

# Scattering and resonances in leaky quantum-wire systems

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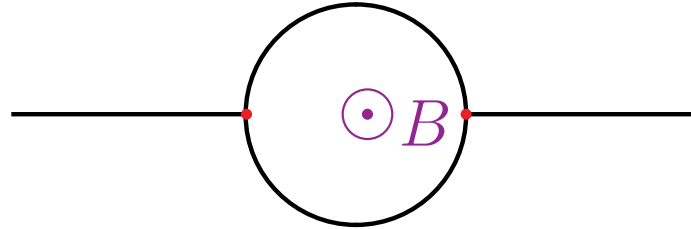
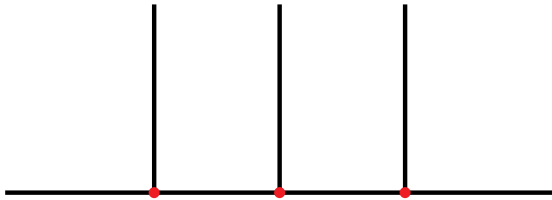
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- Open questions



# Scattering on quantum-wire systems

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

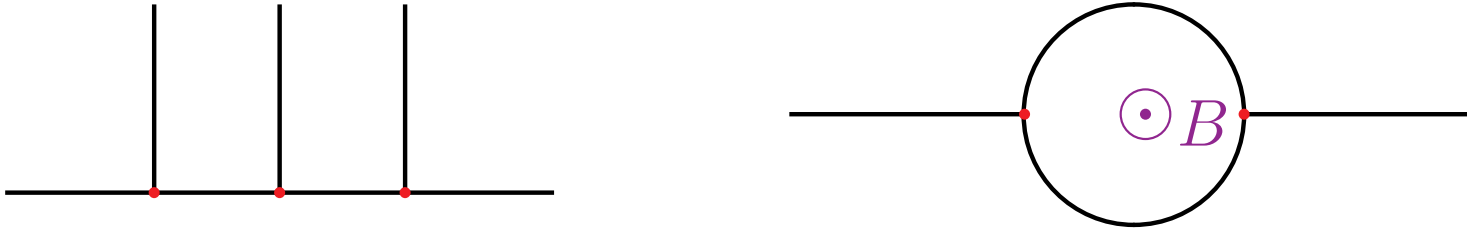


Here we study Schrödinger operator on graph, with appropriate b.c. at vertices. Scattering is an *ODE problem* and it is easy to study resonances; for reviews see, e.g., [Kuchment'04], the forthcoming [INI AGA Proc.'08], etc.



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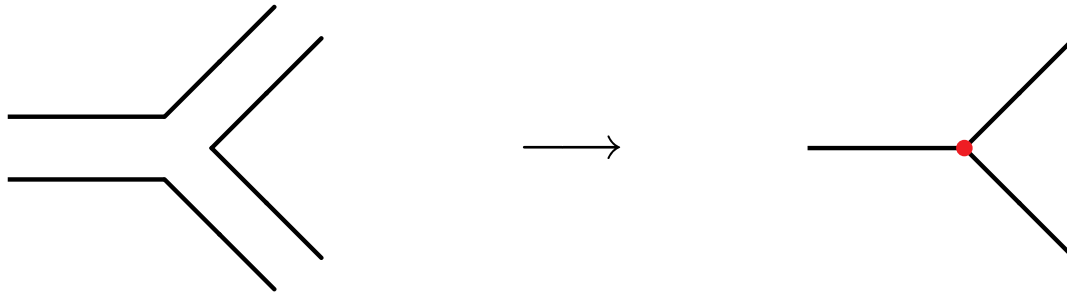
More realistic models of quantum wires treat them as *finite-width channels*, typically with Dirichlet b.c. Various scattering problems studied numerically in many papers.

