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Stark resonances for a double δ quantum well: crossing scenarios, exceptional points and geometric phases

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Abstract

The complex energy resonances of a double δ potential well in a constant (Stark) field are studied. Varying the two system parameters (well distance and field strength) we investigate the behaviour of the resonance energies and wavefunctions both analytically and numerically. Different crossing scenarios for the real and imaginary parts of two resonance energies are observed and compared with a simple two-state model. In addition, a point in parameter space where both the real and imaginary parts of the two energies degenerate, an exceptional point, is found. Varying the system parameters around this exceptional point, the behaviour of energies and wavefunctions is discussed and the corresponding geometric phases, or Berry phases, for this non-Hermitian system are considered.

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1. Introduction

A particle bound by an attractive δ potential is one of the simplest models in introductory quantum mechanics [1]. In more advanced applications, this system can be used to model an electron in an ultra-thin quantum well or a zero-range 'atom' in a laser field. As an example, the generation of high-order harmonic emission (HHG) can be described in such a model in a very elegant way, reproducing most of the experimentally observed features [2–4]. It is also possible to describe ionization processes in strong laser fields of such zero-range 'atoms' with an effective double δ potential [5, 6]. In a number of papers a δ potential in a constant field is investigated modelling the Stark effect in a one-dimensional atom [7], tunnelling from an ultra-thin quantum well in a strong electrostatic field [8, 9] or simply as a model of a decaying quantum-mechanical state [10].

Systems with two attractive δ potentials are also found as exercises in textbooks [1] and provide a simplistic model of a 'molecule' formed by two zero-range 'atoms'. Systems of two (different) repulsive δ potentials have been used in studies of degeneracies of resonances [11, 12].

In the present paper, we study a system of two equal attractive δ potentials in a constant field. This system can be considered as a model of a homonuclear diatomic molecule in a Stark field. Here, however, we are interested in this system as a convenient model to investigate some characteristic properties of resonance states when the system parameters are varied. In particular, we demonstrate the occurrence of two types of crossing scenarios, degenerate (exceptional) points and we investigate the resonance eigenfunctions for a cyclic variation of the system parameters, when geometric (Berry) phases can be observed. Such phenomena attracted much interest in recent studies of non-Hermitian Hamiltonian systems, for example in microcavities [13] or periodic lattices in fields (Wannier–Stark systems) [14, 15] as discussed in more detail in the companion article [16].

The organization of the paper is as follows: first, we give a brief introduction to the resonance crossing scenarios. Section 3 discusses the resonance states of a single δ potential in a Stark field and section 4 contains the main results of this paper, an analysis of the resonance structure of the double δ potential in a Stark field. The final section contains a concluding discussion.

2. Crossing scenarios

In the subsequent study of the Stark resonances for the double δ well, we will observe both of the two characteristic (avoided) crossing scenarios, a familiar one and a second one, which is much less known. To simplify the discussion, we will first give a brief outline of the basic features of the crossing scenario for resonance states [16] (see also [12, 17–19]).

This crossing behaviour can be most easily discussed in terms of a simple two-state model. In addition, we can restrict ourselves in the present context to a symmetric interaction. Assuming for simplicity that only one of the states can decay, i.e. it has a width γ, the Hamilton matrix is

$$H = \begin{pmatrix} \epsilon - 2\mathrm{i}\gamma & V \\ V & -\epsilon \end{pmatrix} \qquad \epsilon, V \in \mathbb{R} \qquad \gamma \geqslant 0 \tag{1}$$

with the complex energy eigenvalues

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

In the Hermitian limit, $\gamma = 0$, the system shows the celebrated diabolic crossing scenario [20]: the eigenvalues cross for $\epsilon = V = 0$; note that even at the degeneracy two (orthogonal) eigenvectors exist. Changing a system parameter, the eigenvalues show typically an avoided crossing. Varying the system parameters ϵ and V along a closed curve, the states undergo a characteristic geometric phase change (the geometric or Berry phase) which equals π or 0 in the present case, if the crossing point is encircled or not. In the non-Hermitian case, we observe a richer scenario. We can distinguish two cases.

Type I. For small width γ, i.e. for $|V| > \gamma$, we find the well-known avoided crossing scenario illustrated in figure 1: the real parts $E_\pm$ avoid each other; for $\epsilon = 0$ their distance is smallest, given by $E_+ - E_- = 2\sqrt{V^2 - \gamma^2}$. The imaginary parts $\Gamma_\pm$ cross. Going from $\epsilon = -\infty$ to $\epsilon = +\infty$ the lower state, E_-, is first stable and the upper one, E_+, is unstable; passing through the crossing region exchanges the stability of the states.

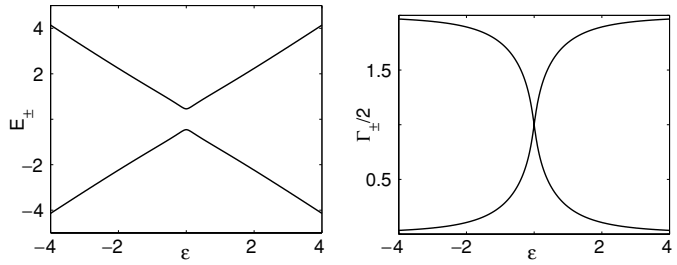

Figure 1. Type I crossing for the two-state model with decay, equation (1), for $|V| > \gamma$ and varying parameter ϵ ($\gamma = 1$, $V = 1.1$). At $\epsilon = 0$ the real parts $E_\pm$ show an avoided crossing, the imaginary parts $\Gamma_\pm$ cross.

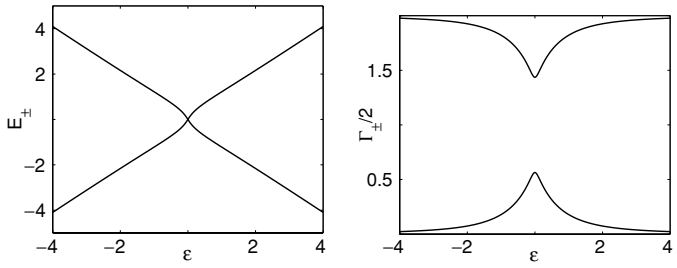

Figure 2. Type II crossing for the two-state model with decay, equation (1), for $|V| < \gamma$ and varying parameter ϵ ($\gamma = 1$, $V = 0.9$). At $\epsilon = 0$ the real parts $E_\pm$ cross and the imaginary parts $\Gamma_\pm$ show an avoided crossing.

