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Appendix resonances on a simple graph

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Abstract. We study the scattering problem on a graph consisting of a line with a finite-length appendix. The two parts are coupled through boundary conditions depending on three parameters; the motion on the line is free while the appendix supports a potential. The appendix bound states give rise to a ladder of resonances; we construct the resolvent and solve the corresponding pole condition for a weak coupling. In general, the condition only admits an analytic solution in particular cases. We find the pole positions numerically for a linear potential and show that the poles eventually return to the real axis when the coupling strength increases.

1. Introduction

New developments in the fabrication of semiconductor microstructures are interesting not only in view of potential device applications, but simply because they give quantum mechanics certain classical features, namely they allow us to test its predictions in a variety of situations where it is us and not nature who chooses the shape of the playground. This particularly concerns scattering on graph-like structures—references to this subject are nowadays so plentiful that we shall restrict ourselves to only mentioning [4, 5, 9, 11–13, 15–17] as a small sample related to the contents of this paper.

While simple conceptually, such systems are not easy to handle. In the usual approximation, low-energy electrons are described as free particles with an effective mass moving in the spatial region (system of tubes) which form the microstructure. The resulting partial differential equations are mostly treated numerically; only a few systems allow us to draw more general conclusions. This is why one usually makes another simplification. If the 'quantum wires' under consideration are sufficiently thin, their transverse modes are well separated in energy and weakly coupled; then it is reasonable to use the one-mode approximation in which the wire system is replaced by the corresponding graph structure.

In this paper we are going to discuss a very simple model describing a quantum particle which lives on a graph consisting of one finite and two semi-infinite links. A particular case is a line with a stub, or a segment connected to it at a point. Such a system has been considered recently by several authors. In [13] the transmission amplitude was derived for a particular choice of coupling between the line and the stub. The authors of [17] extended this result to a two-parameter family of boundary conditions. This is important because it is natural to conjecture that the parameters are related to the geometry of the junction, which we usually do not know much about; recall that this intriguing mathematical problem remains open [10].

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Here we are going to treat a more general three-parameter family of couplings. A more important generalization is that we consider the finite link of an arbitrary shape (we therefore call it an *appendix*) provided it is coupled to the line at only one point, and suppose that the particle is exposed to a general potential on it. It is not difficult to extend our results to the situation where the line also supports a potential, but for the sake of simplicity we refrain from doing that. One naturally expects the appendix bound states to give rise to resonances of the coupled system; we shall show that the model is completely solvable in the sense that the resonance pole positions can be found from a simple transcendental equation.

Let us briefly summarize the contents of this paper. In the next section we describe the model and derive the transmission amplitude. The main results are contained in section 3. Using the Krein formula, we first derive an explicit expression for the resolvent of the Hamiltonian which yields the pole condition. We solve the latter perturbatively for a weak coupling. In general, it admits an analytic solution only in particular cases; we present an example showing that the resonance poles may not exist at all. Numerical analysis of pole trajectories has been performed for the case of a linear potential considered in [15, 16], which is important from the viewpoint of applications. The results show, in particular, that the poles eventually return to the real axis when the coupling strength increases, independently of the intensity of the external field.

2. Description of the model

The graph we consider consists of a line to which we couple at a point (chosen to be $x = 0$) a curve of a finite length ℓ (see figure 1). Consequently, the Hilbert state space of the problem will be $\mathcal{H} := L^2(\mathbb{R}) \oplus L^2(0, \ell)$; we will write its elements as columns $\psi = \binom{f}{u}$. The particle motion on the graph is governed by a Hamiltonian which acts as a standard Schrödinger operator

$$(H\psi)_1(x) = -f''(x) \qquad (H\psi)_2(x) = (-u'' + Vu)(x) \tag{1}$$

provided the connection point is not contained in the support of the wavefunction, $x \neq 0$. In the following we shall specify how the two parts of the graph are coupled.

