Magnetoresonances on a lasso graph

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We consider a charged spinless quantum particle confined to a graph consisting of a loop to which a halfline lead is attached; this system is placed into a homogeneous magnetic field perpendicular to the loop plane. We derive the reflection amplitude and show that there is an infinite ladder of resonances; analyzing the resonance pole trajectories we show that half of them turn into true embedded eigenvalues provided the flux through the loop is an integer or halfinteger multiple of the flux unit hc/e. We also describe a general method to solve the scattering problem on graphs of which the present model is a simple particular case. Finally, we discuss ways in which a state localized initially at the loop decays.

I begun my career at times when the world was much less connected, and of most parts we knew only from journals arriving not quite regularly. My first encounter with the mathematical theory of unstable quantum systems and related scattering problems occurred in this way, particularly through [24, 25] and related papers by Larry Horwitz; the subject remained for me as well as for him an old love to which we return regularly from time to time. Only many years later I had an opportunity to met him in person and to appreciate also his charisma. A distinguished birthday is a good opportunity to come with another decay scattering system; I should say that I prefer presents which are amusing rather than expensive.

1 Introduction

Quantum mechanics for a nonrelativistic particle whose configuration space is a graph has been studied already a long time ago in connection with models of organic molecules [33]. A recent new interest to these problems [1, 4, 5, 6, 11, 12, 16, 17, 20, 23] has been stimulated, in particular, by the progress of experimental solid state

Figure 1: A lasso graph

physics which allows us to produce semiconductor "quantum wire" structures and other "mesoscopic devices"; quantum mechanical graphs represent a natural model for many of them.

Graph systems provide a convenient mean to study various quantum effects both from the theoretical and experimental points of view, because the freedom in setting the geometry of the configuration space allows us to create different dynamics; at the same time, models of this type are often explicitly solvable. This concerns, in particular, resonance scattering effects associated with the existence of quasi-stationary states in graph loops and appendices — see, *e.g.*, [18]. These effects fit well, of course, into the general theory of decay scattering systems as exposed in [10, Chaps. 1,3], [28], or [32, Sec.XII.6], but they also make it possible to illustrate it and to draw fully specific conclusions.

Our aim here is to investigate one more solvable model of this type. It consists of a halfline attached to a loop placed into a magnetic field; the parameters are the magnetic flux through the loop and "coupling strengths" between the graph links at the junction. Our analysis differs from an earlier treatment of similar systems [8, 30] in several aspects. First of all, we consider a different and more general coupling between the loop and the halfline, and we put emphasis on the analytical solution of the problem. Furthermore, we shall be concerned with the decay and scattering properties of the system rather than with persistent currents induced by the magnetic field.

Let us review briefly the contents of the paper. The Hamiltonian of the model we are going to study is introduced in the following section. Next, we derive in Section 3 its spectral and scattering properties. Then we make a digression and describe a general method to treat scattering problem on an arbitrary graph by "discretizing" it, *i.e.*, transforming the corresponding Schrödinger equation into a set of linear equations involving just the wavefunction values at the graph nodes. Returning to our model, we analyze in Section 5 its resonance structure by deriving an explicit expression for the resolvent and finding the resonance–pole trajectories. Finally, in the concluding section we treat our model as a decay system and show how a state localized initially at the loop decays (or does not decay) in the course of time.

2 Description of the model

Consider a quantum particle confined to the lasso–shaped graph Γ sketched on Figure 1, *i.e.*, a circular loop of radius R to which a halfline lead is attached. We suppose that the particle is nonrelativistic, spinless, and charged. To be specific we assume that its charge is $q=-1$; we adopt the usual rational system of units, $e=c=2m=\hbar=1$. The system is placed into a homogeneous magnetic field of intensity B; the vector potential $\vec{A}$ can be chosen tangent to the loop with the modulus

$$A = \frac{1}{2} BR = \frac{\Phi}{L}, \tag{2.1}$$

where Φ is the magnetic flux through the loop and L is the loop perimeter. Under the convention we have adopted the natural flux unit [8] is $hc/e = 2\pi$, so the *rhs* of (2.1) can be also written as ϕ/R where ϕ is the flux value in this scale.

The state Hilbert space of the model is $\mathcal{H} \equiv L^2(\Gamma) := L^2(0,L) \oplus L^2(\mathbb{R}_+)$; the wave functions will be written as columns, $\psi = \binom{u}{f}$. To construct the Hamiltonian we begin with the operator describing the free motion on the loop and the lead under the condition that the graph vertex is "fully disconnected", so $H_\infty = H_{\mathrm{loop}}(B) \oplus H_{\mathrm{halfline}}$, where

$$H_{\mathrm{loop}}(B) = (-i\partial_x + A)^2 , \qquad H_{\mathrm{halfline}} = -\partial_x^2 \tag{2.2}$$

with the Dirichlet condition, $u(0) = u(L) = f(0) = 0$; if there is no danger of misunderstanding we abuse the notation and employ the same symbol for the arc–length variable on both parts of the graph. The operator H_{loop} has a simple discrete spectrum; the eigenfunctions

$$\chi_n(x) = \frac{e^{-iAx}}{\sqrt{\pi R}} \sin\left(\frac{nx}{2R}\right) , \qquad n = 1, 2, \dots \tag{2.3}$$

correspond to the eigenvalues $\left(\frac{n}{2R}\right)^2$, which are embedded into the continuous spectrum of H_{halfline} covering the interval $[0,\infty)$. Notice that the effect of the magnetic field on the *disconnected* loop amounts to a unitary equivalence,

$$H_{\mathrm{loop}}(B) = U_{-A} H_{\mathrm{loop}}(0) U_A , \tag{2.4}$$

where $(U_A u)(x) := e^{iAx} u(x)$.

