Spectral and resonance properties of Smilansky Hamiltonian

Pavel Exner[a,b], Vladimir Lotoreichik[a,*], Miloš Tater[a]

[a] *Department of Theoretical Physics, Nuclear Physics Institute, Czech Academy of Sciences, 25068 Řež near Prague, Czechia*
[b] *Doppler Institute for Mathematical Physics and Applied Mathematics, Czech Technical University, Břehová 7, 11519 Prague, Czechia*

Abstract

We analyze the Hamiltonian proposed by Smilansky to describe irreversible dynamics in quantum graphs and studied further by Solomyak and others. We derive a weak-coupling asymptotics of the ground state and add new insights by finding the discrete spectrum numerically. Furthermore, we show that the model has a rich resonance structure.

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1. Introduction

While the fundamental equations of motion, both in classical and quantum mechanics, are invariant with respect to time reversal, the world around us is full of irreversible processes. On a microscopic level, it is enough to recall spontaneous decays of particles, nuclei, inelastic scattering processes, etc. And, of course, an irreversible process *par excellence* is the wave packet reduction which is the core of Copenhagen description of a measuring process performed on a quantum system.

[*] Corresponding author
Email address: `tater@ujf.cas.cz` (Miloš Tater)
URL: `gemma.ujf.cas.cz/~exner/` (Pavel Exner), `gemma.ujf.cas.cz/~lotoreichik/` (Vladimir Lotoreichik)

A description of such processes in quantum mechanics is typically associated with enlarging the state Hilbert space, conventionally referred to as coupling the system to a heat bath [4, 7]. As a rule, it is assumed that (i) the bath is a system with infinite number of degrees of freedom, (ii) the bath Hamiltonian has a continuous spectrum, and (iii) the presence (or absence) of irreversible modes is determined by the energies involved rather than the coupling strength. While this all is true in many cases, situations may exist where the system has neither of the listed properties. This was the motivation which led Uzy Smilansky to formulation a simple model [16] of a quantum graph coupled to a heat bath consisting of a single harmonic oscillator which exhibits an irreversible behavior. The easiest way to describe the model is to phrase it in PDE terms, then its Hamiltonian is a Schrödinger operator,

$$H_\lambda = -\frac{\partial^2}{\partial x^2} + \frac{1}{2}\left(-\frac{\partial^2}{\partial y^2} + y^2\right) + \lambda y \delta(x) \tag{1}$$

on $L^2(\mathbb{R}^2)$, with a singular interaction supported by the line $x = 0$ the strength of which depends on the coordinate y.

The system governed by the Hamiltonian (1) undergoes an abrupt spectral transition at the critical value $\lambda = \sqrt{2}$; while for $|\lambda| < \sqrt{2}$ the Hamiltonian is positive above this value its spectrum covers the whole real axis. The mechanism of this effect is easy to understand. The first and the last term in (1) represent Hamiltonian of a one-dimensional system with a point interaction which has a single eigenvalue equal to $-\frac{1}{4}\lambda^2 y^2$ [1]. This negative contribution to the energy competes with the oscillator potential with the balance flipping exactly at the said critical value of λ.

The model was subsequently an object of investigations, generalizations and modifications in a series of mathematically rigorous papers. The discrete spectrum in the subcritical case and its behavior as $\lambda \to \sqrt{2}$ were analyzed in [17], the absolute continuity of the other spectral component was established in [13], an extension to the situation when the 'heat bath' consists of two or more oscillators was discussed in [5, 6]. Other modifications consisted of replacing the oscillator by a potential well of a different shape [19] or by replacing the line by a more general graph [18] corresponding to the original Smilansky proposal. It is also possible to have the motion in the x direction restricted to an interval with periodic boundary conditions [11, 15]; in the first named of these papers time evolution of wave packets is investigated confirming the idea that spectral change in the supercritical case corresponds to the possibility of 'escape to infinity'. Let us also mention a modification in which the singular interaction is replaced by a regular potential channel which gets deeper and more narrow as the distance from a fixed point increases [2].