Here the function V is a potential which represents an input of the model. It can be generated, for example, by a homogeneous electric field perpendicular to the line. A particular case, which is of interest in connection with the T-graph studies mentioned in the introduction, is represented by a linear potential which corresponds to the case where the appendix is straight (a line segment). This is not the only possibility, however. The potential may come from another external field or from the geometry of the appendix itself. Recall that bends in thin tubes generate an attractive potential [8]; in the limit of zero radius it is just a negative multiple of the squared curvature.

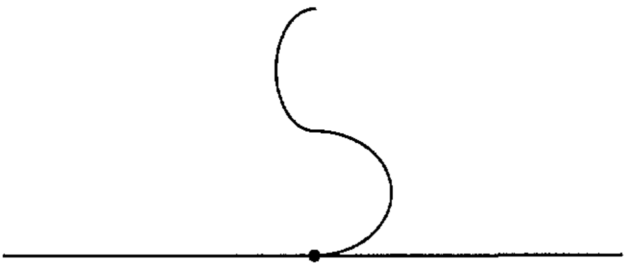

Figure 1. A line with an appendix.

For the model the nature of V is irrelevant; throughout the paper suppose we only that it is a measurable real-valued function of $L^1_{\text{loc}}(0, \ell)$ having finite limits at both endpoints of the appendix; this means, in particular, that the corresponding deficiency indices are $(2, 2)$.

2.1. Boundary conditions

The problem of constructing self-adjoint Schrödinger operators on branching graphs was discussed extensively in [9]; see also [1, 6, 11, 12]. The key idea was that restricting the sum of Hamiltonians of disconnected graph links to functions which vanish in the vicinity of the branching points yields an operator which is symmetric but not self-adjoint; the 'coupled' operators sought are then constructed as self-adjoint extensions. The most suitable way to describe them is local, i.e. through boundary conditions which have a transparent meaning as the requirement of probability flow conservation at the junctions.

The analysis was performed for the case where the motion outside the branching is free; however, addition of a potential of the type described does not alter the boundary conditions. Among the operators on a three-link graph we choose the family of those having the wavefunction continuous between a pair of links [9, section 5]; in the present case we shall suppose that the 'line component' f of ψ is continuous at $x = 0$. Since we want to have parameters which would allow us to easily switch off the coupling between the line and the appendix, we linearly transform the mentioned conditions to the form

$$\begin{aligned} &f(0+) = f(0-) =: f(0) \\ &u(0) = bf(0) + cu'(0) \\ &f'(0+) - f'(0-) = df(0) - bu'(0) \\ &u(\ell) = 0\,. \end{aligned} \tag{2}$$

We have added the Dirichlet condition at the outer end of the appendix. The coefficient matrix $\mathbb{K} = \left(\begin{smallmatrix} b & d \\ c & -b \end{smallmatrix}\right)$ is real; from the start we restrict our attention to Hamiltonians which are time-reversal invariant. The operator specified by the boundary conditions (2) will be denoted as $H(\mathbb{K})$.

The particular case of boundary conditions with fully continuous wavefunctions used by most authors corresponds to $b = 1$ and $c = 0$; we then have $f(0+) = f(0-) = u(0)$ and

$$f'(0+) - f'(0-) + u'(0) = df(0)\,.$$

The advantage of the boundary conditions (2) is that they allow us to disconnect the appendix without breaking the line; putting $b = 0$, we get have the δ-interaction Hamiltonian on the line, $f'(0+) - f'(0-) = df(0)$ (in particular, the free motion for $d = 0$), while the appendix is described by the operator $h_c := -\mathrm{d}^2/\mathrm{d}x^2 + V$ specified by the decoupled condition

$$u(0) - cu'(0) = 0 \tag{3}$$

at the junction. Hence b is the parameter which controls the coupling between the two parts of the graph.