To couple the graph parts one has to follow the standard strategy [17] which means to replace Dirichlet by a "connected" boundary condition at the vertex. In general, there is a nine–parameter family of such conditions. This is too many; we will be concerned with its three–parameter subfamily [17, 18], in particular, with a one–parameter set of boundary conditions known as δ–coupling [12]. Hence the Hamiltonian of our model acts as the free operator specified by (2.2),

$$H_{\alpha,\mu,\omega}(B) \begin{pmatrix} u \\ f \end{pmatrix} = \begin{pmatrix} -u'' - 2iAu' + A^2 u \\ -f'' \end{pmatrix} ; \tag{2.5}$$

the wave function is continuous on the loop,

$$u(0) = u(L) , \tag{2.6}$$

and satisfies the requirements

$$\begin{aligned} f(0) &= \omega u(0) + \mu f'(0) , \\ u'(0) - u'(L) &= \alpha f(0) - \omega f'(0) , \end{aligned} \tag{2.7}$$

for an $\alpha, \mu \in I\!R$ and $\omega \in \mathbb{C}$; the values of $u,\ f$ and their derivatives at the vertex are understood as the appropriate one–sided limits. However, we shall restrict ourselves to the case of time–reversal invariant couplings which means to assume that ω is also real; it has the meaning of a coupling constant between the loop (with a point interaction) and the halfline. In physical terms the conditions (2.6) and (2.7) express the conservation of probability flow at the junction.

The δ–coupling corresponds to the choice $\mu = 0$ and $\omega = 1$ in which case the wavefunction is fully continuous,

$$u(0) \,=\, u(L) \,=\, f(0)\,, \tag{2.8}$$

and

$$u'(0) - u'(L) + f'(0) \,=\, \alpha f(0)\,; \tag{2.9}$$

for the sake of simplicity we shall write $H_\alpha \equiv H_{\alpha,0,1}$. The parameter α is a coupling constant between the *disconnected* loop and the halfline; the fully decoupled case corresponds to $\alpha = \infty$ as the notation suggests.

Remarks. (a) The choice of the coupling at the vertex corresponds to a conceivable quantum–wire experiment. There is an approximation result [13] which means that the δ–coupling constant α can be regarded as a mean value of a sharply localized potential. This corresponds, *e.g.*, to a screened electrode placed at the vicinity of the junction; in a similar way one can model some of the more general boundary conditions (2.6) and (2.7) relating the parameters to physical quantities which an experimentalist can tune.

(b) In general, the vector potential enters the boundary conditions — see [6] and the remarks in Section 4.3 below. In the present case, however, the outward tangent components of $\vec{A}$ at the junction have opposite signs, so their contributions cancel. This may not be true if the loop is noncircular and has corners or cusps, but one can always achieve a cancellation by a suitable gauge choice. If the loop is viewed from outside as in the scattering process, the only quantity which matters is the magnetic flux Φ threading it.

(c) The S–matrix for a coupling of three semiinfinite wires equivalent to (2.6) and (2.7) was derived in [17]. This comparison shows, in particular, that choosing $\alpha = \mu = 0$ and putting $\epsilon := \left(\frac{2\omega}{2+\omega^2}\right)^2$, we obtain the coupling used in [8]. On the other hand, the authors of [30] worked with the ideal δ–coupling, $\alpha = 0$.

3 Scattering and bound states

Consider now the scattering problem on Γ, *i.e.*, the reflection of a particle traveling along the halfline from the magnetic–loop end. We limit ourselves to the stationary formulation looking for generalized eigenvectors, in other words, solutions of the equation $H_\alpha(B)\psi = k^2\psi$ which satisfy the definition domain requirements with exception of global square integrability. In view of (2.5), the most general Ansatz for such a solution is

$$u(x) \,=\, \beta\, e^{-iAx} \sin(kx+\gamma)\,, \qquad f(x) \,=\, e^{-ikx} + r\, e^{ikx} \tag{3.1}$$

with (k–dependent) parameters r, β, and γ; the latter is generally complex.

To find them we employ the boundary conditions. The identity (2.6) in combination with (2.1) leads to the relation

$$\tan\gamma \,=\, \frac{\sin kL}{e^{i\Phi} - \cos kL}\,. \tag{3.2}$$

The conditions (2.7) yield then a system of two linear equations for r, β which is solved by

$$r \,=\, -\,\frac{(1+ik\mu)\left[\alpha\,-\,\frac{\mathcal{R}}{\sin\gamma}\right] + i\omega^2 k}{(1-ik\mu)\left[\alpha\,-\,\frac{\mathcal{R}}{\sin\gamma}\right] - i\omega^2 k}$$

with

$$\frac{\mathcal{R}}{\sin\gamma} \,=\, k\,\cos\gamma - iA\,\sin\gamma - \,e^{-\Phi}\left[k\,\cos(kL+\gamma) - iA\,\sin(kL+\gamma)\right]\,.$$

