Scattering and resonances in leaky quantum wires

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Talk overview

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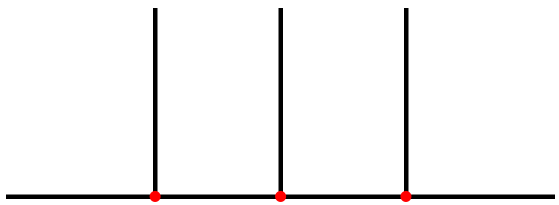
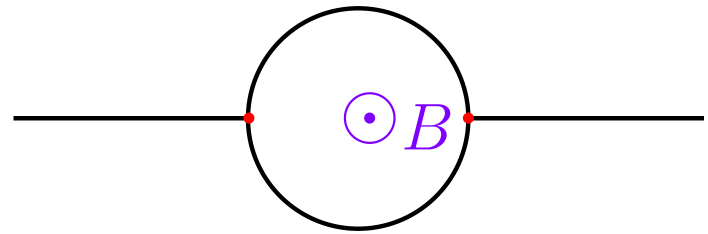
- Open questions

Scattering on quantum-wire systems

Widely used: scattering on “ideal” graphs, e.g.





Here we study Schrödinger operator on graph, with appropriate b.c. at vertices. Scattering is an *ODE problem* and it is easy to study resonances; for reviews see, e.g., [Kostrykin-Schrader’99], [Kuchment’04], etc.

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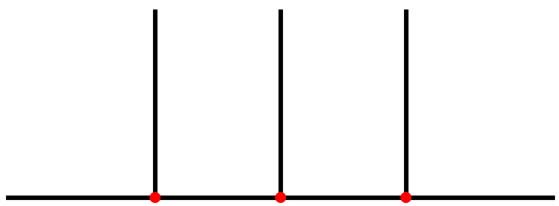

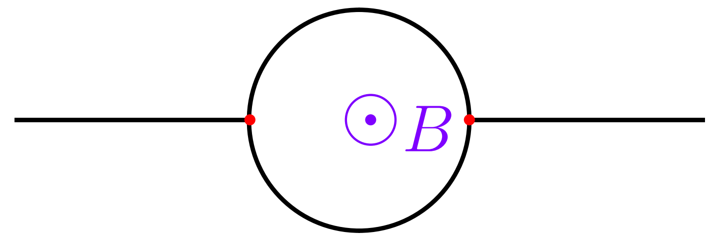

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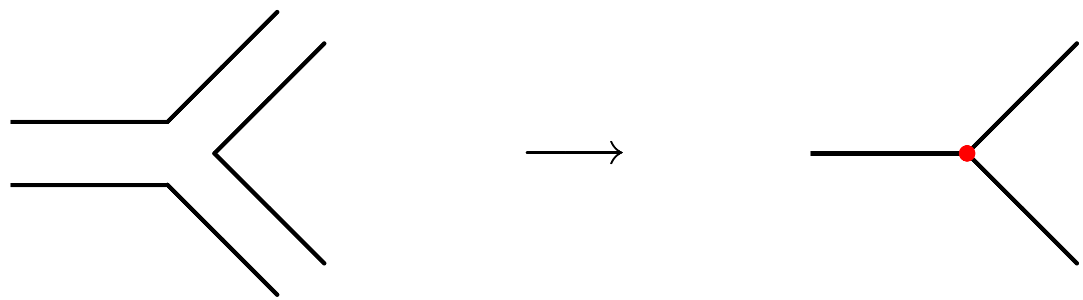
More realistic models of quantum wires treat them as *finite-width channels*, typically with Dirichlet b.c. Various scattering problems studied numerically in many papers.

Rigorous results not so common, for instance, resonances existence in smoothly bent tubes was demonstrated in [Duclos-E.-Šťovíček’95], [Duclos-E.-Meller’98].

Drawbacks of these models

- Presence of ad hoc parameters in the b.c. describing branchings. A natural remedy: use a zero-width limit in a more realistic description



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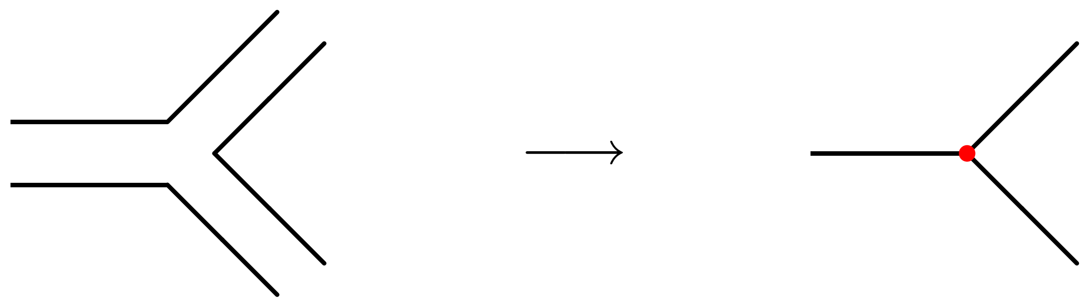

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- *Quantum tunneling is neglected*: recall that a true quantum-wire boundary is a finite potential jump

Leaky quantum graphs

We consider "leaky" graphs with an *attractive interaction supported by graph edges*. Formally we have

$$H_{\alpha,\Gamma} = -\Delta - \alpha\delta(x - \Gamma)\,, \quad \alpha > 0\,,$$

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A proper definition of $H_{\alpha,\Gamma}$: it can be associated naturally with the quadratic form,

$$\psi \mapsto \|\nabla\psi\|^2_{L^2(\mathbb{R}^n)} - \alpha \int_\Gamma |\psi(x)|^2 \mathrm{d}x\,,$$

which is closed and below bounded in $W^{1,2}(\mathbb{R}^n)$; the second term makes sense in view of Sobolev embedding. This definition also works for various “wilder” sets Γ

Leaky quantum-graph Hamiltonians

For Γ with locally finite number of smooth edges and *no cusps* we can use an *alternative definition* by boundary conditions: $H_{\alpha,\Gamma}$ acts as $-\Delta$ on functions from $W^{1,2}_{\mathrm{loc}}(\mathbb{R}^2 \setminus \Gamma)$, which are continuous and exhibit a normal-derivative jump,

$$\frac{\partial\psi}{\partial n}(x)\Big|_{+} - \frac{\partial\psi}{\partial n}(x)\Big|_{-} = -\alpha\psi(x)$$

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Remarks:

- for graphs in $\mathbb{R}^3$ we use generalized b.c. which define a two-dimensional point interaction in normal plane
- one can combine "edges" of different dimensions as long as $\operatorname{codim}\Gamma$ does not exceed three

Geometrically induced spectrum

(a) *Bending means binding*, i.e. it may create isolated eigenvalues of $H_{\alpha,\Gamma}$. Consider a *piecewise* C^1*-smooth* $\Gamma:\ \mathbb{R} \to \mathbb{R}^2$ parameterized by its arc length, and assume:

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- $|\Gamma(s)-\Gamma(s')| \ge c|s-s'|$ holds for some $c\in(0,1)$
- Γ is asymptotically straight: there are $d>0,\ \ \mu>\frac{1}{2}$ and $\omega\in(0,1)$ such that

$$1-\frac{|\Gamma(s)-\Gamma(s')|}{|s-s'|} \le d\left[1+|s+s'|^{2\mu}\right]^{-1/2}$$

in the sector $S_\omega := \left\{(s,s')\,:\ \omega<\frac{s}{s'}<\omega^{-1}\right\}$

- straight line is excluded, i.e. $|\Gamma(s)-\Gamma(s')|<|s-s'|$ holds for some $s,s'\in\mathbb{R}$

Bending means binding

Theorem [E.-Ichinose, 2001]: Under these assumptions, $\sigma_{\rm ess}(H_{\alpha,\Gamma}) = [-\frac{1}{4}\alpha^2, \infty)$ and $H_{\alpha,\Gamma}$ has at least one eigenvalue below the threshold $-\frac{1}{4}\alpha^2$

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- The same for *curves in* $\mathbb{R}^3$, under stronger regularity, with $-\frac{1}{4}\alpha^2$ is replaced by the corresponding 2D p.i. ev
- For *curved surfaces* $\Gamma \subset \mathbb{R}^3$ such a result is proved in the strong coupling asymptotic regime only
- *Implications for graphs:* let $\tilde{\Gamma} \supset \Gamma$ in the set sense, then $H_{\alpha,\tilde{\Gamma}} \leq H_{\alpha,\Gamma}$. If the essential spectrum threshold is the same for both graphs and Γ fits the above assumptions, we have $\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma}) \neq \emptyset$ by minimax principle

Geometrically induced spectrum, contd

(b) *Strong coupling asymptotics:* let $\Gamma : \mathbb{R} \to \mathbb{R}^2$ be as above, now supposed to be C^4*-smooth*

Theorem [E.-Yoshitomi, 2001]: The j-th ev of $H_{\alpha,\Gamma}$ is

$$\lambda_j(\alpha) = -\frac{1}{4}\alpha^2 + \mu_j + \mathcal{O}(\alpha^{-1}\ln\alpha) \quad \text{as} \quad \alpha \to \infty\,,$$

where μ_j is the j-th ev of $K_\Gamma := -\frac{\mathrm{d}}{\mathrm{d}s^2} - \frac{1}{4}\gamma(s)^2$ on $L^2(\mathbb{R})$ and γ is the curvature of Γ.