2.2. Scattering

The existence of the wave operators for the scattering system under consideration is easily established because—as we shall see below—the coupling represents a rank-2 perturbation in the resolvent, so the Kato–Rosenblum theorem applies [14, section XI.3]. What is more interesting, however, is the explicit form of the scattering matrix. To find it we take the following ansatz:

$$f(x) := \begin{cases} e^{ikx} + r\,e^{-ikx} & x < 0 \\ t e^{ikx} & x > 0 \end{cases} \qquad u(x) = \beta u_\ell(x)$$

where u_ℓ is a solution to $-u'' + Vu = k^2 u$ corresponding to the boundary conditions $u_\ell(\ell) = 0$, unique up to a multiplicative constant. These functions should belong *locally* to the domain of the Hamiltonian so they have to satisfy the boundary conditions (2). This yields a system of equations for r, t and β which is solved by

$$\begin{aligned} t(k) &= \frac{-2ik(cu'_\ell - u_\ell)(0)}{b^2 u'_\ell(0) + (d - 2ik)(cu'_\ell - u_\ell)(0)} \\ r(k) &= -\frac{b^2 u'_\ell(0) + d(cu'_\ell - u_\ell)(0)}{b^2 u'_\ell(0) + (d - 2ik)(cu'_\ell - u_\ell)(0)}\,. \end{aligned} \tag{4}$$

For $b = 0$ we recover the standard δ-scattering reflection and transmission amplitudes [2, section I.3]. It is straightforward to check that the scattering matrix is unitary,

$$|t(k)|^2 + |r(k)|^2 = 1\,.$$

The transmission probability is

$$|t(k)|^2 = \frac{4k^2(cu'_\ell(0) - u_\ell(0))^2}{\left[(b^2 + cd)u'_\ell(0) + du_\ell(0)\right]^2 + 4k^2(cu'_\ell(0) - u_\ell(0))^2}\,. \tag{5}$$

Examples of its behaviour will be given in section 3.3 below.

Let us remark that due to the presence of the δ-interaction on the line, the system may have a bound state. We find it by replacing the line part in the above ansatz by $f(x) = \alpha\,e^{-\kappa|x|}$. This leads to a system of equations which is solvable provided

$$b^2 u'_\ell(0) + (d + 2\kappa)(cu'_\ell - u_\ell)(0) = 0$$

(the LHS is the denominator of (4) with $k = i\kappa$). If $b = 0$, an isolated eigenvalue exists, provided $d < 0$, and equals $-\frac{1}{4}d^2$; it remains isolated, at least for $|b|$ small enough.

3. Resonance poles

At this point, let us turn to the resonance scattering. If $b = 0$, the appendix has a simple purely discrete spectrum; the eigenvalues are positive and therefore embedded into the continuous spectrum of the line Hamiltonian. If the coupling is switched on, we expect them to turn into resonances. To confirm this conjecture and to find positions of the resonance poles, we need to find the resolvent of $H(\mathbb{K})$.

3.1. The resolvent

Since all the operators $H(\mathbb{K})$ are obtained as self-adjoint extensions of the same symmetric operator with the deficiency indices $(2, 2)$, the resolvent can be obtained easily from Krein's formula [2, appendix A]. We denote by $\mathbb{K}_0$ the zero matrix and choose the corresponding decoupled Hamiltonian as a reference operator. The line part of the resolvent is then an integral operator with the kernel

$$R_1(x, y; z) = \frac{i}{2k}\,e^{ik|x-y|} \tag{6}$$

where $k := \sqrt{z}$; conventionally we associate the upper half-plane, $\operatorname{Im} k > 0$, with the 'physical' sheet of the complex energy. On the other hand, the appendix resolvent kernel is

$$R_2(x, y; z) = -\frac{u_0(x_<)u_\ell(x_>)}{W(u_0, u_\ell)} \tag{7}$$

where $x_>, x_<$ means respectively the greater (smaller) of x, y, u_ℓ has been introduced above, u_0 *is similarly a solution corresponding to the conditions* $u_0(0) = cu_0'(0)$, and $W(u_0, u_\ell)$ is the Wronskian of the two functions. In particular, if the appendix motion is free, $V = 0$, the last expression simplifies to

$$R_2(x, y; z) = -\frac{\sin(kx_<)\sin(k(x_> - \ell))}{k\sin(k\ell)}. \tag{8}$$

More generally, if a and b are linearly independent solutions of $-u'' + Vu = k^2u$, we can set