Using again (2.6) and (3.2), we arrive after a simple algebra at the expression

$$r(k) \,=\, -\,\frac{(1+ik\mu)\left[\alpha\,-\,\frac{2k}{\sin kL}\,(\cos\Phi\,-\,\cos kL)\right] + i\omega^2 k}{(1-ik\mu)\left[\alpha\,-\,\frac{2k}{\sin kL}\,(\cos\Phi\,-\,\cos kL)\right] - i\omega^2 k} \tag{3.3}$$

for the reflection amplitude, in particular,

$$r(k) \,=\, -\,\frac{(\alpha+ik)\sin kL - 2k(\cos\Phi\,-\,\cos kL)}{(\alpha-ik)\sin kL - 2k(\cos\Phi\,-\,\cos kL)} \tag{3.4}$$

in the δ–coupling case. This (1×1) S–matrix can be also written by means of the phase shift. For instance, denoting

$$\Delta(k) \,\equiv\, \Delta(\alpha,\Phi;k) \,:=\, (\alpha-ik)\sin kL - 2k(\cos\Phi\,-\,\cos kL)\,, \tag{3.5}$$

we can write the *rhs* of (3.4) as $e^{2i\delta(k)}$ with

$$\delta(k) \,=\, \frac{\pi}{2} \,+\, \arctan\frac{k\,\sin kL}{\mathrm{Re}\,\Delta(k)}\,. \tag{3.6}$$

As usual the growth of the phase shift is related to the number of scattering resonances within a given energy interval. It is clear from (3.6) that $\delta(k)$ passes odd multiples of $\pi/2$ whenever the denominator (3.5) passes zero, of course, when there is not a simultaneous zero in the numerator. The last named situation occurs if and only if the flux Φ through the loop is a multiple of π. Hence "one half" of resonances is missing in that case; similar conclusions can be made in the general case of boundary conditions (3.3) when

$$\delta(k) \,=\, \frac{\pi}{2} + \arctan\left\{ \mu k + \frac{\omega^2 k}{\alpha - \frac{2k}{\sin kL}\left(\cos\Phi - \cos kL\right)} \right\} . \tag{3.7}$$

This is related to the existence of embedded eigenvalues at integer/halfinteger values of ϕ which will be clearly seen from the resonance pole trajectories discussed below. The bound states can also be found directly:

(a) It is clear that *positive–energy* bound states may be supported only at the loop. If we restrict our attention to the nontrivial case $\omega \neq 0$, this is possible in view of (2.7) when $u(0) = u'(0) - u'(L) = 0$. Hence such bound states exist only at integer/halfinteger values of the magnetic flux (in the natural units) and the corresponding eigenfunctions are given by (2.3) with an even n for ϕ integer and odd n for ϕ halfinteger.

(b) In addition, there can be *negative* eigenvalues. To find them we suppose that the loop wavefunction is given by the first part of (3.1) with $k = i\kappa$ and the halfline part is $\rho\, e^{-\kappa x},\ \kappa > 0$. The boundary conditions then yield a system of equations for β, ρ which can be solved provided

$$\frac{2\kappa}{\sinh \kappa L}\left(\cos\Phi - \cos\kappa L\right) \,=\, \alpha + \frac{\omega^2 \kappa}{1 + \mu\kappa} . \tag{3.8}$$

It is easy to see that under the condition $\alpha \geq \frac{2}{L}\left(\cos\Phi - 1\right)$ has no solution if $\mu \geq 0$ and a single root otherwise; in the case $\alpha < \frac{2}{L}\left(\cos\Phi - 1\right)$ one more eigenvalue is added.

4 A digression: a duality for graph scattering

At this point we want to make a small detour to describe a general method to treat scattering problem on graphs. Recall that there is an equivalence between the spectral problem for one–dimensional Schrödinger operators with point interactions and certain Jacobi matrices which is known in the literature as a "French connection" [2, 7, 9, 21, 22, 31]. We have been able to extend this duality recently to a wide class of Schrödinger operators on graphs [14]; here we want to illustrate that the same method is applicable to scattering problems.

4.1 Schrödinger operators on a general graph

Let us first collect some notion we shall need to formulate the result; for more details we refer to [14]. A graph Γ consists of a finite or countably infinite number of *vertices* $\mathcal{V} = \{\mathcal{X}_j : j \in I\}$ and *links (edges)* $\mathcal{L} = \{\mathcal{L}_{jn} : (j,n) \in I_{\mathcal{L}} \subset I \times I\}$. Without loss of generality we may suppose that each pair of vertices is connected by not more than one link; otherwise we just add some number of extra vertices. We assume that Γ is connected, so the set $\mathcal{N}(\mathcal{X}_j) = \{\mathcal{X}_n : n \in \nu(j) \subset I \setminus \{j\}\}$ of *neighbors* of $\mathcal{X}_j$, *i.e.*, the vertices connected with $\mathcal{X}_j$ by a single link, is nonempty. Throughout we shall assume that $\mathcal{N}(\mathcal{X}_j)$ is *finite* for any $j \in I$.

The graph *boundary* $\mathcal{B}$ is the subset of vertices having a single neighbor; it may be empty. We use the symbols $I_{\mathcal{B}}$ and $I_{\mathcal{I}}$ for the index subsets in I corresponding to $\mathcal{B}$ and the graph *interior* $\mathcal{I} := \mathcal{V}\setminus\mathcal{B}$, respectively. Γ has a *local* metric structure coming from the fact that each link $\mathcal{L}_{jn}$ can be mapped to a line segment $[0, \ell_{jn}]$. It is also possible to equip the graph naturally with a *global* metric by identifying it with a subset of a plane or a higher dimensional Euclidean space. The two metrics may differ at a single link; the local one which is important for us is usually given by the arc length of the curve segment representing $\mathcal{L}_{jn}$.

