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Perturbation theory for the Stark effect in a double δ quantum well

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Abstract

We study the Stark effect in a symmetric double δ quantum well, for which there are two kinds of resonances: the familiar resonances stemming from the bound states, and a doubly infinite family of resonances stemming from the zero-field continuum threshold. We derive explicit expressions for the Borel-summable Rayleigh–Schrödinger perturbation series for the resonances stemming from the bound states, for the imaginary part of these same resonances and for all the resonances stemming from the zero-field continuum threshold. The techniques used in this paper are directly applicable to realistic models of quantum square well potentials with or without barriers.

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1. Introduction

Besides its interest as a simple almost exactly solvable model in quantum mechanics [1, 2], the one-dimensional δ quantum well has attracted attention as a realistic model in several physical situations, usually in the context of photodetachment or photoionization in the presence of electric fields. For example, it is well-known that in the presence of a static electric field the unique bound state of a δ potential well turns into a resonance and Elberfeld and Kleber [3] used this resonance as a model for tunnelling in ultrathin $\mathrm{GaAs}/\mathrm{Ga}_x\mathrm{Al}_{1-x}\mathrm{As}$ quantum wells, deriving low and high-field asymptotic expansions for both its real part and its imaginary part.

But already in 1987 Ludviksson [4] had shown that in addition to this well-known resonance stemming from the bound state, there is a doubly infinite family of resonances originating from the zero-field continuum threshold. In this same paper, Ludviksson also derived lowest-order asymptotic formulae for the positions of these resonances in the complex energy plane as the applied electric field tends to zero. The role of these resonances in photodetachment of H^- by weak periodic fields has been discussed recently by Emmanouilidou and Reichl [5], who showed that the model reproduces several qualitative features of the experimental cross section. Also very recently, Álvarez and Sundaram [6] discussed the systematic derivation of low and high-field asymptotic expansions for all these resonances, and tracked them numerically as functions of the electric field, thus giving a complete picture of their behaviour in the complex energy plane. Apparently unaware of Ludviksson's paper, Cavalcanti, Giacconi and Soldati [7] have given an independent proof of the existence of the threshold resonances and, with due care of the required regularization, extended the results to two and three dimensions. We would like to mention also that the appearance of Stark resonances without bound-state predecessors in the local short-range Hulthén and Yukawa potentials has been studied numerically by González-Férez and Schweizer [8].

The double δ quantum well to which this paper is devoted was initially studied as a model for the hydrogen molecular ion H_2^+. This model, although clearly less realistic, permits simplified treatments of typical double well phenomena as the exponentially small splitting between pairs of quasi-degenerate energy levels [9–13], and appears naturally in dimensional perturbation theory [14]. From the scattering theory point of view [1, 2], the main difference between the single δ and the double δ quantum wells is the appearance in the latter of intrinsic (i.e. not induced by the external field) resonances. These resonances have been studied theoretically by Albeverio and Høegh-Krohn [15], who used them as an example in their general perturbation theory for resonances, while their physical consequences were quantified by Álvarez and Silverstone [16], who derived an exact expansion of the photoionization cross section of a particle in a double δ quantum well by a weak periodic field as a sum over these resonances plus a slowly varying background term.

Less studied, however, is the Stark effect in the double δ quantum well, despite an ongoing interest in resonances induced by electric fields in quantum wells [17, 18]. The most relevant contribution seems to be a recent paper by Korsch and Mossmann [19] in a different context: as we will show in the next section, there are two independent parameters in the corresponding Hamiltonian, and Korsch and Mossmann use it as a convenient model to study the properties of resonance states as these parameters are varied. Concretely, they derive the condition for the existence of resonances, demonstrate the existence of two types of crossing scenarios and investigate the resonance eigenfunctions for cyclic variations of the parameters where geometric phases can be observed. However, a systematic study of the Stark effect in the double δ quantum well, with a characterization of all the resonances and their behaviours as functions of the applied field seems to be lacking.

In this paper we present a complete discussion of the Stark effect in the double δ quantum well from the point of view of perturbation theory. In section 2 we first quickly review the field-free case in a form and with a notation suitable for later use, and then proceed to a straightforward derivation of the condition for the existence of resonances. Section 3 is devoted to the resonances stemming from the bound states: we first show how to calculate explicitly as many terms as desired of the Borel-summable Rayleigh–Schrödinger perturbation theory power series (in which the imaginary part of the resonances appears implicitly in the process of Borel summation), and then we calculate an explicit asymptotic expansion for the exponentially small imaginary part of these resonances. In section 4 we study the two families of resonances stemming from the continuum threshold and show that they can be described either by an 'exact' Puiseux series or by an asymptotic expansion derived from it. The paper ends with a brief summary of the main ideas and of possible applications of the results herein.

2. The Stark effect in a double δ quantum well

The time-independent Schrödinger equation for a particle of mass m and electric charge e in a double δ quantum well and an external uniform electric field F_c reads

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x_c^2} - g_c(\delta(x_c+a)+\delta(x_c-a)) - eF_c x_c\right)\Psi(x_c) = E_c\Psi(x_c) \tag{1}$$

where the subindex 'c' denotes conventional units and we take the distance between the wells $2a > 0$, the coupling constant $g_c > 0$ (so that we have in fact wells and not barriers) and the applied electric field $F_c \geqslant 0$.

By scaling the independent and dependent variables and the parameters in equation (1) according to

$$x = x_c/a \qquad \psi(x) = \Psi(x_c) \tag{2}$$

$$g = mag_c/\hbar^2 \qquad F = mea^3F_c/\hbar^2 \qquad E = ma^2E_c/\hbar^2 \tag{3}$$

we can transform the Schrödinger equation into the form

$$\left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - g(\delta(x+1)+\delta(x-1)) - Fx\right)\psi(x) = E\psi(x) \tag{4}$$

where $g > 0$ and $F \geqslant 0$. In this section we will first review the analytic structure of the unperturbed case $F = 0$ and then proceed to a straightforward derivation of the condition for the existence of resonances in the perturbed case $F > 0$.

