Singularities Caused by Coalesced Complex Eigenvalues of an Effective Hamilton Operator

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The S matrix theory with use of the effective Hamiltonian is sketched and applied to the description of the transmission through double quantum dots. The effective Hamilton operator is non-hermitian, its eigenvalues are complex, the eigenfunctions are bi-orthogonal. In this theory, singularities occur at points where two (or more) eigenvalues of the effective Hamiltonian coalesce. These points are physically meaningful: they separate the scenario of avoided level crossings from that without any crossings in the complex plane. They are branch points in the complex plane. Their geometrical features are different from those of the diabolic points.

1. INTRODUCTION

The advances in the nanotechnology make it possible to produce small quantum dots and to use them for transport processes. In order to construct dots with desired controllable effects, the theory has to meet the challenge to describe, in a consistent manner, quantum systems that are coupled to an environment. The main problem is caused by the different mathematical properties of the discrete states of the system, on the one hand, and of the scattering states of the environment, on the other hand.

During the last about fifty years several methods were developed in order to obtain a solution of the problem. One of the most powerful methods is the S matrix approach that allows to describe physical observables such as e.g. the scattering cross section of nuclei, see e.g. Feshbach (1958, 1962). In the standard approach, information on the resonance states is obtained from the poles of the S matrix that provide the positions as well as the widths of the resonance states. This

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method gives reliable results when the resonances appear well isolated from one another. When, however, the resonances start to overlap each other or (and) when they lie in the neighborhood of decay thresholds, the standard method ceases to be applicable. This drawback plays a role especially when the spectrum of the system is determined by the propagation band of electrons as it is the case for the transmission through quantum dots. In such a case, the widths of the resonance states depend on energy in a natural manner, see e.g. Sadreev and Rotter (2003). In order to construct quantum dots with special properties, more exact theoretical methods must therefore be used that allow to take into account the influence of neighboring resonance states and of decay thresholds onto each resonance state.

Based on the Feshbach projection operator technique (Feshbach, 1958, 1962), it is possible today to use the S matrix formalism without continuing into the complex plane (Okołowicz *et al.*, 2003; Rotter, 1991). The spectroscopic properties of the discrete states of the system as well as their coupling matrix elements to the environment are contained in the effective Hamiltonian of the system. Its eigenvalues and eigenfunctions are complex and energy dependent and contain the influence of the neighborhood onto every resonance state. They provide the positions and widths of the resonance states and ensure the unitarity of the S matrix also in the overlapping regime and near to thresholds (Rotter, 2003). A continuation of the energy into the complex plane is therefore not necessary, and the poles of the S matrix need not to be considered.

Meanwhile, the effective Hamiltonian has been derived for different systems such as nuclei (Okołowicz *et al.*, 2003), atoms (Magunov *et al.*, 1999, 2001, 2003a) and quantum dots (Sadreev and Rotter, 2003; Rotter and Sadreev, 2004). The S matrix has been calculated in all cases, and the influence of overlapping with neighboring resonance states and of decay thresholds on observables has been studied. For quantum dots, most interesting is the transmission. It may happen that two (or more) eigenvalues of the effective Hamiltonian coalesce at a point in the parameter space. These points are, generally, different from double poles of the S matrix (Rotter and Sadreev, 2004).

Points with coalesced eigenvalues of a Hamilton operator are discussed in the literature since more than forty years. Originally, the accidental coincidence of two eigenvalues of a complex matrix is considered (Kato, 1966). At this point, the Hilbert space is incomplete since the corresponding two eigenfunctions are not independent from one another. These points are called therefore exceptional points. Later, this concept is applied to non-hermitian matrices describing Gamow states (Hernández *et al.*, 2000, 2003; Moiseyev, 1998; Mondragon and Hernanández, 1993, 1996). In quantum systems embedded in a continuum of scattering states, the points of coalesced eigenvalues of the non-hermitian effective Hamilton operator are singular points (Okołowicz *et al.*, 2003; Rotter, 2001; Rotter and Sadreev, 2004, 2005a). They influence the dynamics of the system in a broad neighborhood of the singularity. They are branch points in the complex plane (BPCP) (Okołowicz *et al.*,

2003; Rotter and Sadreev, 2005a). Here, the crossing scenario of the resonance states changes from an avoided one to a crossing-free one. These singular points are therefore of physical relevance.

The topological structure of a singular point is studied theoretically (Heiss *et al.*, 1998; Heiss, 1999, 2000; Keck *et al.*, 2003; Rotter and Sadreev, 2005a) and also experimentally by encircling it in a microwave cavity (Dembowski *et al.*, 2001, 2004). The singular point itself has a chiral structure (Dembowski *et al.*, 2003). The results for encircling a BPCP show a geometrical phase that differs from the Berry phase. The well-known Berry phase (Berry, 1984; Berry and Wilkinson, 1984) appears by encircling a diabolic point (DP), i.e. the 'crossing point' of two (discrete) eigenstates of a hermitian Hamilton operator. The existence of this geometrical phase is proven in many experimental studies. We mention here only the experiment performed in a microwave cavity (Lauber *et al.*, 1994).