Using the local metric, we are able to introduce the state Hilbert space in the way we did it for the lasso graph and similar problems, namely as $L^2(\Gamma) := \bigoplus_{(j,n)\in I_{\mathcal{L}}} L^2(0, \ell_{jn})$. Its elements, *i.e.*, the wave functions, will be written as $\psi = \{\psi_{jn} : (j, n) \in I_{\mathcal{L}}\}$ or simply as $\{\psi_{jn}\}$. We shall suppose that the particle living on Γ is exposed to a potential; it is only important to know its values on the graph links, *i.e.*, a family of functions $V := \{V_{jn}\}$; since we do not want deal with mathematical subtleties here, we suppose that all of them are *essentially bounded,* $V_{jn} \in L^\infty(0, \ell_{jn})$. Then we are able to define the operator $H_\alpha \equiv H(\Gamma, \alpha, V)$ by

$$H_\alpha\{\psi_{jn}\} := \{ -\psi''_{jn} + V_{jn}\psi_{jn} : (j, n) \in I_{\mathcal{L}} \} \tag{4.1}$$

with the domain consisting of all ψ with $\psi_{jn} \in W^{2,2}(0, \ell_{jn})$ subject to a set α of boundary conditions at the vertices which couple the boundary values

$$\psi_{jn}(j) := \lim_{x\to 0+} \psi_{jn}(x) , \qquad \psi'_{jn}(j) := \lim_{x\to 0+} \psi'_{jn}(x) ; \tag{4.2}$$

we have identified here $x = 0$ with the vertex $\mathcal{X}_j$. In general, there is vast family of boundary conditions which make the operator (4.1) self–adjoint. It can be characterized by $4M^2$ real parameters, where M is the number of graph links [2, 17, 32], and even if we restrict to *local* boundary conditions which do not couple the boundary values belonging to different vertices, the number is still too large.

As above we restrict ourselves to the simplest situation when the links connected in a vertex $\mathcal{X}_j$ satisfy the δ*–coupling* condition, *i.e.*, $\psi_{jn}(j) = \psi_{jm}(j) =: \psi_j$ for all $n, m \in \nu(j)$, and

$$\sum_{n\in\nu(j)} \psi'_{jn}(j) = \alpha_j\psi_j \tag{4.3}$$

with a real–valued parameter $\alpha_j \in I\!R$ (coupling constant). However, the results derived below can be reformulated easily for the case when (4.3) is replaced by a δ'–coupling or another type of local boundary conditions [12, 17].

As in the particular case discussed in the previous sections the relation (4.3) and other local couplings have an illustrative meaning of probability current conservation at the vertex; in a sense they represent an analogy of Kirchhoff's law. This means, in particular, that they are independent of the lengths of the involved links. Moreover, since the probability current is connected with the kinetic part of the Schrödinger equation, the coupling is also independent of the potential V as long as the latter is regular, which is the assumption we have adopted. At the graph boundary we employ the usual conditions

$$\psi_j \cos\omega_j + \psi_j' \sin\omega_j \;=\; 0 \tag{4.4}$$

with a parameter ω_j; integer and halfinteger multiples of π correspond to the Dirichlet and Neumann condition, respectively.

4.2 Coupling two link bundles

In the next step we attach a certain number of semiinfinite links to Γ which will support asymptotic solutions; in the standard stationary picture we shall consider a combination of a falling and transmitted/reflected plane wave on each of them. We might regard these "external" links as a part of the graph boundary; however, it is convenient to treat them separately. A reason for that is the following: while we declared the intention to formulate the result for graphs with δ–couplings, it is desirable to have a coupling between the internal and external links which is slightly more general than (4.3). This could be useful, *e.g.*, if we want to study perturbatively resonances which arise when eigenvalues of the original graph operator become embedded into the continuous spectrum of the leads.

As another preliminary, therefore, consider two bundles of leads which support wavefunctions $\{f_n\}_{n=1}^N$ and $\{g_m\}_{m=1}^M$; the endpoints are placed to the point $x=0$. Suppose first that we have separate δ–couplings for each bundle,

$$f_1(0) = \cdots = f_N(0) =: f(0)\,, \qquad g_1(0) = \cdots = g_M(0) =: g(0)\,, \tag{4.5}$$

together with $\sum_{n=1}^N f_n'(0) = \alpha f(0)$ and $\sum_{m=1}^M g_n'(0) = \tilde\alpha g(0)$. To couple the two bundles, we preserve the separate continuity (4.5) and replace the derivative conditions by

$$f(0) \;=\; \alpha^{-1}\sum_{n=1}^N f_n'(0) + \gamma \sum_{m=1}^M g_n'(0)\,, \quad g(0) \;=\; \bar\gamma \sum_{n=1}^N f_n'(0) + \tilde\alpha^{-1}\sum_{m=1}^M g_n'(0) \tag{4.6}$$

with a complex parameter γ; an elementary integration by parts then shows that the corresponding boundary form vanishes under these conditions. The parameter modulus is the coupling strength; if the coupling is required to be time–reversal invariant, γ has to be real. An overall δ–coupling is achieved, of course, if $\alpha = \tilde\alpha = \gamma^{-1}$.