2.1. The unperturbed double δ well

Since the Schrödinger equation (4) with $F = 0$ is invariant under the parity transformation $x \to -x$, we will look separately for its even and odd solutions. We write the even solutions in the form

$$\psi_k^{(+)}(x) = \begin{cases} (1/2)[F_+(k)\,\mathrm{e}^{\mathrm{i}kx} + F_+(-k)\,\mathrm{e}^{-\mathrm{i}kx}] & x < -1 \\ \cos(kx) & -1 \leqslant x \leqslant 1 \\ (1/2)[F_+(k)\,\mathrm{e}^{-\mathrm{i}kx} + F_+(-k)\,\mathrm{e}^{\mathrm{i}kx}] & 1 < x \end{cases} \tag{5}$$

where

$$E = \tfrac{1}{2}k^2 \tag{6}$$

and the Jost function $F_+(k)$ is determined by the continuity of the wavefunction at $x = \pm 1$ and by the discontinuity of its derivative at the same points, which must be $-2g\psi(\pm 1)$. Since the wavefunction (5) is even by construction, it is enough to require

$$\psi_k^{(+)}(1+) - \psi_k^{(+)}(1-) = 0 \tag{7}$$

$$\psi_k^{(+)\prime}(1+) - \psi_k^{(+)\prime}(1-) = -2g\psi_k^{(+)}(1) \tag{8}$$

from which follows immediately

$$F_+(k) = 1 + \frac{\mathrm{i}g}{k}(-\mathrm{e}^{2\mathrm{i}k} - 1). \tag{9}$$

Likewise, the odd solutions of equation (4) with $F = 0$ can be written in the form

$$\psi_k^{(-)}(x) = \begin{cases} (\mathrm{i}/2)[F_-(-k)\,\mathrm{e}^{-\mathrm{i}kx} - F_-(k)\,\mathrm{e}^{\mathrm{i}kx}] & x < -1 \\ \sin(kx) & -1 \leqslant x \leqslant 1 \\ (\mathrm{i}/2)[F_-(k)\,\mathrm{e}^{-\mathrm{i}kx} - F_-(-k)\,\mathrm{e}^{\mathrm{i}kx}] & 1 < x \end{cases} \tag{10}$$

and by imposing the same matching conditions we find

$$F_-(k) = 1 + \frac{\mathrm{i}g}{k}(\mathrm{e}^{2\mathrm{i}k} - 1). \tag{11}$$

For later reference we point out that the even and odd Jost functions differ in just one sign, and can be written jointly as

$$F_\mp(k) = 1 + \frac{\mathrm{i}g}{k}(\pm\mathrm{e}^{2\mathrm{i}k} - 1). \tag{12}$$

We also note that $F_-(k)$ and $kF_+(k)$ are entire functions of k and that

$$\overline{F_\mp(-\overline{k})} = F_\mp(k). \tag{13}$$

In particular, for k real the wavefunctions are real and

$$\int_{-\infty}^{\infty} \psi_k^{(\pm)}(x)\psi_{k'}^{(\pm)}(x)\,\mathrm{d}x = \pi F_\pm(k)F_\pm(-k)\delta(k-k'). \tag{14}$$

The bound states correspond to solutions of $F_\pm(k) = 0$ of the form $k = \mathrm{i}\kappa$ with $\kappa > 0$, i.e. to the real positive solutions of the equations

$$\frac{\kappa}{g} - 1 = \pm\mathrm{e}^{-2\kappa}. \tag{15}$$

It is immediately verified that the double δ quantum well has exactly one even-parity bound state and, if $2g > 1$, exactly one odd-parity bound state. For large values of g the corresponding solutions $\kappa_\pm$ of equation (15) have the asymptotic behaviours

$$\kappa_\pm \sim g \pm g\,\mathrm{e}^{-2g} + \cdots \qquad g \to \infty \tag{16}$$

and as is typical of double-well potentials, the energy difference between the odd and even bound states is exponentially small in the coupling constant g

$$\Delta E = E_- - E_+ = \tfrac{1}{2}\left(\kappa_+^2 - \kappa_-^2\right) \sim 2g^2\,\mathrm{e}^{-2g} + \cdots \qquad g \to \infty. \tag{17}$$

In addition there are infinitely many nonreal zeros of the even Jost function, all of them in the lower half k plane, and asymptotically given by

$$\begin{aligned} k_+ = \pi\left(n + \frac{1}{2}\right)&\left[1 + \frac{1}{2g} + \frac{1}{(2g)^2} + \frac{1 - \frac{4}{3}\pi^2\left(n + \frac{1}{2}\right)^2}{(2g)^3} + \cdots\right] \\ &- \mathrm{i}\pi^2\left(n + \frac{1}{2}\right)^2\left[\frac{1}{(2g)^2} + \frac{3}{(2g)^3} + \cdots\right] \qquad n = 0, \pm1, \pm2, \ldots \quad g \to \infty \end{aligned} \tag{18}$$

and infinitely many nonreal zeros of the odd Jost function, all of them in the lower half k plane, with asymptotic behaviours

$$\begin{aligned} k_- = \pi n&\left[1 + \frac{1}{2g} + \frac{1}{(2g)^2} + \frac{1 - \frac{4}{3}\pi^2 n^2}{(2g)^3} + \cdots\right] - \mathrm{i}\pi^2 n^2\left[\frac{1}{(2g)^2} + \frac{3}{(2g)^3} + \cdots\right] \\ &n = \pm1, \pm2, \ldots \quad g \to \infty. \end{aligned} \tag{19}$$

Note that as a consequence of equation (13) these resonances can be grouped in pairs of the form $k = \pm\mathrm{Re}\,(k) - \mathrm{i}|\mathrm{Im}\,(k)|$. Some authors [1] apply the term resonance to all the zeros in equations (18) and (19), while others [2] reserve it for the zeros with $\mathrm{Re}\,k > 0$ and $\mathrm{Im}\,k < 0$. The first usage of the term is motivated by considering the resonances as (all) the poles of the resolvent in the lower half k plane; the second, by the fact that if $|\mathrm{Im}\,k|$ is sufficiently small and the resonances are well-separated, each one may give a directly observable peak in, for example, the photoionization cross section [16]. In any event, we want to stress that because they satisfy $F_\pm(k) = 0$, equations (5) and (10) show that these latter intrinsic resonances with $\mathrm{Re}\,k > 0$ correspond to purely outgoing waves in both directions of the real axis.