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where μ_j is the j-th ev of $K_\Gamma := -\frac{\mathrm{d}}{\mathrm{d}s^2} - \frac{1}{4}\gamma(s)^2$ on $L^2(\mathbb{R})$ and γ is the curvature of Γ. The same holds if Γ is a loop; then we also have

$$\#\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma}) = \frac{|\Gamma|\alpha}{2\pi} + \mathcal{O}(\ln\alpha) \quad \text{as} \quad \alpha \to \infty$$

Further extensions

- $H_{\alpha,\Gamma}$ with a *periodic* Γ has a band-type spectrum, but analogous asymptotics is valid for its *Floquet components* $H_{\alpha,\Gamma}(\theta)$, with the comparison operator $K_\Gamma(\theta)$ satisfying the appropriate b.c. over the period cell. It is important that the error term is uniform w.r.t. θ

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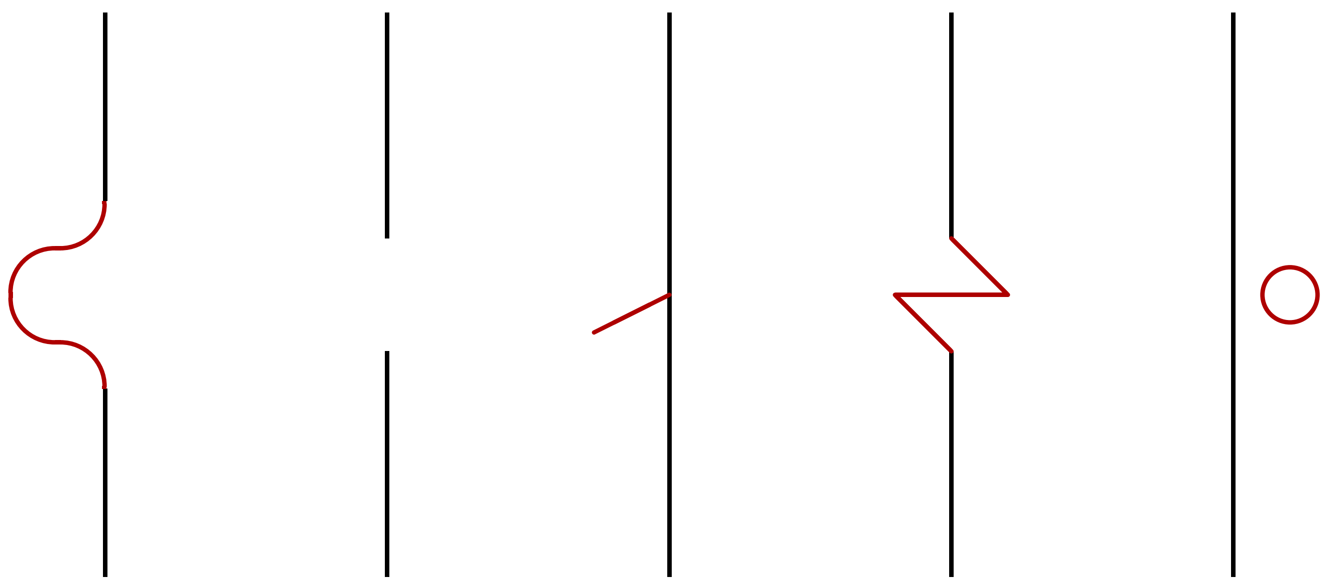
- Similar result holds for planar loops *threaded by mg field*, homogeneous, AB flux line, etc.
- *Higher dimensions:* the results extend to loops, infinite and periodic curves in $\mathbb{R}^3$
- and to *curved surfaces* in $\mathbb{R}^3$; then the comparison operator is $-\Delta_{\mathrm{LB}} + K - M^2$, where K, M, respectively, are the corresponding Gauss and mean curvatures

Scattering on a locally deformed line

Scattering requires to specify a *free dynamics*. In this talk we suppose that the latter is described by $H_{\alpha,\Sigma}$, where Σ is a *straight line*, $\Sigma = \{(x_1, 0) : x_1 \in\}$, and that the graph Γ in question differs from Σ by a *local deformation* only



Assumptions

We will consider the following class of local deformations:

- there exists a *compact* $M \subset \mathbb{R}^2$ such that $\Gamma \setminus M = \Sigma \setminus M$,
- the set $\Gamma \setminus \Sigma$ admits a finite decomposition,

$$\Gamma \setminus \Sigma = \bigcup_{i=1}^{N} \Gamma_i \,, \quad N < \infty \,,$$

where the Γ_i's are finite C^1 curves such that *no pair* of components of Γ *crosses* at their interior points, neither a component has a *self-intersection*; we allow the components to touch at their endpoints but assume they do not form a *cusp* there

As we have said, $H_{\alpha,\Gamma}$ is then well defined

Krein's formula

Our main tool will be a formula comparing the resolvents of $H_{\alpha,\Gamma}$ and $H_{\alpha,\Sigma}$. We will use the decomposition

$$\Lambda = \Lambda_0 \cup \Lambda_1 \quad \text{with} \quad \Lambda_0 := \Sigma \setminus \Gamma\,, \;\; \Lambda_1 := \Gamma \setminus \Sigma = \bigcup_{i=1}^{N} \Gamma_i\,;$$

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the coupling constant of the perturbation will be naturally equal to α on the "subtracted" set Λ_0 and $-\alpha$ on Λ_1
To construct resolvent of $H_{\alpha,\Sigma}$ we use R^k, the one of $-\Delta$, which is for $k^2 \in \rho(-\Delta)$ an integral operator with the kernel

$$G^k(x-y) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{\mathrm{e}^{ip(x-y)}}{p^2 - k^2}\, \mathrm{d}p = \frac{1}{2\pi} K_0(ik|x-y|)\,,$$

where $K_0(\cdot)$ stands for the Macdonald function

Krein's formula, continued

A straightforward computation shows that the resolvent R^k_Σ of $H_{\alpha,\Sigma}$ has the kernel $G^k_\Sigma(x-y)$ given by

$$G^k(x-y) + \frac{\alpha}{4\pi^3}\int_3 \frac{\mathrm{e}^{ipx-ip'y}}{(p^2-k^2)(p'^2-k^2)}\,\frac{\tau_k(p_1)}{2\tau_k(p_1)-\alpha}\,\mathrm{d}p\,\mathrm{d}p'_2\,,$$

where $\tau_k(p_1) := (p_1^2-k^2)^{1/2}$ and $p=(p_1,p_2)$, $p'=(p_1,p'_2)$

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We need embeddings of R^k_Σ to $L^2(\nu)$, where $\nu \equiv \nu_\Lambda$ is the Dirac measure on Λ. It can be written as $\nu_\Lambda = \nu_0 + \sum_{i=1}^N \nu_i$, where ν_0 is the Dirac measure on Λ_0. It convenient also to introduce the space $\mathrm{h} \equiv L^2(\nu)$ which decomposes into

$$\mathrm{h} = \mathrm{h}_0 \oplus \mathrm{h}_1 \quad \text{with} \quad \mathrm{h}_0 \equiv L^2(\nu_0) \quad \text{and} \quad \mathrm{h}_1 \equiv \bigoplus_{i=1}^N L^2(\nu_i)$$

Embeddings

Now we are able to introduce the operator

$$\mathrm{R}^k_{\Sigma,\nu} : \mathrm{h} \to L^2\,, \quad \mathrm{R}^k_{\Sigma,\nu} f = G^k_\Sigma * f\nu \quad \text{for} \quad f \in \mathrm{h}$$

defined for suitable values of k. Similarly, $(\mathrm{R}^k_{\Sigma,\nu})^* : L^2 \to \mathrm{h}$ is its adjoint and $\mathrm{R}^k_{\Sigma,\nu\nu}$ denotes the operator-valued matrix in h with the "block elements" $G^k_{\Sigma,ij} \equiv G^k_{\Sigma,\nu_i\nu_j} : L^2(\nu_j) \to L^2(\nu_i)$

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They have the following properties:

- For any $\kappa \in (\alpha/2, \infty)$ the operator $\mathrm{R}^{i\kappa}_{\Sigma,\nu}$ is bounded. In fact, $\mathrm{R}^{i\kappa}_{\Sigma,\nu}$ is a continuous embedding into $W^{1,2}$
- For any $\sigma > 0$ there exists κ_σ such that for $\kappa > \kappa_\sigma$ the operator $\mathrm{R}^{i\kappa}_{\Sigma,\nu\nu}$ is bounded with the norm less than σ

Krein's formula, continued

Introduce an operator-valued matrix in $\mathrm{h} = \mathrm{h}_0 \oplus \mathrm{h}_1$ as

$$\Theta^k = -(\alpha^{-1}\check{\mathbb{I}} + \mathrm{R}^k_{\Sigma,\nu\nu}) \quad \text{with} \quad \check{\mathbb{I}} = \begin{pmatrix} \mathbb{I}_0 & 0 \\ 0 & -\mathbb{I}_1 \end{pmatrix},$$

where $\mathbb{I}_i$ are the unit operators in h_i. Using the properties of the embeddings we prove the following claim:

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Theorem [E.-Kondej, 2005]: Let Θ^k have inverse in $\mathcal{B}(\mathrm{h})$ for $k \in \mathbb{C}^+$ and let the operator

$$R^k_\Gamma = R^k_\Sigma + \mathrm{R}^k_{\Sigma,\nu}(\Theta^k)^{-1}(\mathrm{R}^k_{\Sigma,\nu})^*$$

be defined everywhere on L^2. Then k^2 belongs to $\rho(H_{\alpha,\Gamma})$ and the resolvent $(H_{\alpha,\Gamma} - k^2)^{-1}$ is given by R^k_Γ

Spectrum of $H_{\alpha,\Gamma}$

Let us first look at the essential spectrum:

Proposition: $\sigma_{\mathrm{ess}}(H_{\alpha,\Gamma}) = \sigma_{\mathrm{ess}}(H_{\alpha,\Sigma}) = [-\frac{1}{4}\alpha^2, \infty)$

Proof: Check that $B^k := \mathrm{R}^k_{\Sigma,\nu}(\Theta^k)^{-1}(\mathrm{R}^k_{\Sigma,\nu})^*$ is compact for some $k \in \mathbb{C}^+$. We know that $(\Theta^{i\kappa})^{-1} \in \mathcal{B}(\mathrm{h})$ and $(\mathrm{R}^{i\kappa}_{\Sigma,\nu})^*$ is bounded if κ is large enough. By [BEKŠ'94] we have $\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} |G^{i\kappa}(x-y)|^2\,\nu_j(\mathrm{d}y)\,\mathrm{d}x < \infty$, and for $\kappa > \frac{1}{2}\alpha$ and $j = 0, \dots, N$ the second component ξ^k of $G^{i\kappa}_{\Sigma}$ satisfies

$$\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} |\xi^k(x,y)|^2\,\nu_j(\mathrm{d}y)\,\mathrm{d}x < CL_j \int_{\mathbb{R}^2} \frac{\mathrm{d}p}{(p^2+\kappa)^2} < \infty\,,$$

where C is a constant and L_j denote the length of Λ_j. This yields compactness of $\mathrm{R}^k_{\Sigma,\nu}$, and thus the same for B^k. $\square$

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Remark: $\sigma_{\text{disc}}(H_{\alpha,\Gamma})$ given by singularities of Θ^k is often non-empty – see above – but it is not our concern here

Wave operators

The existence and completeness of wave operators for the pair $(H_{\alpha,\Gamma}, H_{\alpha,\Sigma})$ follows from the standard trace-class criterion, conventionally called Birman-Kuroda theorem. Specifically, we have

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Proof is inspired by [Brasche-Teta'92]. We use the estimate $(\Theta^{i\kappa})^{-1} \leq C'(\Theta^{i\kappa,+})^{-1}$, where $\Theta^{i\kappa,+} := \alpha^{-1}\mathbb{I} + \mathrm{R}^{i\kappa}_{\Sigma,\nu\nu}$ and $\mathbb{I}$ is the $(N+1)\times(N+1)$ unit matrix, for some $C' > 0$ and all κ sufficiently large; it is clear that $(\Theta^{i\kappa,+})^{-1}$ is positive and bounded. This gives

$$B^{i\kappa} \leq C' B^{i\kappa,+}\,, \qquad B^{i\kappa,+} := \mathrm{R}^{i\kappa}_{\Sigma,\nu}(\Theta^{i\kappa,+})^{-1}(\mathrm{R}^{i\kappa}_{\Sigma,\nu})^*$$

Proof, continued

Define $B_\delta^{i\kappa,+}$ as integral operator with the kernel

$$B_\delta^{i\kappa,+}(x,y) = \chi_\delta(x) B^{i\kappa,+}(x,y) \chi_\delta(y)\,,$$

where χ_δ stands for the indicator function of the ball $\mathcal{B}(0,\delta)$; one has $B_\delta^{i\kappa,+} \to B^{i\kappa,+}$ as $\delta \to \infty$ in the weak sense.