4.3 The S–matrix equation

Suppose now that a bundle of m_j halflines, $0 \le m_j < \infty$, is attached to the point $\mathcal{X}_j$ of Γ; the coupling being given by (4.5), (4.6) with the parameters α_j for the graph links joined at $\mathcal{X}_j$, $\tilde\alpha_j$ for the external links at $\mathcal{X}_j$, and γ_j. We call the j–th bundle $\mathcal{E}_j$ and $\mathcal{E}_{jm}$ will be the m–th halfline in it, so the full state Hilbert space will be now $L^2(\Gamma)\oplus\left(\bigoplus_{j\in I}\bigoplus_{m=1}^{m_j}L^2(\mathcal{E}_{jm})\right)$. For the sake of brevity, the graph extended by the external links will be denoted as $\Gamma_e\equiv\Gamma\cup\mathcal{E}$, for the state Hilbert space we will use the shorthand $L^2(\Gamma_e)$. The symbol $H_\alpha\equiv H(\Gamma_e,\{\alpha_j,\tilde\alpha_j,\gamma_j\},V)$ means a Schrödinger operator on Γ_e with the described coupling; for simplicity we assume that the potentials on the external links are zero.

As usual the stationary scattering problem means finding a generalized eigenvector of H_α with prescribed behavior in the asymptotic region, *i.e.*, a solution to the equation

$$H_\alpha\psi\,=\,k^2\psi\,, \tag{4.7}$$

which belongs *locally* to $D(H_\alpha)$ satisfying all the domain requirement (in particular, the boundary conditions at each vertex) apart of the global square integrability, and such that

$$\psi_{jm}(x)\,=\,a_{jm}e^{-ikx}+b_{jm}e^{ikx} \tag{4.8}$$

holds for $x\in\mathcal{E}_{jm}$. The vectors $a\equiv\{a_{jm}\}$ and $b\equiv\{b_{jm}\}$ of dimension $\mathrm{card}\,\mathcal{E}=\sum_{j\in I}m_j$ represent the incoming and outgoing amplitudes, respectively; we are interested in the operator that maps the former into the latter, $b=Sa$.

To proceed further, we need some more notation. The symbol H_α^D will denote the decoupled operator obtained from H_α by changing the conditions (4.3) at the points of graph interior $\mathcal{I}$ to Dirichlet, while at the boundary they are kept fixed; we also define $\mathcal{K}_\alpha:=\{k\,:\,k^2\in\sigma(H_\alpha^D),\ \mathrm{Im}\,k\geq 0\}$. Next we take an arbitrary link $\mathcal{L}_{nj}\equiv[0,\ell_{jn}]$ of Γ, the right endpoint being identified with $\mathcal{X}_j$, and denote by u_{jn}, v_{jn} the normalized Dirichlet solutions to the corresponding component $-f''+V_{jn}f=k^2f$ of the Schrödinger equation (4.7). In other words, we demand that the following boundary conditions are satisfied,

$$u_{jn}(\ell_{jn})=1-u'_{jn}(\ell_{jn})=0\,,\qquad v_{jn}(0)=1-v'_{jn}(0)=0\,, \tag{4.9}$$

provided $n\in I_{\mathcal{I}}$; at the graph boundary we replace the last requirement by $v_{jn}(0)=\sin\omega_n$ and $v'_{jn}(0)=-\cos\omega_n$. The Wronskian of these solutions equals

$$W_{jn}=-v_{jn}(\ell_{jn})=u_{jn}(0) \tag{4.10}$$

for $n\in I_{\mathcal{I}}$ and $W_{jn}=-u_{jn}(0)\cos\omega_n-u'_{jn}(0)\sin\omega_n$ otherwise. All these quantities depend in general on the spectral parameter k but we shall not indicate this fact explicitly. Now we can formulate the mentioned result:

Proposition. *Let* $k\notin\mathcal{K}_\alpha$ *with* $k^2\in I\!R$, $\mathrm{Im}\,k\geq 0$. *Under the assumptions given above, the corresponding on–shell scattering matrix for the graph* Γ_e *is given by the following system of* $N:=\mathrm{card}\,I+\mathrm{card}\,\mathcal{E}$ *equations*

$$\sum_{n\in\nu(j)\cap I_{\mathcal{I}}}\frac{\psi_n}{W_{jn}}\;-\;\left(\sum_{n\in\nu(j)}\frac{v'_{jn}(\ell_{jn})}{W_{jn}}-\alpha_j\right)\psi_j\,-\,ik\alpha_j\gamma_jm_jb_{j1}$$

$$= -ik\alpha_j\gamma_j \left(m_j\alpha_{j1} - 2\sum_{m=2}^{m_j} a_{jm} \right) \tag{4.11}$$

$$\tilde\alpha_j\bar\gamma_j \left(\sum_{n\in\nu(j)\cap I_{\mathcal{I}}} \frac{\psi_n}{W_{jn}} - \sum_{n\in\nu(j)} \frac{v'_{jn}(\ell_{jn})}{W_{jn}} \right)\psi_j + b_{j1}\,(\tilde\alpha_j - ikm_j)$$

$$= -a_{j1}\,(\tilde\alpha_j + ikm_j) - 2ik\sum_{m=2}^{m_j} a_{jm} \tag{4.12}$$

and

$$b_{jm} = b_{j1} + a_{j1} - a_{jm}\,, \qquad m = 2,\dots,m_j\,. \tag{4.13}$$

Remarks. (a) If $N<\infty$ the above relations represent a system of linear equations. In the opposite case they have to be interpreted as the appropriate operator equation on ℓ^2. This can be done under some additional assumptions on Γ, *e.g.*, if there are positive numbers c_1, c_2 such that $c_1 \le \ell_{jn} \le c_2$ holds for all $(j,n)\in I_{\mathcal{L}}$ — see [14] for more details.