It is interesting to study the relation between the geometrical features of the DPs and those of the BPCP in detail. We will do this in the following by using a double quantum dot as an example. The advantage of using a double quantum dot is that this system mimics, on the one hand, nuclear or atomic scattering and can be controlled, on the other hand, by varying different parameters.

In Section 2, we sketch the formalism of the S matrix with use of the effective Hamilton operator for the description of open quantum systems. We illustrate the appearance of singular points by means of a two-by-two Hamiltonian matrix in Section 3. In the following section, we give the effective Hamiltonian for a double quantum dot and consider the transmission through this dot in Section 5. Also here we focus onto the points of coalesced eigenvalues and their physical relevance. In Section 6, the geometrical features of the singular points of the double quantum dot are studied. They are compared with the geometrical features of DPs and with experimental data. The results are summarized in the last section.

2. THE EFFECTIVE HAMILTONIAN OF AN OPEN QUANTUM SYSTEM

We use the Feshbach projection operator technique (Feshbach, 1958, 1962) in order to solve the Schrödinger equation

$$(H^{\text{full}} - E)\Psi_E^c = 0 \tag{1}$$

in the whole function space (Rotter, 1991; Okołowicz *et al.*, 2003). First, the solutions in the function space of discrete states and those for the scattering states have to be found separately,

$$\left(H_B - E_k^B\right)\Phi_k^B = 0, \quad (H_c - E)\xi_E^{c(+)} = 0. \tag{2}$$

Then, the projection operators are defined by

$$Q = \sum_k |\Phi_k^B\rangle\langle\Phi_k^B|, \quad P = \sum_c \int_{\epsilon_c}^{\epsilon_c'} dE \; |\xi_E^{c(+)}\rangle\langle\xi_E^{c(+)}| \tag{3}$$

and the coupling matrix elements between the two subspaces are

$$\gamma_{kc}^0 = \sqrt{2\pi}\,\big\langle\Phi_k^B|H_{QP}|\xi_E^{c(+)}\big\rangle. \tag{4}$$

Using these operators and the assumption that $P + Q = 1$, the full Hamiltonian reads $H^{\text{full}} = H_{QQ} + H_{QP} + H_{PQ} + H_{PP}$ where $H_{QQ} \equiv QHQ$ and so on. Rewriting Eq. (1), the solution of the Schrödinger equation reads

$$\Psi_E^c = \xi_E^c + \sum_{kj}\big(\Phi_k^B + \omega_k\big)\Big\langle\Phi_k^B\Big|\frac{1}{E - H_{\text{eff}}}\Big|\Phi_j^B\Big\rangle\big\langle\Phi_j^B|H_{QP}|\xi_E^c\big\rangle \tag{5}$$

where

$$H_{\text{eff}} = H_{QQ} + H_{QP}G_P^{(+)}H_{PQ} \tag{6}$$

is the effective Hamilton operator that appears in the Q subspace when the coupling to the P subspace is taken into account. Further, $\omega_k^{(+)} = G_P^{(+)}H_{PQ}\cdot\Phi_k^B$ and $G_P^{(+)} = P(E - H_{PP})^{-1}P$ is the Green function in the P subspace. Diagonalizing H_{eff},

$$H_{\text{eff}}\,\tilde\Phi_k = z_k\,\tilde\Phi_k, \tag{7}$$

the solution in the whole function space reads (Okołowicz *et al.*, 2003; Rotter, 1991)

$$\Psi_E^c = \xi_E^c + \sum_{k=1}^N \big(1 + G_P^{(+)}\,H_{PQ}\big)\tilde\Phi_k \cdot \frac{\langle\tilde\Phi_k^*|H_{QP}|\xi_E^c\rangle}{E - z_k}. \tag{8}$$

According to (8), the wave functions of the resonance states are

$$\tilde\Omega_k = \big(1 + G_P^{(+)}\,H_{PQ}\big)\tilde\Phi_k \tag{9}$$

while their energies and widths follow from the solutions of the fixed-point equations

$$E_k = \text{Re}\,(z_k)|_{E=E_k} \quad \Gamma_k = 2\,\text{Im}\,(z_k)|_{E=E_k}. \tag{10}$$