2.2. The perturbed double δ well

Let us consider now the Schrödinger equation (4) with $F > 0$, which corresponds to a piecewise linear potential whose solutions can be written in terms of Airy functions [20]. It is well-known from functional-analytic methods that the spectrum of the Stark operator is absolutely continuous and fills the real line [21]. Since the linear potential tends to $+\infty$ as $x \to -\infty$, there is only one bounded linearly independent solution of equation (4) for each real value of E. Equivalently, as $x \to -\infty$ we have to use the exponentially decreasing Airy function $\mathrm{Ai}(-(2F)^{1/3}(x + E/F))$, which has to be connected with linear combinations of $\mathrm{Ai}(-(2F)^{1/3}(x + E/F))$ and $\mathrm{Bi}(-(2F)^{1/3}(x + E/F))$ across the two centres $x = \mp 1$ of the δ potentials.

However, anticipating the calculation of resonances, we will write the solution for $1 < x$ directly in terms of the linear combinations of $\mathrm{Ai}(z)$ and $\mathrm{Bi}(z)$ with purely outgoing and incoming behaviour as $z = -(2F)^{1/3}(x + E/F) \to -\infty$, for which we use the notation of reference [22]:

$$\mathrm{Ai}^{(\pm)}(z) = \mathrm{Bi}(z) \pm \mathrm{i}\,\mathrm{Ai}(z) = 2\,\mathrm{e}^{\pm \mathrm{i}\pi/6}\,\mathrm{Ai}(\mathrm{e}^{\pm 2\pi \mathrm{i}/3} z). \tag{20}$$

Summing up, for given values of E and $F > 0$ we write the solution of equation (4) in the form

$$\psi(x) = \begin{cases} \mathrm{Ai}(z(x)) & x < -1 \\ c^{(A)}\,\mathrm{Ai}(z(x)) + c^{(B)}\,\mathrm{Bi}(z(x)) & -1 \leqslant x \leqslant 1 \\ c^{(+)}\,\mathrm{Ai}^{(+)}(z(x)) + c^{(-)}\,\mathrm{Ai}^{(-)}(z(x)) & 1 < x \end{cases} \tag{21}$$

where

$$z(x) = -(2F)^{1/3}(x + E/F). \tag{22}$$

By imposing the continuity of the wavefunction and the discontinuity of its derivative at $x = \mp 1$ we arrive at a set of four linear equations which are readily solved for the four coefficients $c^{(A)}$, $c^{(B)}$, $c^{(+)}$ and $c^{(-)}$ as functions of the energy E (the resulting expressions can be greatly simplified using the Wronskian of the Airy functions $W(\mathrm{Ai}(z), \mathrm{Bi}(z)) = 1/\pi$). In this perturbed case, the resonances correspond to purely outgoing waves as $x \to +\infty$ (and therefore $z(x) \to -\infty$), i.e. to complex solutions of $c^{(-)}(E) = 0$. This condition for the existence of resonances can be conveniently written in terms of the following parameters

$$\gamma = 2^{2/3} g / F^{1/3} \tag{23}$$

$$z_+ = z(1) = -(2F)^{1/3}(1 + E/F) \tag{24}$$

$$z_- = z(-1) = -(2F)^{1/3}(-1 + E/F) \tag{25}$$

and reads

$$\begin{aligned} 1 = \gamma\pi[&\mathrm{Ai}(z_+)\,\mathrm{Ai}^{(+)}(z_+) + \mathrm{Ai}(z_-)\,\mathrm{Ai}^{(+)}(z_-)] \\ &+ (\gamma\pi)^2\,\mathrm{Ai}^{(+)}(z_+)\,\mathrm{Ai}(z_-)[\mathrm{Ai}^{(+)}(z_+)\,\mathrm{Ai}(z_-) - \mathrm{Ai}(z_+)\,\mathrm{Ai}^{(+)}(z_-)]. \end{aligned} \tag{26}$$

Equation (26) with a different scaling has been derived by the equivalent transfer-matrix formalism by Korsch and Mossmann [19], who used it for their numerical studies of the variation of the resonances as the distance between the wells and the applied electric field are varied. We devote the rest of the paper to a systematic analytic study of all the solutions of the resonance condition (26) from the point of view of perturbation theory, and to the ensuing relation with the bound states and resonances of the unperturbed double well discussed at the beginning of this section.

3. Resonances stemming from the bound states

We devote this section to the resonances stemming from the bound states, where the particle, initially confined in the potential well, escapes towards $x = +\infty$ by tunnelling, and we expect an exponentially small width. In other words, we look for solutions $E(F)$ of the resonance condition (26) that in the limit $F \to 0$ tend to the unperturbed bound states $E_\pm < 0$. Therefore, by equations (24) and (25), we have to study the solutions of equation (26) as $z_\pm \to +\infty$. The mathematically rigorous and unambiguous way to solve equation (26) in this limit is to use the concept of Borel summability [6, 23].

The Borel-summable asymptotic expansion for the Airy function $\mathrm{Ai}(z)$ in a sector containing the positive real axis is discussed in [22, 23], in which it is shown that

$$\mathrm{Ai}(z) \sim \tfrac{1}{2}\pi^{-1/2} z^{-1/4} \mathrm{e}^{-\frac{2}{3}z^{3/2}} {}_2F_0\left(\tfrac{1}{6}, \tfrac{5}{6}; ; -\tfrac{3}{4}z^{-3/2}\right) \qquad |\arg z| < \tfrac{2}{3}\pi \tag{27}$$

where

$${}_2F_0(a, b; ; z) = \sum_{k=0}^{\infty} (a)_k (b)_k \frac{z^k}{k!} \tag{28}$$

is a generalized formal hypergeometric series and where $(a)_k$ is the Pochhammer symbol: $(a)_0 = 1$, $(a)_k = a(a+1)\cdots(a+k-1)$ for $k > 0$. Note in particular the sector of validity $|\arg z| < \frac{2}{3}\pi$, which is a proper subset of the sector of validity in the Poincaré sense $|\arg z| < \pi$ given in equation 10.4.59 of [20].