$$u_0(x) = b(0)a(x) - a(0)b(x) \qquad u_\ell(x) = b(\ell)a(x) - a(\ell)b(x).$$

A particular case of interest concerns the case of a linear potential, $V(x) = Ex$, where

$$a(x) = \mathrm{Ai}\left(\frac{E}{|E|^{2/3}}\left(x - \frac{z}{E}\right)\right) \qquad b(x) = \mathrm{Bi}\left(\frac{E}{|E|^{2/3}}\left(x - \frac{z}{E}\right)\right) \tag{9}$$

so

$$W(u_0, u_\ell) = \frac{E}{\pi|E|^{2/3}}\left(b(\ell)a(0) - a(\ell)b(0)\right).$$

According to Krein's formula, the resolvent kernel of $H(\mathbb{K})$ is a 2×2 matrix of the form

$$(H(\mathbb{K}) - z)^{-1}(x, y) = (H(\mathbb{K}_0) - z)^{-1}(x, y) + \sum_{j=1,2} \lambda_{jk}F_j(x)F_k(y) \tag{10}$$

where F_j are vectors from the deficiency subspaces of the maximal common restriction of the two operators; these can be chosen, for example, as

$$F_1(x) := \begin{pmatrix} R_1(x, y) \\ 0 \end{pmatrix} \qquad F_2(x) := \begin{pmatrix} 0 \\ u_\ell(x) \end{pmatrix}$$

(when it is not necessary we will not indicate the dependence on z). To determine the coefficients λ_{jk}, we employ the standard procedure (see, for instance, [3, 7]): the vector $\binom{f}{u} = (H(\mathbb{K}) - z)^{-1}\binom{g}{v}$ should belong to the domain of $H(\mathbb{K})$ for any $\binom{g}{v} \in \mathcal{H}$, hence, in particular, its components have to satisfy the boundary conditions (2). Denoting

$$h_1 := \int_{\mathbb{R}} R_1(0, y)g(y)\,\mathrm{d}y \qquad h_2 := \int_0^\ell u_\ell(y)v(y)\,\mathrm{d}y$$

we get

$$\begin{aligned}
f(0) &= h_1 + \frac{\mathrm{i}}{2k}(\lambda_{11}h_1 + \lambda_{12}h_2) \\
u(0) &= u_\ell(0)(\lambda_{21}h_1 + \lambda_{22}h_2) \\
u'(0) &= u_\ell(0)^{-1}h_2 + u_\ell'(0)(\lambda_{21}h_1 + \lambda_{22}h_2) \\
f'(0\pm) &= -\tfrac{1}{2}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}ky}\operatorname{sgn}(y)g(y)\,\mathrm{d}y \mp \tfrac{1}{2}(\lambda_{11}h_1 + \lambda_{12}h_2)
\end{aligned}$$

where we have used the identity $W(u_0, u_\ell) = -u'(0)u_\ell(0)$. Substituting these boundary values into (2), we get a system of linear equations which is solved by

$$\lambda_{11} = D(k)^{-1}\left[b^2 u_\ell'(0) + d(cu_\ell' - u_\ell)(0)\right]$$
$$\lambda_{12} = \lambda_{21} = \frac{b}{D(k)}$$
$$\lambda_{22} = \frac{u_\ell(0)^{-1}}{D(k)}\left(c + \mathrm{i}\frac{cd + b^2}{2k}\right)$$

with

$$D(k) = -\frac{\mathrm{i}b^2}{2k}u_\ell'(0) - \left(1 + \frac{\mathrm{i}d}{2k}\right)\left(cu_\ell'(0) - u_\ell(0)\right). \tag{11}$$

The last expression coincides up to a factor with the denominator in (4). Zeros of the function D determine singularities of the resolvent.

If $b = 0$ the expression factorizes and solutions to $D(k) = 0$ are easily found. They correspond to the eigenvalues of h_c specified by the condition (3) which are embedded in the continuous spectrum of the line Hamiltonian; for $d \neq 0$ we have, in addition, an imaginary solution referring to the (anti-)bound state of the δ-interaction.