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$$\int_{\mathbb{R}^2} B_\delta^{i\kappa,+}(x,x)\mathrm{d}x = \int_{\mathbb{R}^2} (G_\Sigma^{i\kappa}(\cdot,x)\chi_\delta(x), (\Theta^{i\kappa,+})^{-1} G_\Sigma^{i\kappa}(\cdot,x)\chi_\delta(x))_{\mathrm{h}}\,\mathrm{d}x$$

$$\leq \|(\Theta^{i\kappa,+})^{-1}\| \int_{\mathbb{R}^2} \|G_\Sigma^{i\kappa}(\cdot,x)\chi_\delta(x)\|_{\mathrm{h}}^2\,\mathrm{d}x \leq C\|(\Theta^{i\kappa,+})^{-1}\|\,,$$

hence $B_\delta^{i\kappa,+}$ is trace class for any $\delta > 0$, and the same is true for the limiting operator.

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$$B_\delta^{i\kappa,+}(x,y) = \chi_\delta(x) B^{i\kappa,+}(x,y) \chi_\delta(y)\,,$$

where χ_δ stands for the indicator function of the ball $\mathcal{B}(0,\delta)$; one has $B_\delta^{i\kappa,+} \to B^{i\kappa,+}$ as $\delta \to \infty$ in the weak sense. Then

$$\int_{\mathbb{R}^2} B_\delta^{i\kappa,+}(x,x)\,\mathrm{d}x = \int_{\mathbb{R}^2} (G_\Sigma^{i\kappa}(\cdot,x)\chi_\delta(x), (\Theta^{i\kappa,+})^{-1} G_\Sigma^{i\kappa}(\cdot,x)\chi_\delta(x))_{\mathrm{h}}\,\mathrm{d}x$$

$$\leq \|(\Theta^{i\kappa,+})^{-1}\| \int_{\mathbb{R}^2} \|G_\Sigma^{i\kappa}(\cdot,x)\chi_\delta(x)\|_{\mathrm{h}}^2\,\mathrm{d}x \leq C\|(\Theta^{i\kappa,+})^{-1}\|\,,$$

hence $B_\delta^{i\kappa,+}$ is trace class for any $\delta > 0$, and the same is true for the limiting operator.

Similarly one finds a Hermitian trace class operator $B^{i\kappa,-}$ which provides an estimate from below, $B^{i\kappa,-} \leq B^{i\kappa}$; this means that $B^{i\kappa}$ is a trace class operator too. $\square$

Generalized eigenfunctions

We want to find the S-matrix, $S\psi_\lambda^- = \psi_\lambda^+$, for scattering in the *negative part of the spectrum* with a fixed energy $\lambda \in (-\frac{1}{4}\alpha^2, 0)$ corresponding to the effective momentum $k_\alpha(\lambda) := (\lambda + \alpha^2/4)^{1/2}$. We employ generalized ef's of $H_{\alpha,\Sigma}$,

$$\omega_\lambda(x_1, x_2) = \mathrm{e}^{i(\lambda+\alpha^2/4)^{1/2} x_1} \mathrm{e}^{-\alpha|x_2|/2} \,,$$

their analogues ω_z for complex energies and regularizations $\omega_z^\delta(x) = \mathrm{e}^{-\delta x_1^2}\omega_z(x)$ for $z \in \rho(H_{\alpha,\Sigma})$, belonging to $D(H_{\alpha,\Sigma})$.

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Consider now ψ_z^δ such that $(H_{\alpha,\Gamma} - z)\psi_z^\delta = (H_{\alpha,\Sigma} - z)\omega_z^\delta$. After taking the limit $\lim_{\epsilon\to 0}\psi_{\lambda+i\epsilon}^\delta = \psi_\lambda^\delta$ in the topology of L^2 the function ψ_λ^δ still belongs to $D(H_{\alpha,\Sigma})$ and we have

$$\psi_\lambda^\delta = \omega_\lambda^\delta + \mathrm{R}_{\Sigma,\nu}^{k_\alpha(\lambda)}(\Theta^{k_\alpha(\lambda)})^{-1}I_\Lambda\omega_\lambda^\delta$$

Generalized eigenfunctions, continued

Here $\mathrm{R}_{\Sigma,\nu}^{k_\alpha(\lambda)}$ is integral operator on the Hilbert space h with the kernel $G_\Sigma^{k_\alpha(\lambda)}(x-y) := \lim_{\varepsilon\to 0} G_\Sigma^{k_\alpha(\lambda+i\varepsilon)}(x-y)$ and $\Theta^{k_\alpha(\lambda)} := -\alpha^{-1}\check{\mathbb{I}} - \mathrm{R}_{\Sigma,\nu\nu}^{k_\alpha(\lambda)}$ are the operators on h with $\mathrm{R}_{\Sigma,\nu\nu}^{k_\alpha(\lambda)}$ being the natural embedding . By a direct computation, the kernel is found to be

$$G_\Sigma^{k_\alpha(\lambda)}(x-y) = K_0(i\sqrt{\lambda}|x-y|) + \mathcal{P}\int_0^\infty \frac{\mu_0(t;x,y)}{t-\lambda-\alpha^2/4}\,\mathrm{d}t + s_\alpha(\lambda)\,\mathrm{e}^{ik_\alpha(\lambda)|x_1-y_1|}\,\mathrm{e}^{-\alpha/2(|x_2|+|y_2|)},$$

where $s_\alpha(\lambda) := i\alpha(2^3 k_\alpha(\lambda))^{-1}$ and

$$\mu_0(t;x,y) := -\frac{i\alpha}{2^5\pi}\,\frac{\mathrm{e}^{it^{1/2}(x_1-y_1)}\,\mathrm{e}^{-(t-\lambda)^{1/2}(|x_2|+|y_2|)^{1/2}}}{t^{1/2}((t-\lambda)^{1/2})}\,.$$

Generalized eigenfunctions, continued

Of course, the pointwise limits $\psi_\lambda = \lim_{\delta\to 0}\psi_\lambda^\delta$ cease to L^2, however, they still belong to L^2 locally and provide us with the generalized eigenfunction of $H_{\alpha,\Gamma}$ in the form

$$\psi_\lambda = \omega_\lambda + \mathrm{R}_{\Sigma,\nu}^{k_\alpha(\lambda)}(\Theta^{k_\alpha(\lambda)})^{-1} J_\Lambda \omega_\lambda\,,$$

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To find the S-matrix we have to investigate the behavior of ψ_λ for $|x_1| \to \infty$. By a direct computation, we find that for y of a compact $M \subset \mathbb{R}^2$ and $|x_1| \to \infty$ we have

$$G_\Sigma^{k_\alpha(\lambda)}(x-y) \approx s_\alpha(\lambda)\, \mathrm{e}^{ik_\alpha(\lambda)|x_1-y_1|}\, e^{-\alpha/2(|x_2|+|y_2|)}$$

S-matrix at negative energy

Using this asymptotics we find the sought on-shell S-matrix:

Theorem [E.-Kondej, 2005]: For a fixed $\lambda \in (-\frac{1}{4}\alpha^2, 0)$ the generalized eigenfunctions behave asymptotically as

$$\psi_\lambda(x) \approx \begin{cases} \mathcal{T}(\lambda)\, \mathrm{e}^{ik_\alpha(\lambda)x_1}\, \mathrm{e}^{-\alpha|x_2|/2} & \text{for} \quad x_1 \to \infty \\ \mathrm{e}^{ik_\alpha(\lambda)x_1}\mathrm{e}^{-\alpha|x_2|/2} + \mathcal{R}(\lambda)\, \mathrm{e}^{-ik_\alpha(\lambda)x_1}\mathrm{e}^{-\alpha|x_2|/2} & \text{for} \quad x_1 \to -\infty \end{cases}$$

where $k_\alpha(\lambda) := (\lambda + \alpha^2/4)^{1/2}$ and the *transmission and reflection amplitudes* $\mathcal{T}(\lambda), \mathcal{R}(\lambda)$ are given respectively by

$$\mathcal{T}(\lambda) = 1 - s_\alpha(\lambda)\left((\Theta^{k_\alpha(\lambda)})^{-1} J_\Lambda \omega_\lambda, J_\Lambda \omega_\lambda\right)_{\mathrm{h}}$$

and

$$\mathcal{R}(\lambda) = s_\alpha(\lambda)\left((\Theta^{k_\alpha(\lambda)})^{-1} J_\Lambda \omega_\lambda, J_\Lambda \bar{\omega}_\lambda\right)_{\mathrm{h}}$$

Strong coupling: a conjecture

Consider Γ which is a C^4-*smooth* local deformation of a line. In analogy with the spectral result of [E.-Yoshitomi'01] quoted above one expects that in *strong coupling* case the scattering will be determined in the leading order by the *local geometry* of Γ through the same comparison operator, namely $K_\Gamma := -\frac{\mathrm{d}}{\mathrm{d}s^2} - \frac{1}{4}\gamma(s)^2$ on $L^2(\mathbb{R})$.

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Let $\mathcal{T}_K(k)$, $\mathcal{R}_K(k)$ be the corresponding transmission and reflection amplitudes at a fixed momentum k. Denote by $\mathbf{S}_{\Gamma,\alpha}(\lambda)$ and $\mathbf{S}_K(\lambda)$ the on-shell $S-$matrixes of $H_{\alpha,\Gamma}$ and K at energy λ, respectively.

Conjecture: For a fixed $k \neq 0$ and $\alpha \to \infty$ we have the relation

$$\mathbf{S}_{\Gamma,\alpha}\left(k^2 - \frac{1}{4}\alpha^2\right) \to \mathbf{S}_K(k^2)$$

How to find the spectrum?