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

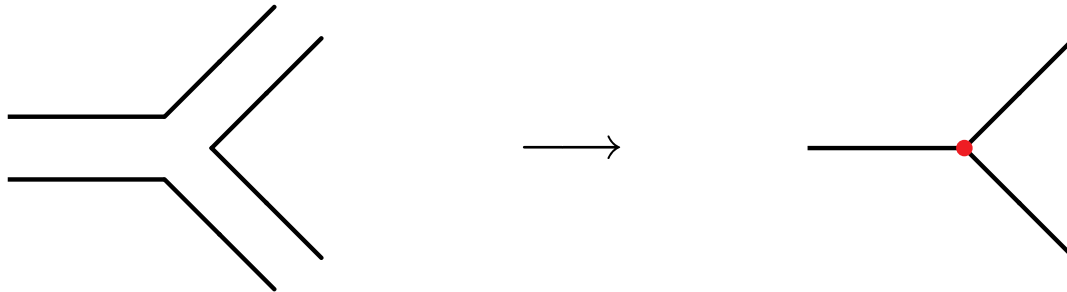
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- after a long effort the *Neumann-like case* is understood, see [Freidlin-Wentzell'93], [Freidlin'96], [Saito'01], [Kuchment-Zeng'01], [Rubinstein-Schatzmann'01], [E.-Post'05, 07], [Post'06], giving basically free b.c. only
- recently a progress achieved in the *Dirichlet case* [Post'05], [Molchanov-Vainberg'07], [Grieser'07], [Cacciapuoti-E.'07].



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- At least in principle, the difficulty with the *ad hoc parameters* can be thus solved
- The “ideal” graph models have, however, another flaw, namely that *quantum tunneling is neglected*:

recall that a true quantum-wire boundary is a finite potential jump, so an electron may pass between different quantum wires by tunneling the classically forbidden region between them

This motivates us to look for an alternative quantum graph model



# 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,

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

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  $\Gamma$



# Leaky quantum-graph Hamiltonians

For  $\Gamma$  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  $W_{\text{loc}}^{1,2}(\mathbb{R}^2 \setminus \Gamma)$ , 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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$$\left. \frac{\partial \psi}{\partial n}(x) \right|_+ - \left. \frac{\partial \psi}{\partial n}(x) \right|_- = -\alpha \psi(x)$$

## 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  $\text{codim } \Gamma$  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*  $\Gamma : \mathbb{R} \rightarrow \mathbb{R}^2$  parameterized by its arc length, and assume:



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

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

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

- 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,  $\sigma_{\text{ess}}(H_{\alpha,\Gamma}) = [-\frac{1}{4}\alpha^2, \infty)$  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  $\Gamma$  fits the above assumptions, we have  $\sigma_{\text{disc}}(H_{\alpha,\Gamma}) \neq \emptyset$  by minimax principle



# Geometrically induced spectrum, contd

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

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

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

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



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



# Further extensions

- $H_{\alpha, \Gamma}$  with a *periodic*  $\Gamma$  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.  $\theta$





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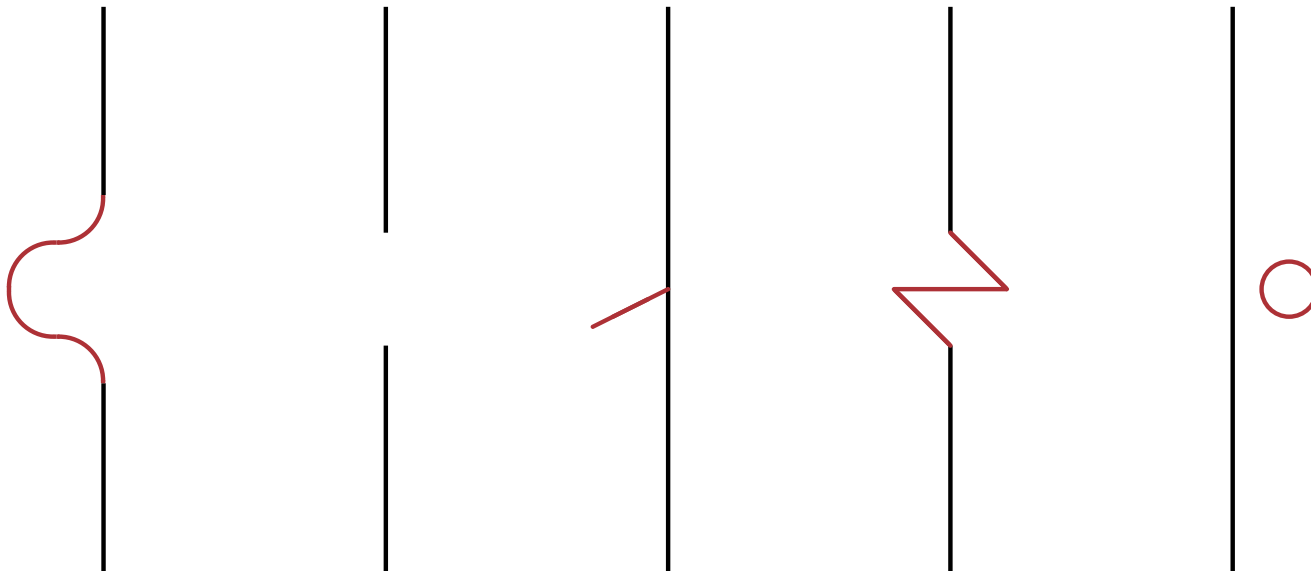
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- *Higher dimensions*: the results extend to loops, infinite and periodic curves in  $\mathbb{R}^3$
- and to *curved surfaces* in  $\mathbb{R}^3$ ; then the comparison operator is  $-\Delta_{LB} + K - M^2$ , where  $K, M$ , respectively, are the corresponding 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  $\Sigma$  is a *straight line*,  $\Sigma = \{(x_1, 0) : x_1 \in \mathbb{R}\}$ , and that the graph  $\Gamma$  in question differs from  $\Sigma$  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  $\Gamma_i$ 's are finite  $C^1$  curves such that *no pair* of components of  $\Gamma$  *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 *cuspl* 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