Type II. For the case $|V| < \gamma$ the behaviour qualitatively changes. At $\epsilon = 0$ the real parts cross and the widths $\Gamma_\pm$ show an avoided crossing (separation $\Gamma_+ - \Gamma_- = 4\sqrt{\gamma^2 - V^2}$). At some distance from the crossing region the state E_- is almost stable and the other one decays. In the vicinity of the crossing, the lower state is destabilized; it can decay via a transition to the upper, unstable one. In the same way, the upper state is stabilized by the coupling to the lower one. This second type of crossings has been described first by Avron [21] in context with an analysis of the Wannier–Stark ladder of resonances (see also [22]) as well as in a more recent study of resonances in biased multiple well potentials [23]. Figure 2 illustrates this crossing type.

For a critical coupling, $V = \pm\gamma$, the two resonances coincide. Such a point in parameter space is called *exceptional point* (see [19, 24], and references given there). In order to achieve such a complex-valued coincidence, at least two real system parameters must be varied. Note, however, that such a degeneracy is *not* the complex equivalent of the real crossing in the Hermitian case. The main difference is that at an exceptional point also the eigenvectors coincide, i.e. when the non-hermiticity parameter γ is increased from zero to positive values, the diabolic point bifurcates into two exceptional ones and each of them carries one of the two eigenvectors of the diabolic degeneracy. Varying ϵ and V for fixed γ the crossings appear at the line $\epsilon = 0$ in the (ϵ, V)-plane (see figure 3). The exceptional points at $\epsilon = 0$, $V = \pm\gamma$ separate this line into different parts: for $|V| < \gamma$ the real parts of the resonance energies coincide, $E_+ = E_-$, i.e. we have type II crossings, and for $|V| > \gamma$ we have type I crossings, $\Gamma_+ = \Gamma_-$.

As can be seen in the following sections for the double δ potential in a Stark field the direct identification of an exceptional point by numerically detecting a crossing point of the

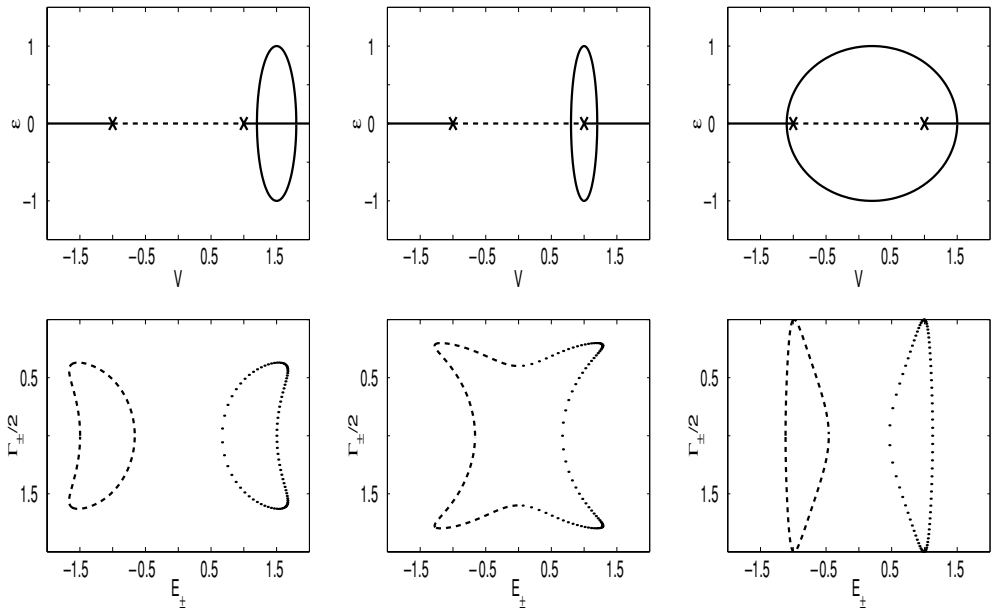

Figure 3. Eigenvalues $\mathcal{E}_+$ (dotted line) and $\mathcal{E}_-$ (dashed line) of system (1) for a curve encircling no (*a*), one (*b*) or both (*c*) exceptional points (×). The upper row shows the curves in parameter space, in the lower line the energies are plotted. At the line $\epsilon = 0$ passing through the exceptional points we have crossings of type I (—) or type II (− −). The parameter γ is set to 1.

resonances in a more realistic situation can be quite demanding and a simple criterion to show the existence of an exceptional point in a certain region is required. This can be achieved by tracing the numerically computed eigenvalues along a closed curve in parameter space.

Figure 3 shows the energies $\mathcal{E}_\pm = E_\pm - \mathrm{i}\Gamma_\pm/2$ for different closed circuits in parameter space for the two-state system (1). Three topologically different cases are shown. In cases (*a*) and (*c*), no or both exceptional points are encircled and the corresponding eigenvalues trace out two disconnected loops. In case (*b*), a single exceptional point is encircled and the two eigenvalues together form a closed curve. This behaviour is a consequence of the sequence of two different types of crossing along the circuit in case (*b*) (types I and II), so that after a full circulation in parameter space the values of the two energies $\mathcal{E}_\pm$ are interchanged.

3. A single δ quantum well

We begin our discussion with a single attractive δ potential located at x_0. The Hamiltonian of this system can be written as

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \lambda\delta(x - x_0) + Fx \tag{3}$$

with $\lambda < 0$ and $F \geqslant 0$ (units with $\hbar = 1$ and mass $m = 1$ are used). In the field-free case ($F = 0$), the spectrum of the Hamiltonian consists of a single bound state with energy

$$E_0 = -\frac{\lambda^2}{2} \tag{4}$$

and a continuous spectrum for $E \geqslant 0$. At the threshold $E = 0$, we observe some special behaviour in the limit $F \to 0$, as will become clear later on.