However, the real positive axis is a Stokes line for the Borel-summable asymptotic expansion of $\mathrm{Bi}(z)$ implicit in the definition of $\mathrm{Ai}^{(+)}(z)$:

$$\begin{aligned}\mathrm{Bi}(z) \sim{}& \pi^{-1/2} z^{-1/4} \mathrm{e}^{\frac{2}{3}z^{3/2}} {}_2F_0\left(\tfrac{1}{6}, \tfrac{5}{6}; ; \tfrac{3}{4}z^{-3/2}\right) \\ &\pm \mathrm{i}\tfrac{1}{2}\pi^{-1/2} z^{-1/4} \mathrm{e}^{-\frac{2}{3}z^{3/2}} {}_2F_0\left(\tfrac{1}{6}, \tfrac{5}{6}; ; -\tfrac{3}{4}z^{-3/2}\right) \qquad 0 < \pm \arg z < \tfrac{2}{3}\pi.\end{aligned} \tag{29}$$

Again, see [22, 23] for the derivation of these Borel-summable expansions of the function $\mathrm{Bi}(z)$ with the ensuing unique determination of the exponentially small subseries, in contrast with the asymptotic expansion in the Poincaré sense given in equation 10.4.63 of [20]. Therefore, due to this Stokes line, the solution of equation (26) by asymptotic methods has to be carried out independently on each side of the positive real axis.

3.1. The Borel-summable Rayleigh–Schrödinger power series

Let us consider first the upper side of the Stokes line $\mathrm{Re}\, F > 0$, $\mathrm{Im}\, F > 0$ and use the abridged notation

$$\Sigma_A(z) = z^{-1/4} {}_2F_0\left(\tfrac{1}{6}, \tfrac{5}{6}; ; -\tfrac{3}{4}z^{-3/2}\right) \tag{30}$$

$$\Sigma_B(z) = z^{-1/4} {}_2F_0\left(\tfrac{1}{6}, \tfrac{5}{6}; ; \tfrac{3}{4}z^{-3/2}\right) \tag{31}$$

$$\Sigma_{AB}(z) = \Sigma_A(z)\Sigma_B(z). \tag{32}$$

By substituting equations (27) and (29) with the minus sign into equation (26) we arrive at the formally real asymptotic equation

$$1 = \frac{\gamma}{2}(\Sigma_{AB}(z_+) + \Sigma_{AB}(z_-)) + \frac{\gamma^2}{4}\left(\mathrm{e}^{\frac{4}{3}(z_+^{3/2} - z_-^{3/2})} \Sigma_B(z_+)^2 \Sigma_A(z_-)^2 - \Sigma_{AB}(z_+)\Sigma_{AB}(z_-)\right). \tag{33}$$

To calculate the expansion of the right-hand side of equation (33) we study first the factor $e^{\frac{4}{3}(z_+^{3/2}-z_-^{3/2})}$. By substituting the relation

$$E = -\tfrac{1}{2}\kappa^2 \tag{34}$$

and the definitions (24) and (25) of $z_\pm$ into this exponential, we find that it can be expanded as a power series in F^2 whose coefficients are a global $e^{-4\kappa}$ factor times rational functions of κ:

$$e^{\frac{4}{3}(z_+^{3/2}-z_-^{3/2})} = e^{-4\kappa}\left(1 + \frac{2}{3\kappa^3}F^2 + \frac{4\kappa+9}{18\kappa^7}F^4 + \cdots\right). \tag{35}$$

Next we note that with the same substitutions for E and $z_\pm$, the remaining terms in equation (33) can be readily expanded as a power series and therefore the right-hand side of equation (33) is in fact a power series in F^2. We absorb the 1 in the left-hand side into this power series and denote it by $P_r(\kappa)$, of which we show explicitly the first two terms to illustrate the pattern:

$$P_r(\kappa) = \left(1 - \frac{\kappa}{g}\right)^2 - e^{-4\kappa} + \frac{gF^2}{4\kappa^8}\left(5g - 5\kappa + 8g\kappa^2 - 12\kappa^3 \right. \\ \left. - g\,e^{-4\kappa}\left(5 + 10\kappa + 8\kappa^2 + \frac{8}{3}\kappa^3\right)\right) + O(F^4). \tag{36}$$

Therefore equation (33) can be written in the form

$$P_r(\kappa) = 0 \tag{37}$$

and solved by writing κ itself as a Borel-summable power series in F^2

$$\kappa = \kappa^{(0)}(F) = \sum_{j=0}^{\infty} \kappa_{2j}F^{2j}. \tag{38}$$

We substitute this expansion into equation (37) and recursively equate to zero the coefficients of the powers of F. To order F^0 we find

$$\left(1 - \frac{\kappa_0}{g}\right)^2 - e^{-4\kappa_0} = F_-(i\kappa_0)F_+(i\kappa_0) = 0 \tag{39}$$

where we have used the definitions (12) of $F_\mp(k)$ and we see that in the limit $F \to 0$ we recover the conditions for the existence of the even and odd bound states (15). Using equation (39) to eliminate $e^{-4\kappa_0}$ from higher perturbation coefficients we can generate the κ_{2j} as explicit rational functions of the coupling constant g and of the first coefficient κ_0, whose two possible values are in turn determined by the equations for the existence of the unperturbed even and odd bound states (39). By way of example,

$$\kappa_2 = \frac{15(\kappa_0 - g) + \left(30 + 8\kappa_0^2\right)(\kappa_0 - g)^2 + 12\kappa_0^2(2\kappa_0 - g)}{24\kappa_0^5(\kappa_0 - g)(2\kappa_0 - 2g + 1)} \tag{40}$$

and although κ_4 is already too unwieldy to be calculated by hand, the procedure can be easily programmed in a computer and the κ_{2j} generated to high order.

In turn, the Borel-summable Rayleigh–Schrödinger perturbation theory series

$$E = \sum_{j=0}^{\infty} E_{2j}F^{2j} \tag{41}$$

can be calculated immediately from equation (34), and since the coefficients E_{2j} are polynomials in the κ_{2j}, the E_{2j} inherit the structure of explicit rational functions of g and κ_0. We want to stress that the formally real Rayleigh–Schrödinger power series (41) is Borel-summable to the *exact* resonances in the upper half plane $\operatorname{Im} F > 0$, and that the imaginary part of the resonances appears implicitly in the process of Borel summation [6].