(b) The results generalizes easily to the situation when Γ as a subset of $I\!R^\nu$ is placed into a magnetic field, not necessarily homogeneous, described by a vector potential A. The boundary conditions (4.3) are modified replacing $\psi'_{jn}(j)$ by $\psi'_{jn}(j) + iA_{jn}(j)$, where $A_{jn}(j)$ is the tangent component of A to $\mathcal{L}_{jn}$ at $\mathcal{X}_j$ [6]. The particle abiding on Γ is supposed here to be an electron; otherwise A has to be replaced by $-qA$ where q is the particle charge. The magnetic case can be handled by means of the unitary operator $U:\, L^2(\Gamma)\to L^2(\Gamma)$ which acts as

$$(U\psi)_{jn}(x) \;:=\; \exp\left(i\int_{x_{jn}}^{x} A_{jn}(y)\,dy \right)\, \psi_{jn}(x)\,;$$

the values x_{jn} are fixed reference points. Then the functions $(U\psi)_{jn}$ satisfy (4.3) and it is sufficient to replace the function values ψ_n in (4.11), (4.12) by $e^{iA_n}\psi_n$ provided the magnetic phase factors A_j are chosen to obey the natural consistency condition

$$A_j - A_n \;=\; \int_{\mathcal{L}_{jn}} A_{jn}(y)\,dy\,.$$

required by the wave function continuity.

(c) Consider a simple situation when a single halfline is attached to every point of Γ and denote the "graph part" of the above system, *i.e.*, the operator represented by the two sums at the *lhs* of (4.11) as h. If the coupling is ideal, $\alpha_j = 0$ for all $j\in I$, the S–matrix is given by

$$S \;=\; -\,\frac{h+ik}{h-ik}\,.$$

It is illustrative to compare this to the the formula used recently by Sadun and Avron [34] in a study of scattering on discrete graphs; the only difference is the replacement of $-ik$ by e^{ik}, the energy being $2\cos k$ in this case.

To prove the proposition, it is sufficient to use the transfer matrices which relate the Schrödinger equation solutions at both ends of each link [14]. Since the Wronskian is nonzero for $k \notin \mathcal{K}_\alpha$, we get

$$\begin{aligned} \psi_j &:= \psi_{jn}(j) = u'_{jn}(0)\psi_n + v_{jn}(\ell_{jn})\psi'_{jn}(n)\,, \\ -\psi'_{jn}(j) &= \frac{1-u'_{jn}(0)v'_{jn}(\ell_{jn})}{W_{jn}}\psi_n + v'_{jn}(\ell_{jn})\psi'_{jn}(n)\,; \end{aligned}$$

the sign change at the *lhs* of the last condition reflects the fact that (4.2) defines the *outward* derivative at $\mathcal{X}_j$. We express $\psi'_{jn}(n)$ from the first relation and substitute to the second one. This yields

$$\psi'_{jn}(j) = -\frac{\psi_n}{W_{jn}} + \frac{v'_{jn}(\ell_{jn})}{W_{jn}}\,\psi_j$$

for $n \in I_\mathcal{I}$, while at the graph boundary we get with the help of (4.4) instead

$$\psi'_{jn}(j) = \frac{v'_{jn}(\ell_{jn})}{W_{jn}}\,\psi_j\,.$$

Now one has just to substitute these values into the boundary conditions at each vertex to arrive at the relations (4.11)–(4.13). ∎

It is not difficult to check that the lasso graph with the δ–coupling can be treated within this general scheme. We use the normalized Dirichlet solutions at both loop "ends", $k^{-1}\sin kx$ and $-k^{-1}\sin k(x-L)$, and add a vertex into an "interior point". Using (4.11) and (4.12) and excluding the function values at the added point, we arrive after a straightforward calculation at the equations

$$\begin{aligned} \left(-k\,\frac{e^{i\Phi}+e^{-i\Phi}}{\sin kL} + 2k\,\frac{\cos kL}{\sin kL} + \alpha\right)\psi - ikb &= -ika\,, \\ \psi &= b+a\,, \end{aligned}$$

from which we recover the reflection amplitude (3.4).

5 Resonances

5.1 The resolvent

Let us return now to our model. The most natural way to study spectral properties of an operator is through its resolvent, and therefore we want to find it for $H_\alpha(B)$.

The "decoupled" resolvent is found easily: it is a matrix integral operator with the kernel

$$G_\infty(x,y;k) \;=\; \begin{pmatrix} e^{-iA(x-y)}\,\frac{\sin kx_<\,\sin k(x_>-L)}{k\,\sin kL} & 0 \\ 0 & \frac{\sin kx_<\,\exp(ikx_>)}{k} \end{pmatrix}, \tag{5.1}$$

where $x_<$ and $x_>$ mean conventionally the smaller and larger of the variables x, y, respectively. We abuse here again the notation and employ the same symbol for the arc–length variable on the loop and the lead as well as for the pair of them.