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

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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

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

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



# Krein's formula, continued

A straightforward computation shows that the resolvent  $R_{\Sigma}^k$  of  $H_{\alpha, \Sigma}$  has the kernel  $G_{\Sigma}^k(x-y)$  given by

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

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  $R_{\Sigma}^k$  to  $L^2(\nu)$ , where  $\nu \equiv \nu_{\Lambda}$  is the Dirac measure on  $\Lambda$ . It can be written as  $\nu_{\Lambda} = \nu_0 + \sum_{i=1}^N \nu_i$ , where  $\nu_0$  is the Dirac measure on  $\Lambda_0$ . It convenient also to introduce the space  $\mathfrak{h} \equiv L^2(\nu)$  which decomposes into

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



# Embeddings

Now we are able to introduce the operator

$$\mathbb{R}_{\Sigma, \nu}^k : \mathfrak{h} \rightarrow L^2, \quad \mathbb{R}_{\Sigma, \nu}^k f = G_{\Sigma}^k * f \nu \quad \text{for } f \in \mathfrak{h}$$

defined for suitable values of  $k$ . Similarly,  $(\mathbb{R}_{\Sigma, \nu}^k)^* : L^2 \rightarrow \mathfrak{h}$  is its adjoint and  $\mathbb{R}_{\Sigma, \nu \nu}^k$  denotes the operator-valued matrix in  $\mathfrak{h}$  with the “block elements”  $G_{\Sigma, ij}^k \equiv G_{\Sigma, \nu_i \nu_j}^k : L^2(\nu_j) \rightarrow L^2(\nu_i)$

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They have the following properties:

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



# Krein's formula, continued

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

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

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

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

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

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  $R_{\Gamma}^k$



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

Let us first look at the essential spectrum:

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

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

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

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



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*Remark:*  $\sigma_{\text{disc}}(H_{\alpha,\Gamma})$  given by singularities of  $\Theta^k$  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  $\Theta^{i\kappa,+} := \alpha^{-1}\mathbb{I} + R_{\Sigma,\nu\nu}^{i\kappa}$  and  $\mathbb{I}$  is the  $(N+1) \times (N+1)$  unit matrix, for some  $C' > 0$  and all  $\kappa$  sufficiently large; it is clear that  $(\Theta^{i\kappa,+})^{-1}$  is positive and bounded. This gives

$$B^{i\kappa} \leq C' B^{i\kappa,+}, \quad B^{i\kappa,+} := R_{\Sigma,\nu}^{i\kappa} (\Theta^{i\kappa,+})^{-1} (R_{\Sigma,\nu}^{i\kappa})^*$$