3.2. Weak coupling

When the parameter $|b|$ which characterizes the coupling strength between the two parts of the graph is small the pole condition can be solved by means of the implicit function theorem. We have the following general result.

Theorem. Let k_n refer to the nth eigenvalue of h_c and denote by χ_n the corresponding *normalized* eigenfunction. Under the assumptions stated above, the condition $D(k) = 0$ has for all sufficiently small $|b|$ just one solution in the vicinity of k_n which is given by

$$k_n(b) = k_n - \frac{\mathrm{i}b^2\chi_n'(0)^2}{2k_n(2k_n + \mathrm{i}d)} + \mathcal{O}(b^4). \tag{12}$$

Proof. By a straightforward application of the implicit function theorem we get the expansion

$$k_n(b) = k_n - \frac{\mathrm{i}b^2\chi_n'(0)^2}{(2k_n + \mathrm{i}d)\,\frac{\mathrm{d}}{\mathrm{d}k}(cu_\ell'(0) - u_\ell(0))_{k=k_n}} + \mathcal{O}(b^4)$$

provided the denominator is non-zero. To complete the proof we modify an argument used in [3]. Denote $\chi := u_\ell$ and let ϕ be the solution to $-u'' + (V - z)u = 0$ fulfilling the boundary conditions $\phi(0) = 1$ and $\phi'(0) = 0$. For $z' \neq z$ we rewrite the last equation in the following inhomogeneous form:

$$-u'' + (V - z)u = (z' - z)u$$

which can be solved by a variation of constants,

$$\chi(x, z') = c_1(z')\chi(x, z) + c_2(z')\phi(x, z) + (z' - z)g(x, z)$$

where

$$g(x, z) = -\frac{\chi(x)}{\chi'(x)}\int_0^x \phi(y)\chi(y)\,\mathrm{d}y - \frac{\phi(x)}{\chi'(x)}\int_x^\ell \chi(y)^2\,\mathrm{d}y$$

(all the functions on the RHS refer to the complex energy z). If we denote by h_∞ the appendix Hamiltonian with the *Neumann* boundary condition at $x=0$, then the last relation may be rewritten as $g=(h_\infty - z)^{-1}\chi$, so that $g\in D(h_\infty)$ and $g'(0,z)=g(\ell,z)=0$.

The spectra of the operators h_0 and h_∞ are disjoint; hence the function $\phi(\cdot,z)$ does *not* satisfy the Dirichlet condition at $x=\ell$. At the same time, $\chi(\ell,z)=0$, by definition, and $g(\ell,z)=0$ as we have pointed out. This means that the function $c_2=0$ and the derivative of $c\chi'-\chi$ with respect to the momentum at $z_n:=k_n^2$ can be expressed as

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}k}(c\chi'-\chi)(x,z_n) &= 2k_n\frac{\mathrm{d}}{\mathrm{d}z}(c\chi'-\chi)(x,z_n)\\ &= \{c_1'(z_n)(c\chi'-\chi)(x,z_n)+(cg'-g)(x,z_n)\}\,.\end{aligned}$$

In particular, the first term on the RHS vanishes in the limit $x\to 0$ and, returning to the original notation, we arrive at the required formula (12) and we get

$$\frac{\mathrm{d}}{\mathrm{d}k}(c\chi'-\chi)(x,z_n) = -2k_n\frac{c\phi'(0)-\phi(0)}{\chi'(0)}\int_0^\ell \chi(y)^2\,\mathrm{d}y = \frac{2k_n}{\chi'(0)}\int_0^\ell \chi(y)^2\,\mathrm{d}y\,.$$

At the same we have justified the use of the implicit function theorem. □

Notice that, for a non-zero b, solutions to the pole condition lie in the lower complex half-plane as required. The relation (12) yields the weak-coupling expansion of the resonance pole positions:

$$z_n(b) = k_n^2 - \frac{\mathrm{i}b^2\chi_n'(0)^2}{2k_n+\mathrm{i}d} + \mathcal{O}(b^4)\,. \tag{13}$$