3.2. Asymptotic expansion for the imaginary part of the resonances

Although the formally real Rayleigh–Schödinger power series (41) encodes both the exact real part and the exact imaginary part of the resonances stemming from the bound states, it is desirable to have an explicit asymptotic expansion for the imaginary part of the resonances. To achieve this goal, we solve equation (26) at the lower side of the Stokes line, i.e. we consider now $\operatorname{Re} F > 0, \operatorname{Im} F < 0$. By substituting equations (27) and (29) with the plus sign into equation (26) we arrive at the explicitly complex asymptotic equation

$$\begin{aligned}1 = \frac{\gamma}{2}\left[\Sigma_{AB}(z_+) + \Sigma_{AB}(z_-) + \mathrm{i}\left(\mathrm{e}^{-\frac{4}{3}z_+^{3/2}}\Sigma_A(z_+)^2 + \mathrm{e}^{-\frac{4}{3}z_-^{3/2}}\Sigma_A(z_-)^2\right)\right]\\ + \frac{\gamma^2}{4}\left[\mathrm{e}^{\frac{4}{3}(z_+^{3/2}-z_-^{3/2})}\Sigma_B(z_+)^2\Sigma_A(z_-)^2 - \Sigma_{AB}(z_+)\Sigma_{AB}(z_-)\right.\\ \left. + \mathrm{i}\left(\mathrm{e}^{-\frac{4}{3}z_-^{3/2}}\Sigma_{AB}(z_+)\Sigma_A(z_-)^2 - \mathrm{e}^{-\frac{4}{3}z_+^{3/2}}\Sigma_A(z_+)^2\Sigma_{AB}(z_-)\right)\right] \qquad (42)\end{aligned}$$

which can be written in the form

$$P_r(\kappa) + \mathrm{i}\,\mathrm{e}^{-2\kappa^3/(3F)}P_i(\kappa) = 0 \qquad (43)$$

where $P_r(\kappa)$ has been defined in equation (36) and $P_i(\kappa)$ is a power series in F whose first two terms are

$$\begin{aligned}P_i(\kappa) = \frac{2g}{\kappa}\left(\frac{g}{\kappa}\sinh(2\kappa) - \cosh(2\kappa)\right) + \frac{gF}{6\kappa^5}((5\kappa + 12\kappa^3)\cosh(2\kappa)\\ - (5g + 12\kappa^2 + 12g\kappa^2)\sinh(2\kappa)) + O(F^2). \qquad (44)\end{aligned}$$

Because of the exponentially small factor that multiplies $P_i(\kappa)$ in equation (43), its Borel-summable solution is indeed the same power series (38) plus a sequence of successively exponentially smaller subseries, alternately formally real and formally imaginary, which we write in the form

$$\kappa = \kappa^{(0)}(F) + \kappa^{(1)}(F) + \kappa^{(2)}(F) + \cdots. \qquad (45)$$

The exponentially small corrections $\kappa^{(p)}(F)$ with $p \geqslant 1$ can be calculated from the already known $\kappa^{(0)}(F)$ by a Taylor expansion. For example, the first exponentially small correction is

$$\kappa^{(1)}(F) = -\mathrm{i}\,\mathrm{e}^{-2\kappa^{(0)}(F)^3/(3F)}\frac{P_i(\kappa^{(0)}(F))}{P_r'(\kappa^{(0)}(F))} \qquad (46)$$

where the prime denotes the derivative of $P_r(\kappa)$ with respect to its argument κ.

At this point note that both asymptotic expansions (38) and (45) represent *the same* analytic (and therefore continuous) function $\kappa(F)$ on adjacent sectors. In particular

$$\kappa(F - \mathrm{i}0) = \kappa(F + \mathrm{i}0) \qquad (47)$$

while in the Borel-sum sense

$$\kappa^{(0)}(F - \mathrm{i}0) = \overline{\kappa^{(0)}(F + \mathrm{i}0)}. \qquad (48)$$

As a consequence we have the following explicit, Borel-summable asymptotic expansion for the imaginary part

$$\mathrm{i}\operatorname{Im}[\kappa(F + \mathrm{i}0)] = \tfrac{1}{2}(\kappa^{(1)}(F - \mathrm{i}0) + \kappa^{(2)}(F - \mathrm{i}0) + \cdots) \qquad (49)$$

where we have used the notation $F \pm \mathrm{i}0$ as a reminder of the sectors in which each term is valid. Equations (34), (38), (46) and (49) lead to the corresponding asymptotic expansion for the imaginary part of the resonance energy

Table 1. Comparison between the asymptotic values of the resonances stemming from the even (+) and odd (−) bound states given by equations (41) with $j = 1$ and (50) with $j = 1$, and the values obtained solving numerically the resonance condition (26) for a double δ quantum well with coupling constant $g = 1$.

F	Parity	Asymptotic	Numerical
0.10	+	$-0.656\,515 - \mathrm{i}0.000\,180$	$-0.653\,616 - \mathrm{i}0.000\,170$
	−	$-0.292\,404 - \mathrm{i}0.009\,303$	$-0.293\,636 - \mathrm{i}0.009\,729$
0.02	+	$-0.616\,452 - \mathrm{i}4.349 \times 10^{-20}$	$-0.616\,446 - \mathrm{i}4.328 \times 10^{-20}$
	−	$-0.316\,453 - \mathrm{i}4.238 \times 10^{-8}$	$-0.316\,478 - \mathrm{i}4.177 \times 10^{-8}$
0.01	+	$-0.615\,200 - \mathrm{i}8.289 \times 10^{-40}$	$-0.615\,199 - \mathrm{i}8.278 \times 10^{-40}$
	−	$-0.317\,204 - \mathrm{i}2.186 \times 10^{-15}$	$-0.317\,206 - \mathrm{i}2.179 \times 10^{-15}$

$$\operatorname{Im} E(F) = -\frac{g\kappa_0^3\,\mathrm{e}^{-2\kappa_0}\mathrm{e}^{-2\kappa_0^3/(3F)}}{4(\kappa_0 - g)^2(2\kappa_0 - 2g + 1)}\sum_{j=0}^{\infty} b_j F^j + O\left(\mathrm{e}^{-4\kappa_0^3/(3F)}\right) \tag{50}$$

$$= \mp\frac{\kappa_0^3\mathrm{e}^{-2\kappa_0^3/(3F)}}{4(\kappa_0 - g)(2\kappa_0 - 2g + 1)}\sum_{j=0}^{\infty} b_j F^j + O\left(\mathrm{e}^{-4\kappa_0^3/(3F)}\right) \tag{51}$$

where $b_0 = 1$ and b_j are explicit rational functions of κ_0 and g. For example,

$$b_1 = -\frac{(\kappa_0 - g)(5 + 6\kappa_0) + (\kappa_0 - g)^2\left(10 + 12\kappa_0 + 8\kappa_0^2\right) + 3\kappa_0^2(\kappa_0 - 1)}{3(\kappa_0 - g)\kappa_0^3(2\kappa_0 - 2g + 1)}. \tag{52}$$