Using the Lippmann-Schwinger-like relation between the wave functions $\tilde\Omega_k$ and $\tilde\Phi_k$ (Rotter, 1991), the coupling matrix elements between the resonance states and the continuum of scattering wave functions are

$$\tilde\gamma_{kc} = \sqrt{2\pi}\,\big\langle\tilde\Phi_k^*|H_{QP}|\xi_E^c\big\rangle = \sqrt{2\pi}\,\big\langle\tilde\Omega_k^*|H_{QP}|\chi_E^c\big\rangle \tag{11}$$

where the χ_E^c are solutions of the uncoupled channel equations $(H_c^{(0)} - E)\chi_E^c = 0$. Using (11), the resonance part of the S matrix reads

$$S_{cc'}^{(\text{res})} = i \sum_{k=1}^{N} \frac{\tilde{\gamma}_{kc'}\,\tilde{\gamma}_{kc}}{E - z_k}. \tag{12}$$

Although (12) has the standard view, there are differences between (12) and the standard expression. These differences are important in the regime of overlapping resonances. In (12)

  – the $\tilde{\gamma}_{kc}$ are calculated by means of the eigenfunctions of H_{eff},
  – the z_k are the eigenvalues of H_{eff},
  – the $\tilde{\gamma}_{kc}$ and the z_k depend on the energy E (and other parameters).

In the calculations with use of the effective Hamiltonian, the energy E of the incident particle is considered to be real, and the positions and widths of the resonance states are determined by the complex eigenvalues z_k of H_{eff}. The poles of the S-matrix are not considered. Furthermore, the S matrix is unitary at all energies also in the regime of overlapping resonances (Rotter, 2003). We underline once more that the part $H_{QQ} \equiv H_B$ of the effective Hamilton operator H_{eff} is diagonalized so that the expression (6) is exact (and not the first part of a perturbation series).

The effective Hamilton operator H_{eff} in the Q subspace is non-hermitian, its eigenvalues z_k and eigenfunctions $\tilde{\Phi}_k$ are complex and energy dependent (Okołowicz *et al.*, 2003). The left and right eigenfunctions, $\tilde{\Phi}_k^{\text{lt}}$ and $\tilde{\Phi}_k^{\text{rt}}$, are different from one another, $\langle \tilde{\Phi}_k^* |\, H_{\text{eff}} = \langle \tilde{\Phi}_k^* |\, z_k$ and $H_{\text{eff}}\, |\tilde{\Phi}_k\rangle = z_k\, |\tilde{\Phi}_k\rangle$, and therefore $\tilde{\Phi}_k^{\text{rt}} \equiv \tilde{\Phi}_k$; $\tilde{\Phi}_k^{\text{lt}} = \tilde{\Phi}_k^{\text{rt}\,*} \equiv \tilde{\Phi}_k^*$. The eigenfunctions of H_{eff} can be orthonormalized according to

$$\left\langle \tilde{\Phi}_k^{\text{lt}} | \tilde{\Phi}_l^{\text{rt}} \right\rangle \equiv (\tilde{\Phi}_k | \tilde{\Phi}_l) = \langle \tilde{\Phi}_k^* | \tilde{\Phi}_l \rangle = \delta_{kl}. \tag{13}$$

From these biorthogonality relations follows

$$A_k \equiv \langle \tilde{\Phi}_k | \tilde{\Phi}_k \rangle \geq 1 , \qquad B_k^{l \neq k} \equiv |\langle \tilde{\Phi}_k | \tilde{\Phi}_{l \neq k} \rangle| \geq 0. \tag{14}$$

It may happen that $|A_k| \to \infty$ and $|B_k^l| \to \infty$, for more details see Okołowicz *et al.* (2003). The properties of these singular points will be discussed in the following.

Thus, an open quantum system is characterized by two Hamilton operators: the hermitian Hamilton operator $H_B = H_0 + V$ of the closed system, see (2), and the non-hermitian Hamilton operator (6) of the system (Q subspace) when embedded in the continuum of decay channels (P subspace). Two (or more) eigenvalues of each Hamilton operator may accidentally coalesce. The corresponding points in the real and complex plane, respectively, have special properties that are different from one another. When two (or more) of the complex eigenvalues of H_{eff} coalesce, $A_k \to \infty$ and $B_k^{l \neq k} \to \infty$.

3. TWO-BY-TWO HAMILTONIAN MATRIX

Let us illustrate the crossing and avoided crossing scenario of discrete and resonance states by using the two-by-two Hamiltonian matrix (Okołowicz *et al.*, 2003; Rotter, 2001)

$$H_{\text{eff}}^{(2)} = \begin{pmatrix} \epsilon_1(a) & 0 \\ 0 & \epsilon_2(a) \end{pmatrix} - \begin{pmatrix} 0 & w \\ w & 0 \end{pmatrix}. \tag{15}$$