3.3. Pole trajectories

If the coupling is not weak, the pole condition could be solved analytically only in particular cases. A notable example is the situation when the motion in the appendix is free and the decoupled operator is specified by the Dirichlet boundary condition, i.e.

$$V=0 \qquad \text{and} \qquad c=d=0\,. \tag{14}$$

In this case the embedded eigenvalues are k_n^2, where $k_n:=n\pi/\ell$ and the equation $D(k)=0$ reduces to $\tan(k\ell)=-\frac{1}{2}\mathrm{i}\beta^2$, which is solved by

$$\begin{aligned} k_n(b) &= \frac{n\pi}{\ell}+\frac{\mathrm{i}}{2\ell}\ln\frac{2-b^2}{2+b^2} \qquad \text{if} \quad |b|<\sqrt{2}\\ k_n(b) &= \frac{(2n-1)\pi}{2\ell}+\frac{\mathrm{i}}{2\ell}\ln\frac{b^2-2}{b^2+2} \qquad \text{if} \quad |b|>\sqrt{2}\,.\end{aligned} \tag{15}$$

Hence the poles travel with the growing $|b|$ down in the k-plane following lines parallel to the imaginary axis. If $|b|=\sqrt{2}$ the resolvent has no poles at all. For larger values of the coupling constant the poles reappear and move towards the real axis; however, their trajectories are now shifted and end in the limit $|b|\to\infty$ at the points $\frac{\pi}{\ell}\left(n+\frac{1}{2}\right)$. This is not surprising, because these values refer to eigenvalues of the operator h_∞ with the Neumann condition at $x=0$; notice that the boundary conditions (2) give, in the limit, the Hamiltonian of the graph decoupled into three parts: the appendix described by h_∞ and two half-lines with the Dirichlet condition at the endpoints. In the z-plane, the trajectories are correspondingly parabolic curves; the poles move to the third quadrant and return following shifted parabolas. For small values of $|b|$ the first of the relations (15) gives

$$k_n(b) = \frac{n\pi}{\ell} - \frac{\mathrm{i}b^2}{2\ell} + \mathcal{O}(b^4) \tag{16}$$

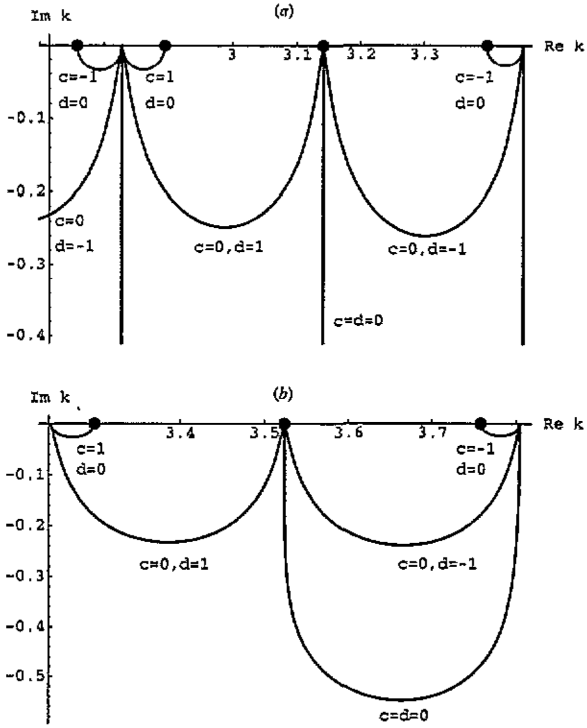

Figure 2. Pole trajectories in the k-plane for various values of the coefficients c and d as functions of the coupling parameter b. The starting value $b = 0$ is marked by full circles; the parameter runs from 0 to $+\infty$, with field strengths (a) $E = 0$ and (b) $E = 1$.