In connection with the last mentioned system let us point out that similar parameter dependent spectral transitions can be also observed in other systems, an example being the one described by the Hamiltonian

$$H = -\Delta + |xy|^p - \lambda(x^2 + y^2)^{p/(p+2)}\,, \qquad p \geq 1, \tag{2}$$

on $L^2(\mathbb{R}^2)$ [3]. In this case the change is even more dramatic, from the spectrum which is below bounded and purely discrete to the whole real line, the transition occurring at the critical value $\lambda = \lambda_p$, the ground state eigenvalue of the appropriate (an)harmonic oscillator. To our knowledge, spectral transitions of this type were for the first time noted in [20].

Our object of interest in the present paper is the original Smilansky Hamiltonian (1). Despite the fact that many of its properties were demonstrated in the papers mentioned above, there is still a room for new insights. The first topic here concerns the discrete spectrum of H_λ and comes from the observation that it is relatively easy to find the eigenvalues and eigenfunctions numerically turning the task into a matrix problem of a sufficiently large dimension.

Another question to be discussed here concerns *resonances* in the system described by the Hamiltonian (1). While the absolute continuity of the spectrum above the threshold and the existence of the wave operators were established in [5], the possible resonance character of the scattering seems to have escaped attention. In our recent paper [10] we have demonstrated how one can find poles of the analytically continued resolvent and derived asymptotic expansions for them, here we focus on the physical meaning of the resonances and illustrate their behavior by numerical results.

2. Survey of results about the spectrum

To make the paper self-contained we summarize first the known facts about the operator that are indicated briefly in the introduction. It is obvious that we can consider the positive values of the coupling constant λ as the opposite case is obtained via a mirror transformation with respect to the axis $x = 0$.

(a) Spectral transition: In the subcritical case, $\lambda < \sqrt{2}$, the particle remains localized in the vicinity of the x axis, while for $\lambda > \sqrt{2}$ it can according to [11] escape to infinity along the singular 'channel' in the y direction. In spectral terms, this corresponds to the switch from a positive spectrum of H_λ to a below unbounded one which occurs at $\lambda = \sqrt{2}$.

(b) The continuous spectrum of H_λ covers the interval $(\frac{1}{2}, \infty)$ for $\lambda < \sqrt{2}$, the positive semi-axis for $\lambda = \sqrt{2}$, and the whole real axis if $\lambda > \sqrt{2}$. Moreover, this spectrum is in fact purely absolutely continuous [14, Sec. VII.2], in particular, the operator is purely absolutely continuous in the supercritical case when $\sigma(H_\lambda) = \sigma_{\rm ac}(H_\lambda) = \mathbb{R}$.

(c) Eigenvalue existence and location: For any $\lambda \in (0, \sqrt{2})$ the discrete spectrum of H_λ is nonempty, simple, and finite, being contained in $(0, \frac{1}{2})$, i.e. the subcritical operator is positive. The eigenvalues are decreasing functions of the coupling constant λ. On the other hand, there are no eigenvalues $\geq \frac{1}{2}$, and in the supercritical case, $\lambda > \sqrt{2}$, the point spectrum of H_λ is empty, in other words, there are no eigenvalues embedded in the continuum.

(d) Near critical asymptotics: The number of eigenvalues in the subcritical regime increases with the coupling constant and explodes as it approaches the critical value $\lambda = \sqrt{2}$ behaving asymptotically as [17]

$$N(\tfrac{1}{2}, H_\lambda) \sim \tfrac{1}{4}\sqrt{\tfrac{1}{\sqrt{2}(\sqrt{2}-\lambda)}} \tag{3}$$

where $N(\mu, A)$ conventionally denotes the number of eigenvalues of the operator A below μ with the multiplicity taken into account.

(e) Weak-coupling asymptotics: For small enough λ there is a single eigenvalue which behaves as

$$\epsilon_1(\lambda) = \frac{1}{2} - \frac{\lambda^4}{64} + \mathcal{O}(\lambda^5) \tag{4}$$

as $\lambda \to 0$ [10]. In fact, due to the mirror symmetry of the spectrum with respect to λ the error term can be replaced by $\mathcal{O}(\lambda^6)$.