Here, the unperturbed energies of the two (resonance) states are denoted by $\epsilon_k = e_k - \frac{i}{2}\gamma_k$, $k = 1, 2$. They are assumed to depend on the parameter a to be tuned in such a manner that the two states may cross ($\epsilon_1 = \epsilon_2$) when $w = 0$. The two states may interact via the non-diagonal matrix elements w. The eigenvalues of (15) are

$$\mathcal{E}_{\pm} \equiv E_{\pm} - \frac{i}{2}\Gamma_{\pm} = \frac{\epsilon_1 + \epsilon_2}{2} \pm \frac{1}{2}\sqrt{F(a, w)} \tag{16}$$

where the difference between the two eigenvalues is determined by

$$F(a, w) = (\epsilon_1 - \epsilon_2)^2 + 4 w^2. \tag{17}$$

For discrete states, $\epsilon_1 - \epsilon_2$ and w are real. Therefore, interacting discrete states ($w \neq 0$) always avoid crossing. In such a case, $F(a, w) > 0$, and the levels repel in energy.

The crossing scenario of resonance states is more interesting since both $\epsilon_1 - \epsilon_2$ and w may be complex. For illustration let us consider the situation when Im (F) is small. When furthermore Im (w) is small, the two states are near to one another ($e_1 \approx e_2$) or (and) have comparable widths ($\gamma_1 \approx \gamma_2$) in this case. The corresponding crossing scenario follows directly from the eigenvalues of (15). The energies and widths of the two resonance states are

$$\text{Re}\,(\mathcal{E}_{\pm}) \equiv E_{\pm} = \frac{e_1 + e_2}{2} \pm \frac{1}{2}\,\text{Re}\,\sqrt{F(a, w)} \tag{18}$$

$$\text{Im}\,(\mathcal{E}_{\pm}) \equiv -\frac{\Gamma_{\pm}}{2} = -\frac{\gamma_1 + \gamma_2}{4} \pm \frac{1}{2}\,\text{Im}\,\sqrt{F(a, w)}. \tag{19}$$

When $F(a, w) > 0$, level repulsion occurs. The two states avoid crossing in the complex plane as well as in the projection onto the real axis. When however $F(a, w) < 0$, width bifurcation occurs. In this case, the two states cross in the projection onto the real (energy) axis. They do not cross in the complex plane due to the different time scales related to them.

When $F(a, w) = 0$, the two states cross in the complex plane, i.e. their energies and widths are equal to one another: $\mathcal{E}_+ = \mathcal{E}_-$. As has been shown in many studies (Okołowicz *et al.*, 2003), the coalescence of two (or more) complex eigenvalues of the effective Hamiltonian causes a singularity, $A_k \to \infty$, $B_k^{l \neq k} \to$

∞. This point is a BPCP that influences strongly the dynamics of open quantum systems.

This example illustrates not only that level repulsion and bifurcation of the widths follow directly from the equations for the eigenvalues of the Hamiltonian (15), but also that resonance states of realistic systems may cross in the complex plane. That means, while interacting discrete states always avoid crossing, interacting resonance states may cross or avoid crossing. At the crossing points, the crossing scenario changes. For a more detailed discussion see Okołowicz *et al.* (2003); Rotter and Sadreev (2004, 2005a).

Additionally, we note that the eigenfunctions of $H_B = H_0 + V$ may be represented by

$$\psi_k^B = \sum a_{kl} \, \psi_l^{B(0)} \tag{20}$$

where the $\psi_l^{B(0)}$ are eigenfunctions of H_0, the a_{kl} are real and $\sum_l |a_{kl}|^2 = 1$. This representation is not always well defined because some arbitrariness in defining H_0 and the corresponding basic set $\{\psi_l^{B(0)}\}$ may appear.

The eigenfunctions of $H_{\text{eff}}^{(2)}$, however, can be represented in a natural manner in relation to a well-defined set of basic wave functions. According to (6), the system is embedded into the continuum. A natural basis is defined by the eigenfunctions ψ_l^B of the Hamiltonian H_B of the closed system,

$$H_{\text{eff}}^{(2)} = H_B + V_{QP} \, G_P^{(+)} \, V_{PQ} = \begin{pmatrix} e_1(a) & 0 \\ 0 & e_2(a) \end{pmatrix} - \begin{pmatrix} \frac{i}{2}\gamma_1(a) & w \\ w & \frac{i}{2}\gamma_2(a) \end{pmatrix}. \tag{21}$$