If a Stark field is present, $F \neq 0$, the bound state is shifted and can decay, i.e. it turns into a resonance with complex energy $\mathcal{E}_0 = E_0 - \mathrm{i}\Gamma_0/2$. Such a resonance state appears as an eigenstate of the Hamiltonian (3) with purely outgoing (Siegert) boundary conditions [25]. In the present case, the solutions for $x \neq x_0$ are linear combinations of Airy functions of types Ai and Bi

$$\psi(x;\mathcal{E}) = A\mathrm{Ai}(z) + B\mathrm{Bi}(z) \tag{5}$$

with

$$z = \alpha(Fx - \mathcal{E}) \qquad \alpha = (2/F^2)^{1/3} \tag{6}$$

(see [26]). The solutions on both sides of the δ well are connected by the conditions

$$\lim_{x\to x_0-} \psi(z(x)) = \lim_{x\to x_0+} \psi(z(x)) \tag{7}$$

$$\lim_{x\to x_0-} \psi'(z(x)) = \lim_{x\to x_0+} \psi'(z(x)) - 2\lambda \lim_{x\to x_0+} \psi(z(x)) \tag{8}$$

or, in terms of the coefficients A_-, B_- and A_+, B_+ of the solution (5) on the left-hand and the right-hand sides, respectively, as the matrix equation

$$\begin{pmatrix} \mathrm{Ai}(z_0) & \mathrm{Bi}(z_0) \\ \alpha F\mathrm{Ai}'(z_0) & \alpha F\mathrm{Bi}'(z_0) \end{pmatrix} \begin{pmatrix} A_- \\ B_- \end{pmatrix} \tag{9}$$

$$= \begin{pmatrix} \mathrm{Ai}(z_0) & \mathrm{Bi}(z_0) \\ \alpha F\mathrm{Ai}'(z_0) - 2\lambda\mathrm{Ai}(z_0) & \alpha F\mathrm{Bi}'(z_0) - 2\lambda\mathrm{Bi}(z_0) \end{pmatrix} \begin{pmatrix} A_+ \\ B_+ \end{pmatrix} \tag{10}$$

with $z_0 = z(x_0)$. These equations can be written in the form

$$\begin{pmatrix} A_- \\ B_- \end{pmatrix} = T(x_0,\mathcal{E}) \begin{pmatrix} A_+ \\ B_+ \end{pmatrix} \tag{11}$$

where the transfer matrix T is given by

$$T(x_0,\mathcal{E}) = I + \beta \begin{pmatrix} \mathrm{Bi}(z_0) \\ -\mathrm{Ai}(z_0) \end{pmatrix} (\mathrm{Ai}(z_0), \mathrm{Bi}(z_0)) = \begin{pmatrix} 1+\beta\mathrm{Ai}(z_0)\mathrm{Bi}(z_0) & \beta\mathrm{Bi}^2(z_0) \\ -\beta\mathrm{Ai}^2(z_0) & 1-\beta\mathrm{Ai}(z_0)\mathrm{Bi}(z_0) \end{pmatrix} \tag{12}$$

with $\beta = 2\pi\lambda/\alpha F = 2\pi\lambda(2F)^{-1/3}$.

Since the potential Fx increases for $x \to \infty$ and the Bi function diverges [26], the coefficients on the right-hand side must be chosen as $(A_+, B_+) \sim (1, 0)$. In order to satisfy the purely outgoing boundary conditions for the resonance states, the solution on the left-hand side must be of the form [26]

$$\mathrm{i}\,\mathrm{Ai}(z) + \mathrm{Bi}(z) = \mathrm{Ci}^+(z) \tag{13}$$

i.e. $(A_-, B_-) \sim (\mathrm{i}, 1)$ for the coefficient vector. Thus the resonance energies $\mathcal{E}$ can be calculated by solving the equation

$$\begin{pmatrix} \mathrm{i} \\ 1 \end{pmatrix} \sim T(x_0,\mathcal{E}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{14}$$

which is equivalent to

$$T_{11}(x_0,\mathcal{E}) - \mathrm{i}T_{21}(x_0,\mathcal{E}) = 0. \tag{15}$$

This is the general resonance condition for a Stark system which determines the resonance energies $\mathcal{E}_n$.

For two (or more) equal δ potentials located at x_ν, the overall transfer matrix $T(\mathcal{E})$ is simply the ordered product of the individual matrices $T(x_\nu, \mathcal{E})$ which are given in (12).

For the special case of the transfer matrix (12) for a single δ potential at $x_0 = 0$, the resonance condition reads

$$\frac{\alpha F}{2\pi\lambda} + \mathrm{Ai}(-\alpha\mathcal{E})\mathrm{Ci}^{+}(-\alpha\mathcal{E}) = 0 \tag{16}$$

which can be rewritten as

$$\frac{\alpha F}{4\pi\lambda} + \mathrm{e}^{\mathrm{i}\pi/6}\mathrm{Ai}(-\alpha\mathcal{E})\mathrm{Ai}(-\alpha\mathcal{E}\,\mathrm{e}^{\mathrm{i}2\pi/3}) = 0 \tag{17}$$

[7–9, 27, 28]. Note that the scaled energy $\alpha\mathcal{E}$ depends only on a single parameter combination, namely $\alpha F/2\pi\lambda$.

The Stark shift and the width of the bound state $\mathcal{E}_0$ as a function of the field strength F have been discussed in [9]. It is not widely known, however, that there also exist two strings of resonances $\mathcal{E}_n^{(1)}$ and $\mathcal{E}_n^{(2)}$, one along the real axis and the other rotated by an angle of approximately $-2\pi/3$ with respect to the positive real axis. Cancelling the term $\alpha F/(4\pi\lambda)$ in the resonance condition (17) ($F \to 0$), the solutions of (17) are [26]

$$\begin{aligned} \mathcal{E}_n^{(1,0)} &= \alpha^{-1}\left(-\frac{3\pi}{8} + n\frac{3\pi}{2}\right)^{2/3} \\ \mathcal{E}_n^{(2,0)} &= \alpha^{-1}\left(-\frac{3\pi}{8} + n\frac{3\pi}{2}\right)^{2/3}\mathrm{e}^{-2\pi\mathrm{i}/3} \end{aligned} \qquad n = 1, 2, 3, \ldots \tag{18}$$

and for small values of F, a Taylor expansion of (17) yields corrections to the $\mathcal{E}_n^{(k,0)}$, namely

$$\begin{aligned} \mathcal{E}_n^{(1)} &= \mathcal{E}_n^{(1,0)} + \left(\alpha^3\mathcal{E}_n^{(1,0)}\right)^{-1/2}\left(\frac{\mathrm{i}}{2} + \sqrt{\mathrm{i}\frac{\alpha F}{2\lambda}\left(\alpha\mathcal{E}_n^{(1,0)}\right)^{1/2} - \frac{1}{4}}\right) \\ \mathcal{E}_n^{(2)} &= \left[\mathcal{E}_n^{(1,0)} + \left(\alpha^3\mathcal{E}_n^{(1,0)}\right)^{-1/2}\left(-\frac{\mathrm{i}}{2} + \sqrt{-\frac{\alpha F}{2\lambda}\left(\alpha\mathcal{E}_n^{(1,0)}\right)^{1/2}\mathrm{e}^{\mathrm{i}\pi/6} - \frac{1}{4}}\right)\right]\mathrm{e}^{-2\pi\mathrm{i}/3} \end{aligned} \qquad n = 1, \ldots \tag{19}$$