To say something about resonances, let us return to the spectral problem. The general results do not tell us how to find the spectrum for a particular Γ. The options:

- *Direct solution* of the PDE problem $H_{\alpha,\Gamma}\psi = \lambda\psi$ is feasible in a few simple examples only

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- *Direct solution* of the PDE problem $H_{\alpha,\Gamma}\psi = \lambda\psi$ is feasible in a few simple examples only
- Using trace maps of $R^k \equiv (-\Delta - k^2)^{-1}$ and the *generalized BS principle*

$$R^k := R_0^k + \alpha R_{\mathrm{d}x,m}^k [I - \alpha R_{m,m}^k]^{-1} R_{m,\mathrm{d}x}^k \,,$$

where m is δ measure on Γ, we pass to a 1D integral operator problem, $\alpha R_{m,m}^k \psi = \psi$

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  where m is δ measure on Γ, we pass to a 1D integral operator problem, $\alpha R_{m,m}^k \psi = \psi$
- *discretization* of the latter which amounts to a point-interaction approximations to $H_{\alpha,\Gamma}$

2D point interactions

Such an interaction at the point a with the "coupling constant" α is defined by b.c. which change *locally* the domain of $-\Delta$: the functions behave as

$$\psi(x) = -\frac{1}{2\pi} \log|x-a|\, L_0(\psi,a) + L_1(\psi,a) + \mathcal{O}(|x-a|)\,,$$

where the generalized b.v. $L_0(\psi,a)$ and $L_1(\psi,a)$ satisfy

$$L_1(\psi,a) + 2\pi\alpha L_0(\psi,a) = 0\,, \qquad \alpha \in \mathbb{R}$$

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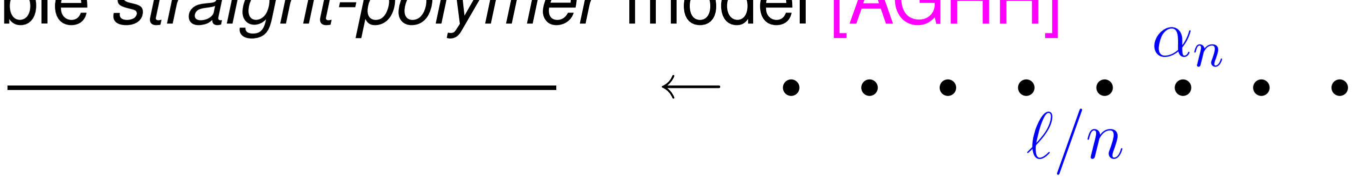
For our purpose, the coupling should depend on the set Y approximating Γ. To see how compare a line Γ with the solvable *straight-polymer* model [AGHH]



2D point-interaction approximation

Spectral threshold convergence requires $\alpha_n = \alpha n$ which means that individual point interactions get *weaker*. Hence we approximate $H_{\alpha,\Gamma}$ by point-interaction Hamiltonians H_{α_n,Y_n} with $\alpha_n = \alpha|Y_n|$, where $|Y_n| := \sharp Y_n$.

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Theorem [E.-Němcová, 2003]: Let a family $\{Y_n\}$ of finite sets $Y_n \subset \Gamma \subset \mathbb{R}^2$ be such that

$$\frac{1}{|Y_n|} \sum_{y \in Y_n} f(y) \;\to\; \int_\Gamma f \,\mathrm{d}m$$

holds for any bounded continuous function $f : \Gamma \to \mathbb{C}$, *together with technical conditions*, then $H_{\alpha_n,Y_n} \to H_{\alpha,\Gamma}$ in the strong resolvent sense as $n \to \infty$.

Comments on the approximation

- A more general result is valid: Γ need not be a graph and the coupling may be non-constant

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Comments on the approximation

- A more general result is valid: Γ need not be a graph and the coupling may be non-constant
- The result applies to finite graphs, however, an infinite Γ can be approximated in strong resolvent sense by a *family of cut-off graphs*
- The idea is due to Brasche, Figari and Teta, 1998, who analyzed point-interaction approximations of measure perturbations with $\operatorname{codim}\Gamma = 1$ in $\mathbb{R}^3$. There are differences, however, for instance in the 2D case we can approximate *attractive* interactions only

Scheme of the proof

Resolvent of H_{α_n,Y_n} is given *Krein's formula*. Given $k^2 \in \rho(H_{\alpha_n,Y_n})$ define $|Y_n| \times |Y_n|$ matrix by

$$\Lambda_{\alpha_n,Y_n}(k^2;x,y) \;=\; \frac{1}{2\pi}\left[2\pi|Y_n|\alpha + \ln\left(\frac{ik}{2}\right) + \gamma_E\right]\delta_{xy} \\ -G_k(x-y)\,(1-\delta_{xy})$$

for $x, y \in Y_n$, where γ_E is *Euler' constant*.

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for $x, y \in Y_n$, where γ_E is *Euler' constant*. Then

$$(H_{\alpha_n,Y_n} - k^2)^{-1}(x,y) = G_k(x-y) \\ + \sum_{x',y' \in Y_n} \left[\Lambda_{\alpha_n,Y_n}(k^2)\right]^{-1}(x',y')G_k(x-x')\,G_k(y-y')$$

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Resolvent of $H_{\alpha,\Gamma}$ is given by the *generalized BS formula* given above; one has to check directly that the difference of the two vanishes as $n \to \infty$ $\square$

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Remarks:

- Spectral condition in the n-th approximation, i.e. $\det \Lambda_{\alpha_n,Y_n}(k^2) = 0$, is a discretization of the integral equation coming from the generalized BS principle
- A solution to $\Lambda_{\alpha_n,Y_n}(k^2)\eta = 0$ determines the approximating ef by $\psi(x) = \sum_{y_j \in Y_n} \eta_j G_k(x - y_j)$
- A *match with solvable models* illustrates the convergence and shows that it is *not fast,* slower than n^{-1} in the eigenvalues. This comes from singular "spikes" in the approximating functions

Finally, the resonances

Consider infinite curves Γ, straight outside a compact, and ask for examples of resonances. Recall the L^2-approach: in 1D potential scattering one explores *spectral properties* of the problem cut to a finite length L. It is time-honored trick that scattering resonances are manifested as avoided crossings in L dependence of the spectrum – for a recent proof see Hagedorn-Meller, 2000. Try the same here:

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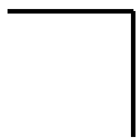
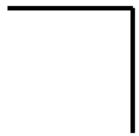
- *Broken line:* absence of "intrinsic" resonances due lack of higher transverse thresholds
- *Z-shaped* Γ*:* if a single bend has a significant reflection, a double band should exhibit resonances
- *Bottleneck curve:* a good candidate to demonstrate tunneling resonances

Broken line



$\alpha = 1$

Broken line



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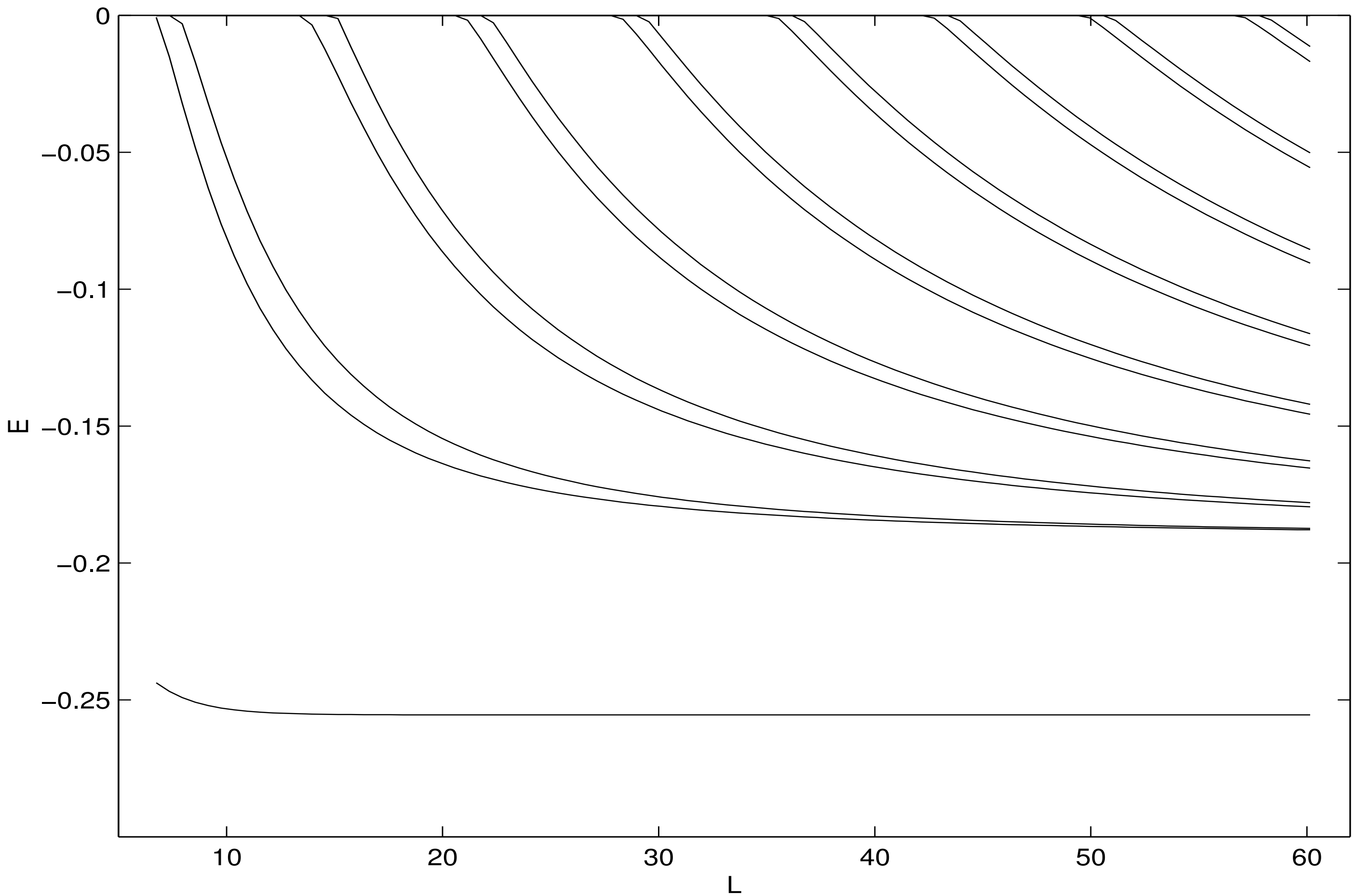
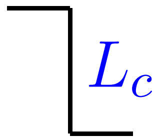