3. Numerical solution of the eigenvalue problem

To find the discrete spectrum we note first that the solutions to the eigenvalue problem can be expanded using the 'transverse' base naturally spanned by the functions

$$\psi_n(y) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}}\, \mathrm{e}^{-y^2/2} H_n(y) \tag{5}$$

corresponding to the oscillator eigenvalues $\nu_n = n + \frac{1}{2}$, $n = 0, 1, 2, \ldots$; here H_n are Hermite polynomials with conventional normalization. Furthermore, the task can be simplified by noting that the problem has a mirror symmetry w.r.t. $x = 0$ which allows us to decompose H_λ into the trivial odd part $H_\lambda^{(-)}$ and the even part $H_\lambda^{(+)}$ which is equivalent to the operator on $L^2(\mathbb{R}^2_+)$, where $\mathbb{R}^2_+ := \mathbb{R} \times (0, \infty)$, with the symbol (1) and the domain consisting of $H^2(\mathbb{R}^2_+)$ functions satisfying the boundary conditions

$$f'_x(0+, y) = \frac{1}{2}\, \lambda y f(0+, y)\,. \tag{6}$$

Substituting the Ansatz

$$f(x, y) = \sum_{n=0}^{\infty} c_n\, \mathrm{e}^{-\kappa_n x} \psi_n(y) \tag{7}$$

with

$$\kappa_n := \sqrt{n + \frac{1}{2} - \epsilon} \tag{8}$$

into (6) and using orthonormality of the basis (5), we get for solution with the energy ϵ the equation

$$B_\lambda c = 0\,, \tag{9}$$

where c is the coefficient vector and B_λ is an operator in ℓ^2, in other words, an infinite matrix with the elements

$$(B_\lambda)_{m,n} = \kappa_n \delta_{m,n} + \frac{1}{2}\lambda(\psi_m, y\psi_n)\,; \tag{10}$$

note that the matrix B_λ is in fact tridiagonal because

$$(\psi_m, y\psi_n) = \frac{1}{\sqrt{2}}\big(\sqrt{n+1}\,\delta_{m,n+1} + \sqrt{n}\,\delta_{m,n-1}\big)\,,$$

in other words, B_λ is a Jacobi matrix.

Note that using a general sequence $\{u_n(x)\}$ instead of $\mathrm{e}^{-\kappa_n x}$ in the Ansatz (7) one can reformulate the problem as an analogue of the Birman-Schwinger principle as first proposed by M. Solomyak in [17], see a detailed discussion in [10]. The same approach works also for some modifications of the original Smilansky model mentioned in the introduction where, however, the structure of the appropriate matrix problem is different and may be more complicated.

To find the values of ϵ for which the secular equation (9) is satisfied for a given λ we solve a truncated matrix problem increasing the cut-off until a numerical stability is reached. The convergence is slower the closer is the value of ϵ to the threshold value $\frac{1}{2}$. We present results for the sizes up to 9000×9000.

The results are plotted below in a series of figures. They are, of course, in agreement with the theoretical predictions listed in the previous section, but they provide additional insights. To begin with, Fig. 1 shows eigenvalues of H_λ as functions of the coupling constant. We see that in the most part of the subcritical region, more than 98% of it, the Hamiltonian has a single eigenstate. The second eigenvalue appears only at $\lambda \approx 1.387559$, the next thresholds are $1.405798, 1.410138, 1.41181626, 1.41263669, \dots$. This does not give a good picture of the spectral behavior near the critical values. Instead we can plot the eigenvalue as functions of λ using a logarithmic scale. The result is shown in Fig. 2. We see that their number indeed grows as we approach the transition point filling the allowed interval so that $\sigma(H_{\sqrt{2}}) = [0,\infty)$, but that the discrete spectrum is asymptotically equidistantly distributed. The same result allows us to illustrate the Solomyak asymptotic formula (3): it is obvious