In this case, the representation is

$$\tilde{\psi}_k = \sum b_{kl} \, \psi_l^B \tag{22}$$

with complex b_{kl} and $\sum_l (b_{kl})^2 = 1$. It can be used, however, also the representation of the eigenfunctions of $H_{\text{eff}}^{(2)}$ according to (15)

$$H_{\text{eff}}^{(2)} = H_{\text{eff}}^0 + W = \begin{pmatrix} e_1(a) - \frac{i}{2}\gamma_1(a) & 0 \\ 0 & e_2(a) - \frac{i}{2}\gamma_2(a) \end{pmatrix} - \begin{pmatrix} 0 & w \\ w & 0 \end{pmatrix} \tag{23}$$

where W describes the interaction of the resonance states via the continuum due to their overlapping. In this case,

$$\tilde{\psi}_k = \sum b'_{kl} \, \tilde{\psi}_l^0 \tag{24}$$

with complex b'_{kl} and $\sum_l (b'_{kl})^2 = 1$. These two representations are completely analogue to one another. Important is the normalization $\sum_l (b'_{kl})^2 = \sum_l (b_{kl})^2 = 1$ for resonance states in contrast to $\sum_l |a_{kl}|^2 = 1$ for discrete states. It causes $|b_{kl}| \to \infty$ (or $|b'_{kl}| \to \infty$) at singular points (Okołowicz *et al.*, 2003; Rotter, 2001; Rotter and Sadreev, 2005a).
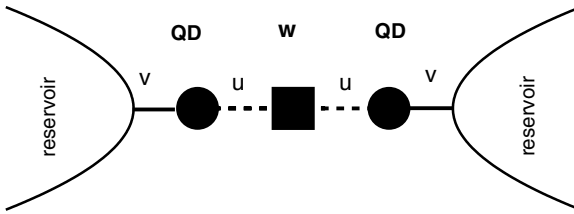
Fig. 1. Two single state quantum dots are connected to the wire w with the coupling constants u and to the reservoirs (continuum of scattering wave functions) with the coupling constants v.

4. REALISTIC EXAMPLE: DOUBLE QUANTUM DOT

We consider now a realistic example: a double quantum dot consisting of two single dots that are connected by a wire of a certain length L, Fig. 1. For simplicity, we assume here that the two single dots are identical and have each only one level at ε_1. The Hamiltonian of the closed double dot is (Rotter and Sadreev, 2005b)

$$H_B = \begin{pmatrix} \varepsilon_1 & u & 0 \\ u & \epsilon(L) & u \\ 0 & u & \varepsilon_1 \end{pmatrix} \tag{25}$$

with the eigenvalues

$$E_{1,3}^B = \frac{\varepsilon_1 + \epsilon(L)}{2} \mp \eta, \quad E_2^B = \varepsilon_1 \tag{26}$$

and eigenfunctions

$$|1\rangle = \frac{1}{\sqrt{2\eta(\eta + \Delta\varepsilon)}} \begin{pmatrix} -u \\ \eta + \Delta\varepsilon \\ -u \end{pmatrix}, \quad |2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix},$$

$$|3\rangle = \frac{1}{\sqrt{2\eta(\eta - \Delta\varepsilon)}} \begin{pmatrix} u \\ \eta - \Delta\varepsilon \\ u \end{pmatrix}. \tag{27}$$

Here, $\epsilon(L)$ characterizes the energy of the wire and u stands for the coupling between the single dots and the wire. Further,

$$\Delta\varepsilon(L) = \frac{\varepsilon_1 - \epsilon(L)}{2}, \quad \eta^2 = \Delta\varepsilon^2 + 2u^2. \tag{28}$$

When the double quantum dot is opened by attaching leads to it, the effective Hamiltonian of the open system is (Rotter and Sadreev, 2004, 2005b)

$$H_{\text{eff}} = H_B + \sum_{C=L,R} V_{BC} \frac{1}{E^+ - H_C} V_{CB}$$

$$= \begin{pmatrix} E_1^B - \frac{v^2 u^2 e^{ik}}{\eta(\eta+\Delta\varepsilon)} & 0 & \frac{v^2 u e^{ik}}{\sqrt{2}\eta} \\ 0 & \varepsilon_1 - v^2 e^{ik} & 0 \\ \frac{v^2 u e^{ik}}{\sqrt{2}\eta} & 0 & E_3^B - \frac{v^2 u^2 e^{ik}}{\eta(\eta-\Delta\varepsilon)} \end{pmatrix} \tag{29}$$

where L and R stand for the left and right lead, V_{BC} and V_{CB} for the coupling between the double dot and the leads, and v characterizes this coupling strength. The eigenvalues and eigenfunctions of H_{eff} are

$$z_2 = \varepsilon_1 - v^2 e^{ik},$$

$$z_{1,3} = \frac{\varepsilon_1 + \epsilon(L) - v^2 e^{ik}}{2} \mp \sqrt{\left(\frac{v^2 e^{ik}}{2} - \Delta\varepsilon\right)^2 + 2u^2} \tag{30}$$

and

$$|1) = \begin{pmatrix} a \\ 0 \\ b \end{pmatrix}, \qquad |2) = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |3) = \begin{pmatrix} b \\ 0 \\ -a \end{pmatrix}. \tag{31}$$