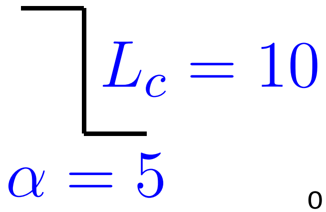
Z shape with $\theta = \frac{\pi}{2}$

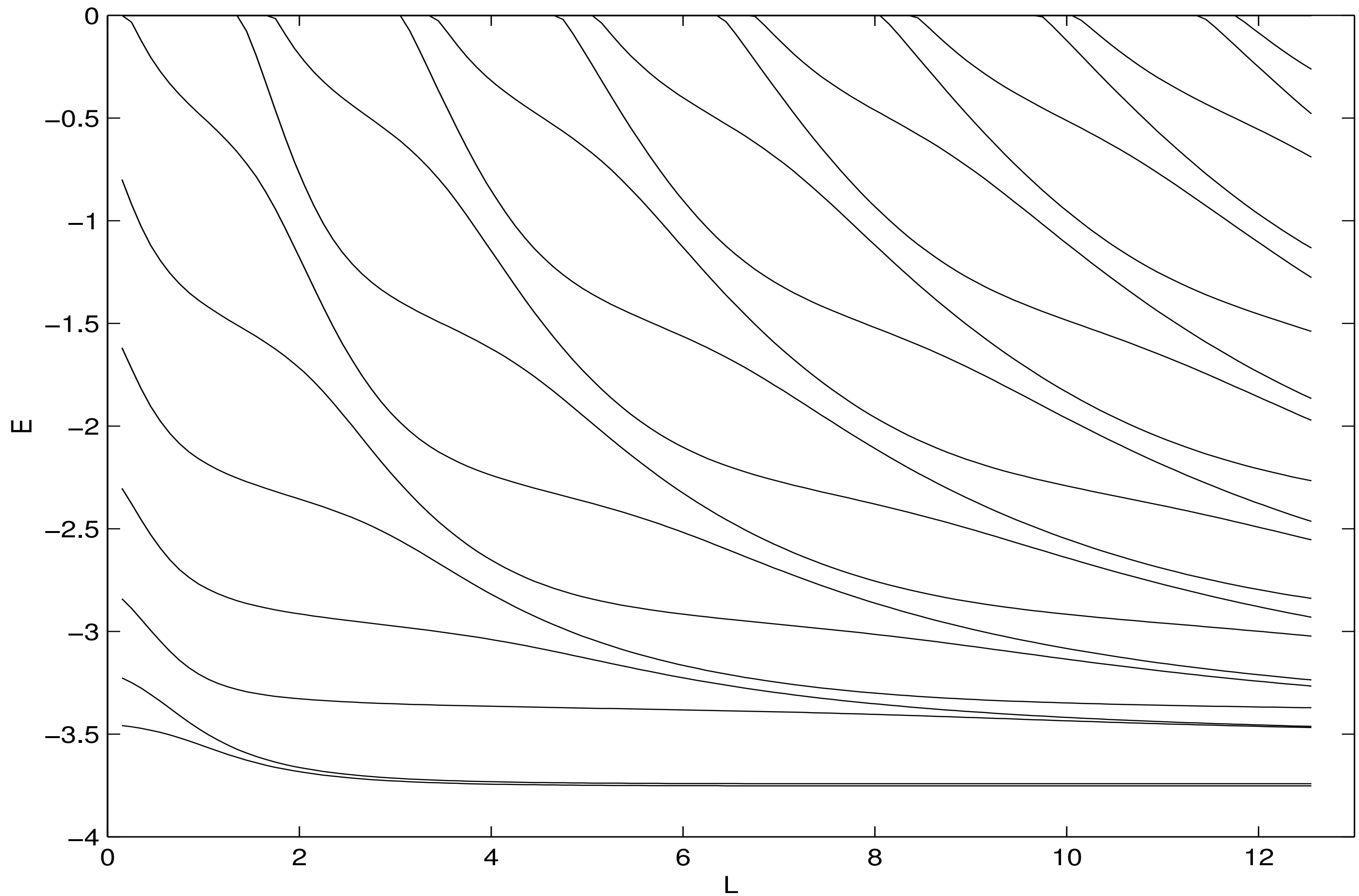


$L_c = 10$

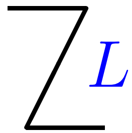
$\alpha = 5$

Z shape with $\theta = \frac{\pi}{2}$





Z shape with $\theta = 0.32\pi$



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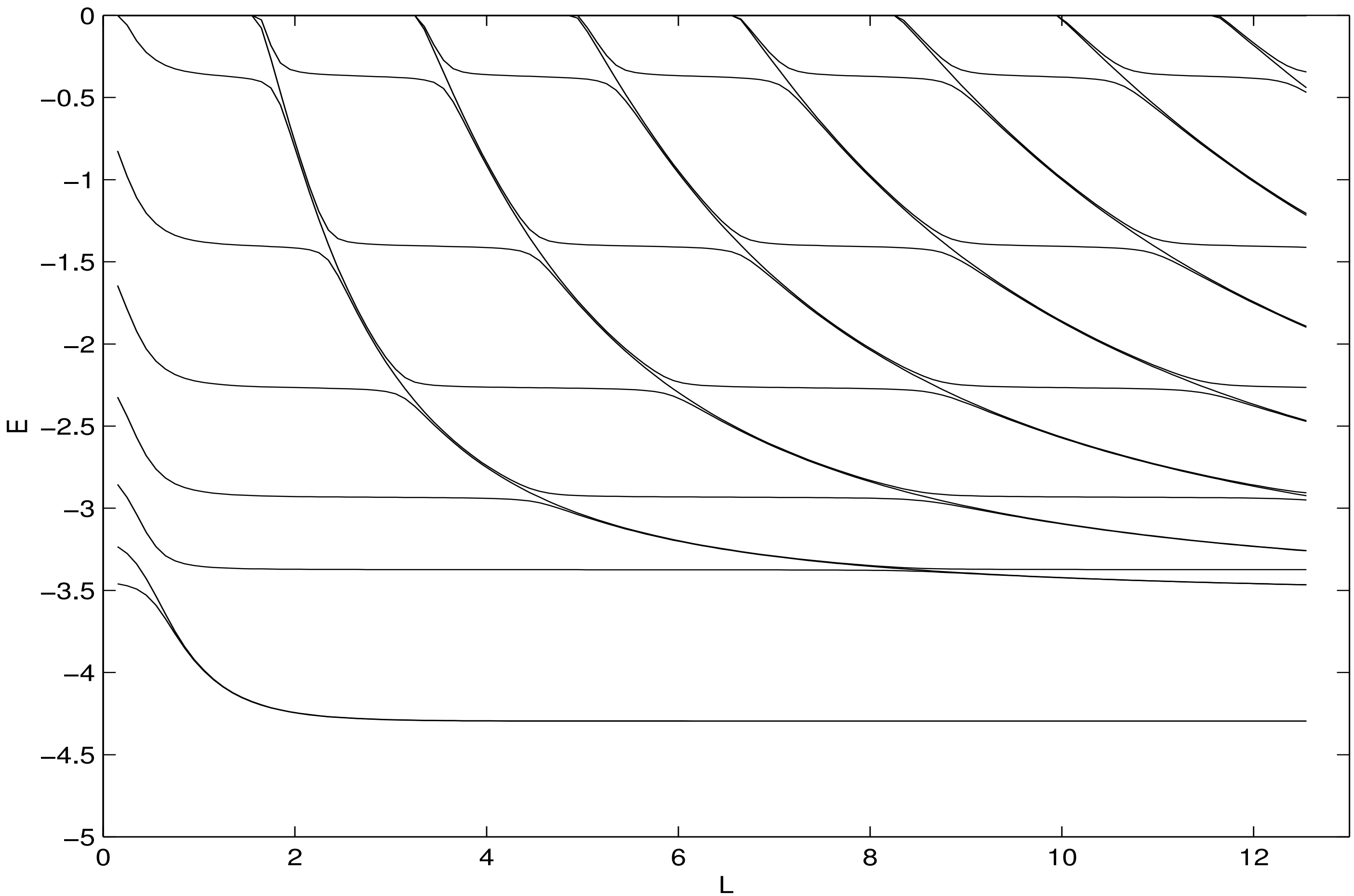
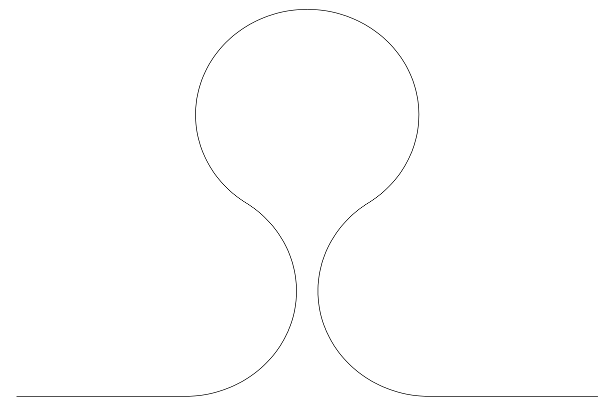


A bottleneck curve

Consider a straight line deformation which shaped as an open loop with a bottleneck the width a of which we will vary



