when a diabolic point is encircled once [21, 31].

(vi) For parameter values near the exceptional points, the two eigenvectors $\mathbf{u}_+$ and $\mathbf{u}_-$ are linearly independent. Approaching an exceptional point, the eigenvectors get linearly dependent with a relative factor of i [34]:

$$\mathbf{u}_+ \longrightarrow \pm\mathrm{i}\mathbf{u}_- \qquad \text{for} \quad (\epsilon, V, \gamma) \to (0, \gamma_0, \pm\gamma_0). \tag{52}$$

This can be seen for example by using the expansion (42). It should be pointed out again that at the exceptional point the normalization fails, and the two eigenvectors are not defined. The relation has only the meaning of a limiting process.

Let us finally discuss the geometric (Berry) phases for a cyclic adiabatic parameter evolution, where an initial state returns to itself up to a factor. The normalization used here has the advantage that the Berry phases can be directly read off from the instantaneous eigenfunctions (see equation (25)), provided that the sign is varied continuously along the path.

For a curve encircling a single exceptional point, the eigenstate returns to itself up to a factor of -1 after two cycles (see equation (46)). The same is true for a path encircling both exceptional points, however for a single cycle (see equation (51)). Hence the geometric phase for these cases is

$$\gamma_\pm^B = \pi. \tag{53}$$

4. Concluding remarks

In this paper, a generalization of the diabolic crossing scenario to non-Hermitian matrix Hamiltonians is analysed. In view of the fact that in many applications such matrices are (or can be constructed to be) symmetric, we restricted ourselves to this case. In this simplified situation, a system of normalized bi-orthogonal eigenstates can be used for constructing systems of (resonance) eigenstates which are free of arbitrary phase factors. Under certain conditions, the resonance eigenstates gain a phase factor, a geometric (or Berry) phase for a cyclic parameter variation. Such phases can be easily calculated using this normalization.

For a symmetric Hermitian Hamiltonian, the behaviour of the eigenvalues and eigenstates in parameter space is governed by the diabolic crossing scenario. In a generalization to a non-Hermitian symmetric Hamiltonian, the real eigenvalues move into the complex plane and

the diabolic point bifurcates into two exceptional ones, where the Hamiltonian is defective, i.e. two eigenstates coalesce. This behaviour is generic for a variation of two real-valued system parameters.

For such a generalized diabolic crossing scenario, the behaviour of eigenvalues and eigenstates has been analysed in terms of a two-state system. When a single parameter is varied, two different crossing types can be distinguished: crossings very similar to the crossings in the diabolic scenario (type I) and different ones (type II). A cyclic variation of the parameters can lead to an interchange of eigenvectors accompanied by additional phase factors depending on the geometry of the cyclic path with respect to the exceptional points.

Finally, we would like to point out that in this paper we basically discussed the topological structure of the Riemann surfaces of the functions

$$f(z) = \sqrt{\lambda(t) - z^2} \tag{54}$$

where $\lambda(t)$ is a (closed) path. In a more abstract setting the interested reader can find an analysis in the book by Arnold *et al* [35].

In a companion paper [33] we will apply the results discussed here to a model system, the Stark resonances of a double δ well.

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