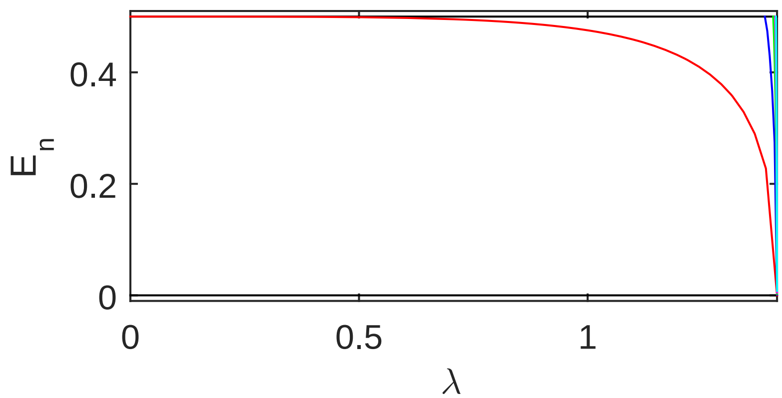

Figure 1: Eigenvalues of H_λ as functions of λ

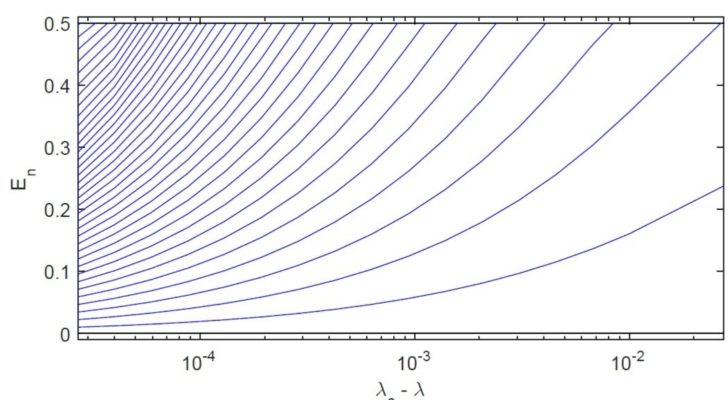

Figure 2: The discrete spectrum near the critical point

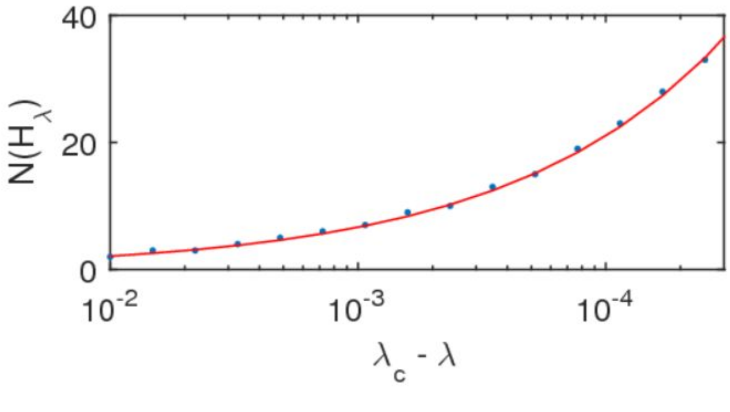

Figure 3: The eigenvalue numbers (indicated by dots) compared with the asymptotics (3)

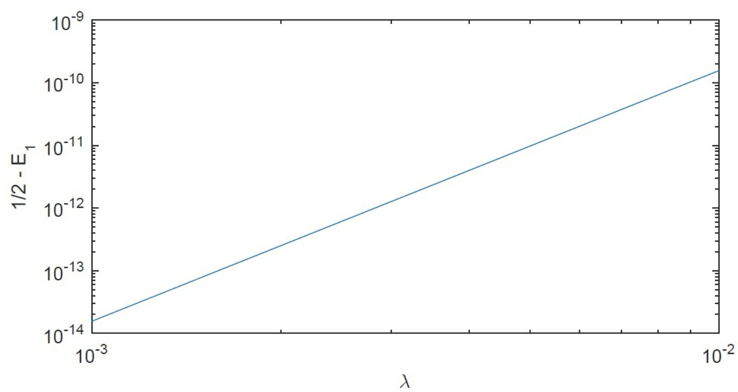

Figure 4: The weak-coupling behavior of the ground-state energy

from Fig. 3 that the leading term of the expansion gives a good approximation as long as $\sqrt{2} - \lambda \lesssim 10^{-2}$.

The opposite asymptotical situation is the weak coupling. In Fig. 4 we plot the ground-state eigenvalue as a function of λ. In the double logarithmic scale the graph is practically indistinguishable from a straight line which allows us to read out the power of the leading term as well as the coefficient $0.015625 = \frac{1}{64}$ appearing in the leading term of (4).

Since, in contrast to points (a)–(d) of the previous section the weak-coupling asymptotics is a new observation it is worth to show a way how it can be derived.