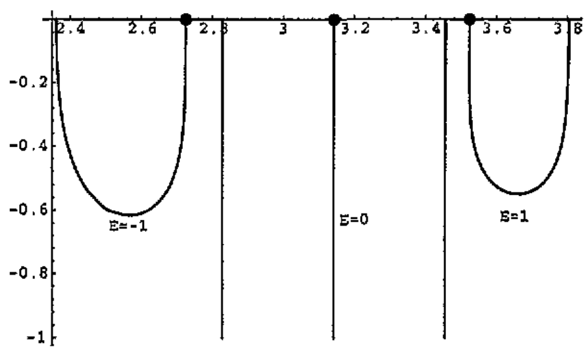

Figure 3. Pole trajectories in the k-plane for different E as functions of the coupling parameter b; the other coefficients are $c = d = 0$.

which is consistent with the above theorem, because the nth Dirichlet eigenfunction is $\chi_n(x) = \sqrt{2/\ell}\cos(k_n x)$.

In the general case the pole condition has to be solved numerically. We shall do that for the particular case of a linear potential, $V(x) = Ex$; the length of the stub is chosen as $\ell = 5$. Figures 2 and 3 illustrate the pole trajectories for several values of the parameters.

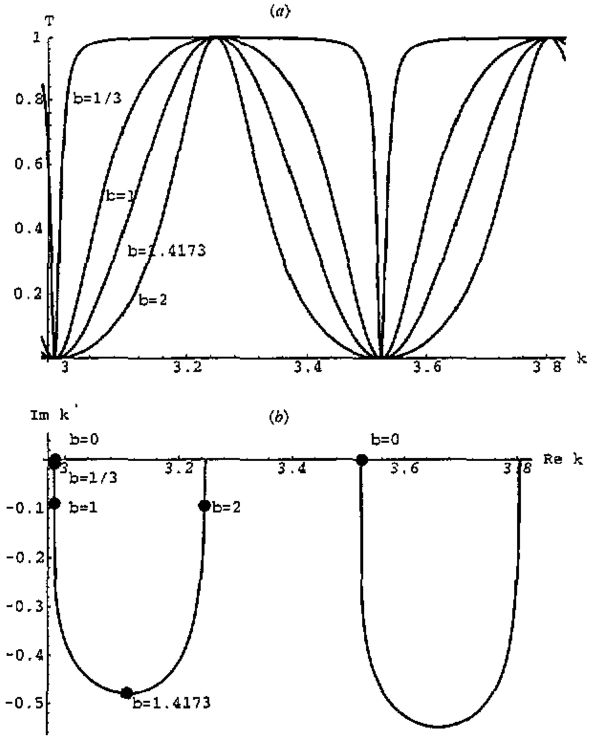

Figure 4. The correspondence between (*a*) the transmission coefficient and (*b*) the pole trajectories for $c = d = 0$ and $E = 1$.

We see that the case described above is rather exceptional; $|\mathrm{Im}\, k_n(b)|$ is generically bounded, but its maximum value is different for different parameters. The 'starting points' $b = 0$ are marked by full circles; they correspond to the embedded eigenvalues and therefore they are only determined by the parameter c. On the other hand, the BC (2) always turns into the Neumann BC at the decoupled end of the appendix as $b \to \infty$. Hence the points at which the trajectories end depend on E, but not on c and d, with the exception that the latter determine whether the pole will travel to the 'Neumann' embedded eigenvalue to the left or to the right of the original one. In figures 2(*a*) and 3 this switching of orientation refers to the sign of d and E, respectively; in the general case one could find the critical values of the parameters by computing the next term in the expansion (12).

In the final figure we compare the pole trajectories with the transmission coefficient as a function of the coupling strength b. We see that while the points of zero transmission and reflection do not move, being given by the embedded eigenvalues and their Neumann counterparts respectively, the transmission plot changes substantially. As one may expect, for weak coupling the resonances are narrow dips: the transmission is almost full with the exception of small neighbourhoods of the embedded eigenvalues. On the other hand, for large b the transmission is only possible in the vicinity of the 'Neumann' eigenvalues; recall that in this case the line is close to full (Dirichlet) decoupling.

Acknowledgments

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