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

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

$$\begin{aligned} \int_{\mathbb{R}^2} B_\delta^{i\kappa,+}(x, x) dx &= \int_{\mathbb{R}^2} (G_\Sigma^{i\kappa}(\cdot, x) \chi_\delta(x), (\Theta^{i\kappa,+})^{-1} G_\Sigma^{i\kappa}(\cdot, x) \chi_\delta(x))_{\mathfrak{h}} dx \\ &\leq \|(\Theta^{i\kappa,+})^{-1}\| \int_{\mathbb{R}^2} \|G_\Sigma^{i\kappa}(\cdot, x) \chi_\delta(x)\|_{\mathfrak{h}}^2 dx \leq C \|(\Theta^{i\kappa,+})^{-1}\|, \end{aligned}$$

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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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  $H_{\alpha,\Sigma}$ ,

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

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



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

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



# Generalized eigenfunctions, continued

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

$$G_{\Sigma}^{k_\alpha(\lambda)}(x-y) = K_0(i\sqrt{\lambda}|x-y|) + \mathcal{P} \int_0^\infty \frac{\mu_0(t; x, y)}{t - \lambda - \alpha^2/4} dt + \frac{i\alpha}{8k_\alpha(\lambda)} e^{ik_\alpha(\lambda)|x_1-y_1|} e^{-\alpha/2(|x_2|+|y_2|)},$$

where

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



# Generalized eigenfunctions, continued

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

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

where  $J_\Lambda \omega_\lambda$  is an embedding of  $\omega_\lambda$  to  $L^2(\nu_\Lambda)$





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

$$G_\Sigma^{k_\alpha(\lambda)}(x-y) \approx \frac{i\alpha}{8k_\alpha(\lambda)} e^{ik_\alpha(\lambda)|x_1-y_1|} e^{-\alpha/2(|x_2|+|y_2|)}$$



# 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

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

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

$$\mathcal{T}(\lambda) = 1 - \frac{i\alpha}{8k_\alpha(\lambda)} \left( (\Theta^{k_\alpha(\lambda)})^{-1} J_\Lambda \omega_\lambda, J_\Lambda \omega_\lambda \right)_h$$

and

$$\mathcal{R}(\lambda) = \frac{i\alpha}{8k_\alpha(\lambda)} \left( (\Theta^{k_\alpha(\lambda)})^{-1} J_\Lambda \omega_\lambda, J_\Lambda \bar{\omega}_\lambda \right)_h$$



# Strong coupling: a conjecture

Consider  $\Gamma$  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  $\Gamma$  through the same comparison operator, namely  $K_\Gamma := -\frac{d}{ds^2} - \frac{1}{4}\gamma(s)^2$  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  $S_{\Gamma,\alpha}(\lambda)$  and  $S_K(\lambda)$  the on-shell  $S$ -matrixes of  $H_{\alpha,\Gamma}$  and  $K$  at energy  $\lambda$ , respectively.

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

$$S_{\Gamma,\alpha}\left(k^2 - \frac{1}{4}\alpha^2\right) \rightarrow S_K(k^2)$$



# 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  $\Gamma$ . The options:

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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*

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

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



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- *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”  $\alpha$  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

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





# 2D point interactions

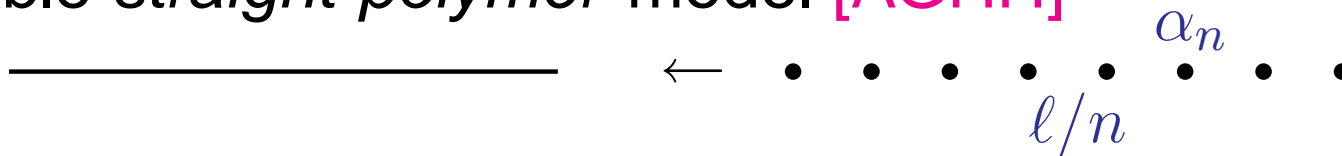
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For our purpose, the coupling should depend on the set  $Y$  approximating  $\Gamma$ . To see how compare a line  $\Gamma$  with the solvable *straight-polymer* model **[AGHH]**



# 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  $H_{\alpha_n, Y_n}$  with  $\alpha_n = \alpha |Y_n|$ , where  $|Y_n| := \#Y_n$ .

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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

$$\frac{1}{|Y_n|} \sum_{y \in Y_n} f(y) \rightarrow \int_{\Gamma} f \, dm$$

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



# Comments on the approximation

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

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- The result applies to finite graphs, however, an infinite  $\Gamma$  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  $\text{codim } \Gamma = 1$  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  $H_{\alpha_n, Y_n}$  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  $\gamma_E$  is *Euler's constant*.