Since $H_{\alpha,\mu,\omega}$ and H_∞ are both self–adjoint extensions of the same symmetric operator with the deficiency indices $(2,2)$, the resolvent of the former is by Krein's formula [2, App.A] given by

$$G_{\alpha,\mu,\omega}(x,y;k) \;=\; G_\infty(x,y;k) + \sum_{j,\ell=1}^{2} \lambda_{j\ell} F_j(x) F_\ell^t(y)\,, \tag{5.2}$$

where the symbol *"t"* means transposition, F_j are vectors of the corresponding deficiency subspaces which we shall choose in the form

$$F_1(x) := \begin{pmatrix} w(x) \\ 0 \end{pmatrix}, \qquad F_2(x) := \begin{pmatrix} 0 \\ e^{ikx} \end{pmatrix} \tag{5.3}$$

with

$$w(x) := e^{iAx}\,\frac{e^{-i\Phi}\sin kx - \sin k(x-L)}{\sin kL}\,,$$

and $\lambda_{j\ell}$ are coefficients to be found. Introducing

$$h_1 := \int_0^L w(y) v(y)\,dy\,, \qquad h_2 := \int_0^\infty e^{iky} g(y)\,dy$$

for a given $\binom{v}{g} \in \mathcal{H}$, we find easily that the boundary values of the function $\binom{u}{f} := (H_{\alpha,\mu,\omega} - k^2)^{-1}\binom{v}{g}$ are in view of (5.2) given by

$$u(0) \;=\; u(L) = \lambda_{11}h_1 + \lambda_{12}h_2\,, \qquad f(0) = \lambda_{21}h_1 + \lambda_{22}h_2\,,$$

$$u'(0) - u'(L) \;=\; h_1 + \frac{2k}{\sin kL}\,(\cos\Phi - \cos kL)\,(\lambda_{11}h_1 + \lambda_{12}h_2)\,,$$

$$f'(0) \;=\; h_2 + ik\,(\lambda_{21}h_1 + \lambda_{22}h_2)\,.$$

However, $\binom{u}{f}$ belongs to $D(H_{\alpha,\mu,\omega})$ for any $\binom{v}{g}$, so substituting these boundary values into (2.7) we get a system of four linear equations which yields the sought coefficients:

$$\begin{aligned} \lambda_{11} \;&=\; -\,\frac{1-i\mu k}{\mathcal{D}}\,, \qquad \lambda_{12} = -\,\frac{\omega}{\mathcal{D}}\,, \\ \lambda_{21} \;&=\; -\,\frac{\omega}{\mathcal{D}}\,, \qquad \lambda_{22} = \frac{\mu\left[2k\,\frac{\cos\Phi-\cos kL}{\sin kL} - \alpha\right] - \omega^2}{\mathcal{D}} \end{aligned} \tag{5.4}$$

with

$$\mathcal{D} \equiv \mathcal{D}(\alpha, \mu\,\omega; k) \;:=\; (1-i\mu k)\left[2k\,\frac{cos\Phi - \cos kL}{\sin kL} - \alpha\right] - i\omega^2 k\,. \tag{5.5}$$

In the case of δ–coupling, $\mu = 0$, $\omega = 1$, the coefficients acquire a particularly simple form, $\lambda_{j\ell} = -\mathcal{D}^{-1}$, $j, \ell = 1, 2$.

5.2 Pole trajectories

As usual in such situations [3, 18] the singularities of $G_\infty(x, y; k)$ cancel with those of the added term in (5.2) and the resolvent poles are given by zeros of the denominator (5.5); the exception is represented by the case of an integer or halfinteger ϕ.

For the sake of simplicity, we shall speak mostly about the δ–coupling situation. If the coupling is ideal, $\alpha = 0$, the pole condition becomes

$$2(\cos\Phi - \cos kL) = -i\,\sin kL \tag{5.6}$$

and one is able to solve it explicitly. No singularities exist in the upper halfplane, hence we write

$$k \;=\; \kappa - i\eta\,. \tag{5.7}$$

Substituting into the above condition, we find that for $|\Phi| < \frac{\pi}{6} \pmod{\pi}$ there is a pair of poles with $\kappa = \pi n/L$ and

$$\eta = \frac{1}{L}\,\ln\left(2(-1)^n\cos\Phi \pm \sqrt{4\cos^2\Phi - 3}\right)\,, \tag{5.8}$$

where $(-1)^n\cos\Phi > 0$. On the other hand, for the remaining values of Φ the poles are found at the line parallel to the real axis with $\eta = -\frac{\ln 3}{2L}$ and

$$\kappa = \pm\frac{1}{L}\,\arccos\left(\frac{2}{\sqrt{3}}\,\cos\Phi\right)\,. \tag{5.9}$$

We see that both poles are in the open lower halfplane with the exception of $\Phi = n\pi$, *i.e.*, ϕ integer or halfinteger, when one of them turns into an embedded–eigenvalue pole at the real axis. The pole trajectories with respect to Φ are not smooth despite the analytic form of the condition (5.6); this is due to the fact that $\mathcal{D} = 0$ at the crossing points $\frac{1}{L}\left(\pi n - \frac{i}{2}\ln 3\right)$, so the implicit–function theorem does not apply there. A similar picture is obtained for the boundary conditions (2.7) with $\alpha = \mu = 0$ and $|\omega| < \sqrt{2}$, in which case the "horizontal" line has $\eta = \frac{1}{2}\,\ln\frac{2+\omega^2}{2-\omega^2}$. On the other hand, in the case $|\omega| \geq \sqrt{2}$ the pole trajectories are "vertical" segments with $\kappa = \pi n/L$ only.