Here,

$$a = -\frac{f}{\sqrt{2\xi(\xi+\omega)}}, \qquad b = \sqrt{\frac{\xi+\omega}{2\xi}} \tag{32}$$

and

$$f = \frac{v^2 u e^{ik}}{\sqrt{2}\,\eta}, \qquad \omega = -\eta + \frac{\Delta\varepsilon v^2 e^{ik}}{2\eta}, \qquad \xi^2 = \omega^2 + f^2. \tag{33}$$

Let us now consider the points at which two (or three) eigenvalues of the Hamiltonian coalesce. The points for the closed system (in the real plane) are defined by

$$\eta^2 = \Delta\varepsilon^2 + 2u^2 = 0 \tag{34}$$

according to (26), where $E_1^B = E_3^B$. At these points, the internal coupling u vanishes. Due to the condition $u = 0$, these points are not meaningful for realistic systems. They are the DPs studied in many different systems.

Two eigenvalues of the effective Hamiltonian H_{eff} coalesce in the complex plane when

$$F \equiv \xi^2 = \omega^2 + f^2 = 0 \tag{35}$$

according to Eq. (30). Here, the internal as well as the external coupling, u and v, are different from zero. These points are meaningful therefore for realistic systems. Everywhere, the wave functions are biorthogonal, $(k|l) \equiv \langle k^*|l\rangle = \delta_{k,l}$, and $\tilde{\psi}_k = \sum b_{kl} \psi_l^B$ without any restriction for the value of $|b_{kl}|$, see (22) and
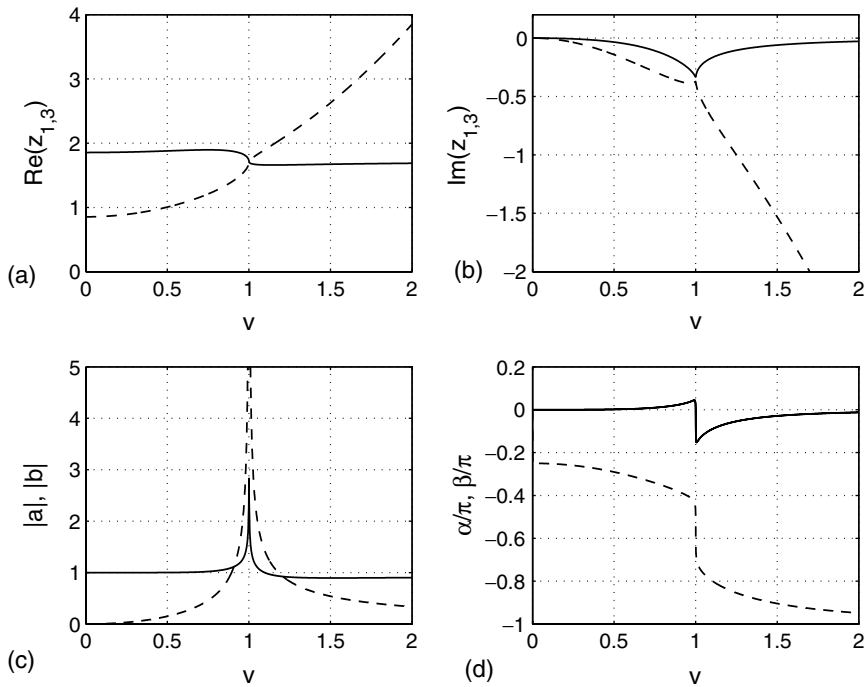
Fig. 2. The evolution of the eigenvalues z_1 (solid lines) and z_3 (dashed lines) (a, b) and of the components $a = |a|\, e^{i\alpha}$ (dashed lines) and $b = |b|\, e^{i\beta}$ (solid lines) of the eigenfunctions $|1\rangle$ and $|3\rangle$ (c, d) of the effective Hamiltonian H_{eff} as a function of v for $E = E_c = \sqrt{2}$. Parameters: $u = u_c = 1/4$, $L = L_c - 0.01$, $L_c = 1.4645$, $\varepsilon_1 = 1$, $\epsilon(L) = 2 - L/5$. At the critical value of v, $|a| \gg 1$, $|b| \gg 1$ and the phases jump by $-\pi/4$. (Rotter and Sadreev, 2005a).

(24). At the points of coalescence, $|b_{kl}| \to \infty$ (Fig. 2). These points are BPCP (Rotter and Sadreev, 2004, 2005a).

5. TRANSMISSION THROUGH DOUBLE QUANTUM DOTS

According to (12), the eigenvalues of the effective Hamilton operator H_{eff} determine the resonance structure of the cross section. The same holds for the transmission through quantum dots which is given by (Sadreev and Rotter, 2003; Rotter and Sadreev, 2004, 2005b)

$$t = -2\pi i \sum_k \frac{\langle L|V|k\rangle (k|V|R\rangle}{E - z_k}. \tag{36}$$

Here the matrix elements $\langle L|V|k\rangle$ and $(k|V|R\rangle$ describe the coupling of the states k to the left (L) and right (R) lead, respectively.