(see [10] for a similar formula). In the limit $F \to 0$ all these resonances approach the limiting value $E = 0$, i.e. the continuum threshold of the field free δ potential. The results of a numerical solution of the exact resonance condition (17) for various values of F are listed in table 1. Up to a field strength of $F = 0.05$ the deviation of the approximation formulae from the exact solution is less than one per cent, for $F = 0.1$ equation (19) gives $\mathcal{E}_1^{(1)} = 0.437 - \mathrm{i}1.31 \times 10^{-2}$ which is still close to the numerically exact value in table 1. For stronger fields the approximation starts to deviate considerably from the exact values.

4. Stark resonances for a double δ well

As outlined in the last section, the properties of a single δ potential show an interesting, however quite simple dependence on the variation of the field strength F. Here we analyse the Stark resonances for a double δ potential, constructed as a combination of two identical δ potentials. Such a system can serve as a simple model for a homonuclear diatomic molecule in a static field. The distance between the two wells appears as an additional parameter of the system and the variation of both parameters, the field strength F and the distance d, provides a comprehensive reservoir of new effects which will be discussed in this section, starting from a brief discussion of the field-free case.

Table 1. Most stable resonances $\mathcal{E}_n^{(k)} = E_n^{(k)} - \mathrm{i}\Gamma_n^{(k)}/2$ for a single attractive δ-well with $\lambda = -1$ in a Stark field as a function of the field strength F. The superscripts denote the two resonance strings.

F	E_0	$\Gamma_0/2$	$E_1^{(1)}$	$\Gamma_1^{(1)}/2$	$E_2^{(1)}$	$\Gamma_2^{(1)}/2$	$E_1^{(2)}$	$\Gamma_1^{(2)}/2$
0.1	−0.5072	5.1015×10^{-4}	0.4405	1.7393×10^{-2}	0.7356	1.8916×10^{-2}	−0.2675	3.8679×10^{-1}
0.2	−0.5269	1.1744×10^{-2}	0.7088	3.8238×10^{-2}	1.1748	3.9951×10^{-2}	−0.4242	6.5635×10^{-1}
0.4	−0.5615	6.3395×10^{-2}	1.1396	8.0870×10^{-2}	1.8752	8.1390×10^{-2}	−0.6502	1.0964×10^{0}
0.6	−0.5837	1.2769×10^{-1}	1.5036	1.2316×10^{-1}	2.4643	1.2151×10^{-1}	−0.8299	1.4698×10^{0}
0.8	−0.5981	1.9560×10^{-1}	1.8298	1.6476×10^{-1}	2.9909	1.6045×10^{-1}	−0.9857	1.8054×10^{0}
1.0	−0.6072	2.6458×10^{-1}	2.1304	2.0564×10^{-1}	3.4755	1.9840×10^{-1}	−1.1260	2.1155×10^{0}

4.1. The double δ well

The field-free Hamiltonian for a symmetric double δ potential reads

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \lambda(\delta(x + d/2) + \delta(x - d/2)) \tag{20}$$

with $\lambda < 0$. It is an elementary exercise to determine the bound state conditions by writing the wavefunction as

$$\psi(x) = \begin{cases} \pm A\mathrm{e}^{+\kappa x} & x < -d/2 \\ B(\mathrm{e}^{+\kappa x} \pm \mathrm{e}^{-\kappa x}) & -d/2 < x < d/2 \\ A\,\mathrm{e}^{-\kappa x} & d/2 < x \end{cases} \tag{21}$$

with symmetry $\psi(-x) = \pm\psi(x)$. Assuming continuity of $\psi(x)$ and a jump of $\psi'(x)/\psi(x)$ by 2λ at $x = \pm d/2$, one obtains the quantization condition

$$\mathrm{e}^{-\kappa d} = \pm\left(-\frac{\kappa}{\lambda} - 1\right). \tag{22}$$

The result of a numerical solution of (22) is shown in figure 4 as a function of the distance d for $\lambda = -1$. We have (normalizable) bound states if condition (22) can be satisfied for $\kappa > 0$. This is always the case for the (even) ground state with energy $E_0 = -\kappa_0^2/2$, which monotonically increases from the combined δ well with strength 2λ for $d = 0$ (energy $E_0 = -2\lambda^2$, according to (4)) to the value $E_0 = -\lambda^2/2$ for the separated single wells for $d \to \infty$.

The situation must be clearly different for the odd state, because the single attractive δ wells for $d = 0$ and $d = \infty$ both support only a single bound state. We observe that the energy E_1 increases from $E_1 = -\lambda^2/2$ with decreasing distance d until it reaches $E_1 = 0$ at a critical distance $d_\mathrm{c} = 1/\lambda$. For smaller distances, E_1 decreases again (see figure 4), however with negative values of κ, i.e. we have a resonance state (more precisely an anti-bound state [29]). In addition, there are many more resonances at complex energies $E_n = -\kappa_n^2/2$. This can be conveniently seen by taking the logarithm of (22):

$$\kappa_n d = \mathrm{i}\pi n - \ln\left(-\frac{\kappa_n}{\lambda} - 1\right) \qquad n = 0, 1, 2, \ldots \tag{23}$$

with complex solutions κ_n. The behaviour of such double δ well resonances, in particular also for complex values of the strength parameter λ, has been investigated by Romo [30] in connection with the closely related problem of s-wave scattering from a surface δ potential.