If $\alpha \neq 0$ the δ–coupling pole condition (5.6) is replaced by

$$2k(\cos\Phi - \cos kL) = (\alpha - ik)\sin kL\,.$$

Figure 2: Pole trajectories from the condition (5.10) for different values of the coupling constant (dashed: $\alpha = 0.5$, full: $\alpha = 0.1$, dotted: $\alpha = 0.05$)

Writing separately the real and imaginary parts with the help of the parametrization (5.7), we find that for $\kappa = \pi n/L$ a zero can exist only at the real axis if $\Phi = m\pi$. For other values of κ the pole condition can be cast into the form

$$\coth \eta L = 2 + \alpha \frac{2\eta - \kappa \cot \kappa L}{\eta(\eta - \alpha) + \kappa^2}, \tag{5.10}$$

which has to be solved numerically. The resulting pole trajectories are shown on Figure 2.

6 Decay of loop states

Up to now we have considered the lasso graph as a scattering system. Now we shall suppose that the system is prepared at an initial instant in a state the wavefunction of which is localized at the loop. It is not so important how such a situation is realized. For instance, one can place an electron at an isolated ring and "switch in" the junction at $t = 0$. The state is generally unstable under the evolution governed by $H_{\alpha,\mu,\omega}$ and we are interested in the way in which it decays.

Since we have an explicit expression for the resolvent, we are able in principle to write the non–decay amplitude explicitly [10, Sec.3.1]. However, instead of trying to evaluate this function we limit ourselves to elucidation of its basic properties.

6.1 Spectral decomposition

The relations (5.2) and (5.4) imply, in particular, that the resolvent form $z \mapsto \left(\psi, (H_{\alpha,\mu,\omega} - z)^{-1}\psi\right)$ is a meromorphic function including its continuation to the second sheet. Its possible poles are associated with the discrete spectrum of $H_{\alpha,\mu,\omega}$ which we also know explicitly. Since these are the only singularities, the function $\left(\psi, (H_{\alpha,\mu,\omega} - \cdot)^{-1}\psi\right)$ is analytic for all ψ belonging to the complement $\mathcal{H}_p(H_{\alpha,\mu,\omega})^{\perp}$. In particular, it is uniformly bounded in any finite part of the strip $|\mathrm{Im}\, z| < 1$, and thus by the basic criterion [32, Thm.XIII.19] such a vector belongs to $\mathcal{H}_{ac}(H_{\alpha,\mu,\omega})$.

Consequently, our Hamiltonian has no singularly continuous spectrum. The initial state can be therefore decomposed into $\psi = \psi_p + \psi_{ac}$ and the corresponding non–decay amplitude equals

$$(\psi, U_t\psi) = (\psi_p, U_t\psi_p) + (\psi_{ac}, U_t\psi_{ac}), \tag{6.1}$$

where $U_t := \exp\{-iH_{\alpha,\mu,\omega}t\}$. The second term on the *rhs* goes to zero as $t \to \infty$ in view of the Riemann–Lebesgue lemma; the first one is a linear combination of exponentials with coefficients coming from the Fourier decomposition of ψ_p . If just one of them is nonzero, then the decay law of the corresponding loop state given by squared modulus of (6.1) has a finite nonzero limit. Such a behavior is typical for unstable systems having bound states with a nonzero Fourier component in a decaying state; it has been observed recently in another context — see [15], and also [19] where, however, the effect may be also related to the threshold violation of the Fermi golden rule discovered by Howland [29].

If the loop state contains a superposition of a larger number of eigenvectors, the nondecay probability does not go to zero as $t \to \infty$ but a limit does not exist. In view of the above discussion, such a situation can occur in the present model only if (a) there are two negative eigenvalues (see Remark (b) at the end of Section 3), or (b) if $\Phi = n\pi$ with $n \in \mathbb{Z}$. The asymptotic behavior of the decay law depends then on the coupling parameters. If all the involved eigenvalues are commensurate, the asymptotics is periodic; this happens always if there is no negative–energy bound state. In the general case the decay law asymptotics is quasiperiodic.

6.2 What has all this in common with neutral kaons?

Concluding this study, let me mention one more topic to which Larry Horwitz made a contribution, namely the decay theory of neutral kaons. This subject attracted attention at the end of the sixties as an example of a system with a substantially nonexponential decay law exhibiting different time scales, as well as the possibility to "recreate" decayed particles by performing a set of noncompatible measurements.

Mesoscopic physics makes it possible to tailor systems in which similar effect can be observed. Consider our lasso graph with the initial wavefunction u on the loop such that $x \mapsto e^{iAx}u(x)$ has no definite symmetry with respect to the connection point $x = 0$ (say, $u(x) = e^{-ix(A-2\pi n/L)}$). If the flux value ϕ is integer, the A–even component represents a superposition of embedded–eigenvalue bound states and thus it survives, while the A–odd one dies out. In a real life experiment, of course, we cannot ensure that ϕ is exactly an integer, hence we shall have rather a fast and a slowly decaying part of the wavefunction; recall the pole trajectories discussed in Section 5.2.

Moreover, consider a loop to which two halfline leads are attached at different points and assume that we are able to switch the coupling in and out independently. We wait until the A–odd part in the above described experiment essentially decays while the longliving component is still preserved, and switch from the first lead to the second one. Now the symmetry with respect to the other junction is important. If the surviving part of the wavefunction is a superposition of an A–even and an A–odd part with respect to the latter, the scenario repeats. Of course, the "second decay" may produce a smaller component A–odd with respect to the first junction, so the analogy is complete.

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Figure captions

Figure 1. A lasso graph

Figure 2. Pole trajectories from the condition (5.10) for different values of the coupling constant (dashed: $\alpha = 0.5$, full: $\alpha = 0.1$, dotted: $\alpha = 0.05$)

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