To this purpose we introduce a symbol for the energy gap

$$\mu_\lambda := 1/2 - \epsilon_1(\lambda) \tag{11}$$

and denote by $c^\lambda = (c_0^\lambda, c_1^\lambda, c_2^\lambda, \dots)$ the normalized eigenfunction of B_λ given by (9) corresponding to zero eigenvalue. Without loss of generality we may assume that c_0^λ is non-negative. Writing the lines of the corresponding infinite system of equation explicitly, we get

$$\begin{aligned} &\sqrt{\mu_\lambda}\, c_0^\lambda + \frac{\lambda}{2\sqrt{2}}\, c_1^\lambda = 0\,, \\ &\frac{\sqrt{k}\lambda}{2\sqrt{2}}\, c_{k-1}^\lambda + \sqrt{k+\mu_\lambda}\, c_k^\lambda + \frac{\sqrt{k+1}\lambda}{2\sqrt{2}}\, c_{k+1}^\lambda = 0\,, \qquad k \geq 1\,. \end{aligned} \tag{12}$$

Using elementary inequalities $\sqrt{k} \leq \sqrt{k+\mu_\lambda}$ and that $\sqrt{k+1} \leq \sqrt{2(k+\mu_\lambda)}$, we get from the second relation in (12) the estimate

$$|c_k^\lambda| \leq \frac{\lambda}{2\sqrt{2}}\, |c_{k-1}^\lambda| + \frac{\lambda}{2}\, |c_{k+1}^\lambda|\,, \qquad k \geq 1\,, \tag{13}$$

which implies

$$|c_k^\lambda|^2 \leq \frac{\lambda^2}{4}\, |c_{k-1}^\lambda|^2 + \frac{\lambda^2}{2}\, |c_{k+1}^\lambda|^2\,, \qquad k \geq 1.$$

and combining it with the normalization assumption, $\|c^\lambda\| = 1$, we arrive at

$$\sum_{k=1}^{\infty} |c_k^\lambda|^2 \leq \frac{\lambda^2}{4} \sum_{k=0}^{\infty} |c_k^\lambda|^2 + \frac{\lambda^2}{2} \sum_{k=2}^{\infty} |c_k^\lambda|^2 \leq \frac{3\lambda^2}{4}.$$

Using $\|c^\lambda\| = 1$ once more, we conclude that

$$c_0^\lambda = \Big(\|c^\lambda\|^2 - \sum_{k=1}^{\infty} |c_k^\lambda|^2 \Big)^{1/2} = 1 + O(\lambda^2)\,, \qquad \lambda \to 0\,; \tag{14}$$

then inequality (13) together with the normalization yield $c_2^\lambda = \mathcal{O}(\lambda)$. In combination with (14) and the second relation of (12) for $k = 1$ this implies further

$$c_1^\lambda = \frac{\lambda}{2\sqrt{2}} + \mathcal{O}(\lambda^2)\,, \qquad \lambda \to 0\,. \tag{15}$$

Using now (14) and (15) we obtain from the first relation in (12) that

$$\mu_\lambda = \frac{\lambda^4}{64} + \mathcal{O}(\lambda^5)\,, \qquad \lambda \to 0\,,$$