Note that in equation (51) we have used the condition for the existence of bound states to eliminate $\mathrm{e}^{-2\kappa_0}$, so that the upper sign corresponds to the even bound state and the lower sign to the odd bound state (both imaginary parts are negative because in the even case $0 < g < \kappa_0$, in the odd case $0 < \kappa_0 < g$, while in both cases $0 < 2\kappa_0 - 2g + 1$).

3.3. Numerical illustration

As a numerical illustration of these results, in table 1 we compare the asymptotic and 'exact' values of the resonances stemming from the even and odd bound states of a double δ quantum well of coupling constant $g = 1$ as functions of the electric field F. The values in the column labelled 'Numerical' have been obtained by direct numerical solution of the resonance condition (26). We stress that particularly for the last two values of F it is necessary to use very high precision to obtain accurate (numerically stable) results. On the other hand, although we have generated the series (41) and (50) to high order, the values in the column labelled 'Asymptotic' have been obtained using only values explicitly given in this paper, which are the only likely to be used in analytic work. Concretely, the real part of the resonances has been calculated using equation (41) with $j = 1$, that is to say, we have used the explicit value of κ_2 given in equation (40) to calculate E_2. Likewise, the imaginary part of the resonances has been calculated using (50) with $j = 1$, that is to say, using the explicit value of b_1 given in equation (52). We see that this simple approximation reproduces accurately both the real parts and the imaginary parts of the resonances, even noting that in the range of fields chosen $\operatorname{Im} E_+(F)$ varies over thirty six orders of magnitude.

4. Resonances stemming from the continuum threshold

The resonances stemming from the even and odd bound states studied in the previous section are not the only solutions of the resonance condition (26). We have to consider also the solutions in which as $F \to 0$, both z_+ and z_- simultaneously tend either to a zero of $\mathrm{Ai}(z)$ or to a zero of $\mathrm{Ai}^{(+)}(z)$. These resonances are analogous to the resonances induced by an electric field in a single δ quantum well first described by Ludviksson [4] and subsequently studied by several authors as we discussed in the introduction [5–7, 19]. Note that from the definitions of $z_\pm$ in equations (24) and (25) it follows that

$$E = -\frac{z_\pm}{2^{1/3}} F^{2/3} \mp F \tag{53}$$

and therefore these resonant energies E tends to 0 (the continuum threshold) as $F^{2/3}$.

4.1. Solutions of $\mathrm{Ai}(z) = 0$

The zeros a_s of the Airy function $\mathrm{Ai}(z)$ are located on the negative real axis, and can be labelled by a positive integer s. From the asymptotic expansion of the Airy $\mathrm{Ai}(z)$ function for negative values of the argument (equation 10.4.60 in [20]) it is easy to derive asymptotic expansions for the zeros (equation 10.4.94 in [20]), expansions which are increasingly accurate as $s \to \infty$. For our purposes it is sufficient to consider the leading term

$$a_s \sim -\left[\frac{3\pi}{8}(4s-1)\right]^{2/3} \qquad s = 1, 2, \ldots. \tag{54}$$

We will use also the following equations

$$\mathrm{Ai}'(a_s) \sim \frac{(-1)^{s-1}}{\pi^{1/2}} \left[\frac{3\pi}{8}(4s-1)\right]^{1/6} \tag{55}$$

$$\mathrm{Bi}(a_s) \sim \frac{(-1)^{s}}{\pi^{1/2}} \left[\frac{3\pi}{8}(4s-1)\right]^{-1/6} \tag{56}$$

$$\mathrm{Bi}'(a_s) \sim \frac{(-1)^{s}}{4\pi^{1/2}} \left[\frac{3\pi}{8}(4s-1)\right]^{-5/6} \tag{57}$$

which are obtained from the corresponding asymptotic expansions for the Airy functions $\mathrm{Ai}(z)$ and $\mathrm{Bi}(z)$ and the trivial result $\mathrm{Ai}''(a_s) = a_s\,\mathrm{Ai}(a_s) = 0$.

4.2. Resonances that tend to solutions of $\mathrm{Ai}(z) = 0$ *as* $F \to 0$

In order to find the behaviour of these resonances as $F \to 0$ we solve the resonance condition (26) by using a Puiseux expansion of the solution (namely, a power series in $F^{1/3}$). Although the expansion can be carried out without difficulty to high order, we show explicitly only the first three terms because, as we will see later, the third term is the lowest term necessary for the imaginary part of the resonance to enter the solution. Therefore we write

$$E = E_0 F^{2/3} + E_1 F + E_2 F^{4/3} + O(F^{5/3}) \tag{58}$$

or, equivalently,

$$z_\pm = -2^{1/3}(E_0 + (E_1 \pm 1)F^{1/3} + E_2 F^{2/3} + O(F)) \tag{59}$$

from which it follows immediately that

$$E_0 = -2^{-1/3} a_s. \tag{60}$$

Substituting the Taylor expansions (59) for $z_\pm$ into equation (26) and using the asymptotic formulas (54)–(57) we find

$$E_s(F) \sim \frac{F^{2/3}}{2^{1/3}}\left[\frac{3\pi}{8}(4s-1)\right]^{2/3} + F\left(1+\frac{1}{4g}+\frac{1}{4g-2}\right) + \frac{F^{4/3}}{(4g)^2(1-2g)^2}\frac{[2-\mathrm{i}3\pi(4s-1)]}{[6\pi(4s-1)]^{2/3}} + O(F^{5/3}) \qquad s=1,2,\ldots. \tag{61}$$

Although this asymptotic formula for the first kind of threshold resonances is increasingly accurate as $s\to\infty$ (i.e. for higher resonances), numerical tests show that it gives accurate results for any value of s. Equation (61) shows that indeed the imaginary part of the resonance enters in the third term of the expansion, and that

$$\mathrm{Im}\,(E_s) \sim -\frac{[\mathrm{Re}\,(E_s)]^2}{g^2(1-2g)^2 3\pi(4s-1)} \qquad F\to 0. \tag{62}$$

Therefore infinitely many resonances approach the origin from the fourth quadrant along a family of increasingly flatter parabolas. This fact explains the sensitivity of a direct numerical solution of equation (26) to initial data in a neighbourhood of the origin. Equation (61) provides the means to identify and track down the results of these numerical calculations.