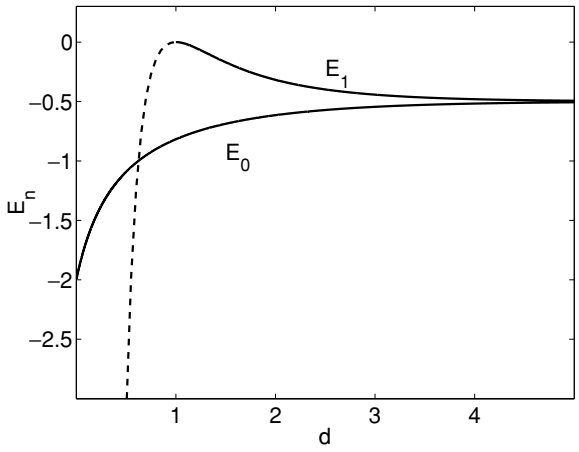

Figure 4. Energy eigenvalues E_0 and E_1 for the lowest even and odd states for the field-free symmetric double δ well ($\lambda = -1$) as a function of the distance d. For $d < d_c = 1/\lambda$, the odd state becomes virtual (dashed line).

4.2. Stark resonances: eigenvalues

For the following discussion of the resonance states of a double δ well in a constant field, it is convenient to choose coordinates centred at one of the wells, i.e. we consider the Hamiltonian

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \lambda(\delta(x) + \delta(x-d)) + Fx \tag{24}$$

($d > 0$) with the transfer matrix (see section 3)

$$T(\mathcal{E}) = T(0,\mathcal{E})T(d,\mathcal{E}) \tag{25}$$

which leads to

$$\begin{aligned} T(\mathcal{E}) = I &+ \beta\begin{pmatrix}\mathrm{Bi}(z_0)\\ -\mathrm{Ai}(z_0)\end{pmatrix}(\mathrm{Ai}(z_0),\mathrm{Bi}(z_0)) + \beta\begin{pmatrix}\mathrm{Bi}(z_d)\\ -\mathrm{Ai}(z_d)\end{pmatrix}(\mathrm{Ai}(z_d),\mathrm{Bi}(z_d)) \\ &+ \beta^2 w\begin{pmatrix}\mathrm{Bi}(z_0)\\ -\mathrm{Ai}(z_0)\end{pmatrix}(\mathrm{Ai}(z_d),\mathrm{Bi}(z_d)) \end{aligned} \tag{26}$$

with $z_0 = -\alpha\mathcal{E}$, $z_d = \alpha(Fd - \mathcal{E})$ and

$$w = (\mathrm{Ai}(z_0),\mathrm{Bi}(z_0))\begin{pmatrix}\mathrm{Bi}(z_d)\\ -\mathrm{Ai}(z_d)\end{pmatrix} = \mathrm{Ai}(z_0)\mathrm{Bi}(z_d) - \mathrm{Bi}(z_0)\mathrm{Ai}(z_d). \tag{27}$$

Explicitly, the matrix elements of the resulting transfer matrix are

$$\begin{aligned} T_{11} &= 1 + \beta\mathrm{Ai}(z_0)\mathrm{Bi}(z_0) + \beta\mathrm{Ai}(z_d)\mathrm{Bi}(z_d) + \beta^2 w\mathrm{Ai}(z_d)\mathrm{Bi}(z_0) \\ T_{12} &= \beta\mathrm{Bi}^2(z_0) + \beta\mathrm{Bi}^2(z_d) + \beta^2 w\mathrm{Bi}(z_0)\mathrm{Bi}(z_d) \\ T_{21} &= -\beta\mathrm{Ai}^2(z_0) - \beta\mathrm{Ai}^2(z_d) - \beta^2 w\mathrm{Ai}(z_0)\mathrm{Ai}(z_d) \\ T_{22} &= 1 - \beta\mathrm{Ai}(z_0)\mathrm{Bi}(z_0) - \beta\mathrm{Ai}(z_d)\mathrm{Bi}(z_d) - \beta^2 w\mathrm{Ai}(z_0)\mathrm{Bi}(z_d) \end{aligned} \tag{28}$$

and the resonance condition (15) reads

$$T_{11} - \mathrm{i}T_{21} = 1 + \beta(\mathrm{Ai}(z_0) + \beta w\mathrm{Ai}(z_d))\mathrm{Ci}^+(z_0) + \beta\mathrm{Ai}(z_d)\mathrm{Ci}^+(z_d) = 0. \tag{29}$$

In the following we will analyse the resonance structures when the parameters of the system, the distance d and the field strength F, are varied. Clearly, there are two limiting

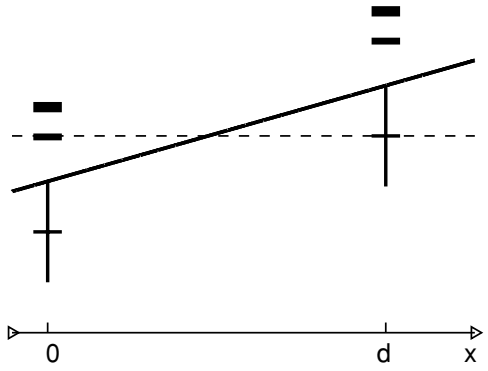

Figure 5. Schematic illustration of a system of two equal attractive δ potentials at a distance d in a Stark potential Fx. For each potential well three resonant states are marked by a line, whose thickness denotes the width. If the field strength F or the distance d is varied, resonant tunnelling phenomena are observed.

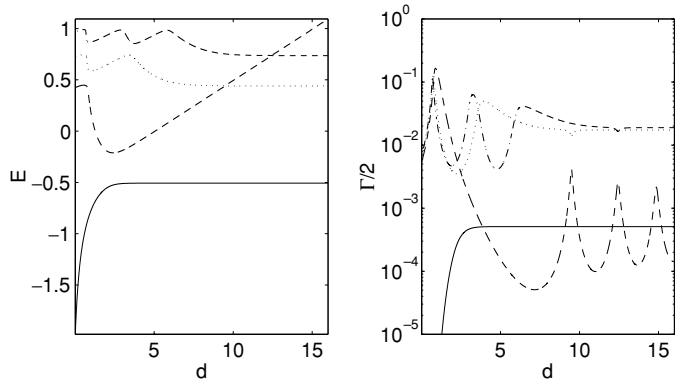

Figure 6. Real and imaginary parts of the four most stable double δ well resonance energies for a field $F = 0.1$ and $\lambda = -1$ as a function of the distance d of the potentials.

cases, where the problem simplifies: for large values of d we have a superposition of two independent δ potentials, and in the limit $d \to 0$ the two δ wells join to a single one with doubled strength parameter 2λ.