Numerical results obtained for the transmission through a double quantum dot by varying different parameters (including the internal and external coupling strengths u and v, respectively) can be found in Rotter and Sadreev (2004a, 2004b). In these calculations, each single dot has only a small number of states while the wire that connects the two single dots is characterized by the energy $\epsilon(L)$ where L is the length of the wire. The numerical results show the following features (Rotter and Sadreev, 2005a).

1. The avoided level crossing scenario appears when the ratio v/u is small. Here the widths of the two resonance states are small and comparable in value (or zero when the states are discrete). The energies show level repulsion.
2. Singular points (BPCP) occur at a critical value of the ratio v/u. At this value, the (complex) eigenvalues of (at least) two eigenstates of H_{eff} accidentally coalesce.
3. No crossing in the complex plane appears for a large ratio v/u. In this case, the widths of the two states are different from one another due to the bifurcation. The energies show level clustering.
4. The transmission is resonant for any ratio v/u between external and internal coupling strength.

These numerical results fit into the picture received for other open quantum systems in the overlapping regime, e.g. for nuclei (Okołowicz *et al*., 2003), atoms (Magunov *et al*., 1999, 2001, 2003a) and molecules (Peskin *et al*., 1994, 1997; Rotter, 1997), see also Rotter (2004). While the Re (z_k) have some relation to the discrete eigenvalues E_k of the Hamiltonian H_B, the Im (z_k) express a new degree of freedom of the open quantum system. They are, as a rule, strongly parameter dependent. They may even vanish also when the decay is not forbidden by any selection rule (Magunov *et al*., 1999, 2001; Rotter and Sadreev, 2004, 2005b). Resonance states with vanishing width ('ghost resonances' (Ladron de Guevara *et al*., 2003)) may cause, in a natural manner, zeros in the transmission through double quantum dots (and double microwave billiards) when this is required by the unitarity condition (Rotter and Sadreev, 2004, 2005b). Furthermore, the line shape of resonances is strongly influenced by interferences between neighboring resonances (Magunov *et al*., 2003b). It may be fitted even by a complex Fano parameter as suggested by experimental results (Kobayashi *et al*., 2002).

A generic feature of open quantum systems in the overlapping regime is the counterintuitive phenomenon of resonance trapping: with increasing coupling strength between system and environment, some resonance states decouple from the continuum of scattering wave functions while a few resonance states align with the continuum channels (Rotter, 1991; Okołowicz *et al*., 2003). For an experimental proof see Persson *et al*. (2000); Stöckmann *et al*. (2002). This phenomenon is caused by the BPCP where a bifurcation of the widths occurs. Only at small

coupling strength between system and channels, the states remain almost unchanged by the coupling to the channels. In this case the most important part of H_{eff} is the Hamilton operator H_B whose rank is N (number of resonance states). At large coupling strength between system and channels, however, the states are strongly changed by the coupling to the channels: most important part of H_{eff} is the coupling matrix between system and channels whose rank is K (number of decay channels). The transition between these two limiting cases takes place in a comparably small parameter range in the neighborhood of the BPCP, see Rotter and Sadreev (2004, 2005a) for double quantum dots as an example.

In any case, the effective Hamiltonian operator H_{eff} of an open quantum system reflects the spectral properties of the closed system as well as the coupling to the environment. In the overlapping regime, non-diagonal matrix elements of H_{eff} arise from the interaction of the different resonance states via the continuum, see the representation (23) of the effective Hamiltonian $H_{\text{eff}}^{(2)}$. In an open quantum system different time scales exist in parallel.

6. GEOMETRICAL FEATURES OF THE SINGULAR POINTS OF THE DOUBLE QUANTUM DOT

The geometrical features of singular points can be studied best by encircling them. Let us first encircle the BPCP where two (or more) eigenvalues of H_{eff} coalesce. Here $F = (\frac{v^2 e^{ik}}{2} - \Delta\varepsilon)^2 + 2u^2 = 0$ according to (35). The encircling can be performed according to $X = |F|\cos\phi$, $Y = |F|\sin\phi$. As a result, the difference $z_1 - z_3$ of the eigenvalues varies as $\exp(i\phi/2)$ and the components a, b of the eigenvectors vary as $\exp(-i\phi/4)$, for details see Rotter and Sadreev, 2005. This means that the eigenvalues are restored after two loops while the eigenvectors are restored after four loops. The same result is obtained when the singular points are encircled by varying physical parameters (that are independent from one another) such as $L = L_c + r\cos\theta$ together with $E = E_c + r\sin\theta$ or $v = v_c + r\sin\theta$ (Rotter and Sadreev, 2005a).