4.3. Resonances that tend to solutions of $\mathrm{Ai}^{(+)}(z)=0$ *as* $F\to 0$

The expressions for the second kind of threshold resonances, which correspond to solutions of the resonance condition (26) in which $z_\pm$ tend to a zero of $\mathrm{Ai}^{(+)}(z)$, can be almost read off from the expansions by drawing on equation (20). Indeed, if we set

$$z_\pm = w_\pm\,\mathrm{e}^{-2\pi\mathrm{i}/3} \tag{63}$$

the resonance condition (26) can be written in the form

$$1 = \gamma\,\mathrm{e}^{\mathrm{i}\pi/3}\pi[\mathrm{Ai}(w_+)\,\mathrm{Ai}^{(-)}(w_+) + \mathrm{Ai}(w_-)\,\mathrm{Ai}^{(-)}(w_-)] + (\gamma\,\mathrm{e}^{\mathrm{i}\pi/3}\pi)^2\,\mathrm{Ai}(w_+)\,\mathrm{Ai}^{(-)}(w_-)[\mathrm{Ai}(w_+)\,\mathrm{Ai}^{(-)}(w_-) - \mathrm{Ai}^{(-)}(w_+)\,\mathrm{Ai}(w_-)] \tag{64}$$

which leads immediately to

$$\hat{E}_s(F) \sim \frac{(F\mathrm{e}^{-\mathrm{i}\pi})^{2/3}}{2^{1/3}}\left[\frac{3\pi}{8}(4s-1)\right]^{2/3} + (F\mathrm{e}^{-\mathrm{i}\pi})\left(1+\frac{1}{4g}+\frac{1}{4g-2}\right) + \frac{(F\mathrm{e}^{-\mathrm{i}\pi})^{4/3}}{(4g)^2(1-2g)^2}\frac{[2+\mathrm{i}3\pi(4s-1)]}{[6\pi(4s-1)]^{2/3}} + O(F^{5/3}) \qquad s=1,2,\ldots. \tag{65}$$

Equation (65) describes the second kind of threshold resonances, all of which approach the origin along the ray $\arg(\hat{E}_s) = -2\pi/3$ in the third quadrant as $F\to 0$.

4.4. Numerical illustration

These results are illustrated by a numerical example in table 2, where we compare the asymptotic, 'Puiseux' and numerical values of the resonances $E_1(F)$ and $\hat{E}_1(F)$ for the same values of the electric field F used in table 1. The values in the column labelled 'Asymptotic' have been obtained with the explicit equations (61) and (65) with $s=1$, while the values in the column labelled 'Numerical' have been calculated by direct numerical solution of the resonance condition (26). As we mentioned earlier, the main problem of a numerical solution in this case is to give a sufficiently accurate initial approximation to the desired root. In

Table 2. Comparison among the asymptotic, Puiseux and numerical values of the first ($s = 1$) resonance of each kind stemming from the continuum threshold for a double δ quantum well with coupling constant $g = 1$. The asymptotic values have been obtained with equations (61) and (65); the Puiseux values, with five exact terms of the series (58) and the numerical values by direct numerical solution of the resonance condition (26).

F		Asymptotic	Puiseux	Numerical
0.10	E_1	$0.572\,151 - \mathrm{i}0.005\,567$	$0.524\,922 - \mathrm{i}0.000\,993$	$0.545\,526 - \mathrm{i}0.003\,750$
	$\hat{E}_1$	$-0.378\,397 - \mathrm{i}0.346\,045$	$-0.401\,306 - \mathrm{i}0.381\,005$	$-0.365\,334 - \mathrm{i}0.393\,499$
0.02	E_1	$0.170\,735 - \mathrm{i}0.000\,651$	$0.168\,670 - \mathrm{i}0.000\,541$	$0.169\,280 - \mathrm{i}0.000\,546$
	$\hat{E}_1$	$-0.103\,432 - \mathrm{i}0.117\,796$	$-0.105\,419 - \mathrm{i}0.120\,914$	$-0.105\,374 - \mathrm{i}0.122\,222$
0.01	E_1	$0.102\,997 - \mathrm{i}0.000\,258$	$0.102\,706 - \mathrm{i}0.000\,243$	$0.102\,831 - \mathrm{i}0.000\,238$
	$\hat{E}_1$	$-0.060\,472 - \mathrm{i}0.074\,140$	$-0.061\,263 - \mathrm{i}0.075\,408$	$-0.061\,322 - \mathrm{i}0.075\,657$

fact, in the calculations displayed in table 2 we have used the asymptotic values as initial approximations for the numerical solution. The main difference with respect to table 1 is that now the asymptotic values do not tend to the exact ones as $F \to 0$, because in the derivation of equations (61) and (65) we have not used the exact values a_s for the zeros of the Airy function, but their approximate values (54) which are increasingly accurate as $s \to \infty$ (therefore, the example shows the worst possible case). To illustrate this fact we have included in the table the column labelled 'Puiseux' which has been calculated using five 'exact' terms of the series (58) where by 'exact' we mean that accurate numerical values of the zeros a_s, of $\mathrm{Bi}(a_s)$ and of the derivatives $\mathrm{Ai}'(a_s)$ and $\mathrm{Bi}'(a_s)$ have been used to calculate the coefficients instead of the asymptotic formulae (54)–(57). Note that from the physical point of view these resonances are much wider than the resonances stemming from the bound states and that their main effect in the photoionization cross section will be to contribute to the background by raising the baseline before the threshold and to increase the asymmetry of the peaks [5, 16, 24].