Figure 5 shows a schematic illustration of the situation. The two attractive δ peaks in the Stark field are shown with three resonance states, respectively. A variation of the field strength F and the distance d produces, in a first approximation, a shift of the energies by $d\Delta F$ or $F\Delta d$, respectively. Interesting effects are expected in the vicinity of the crossings of the resonances, where resonant tunnelling occurs.

Results of a numerical solution of the resonance condition (29) for $\lambda = -1$ and $F = 0.1$ are shown in figure 6. The real and imaginary parts of the four most stable resonances are shown as a function of the distance d. Both type I and type II crossings are observed. In the limit $d \to 0$, the lowest resonance tends to $E \approx -2\lambda^2 = -2$, i.e. the field-free bound for a single δ potential with strength 2λ, while the energies E of the others remain positive. For large values of d, the three lowest states, which are almost independent of the distance in this region, can be identified with the resonances $\mathcal{E}_0$, $\mathcal{E}_1^{(1)}$ and $\mathcal{E}_2^{(1)}$ in the case of one δ potential (compare table 1). Whereas the fourth state corresponds to the ground state of the right hand

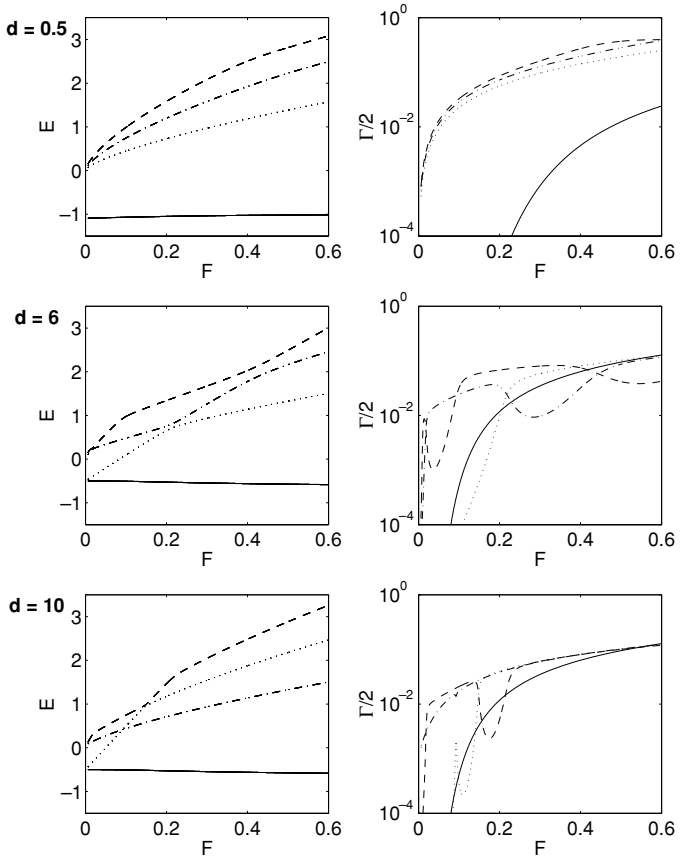

Figure 7. Real and imaginary parts of the four most stable double δ well resonance energies for potential distances of $d = 0.5$, $d = 6$ and $d = 10$ as a function of the Stark field.

δ well at $x = d$. Its real part decreases as $E_0 + Fd$ with decreasing distance d, so that this state shows a sequence of crossings with the resonances of the δ well at $x = 0$. The coupling between these states is weak and the crossings are of type II (compare section 2). The width of this state is increased by two orders of magnitude at these crossings which is known as the phenomenon of resonant tunnelling [22]. If the distance is furthermore decreased, the two most stable resonances approach each other and show a crossing in the region $d \approx 3$. This value can be understood by the following argument: considering the case of one δ potential at x_0 for $F = 0$, the wavefunction reads $\psi(x) = \sqrt{-\lambda}\exp\{\lambda(x - x_0)\}$. So if the two peaks have a distance of the order $2/|\lambda|$, the states start to interact noticeably and show a crossing scenario. Here, the coupling of the two ground states is strong compared to the width and the crossing is of type I (see section 2). More such type I crossings can be seen for the higher resonances in this region.

Figure 7 shows the behaviour of the resonances for a varying field strength F for three distances $d = 0.5, 6, 10$, which show qualitatively different trends. For small distances, $d = 0.5$, the real part of the lowest resonance tends to a negative value for $F \to 0$ while the others converge to 0 (see also figure 4). There are exclusively type I crossings. For an intermediate distance, $d = 6$, a second resonance converges to a negative value for $F \to 0$.