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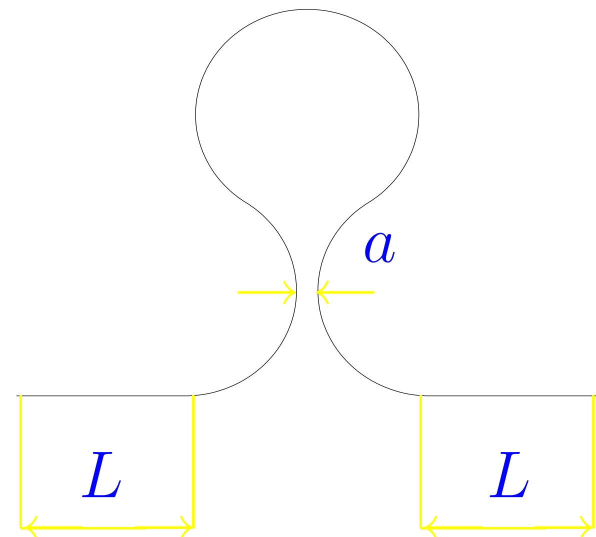
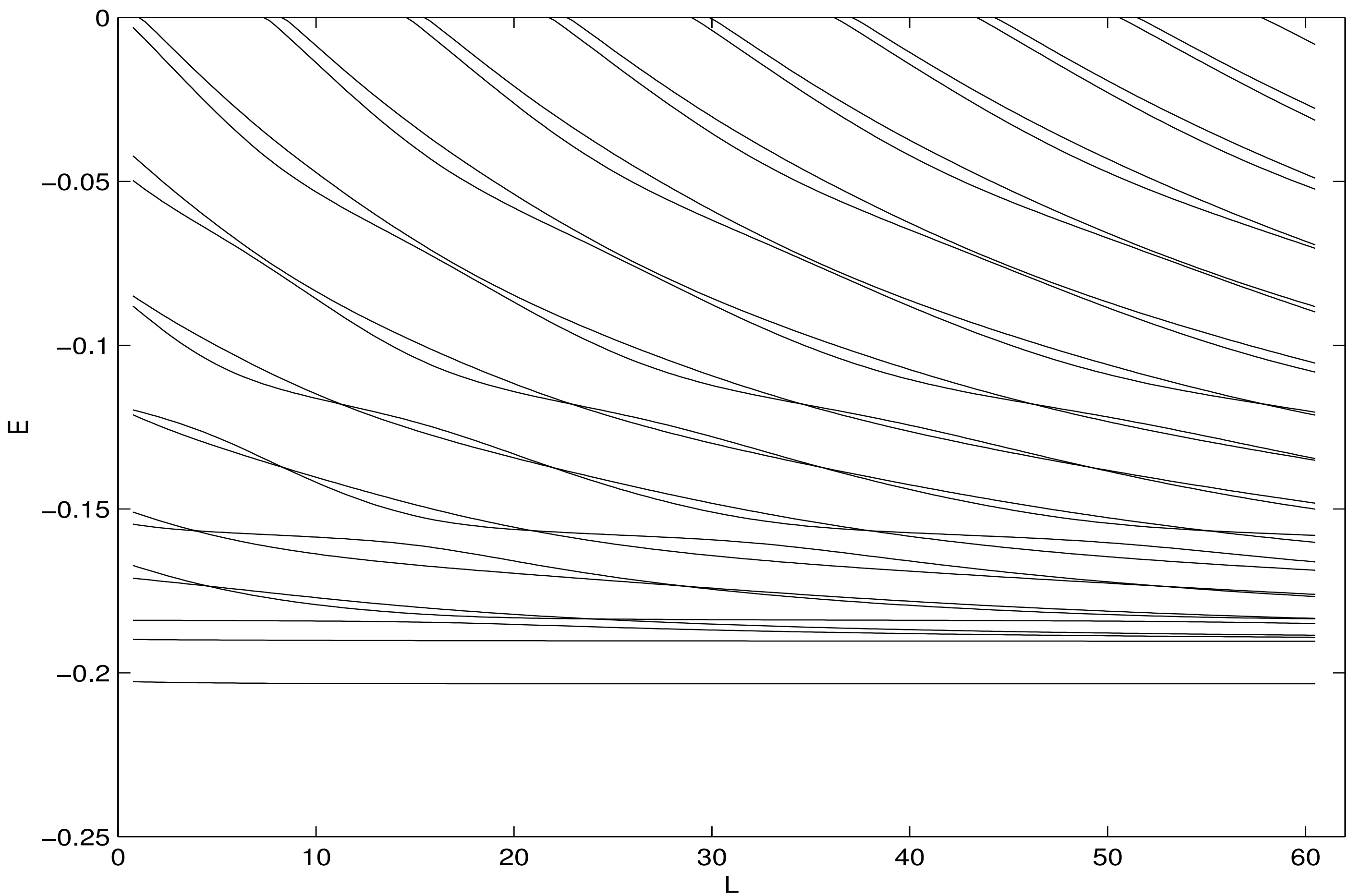
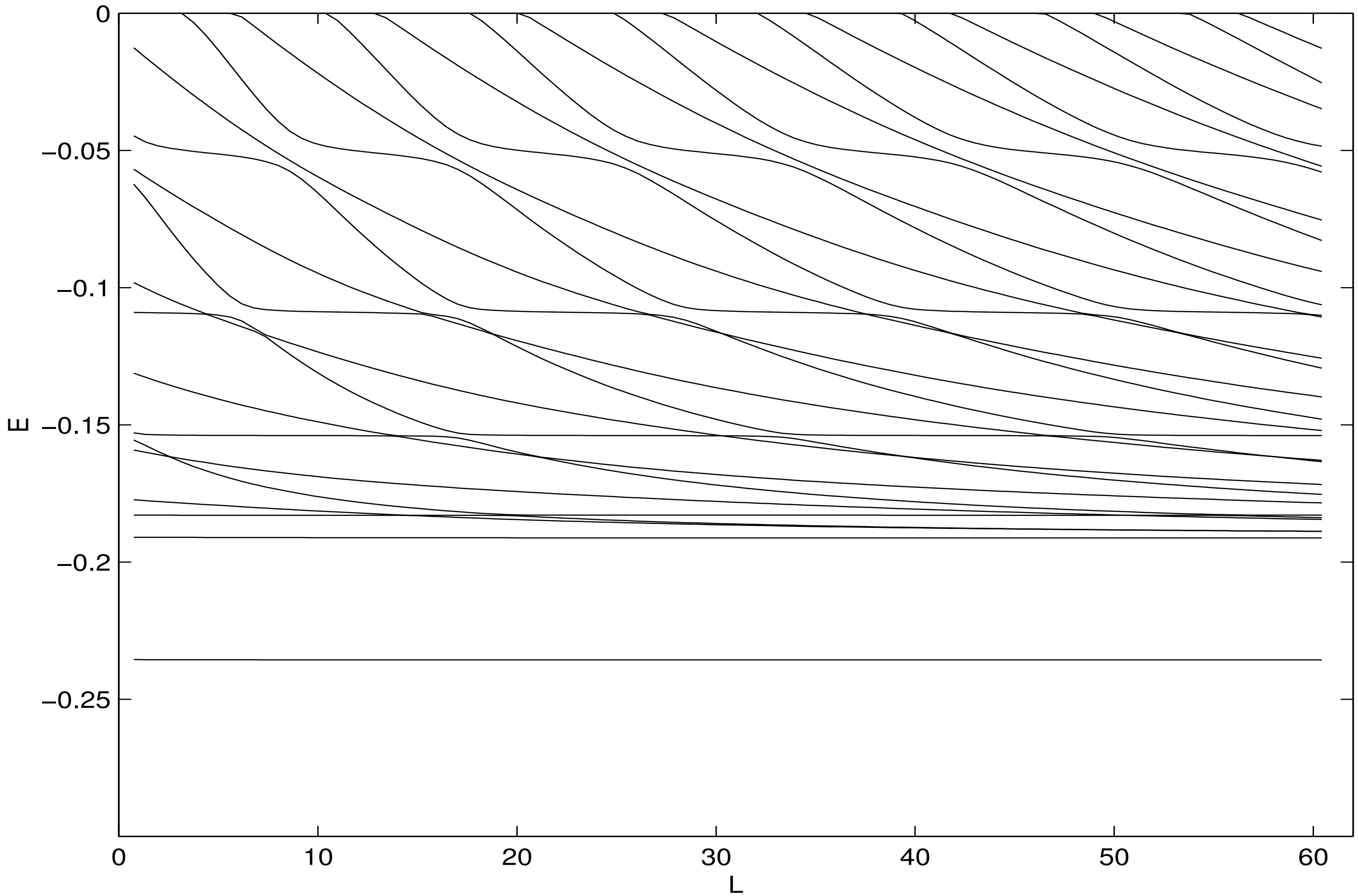


If Γ is a straight line, the transverse eigenfunction is $\mathrm{e}^{-\alpha|y|/2}$, hence the distance at which tunneling becomes significant is $\approx 4\alpha^{-1}$. In the example, we choose $\alpha = 1$

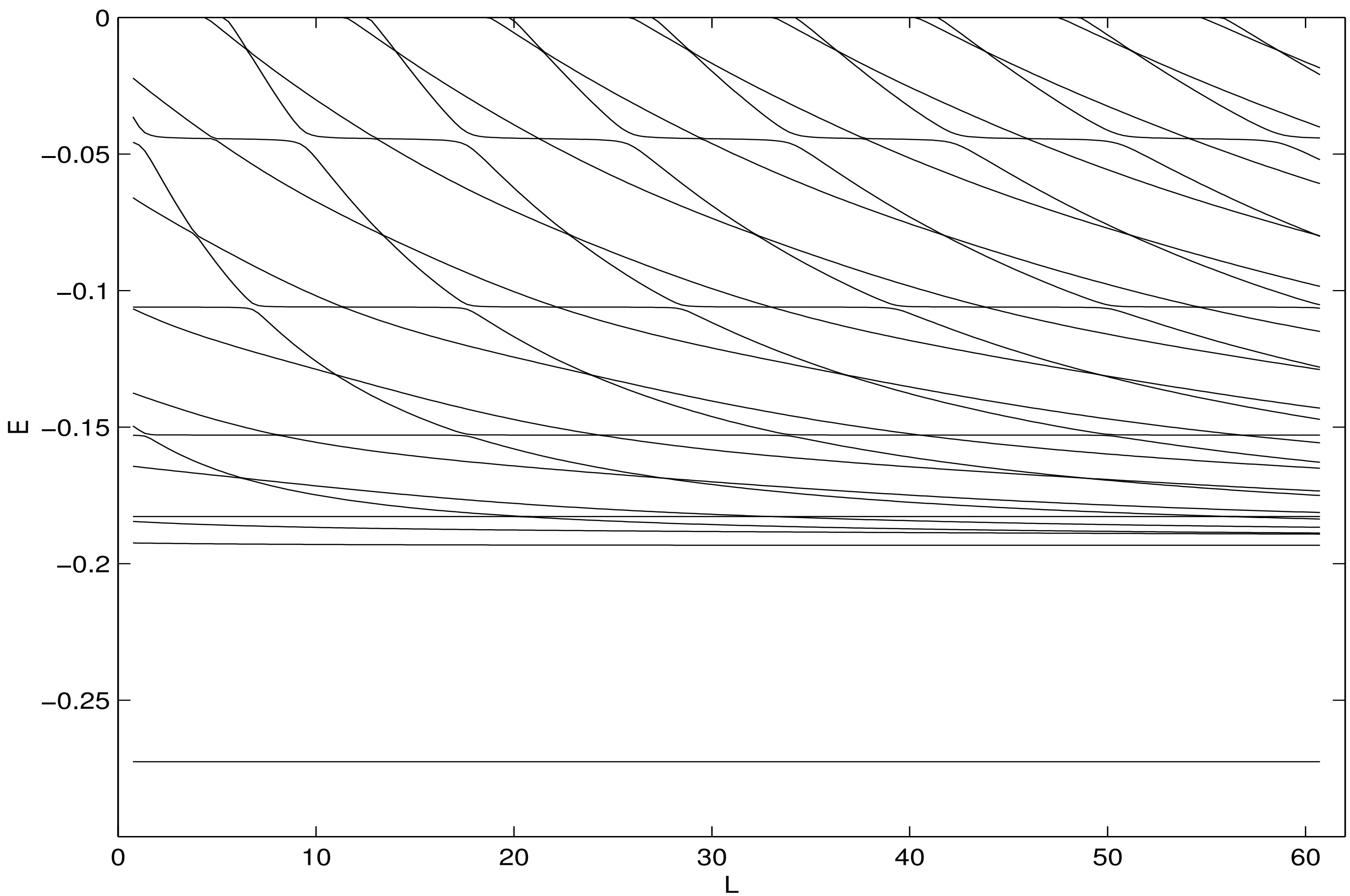
Bottleneck with $a = 5.2$



Bottleneck with $a = 2.9$



Bottleneck with $a = 1.9$



Line and points – a solvable model

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$$-\Delta - \alpha\delta(x-\Sigma) + \sum_{i=1}^{n} \tilde{\beta}_i \delta(x - y^{(i)})$$

in $L^2(\mathbb{R}^2)$ with $\alpha > 0$. The 2D point interactions at $\Pi = \{y^{(i)}\}$ with couplings $\beta = \{\beta_1, \dots, \beta_n\}$ are properly introduced through b.c. mentioned above, giving Hamiltonian $H_{\alpha,\beta}$