4.5. Final remarks on the existence of resonances

Finally, let us consider the asymptotic expansion for large k of the resonance condition (26) in the sector $\mathrm{Re}\,k > 0$, $-\pi/3 < \mathrm{Im}\,k < 0$ which contains the first family of threshold resonances (61). This asymptotic expansion can be easily derived from the fundamental asymptotic expansions (27) and (29) and the 'relations between solutions' of the Airy differential equation given in equations 10.4.6–10.4.9 of [20]. The full expansion has the form $Q_1(k) + \mathrm{e}^{\mathrm{i}2k^3/(3F)} Q_2(k) = 0$, where $Q_1(k)$ and $Q_2(k)$ are power series in F^2 and F respectively, but for the purposes of these final remarks it will be enough to show the leading terms of each series:

$$\left[\left(1 - \frac{\mathrm{i}g}{k}\right)^2 - \left(\frac{\mathrm{i}g}{k}\mathrm{e}^{2\mathrm{i}k}\right)^2 + O(F^2)\right] + \mathrm{e}^{\mathrm{i}2k^3/(3F)}\left[\frac{2g^2}{k^2}\sin(2k) - \frac{2g}{k}\cos(2k) + O(F)\right] = 0. \tag{66}$$

The leading term of $Q_1(k)$ is readily identified with $F_+(k)F_-(k)$ (whose zeros are the intrinsic resonances of the unperturbed problem), but note that this is now the subdominant contribution. The presence of the dominant exponential and the corresponding leading term of $Q_2(k)$ shows that there are not solutions of equation (66) that in the limit $F \to 0$ tend to $k = k_r - \mathrm{i}k_i$ with $k_i > 0$ in the given sector. Incidentally, the leading term of $Q_2(k)$ is also easy to identify: if instead of looking for the even and odd solutions of the unperturbed double δ well we look for the solution that represents for $x < -1$ a pure plane wave moving to the right

$$\psi_k^{(r)}(x) = F_-(-k)\psi_k^{(+)}(x) + \mathrm{i}F_+(-k)\psi_k^{(-)}(x) \tag{67}$$

or more explicitly

$$\psi_k^{(r)}(x) = \begin{cases} \mathrm{e}^{\mathrm{i}kx} & x < -1 \\ (1 + \mathrm{i}g/k)\,\mathrm{e}^{\mathrm{i}kx} - (\mathrm{i}g/k)\,\mathrm{e}^{-2\mathrm{i}k}\,\mathrm{e}^{-\mathrm{i}kx} & -1 \leqslant x \leqslant 1 \\ \rho(k)\,\mathrm{e}^{-\mathrm{i}kx} + \sigma(k)\,\mathrm{e}^{\mathrm{i}kx} & 1 < x \end{cases} \tag{68}$$

where

$$\rho(k) = \frac{1}{2}[F_+(k)F_-(-k) - F_+(-k)F_-(k)] = \frac{2\mathrm{i}g^2}{k^2}\sin(2k) - \frac{2\mathrm{i}g}{k}\cos(2k) \tag{69}$$

$$\sigma(k) = F_+(-k)F_-(-k) = \left(1 + \frac{\mathrm{i}g}{k}\right)^2 - \left(\frac{\mathrm{i}g}{k}\mathrm{e}^{-2\mathrm{i}k}\right)^2 \tag{70}$$

we see that the leading term of $Q_2(k)$ is (minus i times) the coefficient $\rho(k)$, and that its real zeros correspond to the k values for which there is maximum transmission (i.e. no wave moving to the left in the region $1 < x$) in the unperturbed double δ well. Furthermore, note that asymptotically these real values of k are given by

$$k = \frac{n\pi}{2}\left[1 + \frac{1}{2g} + \frac{1}{(2g)^2} + \frac{1 - \frac{4}{3}(n\pi/2)^2}{(2g)^3} + \cdots\right] \qquad g \to \infty \tag{71}$$

and are asymptotically equal to the real parts of both the even and odd resonances in equations (18) and (19).

5. Summary

In this paper we have studied the Stark effect in the double δ quantum well from the point of view of perturbation theory. We have shown that there are two kinds of resonances: the familiar resonances stemming from the bound states and a doubly infinite family of resonances stemming from the continuum threshold. These resonances were first described by Ludviksson [4] in the simpler context of the single δ quantum well and there is also numerical evidence of their existence in short range potentials [8].

We have derived explicit expressions for the coefficients of the Borel-summable Rayleigh–Schrödinger perturbation theory series for the resonances stemming from the bound states, as well as explicit asymptotic expansions for the imaginary part of these resonances. The key idea for an efficient derivation of these results is to use in effect perturbation theory not on the resonance energy directly but on the wavenumber. Likewise, we have derived asymptotic expansions for both kinds of resonances stemming from the unperturbed continuum threshold. These expansions show that resonances of the first kind approach the origin from the fourth quadrant along increasingly flatter parabolas, while resonances of the second kind approach the origin along the ray $\arg E = -2\pi/3$ in the third quadrant. Moreover, while the width of the resonances stemming from the bound states is exponentially small in F, the width of the threshold resonances of the first kind of threshold resonances behaves as $F^{4/3}$ while the width of the second kind behaves as $F^{2/3}$ when $F \to 0$.

But beyond the concrete results pertaining to the double δ model we would like to stress the applicability of the method in a situation which, albeit slightly more complicated from the computational point of view, has direct physical interest: the extraction of electrons by an electric field in (effectively one-dimensional) quantum wells [17, 18]. Since these wells are usually modelled by square well potentials without or with barriers [24], the solution of the corresponding Stark problem reduces again to the matching of Airy wavefunctions in piecewise linear potentials, which leads to an explicit condition for the existence of resonances analogous to our equation (26), to which the techniques developed in this paper can be directly applied. In particular, we consider of special interest the calculation of the photoionization cross section of a realistic $\mathrm{GaAs/Ga}_x\mathrm{Al}_{1-x}\mathrm{As}$ well by the method of [24] but in the presence of an applied electric field.

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