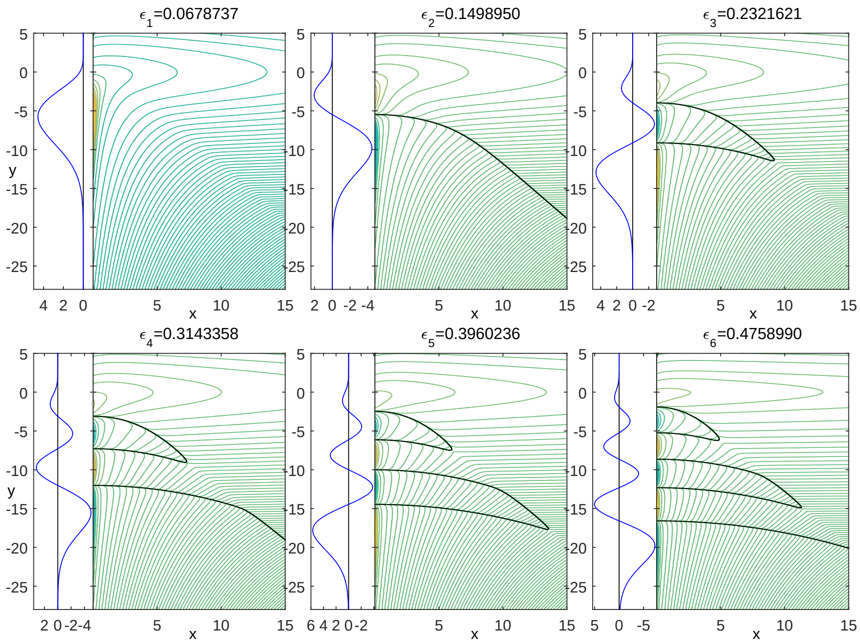

Figure 5: The first six eigenfunctions of H_λ for $\lambda = 1.4128241$

which is nothing else but the formula (4). In the counterpart to this paper [10] we give a modified version of this argument which allows, at least in principle, to compute higher terms of this asymptotic expansion.

Before proceeding further, let us also look at the eigenfunctions. In Fig. 5 we show a contour plot of the first six eigenfunctions of H_λ for $\lambda = 1.4128241$, in other words, $\lambda = \sqrt{2} - 0.0086105$. In the side plots we feature restrictions of the eigenfunctions on the y-axis. As expected the eigenfunctions are concentrated in the vicinity of the 'escape channel', i.e. the negative part of the y-axis. The plots also show that they obey the usual restriction, commonly referred to as Courant nodal domain theorem; the inequality becomes sharp from the third eigenfunction. The pattern is interesting, the odd eigenfunctions (except the ground state) have closed nodal lines only, the even ones have an unbounded nodal line. One wonders whether this property holds for the discrete spectrum generally.

4. Resonances

Our second main point is to show that Smilansky model also exhibits interesting resonance behavior. Having said that, one has to explain first what is meant by a resonance. There are different definitions, the two main being the *resolvent resonances* associated with poles in the analytic continuation of the resolvent over the cut(s) corresponding to the continuous spectrum, and *scattering resonances* associated with singularities of the scattering matrix. While these two can often be identified, this property has to be checked in each particular case; recall that the former are determined by a single operator, the latter come from comparison of the free and interacting dynamics.

From the differential equation point of view finding poles of the analytically continued resolvent means to solve the eigenvalue equation for looking for a complex 'eigenvalue' corresponding to an 'eigenfunction' which does not belong to L^2 being exponentially increasing with $|x|$. Modifying the argument of the previous section which led to the infinite matrix problem the task is again reduced to the equation (9). A subtle point in this case, as with other 'guiding channel' systems with infinite number of transverse modes [9] producing infinite number of cuts in the continuous spectrum, is that the Riemann surface of energy has infinite number of sheets, in fact an uncountable one. We are interested in those of them neighboring with the physical sheet which in the present context means that looking for resonances on the n-th sheet we have to flip sign of the first $n-1$ signs of the square roots in (9); for a more thorough discussion of this problem we refer the reader to [10].

Let us turn to scattering resonances. Suppose that the incident wave comes in the m-th channel from the left with the energy k^2. We use the Ansatz

$$f(x,y) = \begin{cases} \sum_{n=0}^{\infty} \Big(\delta_{mn} \mathrm{e}^{-ip_m x} \psi_n(y) + r_{mn}\, \mathrm{e}^{ip_n x} \psi_n(y) \Big), & x < 0, \\ \sum_{n=0}^{\infty} t_{mn}\, \mathrm{e}^{-ip_n x} \psi_n(y), & x > 0. \end{cases} \tag{16}$$

where we have denoted $p_n = p_n(k) := \sqrt{k^2 - \nu_n}$. Let us note that the on-shell scattering matrix with the elements has the size $M \times M$ where $M := \left[k^2 - \frac{1}{2}\right]$, the other 'reflection' and 'transmission' amplitudes correspond to the evanescent modes present in the scattering solution. The sign choice of the square roots signifying the Riemann sheet choice is the same as in the previous case.