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Resolvent by Krein-type formula: given $z \in \mathbb{C} \setminus [0,\infty)$ we start from the free resolvent $R(z) := (-\Delta - z)^{-1}$, also interpreted as unitary $\mathbf{R}(z)$ acting from L^2 to $W^{2,2}$. Then

Resolvent by Krein-type formula

- we introduce auxiliary Hilbert spaces, $\mathcal{H}_0 := L^2(\mathbb{R})$ and $\mathcal{H}_1 := \mathbb{C}^n$, and trace maps $\tau_j : W^{2,2}(\mathbb{R}^2) \to \mathcal{H}_j$ defined by $\tau_0 f := f \upharpoonright_\Sigma$ and $\tau_1 f := f \upharpoonright_\Pi$,

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- then we define canonical embeddings of $\mathbf{R}(z)$ to $\mathcal{H}_i$ by $\mathbf{R}_{i,L}(z) := \tau_i R(z) : \; L^2 \to \mathcal{H}_i$, $\mathbf{R}_{L,i}(z) := [\mathbf{R}_{i,L}(z)]^*$, and $\mathbf{R}_{j,i}(z) := \tau_j \mathbf{R}_{L,i}(z) : \mathcal{H}_i \to \mathcal{H}_j$, and

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- operator-valued matrix $\Gamma(z) : \mathcal{H}_0 \oplus \mathcal{H}_1 \to \mathcal{H}_0 \oplus \mathcal{H}_1$ by

$$
\begin{aligned}
\Gamma_{ij}(z)g &:= -\mathbf{R}_{i,j}(z)g \quad \text{for} \quad i \neq j \quad \text{and} \quad g \in \mathcal{H}_j \,, \\
\Gamma_{00}(z)f &:= \left[\alpha^{-1} - \mathbf{R}_{0,0}(z)\right] f \quad \text{if} \quad f \in \mathcal{H}_0 \,, \\
\Gamma_{11}(z)\varphi &:= \Big(s_\beta(z)\delta_{kl} - G_z(y^{(k)}, y^{(l)})(1-\delta_{kl}) \Big)\, \varphi \,,
\end{aligned}
$$

with $s_\beta(z) := \beta + s(z) := \beta + \frac{1}{2\pi}(\ln \frac{\sqrt{z}}{2i} - \psi(1))$

Resolvent by Krein-type formula

To invert it we define the “reduced determinant”

$$D(z) := \Gamma_{11}(z) - \Gamma_{10}(z)\Gamma_{00}(z)^{-1}\Gamma_{01}(z) \; : \; \mathcal{H}_1 \to \mathcal{H}_1 \,,$$

Resolvent by Krein-type formula

To invert it we define the “reduced determinant”

$$D(z) := \Gamma_{11}(z) - \Gamma_{10}(z)\Gamma_{00}(z)^{-1}\Gamma_{01}(z) \;:\; \mathcal{H}_1 \to \mathcal{H}_1\,,$$

then an easy algebra yields expressions for “blocks” of $[\Gamma(z)]^{-1}$ in the form

$$\begin{aligned}
[\Gamma(z)]_{11}^{-1} &= D(z)^{-1}\,,\\
[\Gamma(z)]_{00}^{-1} &= \Gamma_{00}(z)^{-1} + \Gamma_{00}(z)^{-1}\Gamma_{01}(z)D(z)^{-1}\Gamma_{10}(z)\Gamma_{00}(z)^{-1}\,,\\
[\Gamma(z)]_{01}^{-1} &= -\Gamma_{00}(z)^{-1}\Gamma_{01}(z)D(z)^{-1}\,,\\
[\Gamma(z)]_{10}^{-1} &= -D(z)^{-1}\Gamma_{10}(z)\Gamma_{00}(z)^{-1}\,;
\end{aligned}$$

thus to determine singularities of $[\Gamma(z)]^{-1}$ one has to find the null space of $D(z)$

Resolvent by Krein-type formula

With this notation we can state the sought formula:

Theorem [E.-Kondej, 2004]: For $z \in \rho(H_{\alpha,\beta})$ with $\mathrm{Im}\, z > 0$ the resolvent $R_{\alpha,\beta}(z) := (H_{\alpha,\beta} - z)^{-1}$ equals

$$R_{\alpha,\beta}(z) = R(z) + \sum_{i,j=0}^{1} \mathbf{R}_{L,i}(z)[\Gamma(z)]_{ij}^{-1}\mathbf{R}_{j,L}(z)$$

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Remark: One can also compare resolvent of $H_{\alpha,\beta}$ to that of $H_\alpha \equiv H_{\alpha,\Sigma}$ using trace maps of the latter,

$$R_{\alpha,\beta}(z) = R_\alpha(z) + \mathbf{R}_{\alpha;L1}(z)D(z)^{-1}\mathbf{R}_{\alpha;1L}(z)$$

Spectral properties of $H_{\alpha,\beta}$

It is easy to check that

$$\sigma_{\mathrm{ess}}(H_{\alpha,\beta}) = \sigma_{\mathrm{ac}}(H_{\alpha,\beta}) = [-\frac{1}{4}\alpha^2, \infty)$$

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σ_{disc} given by *generalized Birman-Schwinger principle:*

$$\begin{aligned} \dim\ker\Gamma(z) &= \dim\ker R_{\alpha,\beta}(z)\,, \\ H_{\alpha,\beta}\phi_z = z\phi_z \;\Leftrightarrow\; \phi_z &= \sum_{i=0}^{1} \mathbf{R}_{L,i}(z)\eta_{i,z}\,, \end{aligned}$$

where $(\eta_{0,z}, \eta_{1,z}) \in \ker\Gamma(z)$. Moreover, it is clear that $0 \in \sigma_{\mathrm{disc}}(\Gamma(z)) \Leftrightarrow 0 \in \sigma_{\mathrm{disc}}(D(z))$; this reduces the task of finding the spectrum to an algebraic problem

Spectral properties of $H_{\alpha,\beta}$

Theorem [E.-Kondej, 2004]: (a) Let $n = 1$ and denote $\operatorname{dist}(\sigma, \Pi) =: a$, then $H_{\alpha,\beta}$ has one isolated eigenvalue $-\kappa_a^2$. The function $a \mapsto -\kappa_a^2$ is increasing in $(0, \infty)$,

$$\lim_{a\to\infty}(-\kappa_a^2) = \min\left\{\epsilon_\beta,\, -\frac{1}{4}\alpha^2\right\},$$

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Remark: Embedded eigenvalues due to mirror symmetry w.r.t. Σ possible if $n \ge 2$

Resonance for $n = 1$

Assume the point interaction eigenvalue *becomes embedded* as $a \to \infty$, i.e. that $\epsilon_\beta > -\frac{1}{4}\alpha^2$

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Observation: Birman-Schwinger works in the complex domain too; it is enough to look for analytical continuation of $D(\cdot)$, which acts for $z \in \mathbb{C} \setminus [-\frac{1}{4}\alpha^2, \infty)$ as a multiplication by

$$d_a(z) := s_\beta(z) - \phi_a(z) = s_\beta(z) - \int_0^\infty \frac{\mu(z,t)}{t - z - \frac{1}{4}\alpha^2}\,\mathrm{d}t\,,$$

$$\mu(z,t) := \frac{i\alpha}{16\pi}\,\frac{(\alpha - 2i(z-t)^{1/2})\,\mathrm{e}^{2ia(z-t)^{1/2}}}{t^{1/2}(z-t)^{1/2}}$$

Thus we have a situation reminiscent of Friedrichs model, just the functions involved are more complicated

Analytic continuation

Take a region Ω_- of the other sheet with $(-\frac{1}{4}\alpha^2, 0)$ as a part of its boundary. Put $\mu^0(\lambda, t) := \lim_{\varepsilon\to 0} \mu(\lambda+i\varepsilon, t)$, define

$$I(\lambda) := \mathcal{P} \int_0^\infty \frac{\mu^0(\lambda, t)}{t-\lambda-\frac{1}{4}\alpha^2}\, \mathrm{d}t\,,$$

and furthermore, $g_{\alpha,a}(z) := \frac{i\alpha}{4} \frac{\mathrm{e}^{-\alpha a}}{(z+\frac{1}{4}\alpha^2)^{1/2}}$.

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Lemma: $z \mapsto \phi_a(z)$ is continued analytically to Ω_- as

$$\phi_a^0(\lambda) = I(\lambda) + g_{\alpha,a}(\lambda) \quad \text{for} \quad \lambda \in \left(-\frac{1}{4}\alpha^2, 0\right)\,,$$

$$\phi_a^-(z) = -\int_0^\infty \frac{\mu(z,t)}{t - z - \frac{1}{4}\alpha^2}\, \mathrm{d}t - 2g_{\alpha,a}(z)\,, \;\; z \in \Omega_-$$

Analytic continuation

Proof: By a direct computation one checks

$$\lim_{\varepsilon \to 0^+} \phi_a^{\pm}(\lambda \pm i\varepsilon) = \phi_a^0(\lambda)\,, \qquad -\frac{1}{4}\alpha^2 < \lambda < 0\,,$$

so the claim follows from edge-of-the-wedge theorem. $\square$

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The continuation of d_a is thus the function $\eta_a : M \mapsto \mathbb{C}$, where $M = \{z : \operatorname{Im} z > 0\} \cup (-\frac{1}{4}\alpha^2, 0) \cup \Omega_-$, acting as

$$\eta_a(z) = s_\beta(z) - \phi_a^{l(z)}(z)\,,$$

and our problem reduces to solution if the implicit function problem $\eta_a(z) = 0$.

Resonance for $n = 1$

Theorem [E.-Kondej, 2004]: Assume $\epsilon_\beta > -\frac{1}{4}\alpha^2$. For any a large enough the equation $\eta_a(z) = 0$ has a unique solution $z(a) = \mu(b) + i\nu(b) \in \Omega_-$, i.e. $\nu(a) < 0$, with the following asymptotic behaviour as $a \to \infty$,

$$\mu(a) = \epsilon_\beta + \mathcal{O}(\mathrm{e}^{-a\sqrt{-\epsilon_\beta}})\,, \quad \nu(a) = \mathcal{O}(\mathrm{e}^{-a\sqrt{-\epsilon_\beta}})$$

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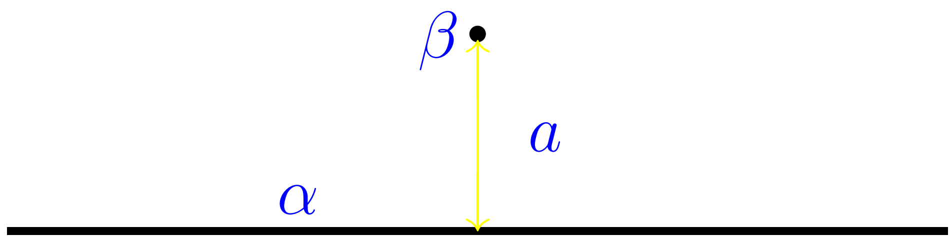
Remark: We have $|\phi_a^-(z)| \to 0$ uniformly in a and $|s_\beta(z)| \to \infty$ as $\operatorname{Im} z \to -\infty$. Hence the imaginary part $z(a)$ is bounded as a function of a, in particular, *the resonance pole survives* as $a \to 0$.