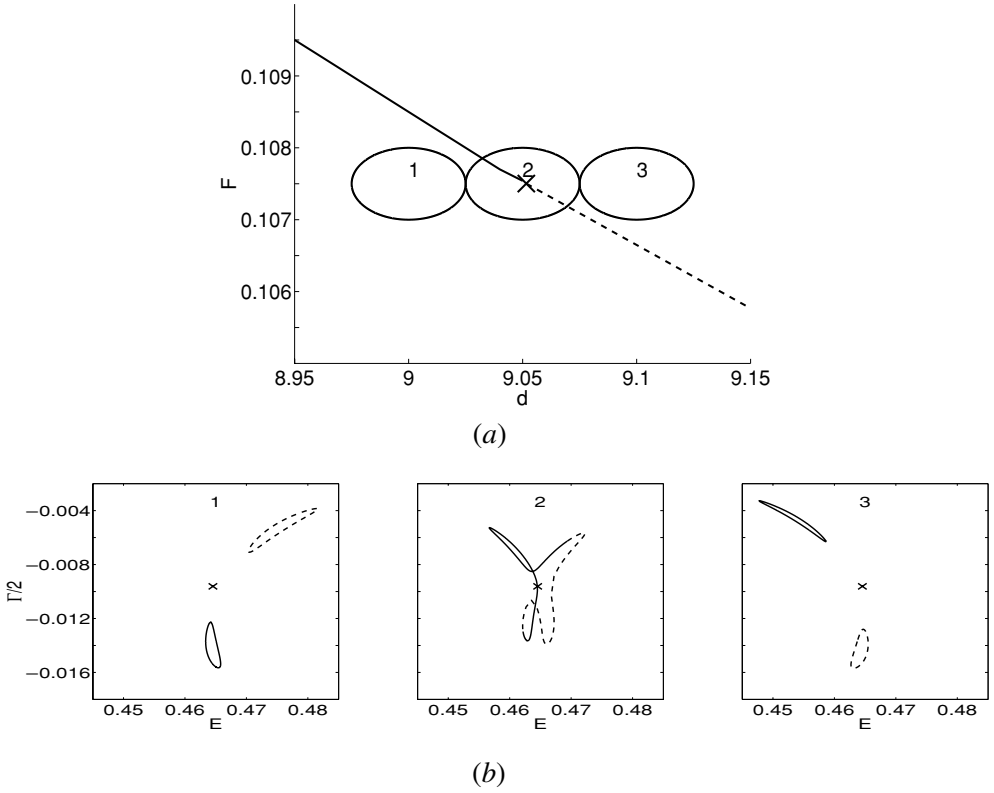

Figure 8. For a cyclic variation of the system parameters F and d shown in (a) the energy eigenvalues $\mathcal{E}_1$ and $\mathcal{E}_2$ shown in (b) trace out a single closed curve (case 2) or two separate ones (cases 1 and 3) in the complex plane, if the exceptional point ($\times$) is encircled or not. On the full line and the dashed line in (a) the states undergo a type I or type II crossing, respectively.

Again, only type I crossings are observed. At large distances, $d = 10$, crossings of type II dominate. For example, the second resonance, labelled $\mathcal{E}_1$ in the following, and the third, labelled $\mathcal{E}_2$, printed as a dotted and a dashed dotted curve in figure 7, show a type II crossing at $F \approx 0.1$ instead of a type I crossing at $F \approx 0.2$ for $d = 6$. Hence, for this pair of resonances the crossing behaviour changes from type I for $d = 0.5$ and $d = 6$ to type II for $d = 10$ and from the discussion in section 2 the existence of an exceptional point can be conjectured. It is quite easy to estimate this exceptional point at $F_c \approx 0.1$, $d_c \approx 9$. (Note that in figure 6 the spikes of the imaginary part almost touch each other at this point.)

In figure 8 the motion of this pair of energy eigenvalues is shown for cyclic variation of the parameters (see figure 8(a)). As in figure 3, the two energies together trace out a single closed curve when the exceptional point is encircled in parameter space (cycle 2) and two separated curves if this is not the case (cycles 1 and 3). It should be pointed out that such an identification is simple, in particular it does not require an identification of the two states or the corresponding eigenstates. Based on this technique, the exceptional point can be numerically localized at

$$d_c \approx 9.051\,59 \qquad F_c \approx 0.107\,50 \tag{30}$$

for this double δ system. Note that these values obtained for a potential strength parameter $\lambda = -1$ are in fact general, because any other (negative) value of $\lambda < 0$ can be mapped to this

case by scaling the coordinate $x' = ax$ using $a = -1/\lambda$, which implies $\lambda' = a\lambda$, $F' = a^3 F$ and $H' = a^2 H$.

The line through the exceptional point (marked by a cross in figure 3(*a*)) is the curve where crossings appear, more specifically we have type I (—) or type II (−−) crossings.

4.3. Stark resonances: eigenvectors

So far we have only discussed the eigenvalues of the Hamiltonian. But the eigenvectors also show an interesting behaviour when passing through a curve in parameter space, especially if an exceptional point is encircled. This case is the subject of the following section.

First of all, since the eigenvalues of the Hamiltonian interchange after a full circulation around the exceptional point, the eigenvectors have a periodicity of at least 4π. But before we can make precise statements, we have to go into a detailed discussion about eigenfunctions of non-Hermitian operators. For such an operator it is convenient to use besides the right eigenvectors $H\psi = \mathcal{E}\psi$ of the Hamiltonian the left eigenvectors, defined by

$$H^\dagger \chi = \mathcal{E}^* \chi. \tag{31}$$

$H^\dagger$ is the adjoint operator of H with the boundary condition

$$\chi(x) \underset{x\to-\infty}{\longrightarrow} c[-\mathrm{iAi}(z(x)) + \mathrm{Bi}(z(x))] \tag{32}$$

(cp [31]). This condition describes a purely *incoming* wavefunction. It can be directly seen that, if ψ is a right eigenvector of H, ψ^* is an eigenvector of $H^\dagger$ with eigenvalue $\mathcal{E}^*$ and fulfills the boundary condition (32). So we get for this Hamiltonian

$$\chi = \psi^*. \tag{33}$$

Finally, the normalization of the eigenstates has to be considered. We choose our eigenstates to satisfy a box normalization

$$\int_{-L}^{L} \chi_n^*(x)\psi_n(x)\,\mathrm{d}x = \int_{-L}^{L} \psi_n^2(x)\,\mathrm{d}x = 1 \qquad n = 1, 2 \tag{34}$$

where the value of L is chosen large enough, so that all the essential physics is captured. We do not consider the limit $L \to \infty$ here, because of the lack of convergence of the integrals for a Stark system. In particular, a regularization of the integral may be required to define a generalized scalar product similar to the one developed by Berggren [32, 33] in conventional scattering theory without a Stark field (see also [34, 35]). Here we used $L = 30$. With this value, the two states ψ_1 and ψ_2 belonging to the energies $\mathcal{E}_1$ resp. $\mathcal{E}_2$ are almost orthogonal,

$$\left|\int_{-L}^{L} \chi_1^*(x)\psi_2(x)\,\mathrm{d}x\right| = \left|\int_{-L}^{L} \psi_1(x)\psi_2(x)\,\mathrm{d}x\right| < 10^{-3} \tag{35}$$

i.e. the sets of eigenvectors ψ_1, ψ_2 and χ_1, χ_2 form (almost) bi-orthogonal sets [31].

It is important to note that the condition (34) determines the eigenfunction up to a sign, and not only up to a phase factor as usual. This eliminates the notorious problem of defining the phase as a function of the system parameters because the sign can be easily chosen to make the eigenstates continuous. An exception is the points in parameter space, where only a single eigenstate exists, i.e. where the eigenstates coalesce, the exceptional points (see section 2). Obviously, such an unambiguous phase assignment provides a convenient basis for calculating the geometric Berry phases as discussed in detail in [16].