These theoretical results obtained for the singular points of a double quantum dot are in agreement with experimental data that are received by encircling a singular point in a microwave cavity (Dembowski *et al*., 2001).

The geometrical properties of the DPs, where $\eta^2 = \Delta\varepsilon^2 + 2u^2 = 0$ according to (34), are different from those of the BPCP. The encircling can be performed according to $\Delta\varepsilon = \eta\cos\theta$, $\sqrt{2}u = \eta\sin\theta$. The result is the following: the eigenvalues E_1^B and E_3^B vary as $\cos\theta$ and the components of the eigenvectors contain $\sin\theta/2$ or $\cos\theta/2$. That means, the eigenvalues are restored after each loop while the eigenvectors are restored only after two loops. Encircling in the space of physical parameters such as L and u gives the same result. The phase appearing after one loop is the well-known Berry phase that is obtained by encircling a DP. Among

many other experimental proofs, the Berry phase is found also in a microwave cavity when a DP is encircled (Lauber *et al.*, 1994).

Additionally it has been shown (Rotter and Sadreev, 2005a) that the geometrical features of the DPs in the real plane and those of the BPCP are completely different from one another:

- encircling a DP in the real plane causes a geometric phase in the closed system but no phase in the open system
- encircling a BPCP causes a geometric phase in the open system but has no effect in the closed system.

The DP in the real plane ($v = 0$) is understood to unfold into two BPCP with different chirality each, when v becomes different from zero (Keck *et al.*, 2003). It is interesting therefore to compare the encircling of a DP in the real plane ($v = 0$) with that of the two corresponding BPCP ($v \neq 0$). In the first case, the Berry phase is obtained while there is no phase at all in the second case (Rotter and Sadreev, 2005a). The reason is that two BPCP with different chirality are encircled in the second case so that the phases compensate each other. There is, however, a strong angle dependence of the widths of the states in this latter case: the difference between the widths of the two states varies twice in each loop from 0 to its maximal value (Rotter and Sadreev, 2005a). A width bifurcation appears every time when $u = 0$ is passed. Thus, the encircling of the two BPCP with different chirality differs from the encircling of the DP into which both BPCP coalesce when $v \to 0$. The difference exists already at infinitesimal small values of v. The reason for this behavior is the new freedom degree of every state when it is embedded into the continuum, i.e. its decay width. By means of the parameter dependence of the widths, the system is able to fulfill constraints of different type onto the system. This holds also for the unitarity of the S matrix (Rotter, 2003).

The different topological structure of the DPs and of the BPCP corresponds to their different physical meaning. At the DPs, the interaction between the levels is vanishing ($u = 0$). These points are therefore not met in realistic systems where $u \neq 0$. Instead, the discrete states of realistic systems avoid crossing. The Berry phase is a signature of the DP.

At BPCP, however, the interaction between the levels is nonvanishing ($v \neq 0$, $u \neq 0$). These points can therefore be met in realistic systems by controlling certain parameters (Rotter and Sadreev, 2005a). When the ratio v/u between external and internal coupling strength is small, the resonance states avoid crossing. When it is large, the resonance states exist at different times and they do not cross at all. Thus, the BPCP are physically meaningful: they separate the avoided level crossing scenario from that without any crossings (Rotter and Sadreev, 2005a).

7. SUMMARY

The *S* matrix formalism with the effective Hamilton operator is a powerful method for the study of open quantum systems. It gives reliable results also in the neighborhood of decay thresholds and in the overlapping regime. While the parameter dependence of the energies of the resonance states is comparably small, that of the widths may be very large. The widths, having no counterpart in the corresponding closed system, play an important role in order to fulfill constraints of different type onto the system. The widths of resonance states may even vanish also when the decay is not forbidden by any selection rule.

In the *S* matrix formalism with effective Hamilton operator (6), a new type of singular points appears. These points are BPCP. They are physically meaningful and influence the properties of an open quantum system in a large neighborhood. They separate the scenario with avoided level crossing from that without any crossing. The scenario with level repulsion is realized for discrete states as well as for long-lived resonance states the widths of which differ from one another only slightly. At the BPCP, the widths of the resonance states bifurcate and the resonance states do no longer cross or avoid crossing in the complex plane. They cross in the projection onto the real energy axis corresponding to a certain level clustering.

The geometrical features of the BPCP differ from those of the DPs. While the well-known Berry phase appears by encircling the DPs, the phase obtained by encircling the BPCP is another one. It reflects the change of the crossing scenario at these points: the eigenvalues are restored only after two full loops and the eigenfunctions are restored after four full loops. The DPs, however, lie within the avoided level crossing scenario: the eigenvalues are restored after each full loop and the eigenfunctions after two full loops. The different geometrical features of the BPCP and of the DPs in the real plane correspond to their different physical meaning.

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