Scattering for $n = 1$

The same as scattering problem for $(H_{\alpha,\beta}, H_\alpha)$



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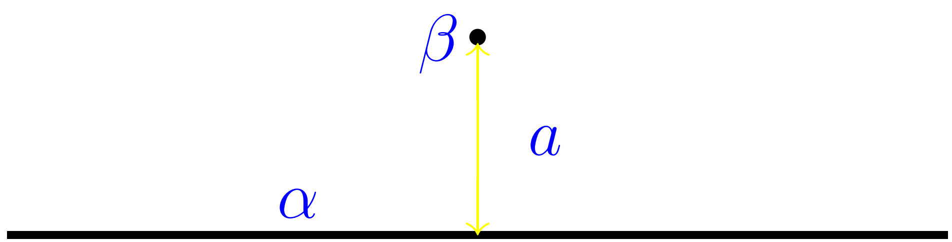

Existence and completeness by Birman-Kuroda theorem; we seek on-shell S-matrix in $(-\frac{1}{4}\alpha^2, 0)$. By Krein formula, resolvent for $\operatorname{Im} z > 0$ expresses as

$$R_{\alpha,\beta}(z) = R_\alpha(z) + \eta_a(z)^{-1}(\cdot, v_z)v_z,$$

where $v_z := R_{\alpha;L,1}(z)$

Scattering for $n = 1$

Apply this operator to vector

$$\omega_{\lambda,\varepsilon}(x) := \mathrm{e}^{i(\lambda+\alpha^2/4)^{1/2}x_1-\varepsilon^2 x_1^2}\, \mathrm{e}^{-\alpha|x_2|/2}$$

and take limit $\varepsilon \to 0+$ in the sense of distributions; then a straightforward calculation give generalized eigenfunction of $H_{\alpha,\beta}$. In particular, we have

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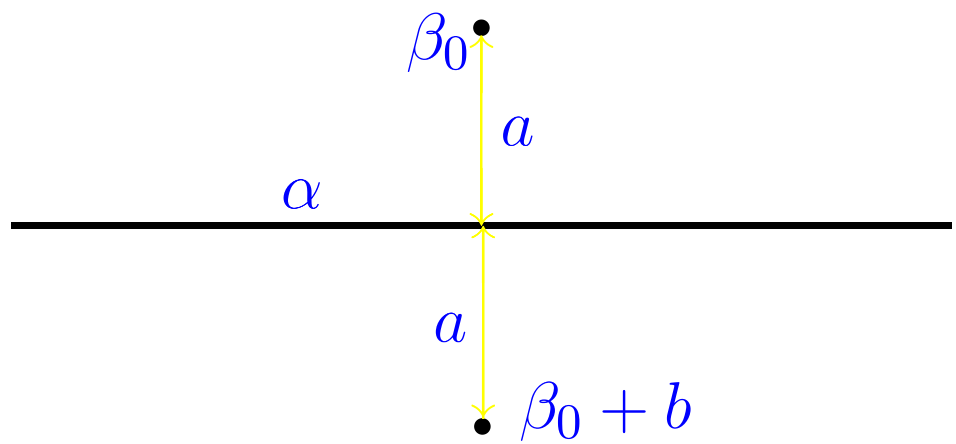
Proposition: For any $\lambda \in (-\frac{1}{4}\alpha^2, 0)$ the reflection and transmission amplitudes are

$$\mathcal{R}(\lambda) = \mathcal{T}(\lambda) - 1 = \frac{i}{4}\,\alpha\eta_a(\lambda)^{-1}\,\frac{\mathrm{e}^{-\alpha a}}{(\lambda+\frac{1}{4}\alpha^2)^{1/2}}\,;$$

they have the same pole in the analytical continuation to Ω_- as the continued resolvent

Resonances from perturbed symmetry

Take the simplest situation, $n = 2$



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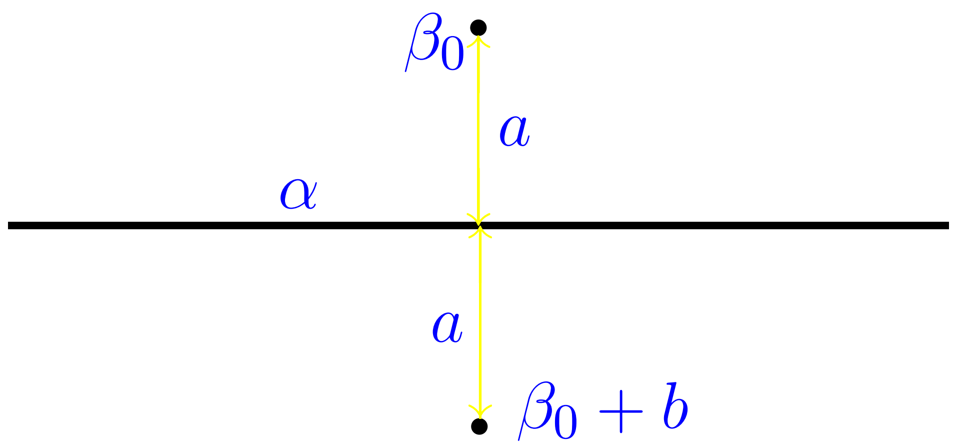

Let $\sigma_{\mathrm{disc}}(H_{0,\beta_0}) \cap \left(-\frac{1}{4}\alpha^2, 0\right) \neq \emptyset$, so that Hamiltonian H_{0,β_0} has two eigenvalues, the larger of which, ϵ_2, exceeds $-\frac{1}{4}\alpha^2$. Then H_{α,β_0} has the same eigenvalue ϵ_2 embedded in the negative part of continuous spectrum

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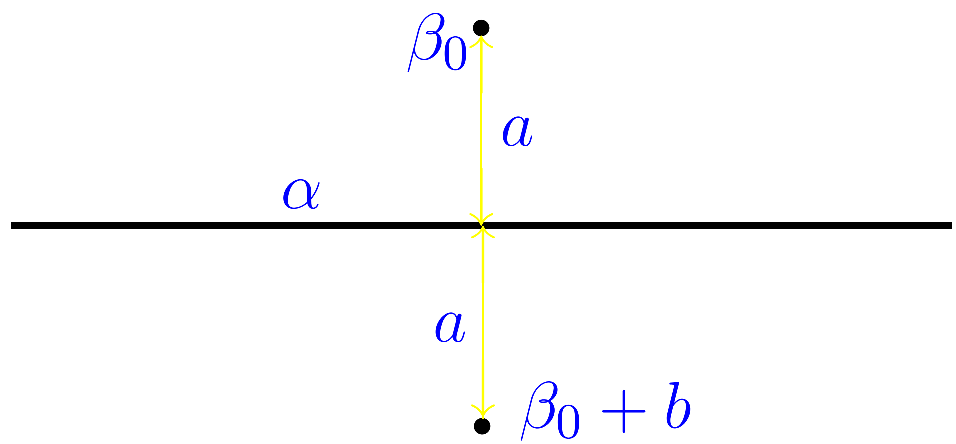

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One has now to continue analytically the 2×2 matrix function $D(\cdot)$. Put $\kappa_2 := \sqrt{-\epsilon_2}$ and $\breve{s}_\beta(\kappa) := s_\beta(-\kappa^2)$

Resonances from perturbed symmetry

Proposition: Assume $\epsilon_2 \in (-\frac{1}{4}\alpha^2, 0)$ and denote $\tilde{g}(\lambda) := -ig_{\alpha,a}(\lambda)$. Then for all b small enough the continued function has a unique zero $z_2(b) = \mu_2(b) + i\nu_2(b) \in \Omega_-$ with the asymptotic expansion

$$\begin{aligned}
\mu_2(b) &= \epsilon_2 + \frac{\kappa_2 b}{\breve{s}'_\beta(\kappa_2) + K'_0(2a\kappa_2)} + \mathcal{O}(b^2)\,, \\
\nu_2(b) &= -\frac{\kappa_2 \tilde{g}(\epsilon_2) b^2}{2(\breve{s}'_\beta(\kappa_2) + K'_0(2a\kappa_2))|\breve{s}'_\beta(\kappa_2) - \phi^0_a(\epsilon_2)|} + \mathcal{O}(b^3)
\end{aligned}$$

Open questions

- *Strong coupling asymptotics of* $\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma})$ is not known for curves with *open ends* (manifolds with boundaries). For *smooth* Γ, one conjectures similar asymptotics, where S_Γ has *Dirichlet b.c.* For *non-smooth* Γ the leading term is expected to be different

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- *More:* random and magnetic graphs, justification of the L^2 approach for leaky-graph resonances, etc.

The talk was based on

[EI01] P.E., T. Ichinose: Geometrically induced spectrum in curved leaky wires, *J. Phys.* **A34** (2001), 1439-1450.

[EK02] P.E., S. Kondej: Curvature-induced bound states for a δ interaction supported by a curve in $\mathbb{R}^3$, *Ann. H. Poincaré* **3** (2002), 967-981.

[EK03] P.E., S. Kondej: Bound states due to a strong δ interaction supported by a curved surface, *J. Phys.* **A36** (2003), 443-457.

[EK04] P.E., S. Kondej: Schrödinger operators with singular interactions: a model of tunneling resonances, *J. Phys.* **A37** (2004), 8255-8277.

[EK05] P.E., S. Kondej: Scattering by local deformations of a straight leaky wire, *J. Phys.* **A38** (2005), to appear

[EN03] P.E., K. Němcová: Leaky quantum graphs: approximations by point interaction Hamiltonians, *J. Phys.* **A36** (2003), 10173-10193.

[EY01] P.E., K. Yoshitomi: Band gap of the Schrödinger operator with a strong δ-interaction on a periodic curve, *Ann. H. Poincaré* **2** (2001), 1139-1158.

[EY02a] P.E., K. Yoshitomi: Asymptotics of eigenvalues of the Schrödinger operator with a strong δ-interaction on a loop, *J. Geom. Phys.* **41** (2002), 344-358.

[EY02b] P.E., K. Yoshitomi: Persistent currents for 2D Schrödinger operator with a strong δ-interaction on a loop, *J. Phys.* **A35** (2002), 3479-3487.

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