Here we follow the eigenfunctions ψ_1 and ψ_2 (normalized as described above) for a variation of the two system parameters F and d along a cyclic path around the exceptional point (30) in parameter space. The curve is parametrized by an angle ϕ, where for $\phi = 2\pi$ a

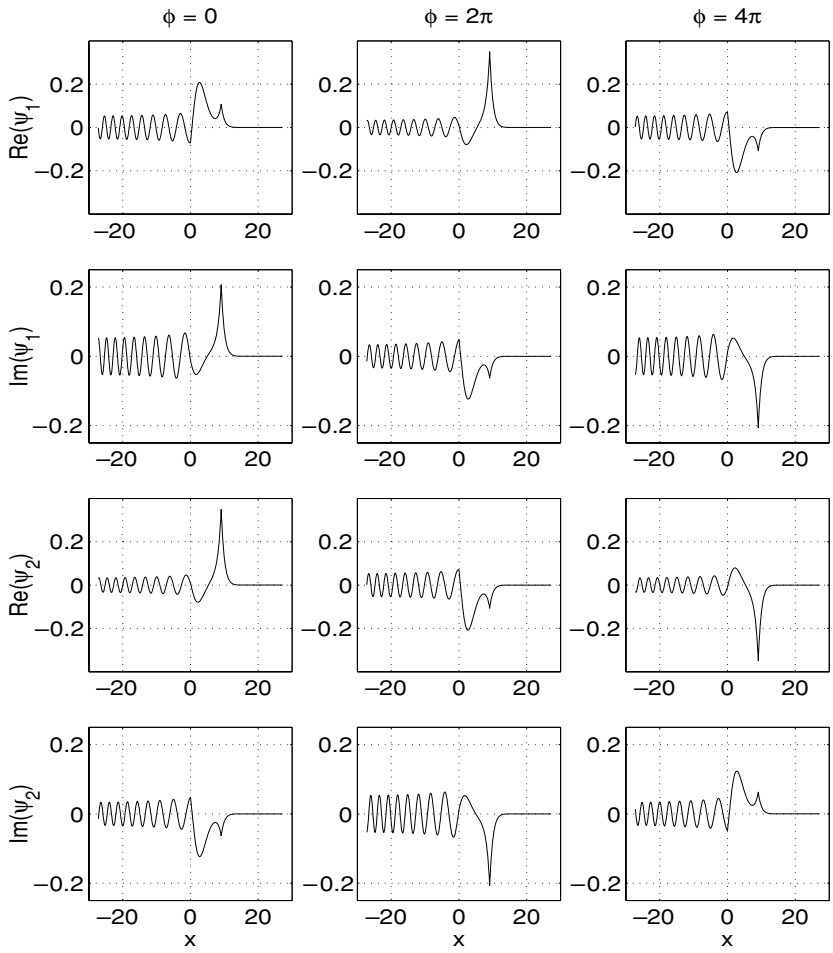

Figure 9. Real and imaginary parts of the normalized wavefunctions ψ_1 and ψ_2 for a cyclic variation of the system parameters for $\phi = 0, 2\pi$ and 4π if the exceptional point is enclosed. The path is circle 2 shown in figure 8(*a*).

single cycle is completed and the initial parameter values are reached again, after an additional increase of ϕ by 2π the exceptional point is encircled twice, and so on.

The result of the numerical computations shown in figure 9 exhibits the scenario analysed in [16] for the eigenvectors of a symmetric non-Hermitian 2×2 Hamiltonian. After a single cycle (2π) the two states are interchanged with a relative sign change, after another cycle of 2π the original states are recovered, however up to a sign factor:

$$\psi_1 \xrightarrow{2\pi} \quad \psi_2 \xrightarrow{2\pi} -\psi_1 \tag{36}$$

$$\psi_2 \xrightarrow{2\pi} -\psi_1 \xrightarrow{2\pi} -\psi_2. \tag{37}$$

Four cycles are required to reach the initial configuration again.

Of special interest are the wavefunctions after two cycles around the exceptional point. There the wavefunctions reproduce each other up to a phase factor of $\exp\{-\mathrm{i}\pi\}$. This factor directly corresponds to the *geometric* or Berry phase γ for an adiabatic evolution of the system

parameters, i.e. the initial state is reproduced up to a phase factor $\exp\{-i\gamma\}$ [20, 36, 37]. As shown in [16], the geometric phase can be written as

$$\gamma_n = i\int_{\mathbf{C}} \langle\chi_n|\nabla_{\mathbf{C}}\psi_n\rangle d\mathbf{C} - i\ln\langle\chi_n(T)|\psi_n(0)\rangle \qquad n = 1, 2 \tag{38}$$

where $\mathbf{C}(t), 0 \leqslant t \leqslant T$ describes a closed curve in parameter space and $\langle\cdot|\cdot\rangle$ is the intrinsic scalar product of $\mathbb{C}^2$. For the special case $\chi = \psi^*$, the normalization $\langle\chi|\psi\rangle = 1$ gives $\langle\chi|\nabla_{\mathbf{C}}\psi\rangle = 0$ and the geometric phase is determined by

$$\gamma_n = -i\ln\langle\chi_n(T)|\psi_n(0)\rangle. \tag{39}$$

Applied to the case of two cycles around the exceptional point, this gives

$$\gamma_n = \pi \qquad n = 1, 2 \tag{40}$$

in agreement with the numerical results shown in figure 9.

5. Conclusions

We have presented a detailed investigation of the resonance states of a symmetric double δ well in a constant (Stark) field. In particular, the dependence on the (two) system parameters, the distance of the δ potentials and the field strength is discussed. We have shown that this simple model exhibits several interesting effects, as for instance a clear exceptional point in the parameter space, where two of the low-lying resonance states are degenerate. Varying a single-system parameter, the two different types of eigenvalue crossing scenarios can be observed. Characteristic properties concerning these two isolated resonances can be described in a simple two-state model. Especially, the behaviour of energies and wavefunctions in the vicinity of the exceptional point is well understood.

Finally, it should be mentioned that there is still an open general problem related to Stark resonances, namely the proper normalization of resonance states or, more generally, the proper scalar product for resonance states (compare with the discussion in section 4.3). This basic problem has apparently not been considered in previous studies and we hope that the present paper will stimulate further studies in this direction.

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Note added in proof. The authors thank the referee for drawing their attention to the rigged Hilbert space formulation of quantum mechanics which provides an alternative (and more rigorous) treatment of resonance states. For references, see the paper by Bohm *et al* [38], where also a discussion of degeneracies of unbound states in the rigged Hilbert space formulation can be found.

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