It is straightforward to compute from here the boundary values $f(0\pm, y)$ and $f'_x(0\pm, y)$. The continuity requirement at $x = 0$ together with the orthonormality of the basis $\{\psi_n\}$ yields

$$t_{mn} = \delta_{mn} + r_{mn}\,. \tag{17}$$

Furthermore, substituting the boundary values from the Ansatz (16) into

$$f'_x(0+, y) - f'_x(0-, y) - \lambda y f(0, y) = 0 \tag{18}$$

and integrating the obtained expression with $\int \mathrm{d}y\, \psi_l(y)$ we obtain

$$\sum_{n=0}^{\infty} \Big(2p_n \delta_{ln} - i\lambda(\psi_l, y\psi_n) \Big) r_{mn} = i\lambda(\psi_l, y\psi_m)\,. \tag{19}$$

The requirement of solvability of this system leads to the same condition as before which allows us to conclude that the *resolvent and scattering resonances in Smilansky model coincide.*

The next question concerns the existence of resonances and their behavior as the coupling constant λ changes. There are some standard mechanisms producing resonances. One is a perturbation of embedded eigenvalues of the Hamiltonian, however, we have seen that in the present case there are no such eigenvalues. Another possibility comes from perturbation of the singularities associated with the thresholds of the transverse channels, i.e. the branching points of the energy surface cuts

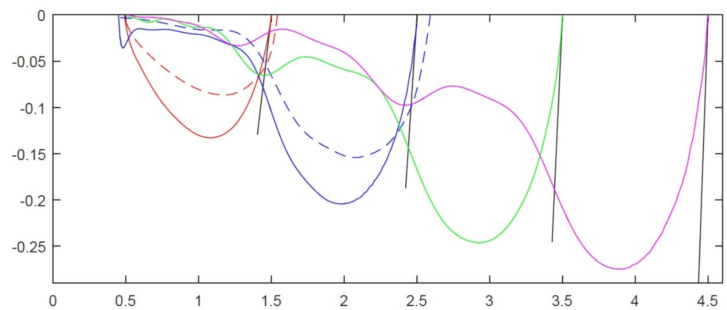

Figure 6: Resonance trajectories as λ runs through the interval $(0, \sqrt{2})$. Resonances that do not depart from thresholds are marked by dashed lines

The weak-coupling analysis follows the route as for the discrete spectrum and shows that for small λ a resonance pole splits of each threshold according to the asymptotic expansion. This indeed leads to emergence of complex poles in the vicinity of thresholds which behave as

$$\rho_m(\lambda) = -\frac{\lambda^4}{64}\big(2m+1+2im(m+1)\big) + \mathcal{O}(\lambda^5) \tag{20}$$

as one can readily check repeating the argument of the previous section, in fact, the weak coupling of the bound state is included if we put $m=0$ in (20). For $m=1,2,\dots$ we get genuine complex poles the distance for the corresponding threshold is proportional to λ^4 and the trajectory asymptote is the 'steeper' the larger m is. A more detailed discussion of the weak-coupling behavior of these resonances and also of resonances lying on the sheets that are not adjacent to the physical sheet can be again found in [10].

However, this tells us nothing about the pole behavior for larger λ. To get a more complete picture, we again analyze the problem numerically.

As described above, we look for complex values of ϵ for which the secular equation (9) is satisfied for a given λ. Now, however, B_λ is modified by flipping sign of the first $n-1$ signs of the square roots. Then, a truncated matrix problem ia solved, tuning the cut-off until a numerical stability is reached.

The results are shown in Fig. 6 where we demonstrate resonances splitting from the lowest thresholds, from the second to the fifth one together with their weak-coupling asymptotes according to (20). We see that the behavior beyond the weak-coupling regime is different, the pole trajectories return to the real axis and they may even end up as an isolated eigenvalue. This is not surprising, however, since a similar behavior is known from other resonance models [8] being first observed in the classical Lee-Friedrichs model [12].

What is even more interesting, the numerical analysis shows that the system has other resonances that do not emerge from thresholds and appear when the coupling surpasses a critical value. In Fig. 6 we show two such trajectories located at the second and third sheet of the energy surfaces and emerging at $\lambda = 1.287$ and $\lambda = 1.19$, respectively. One can conjecture naturally that these are not the only ones and that the system governed by Smilansky Hamiltonian has a rich family of resonances of different kinds which deserve a separate investigation.

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