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

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





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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  $n \rightarrow \infty$   $\square$

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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  $\Gamma$ , 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  $\Gamma$* : if a single bend has a significant reflection, a double band should exhibit resonances
- *Bottleneck curve*: a good candidate to demonstrate tunneling resonances



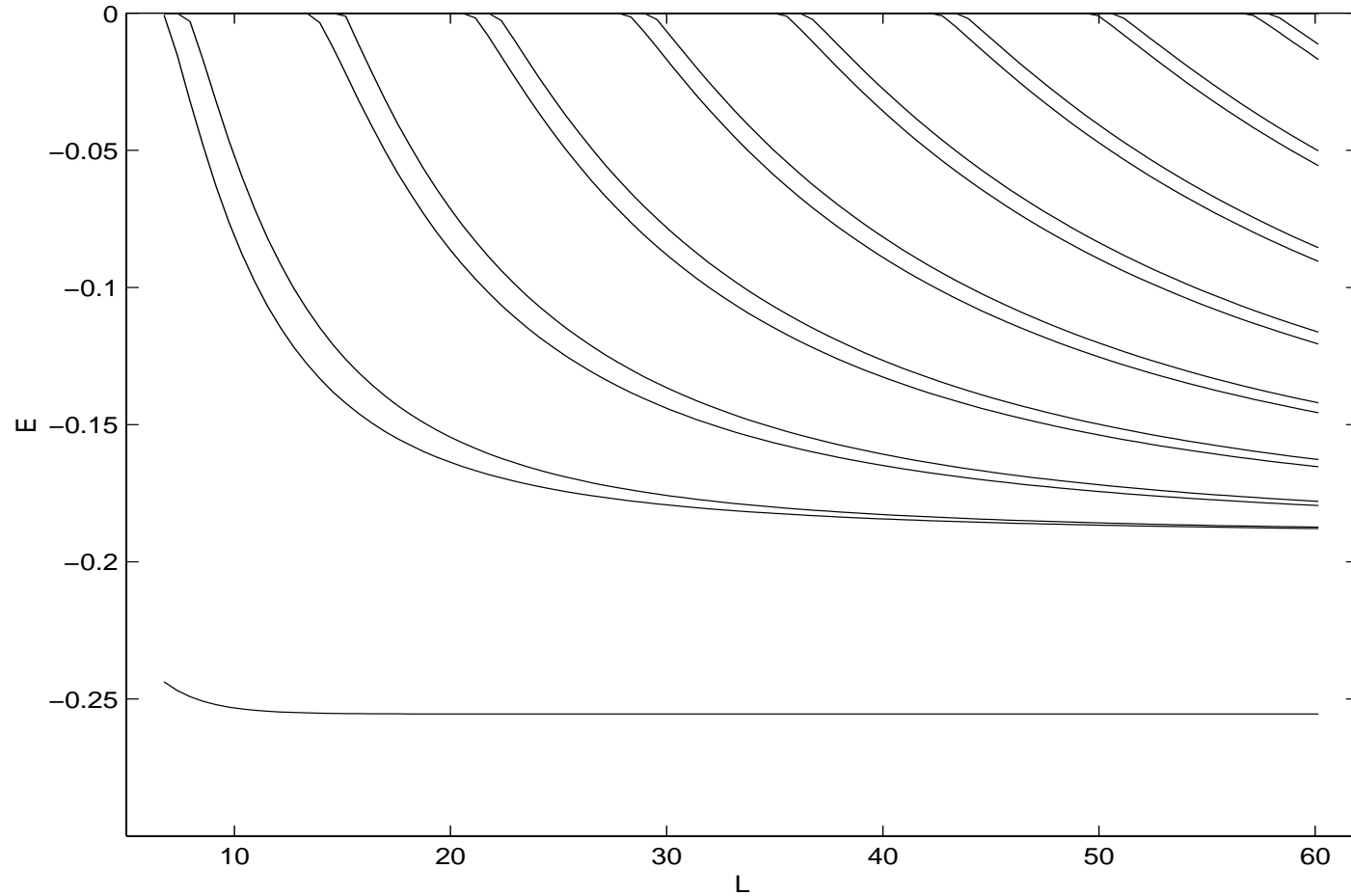
# Broken line


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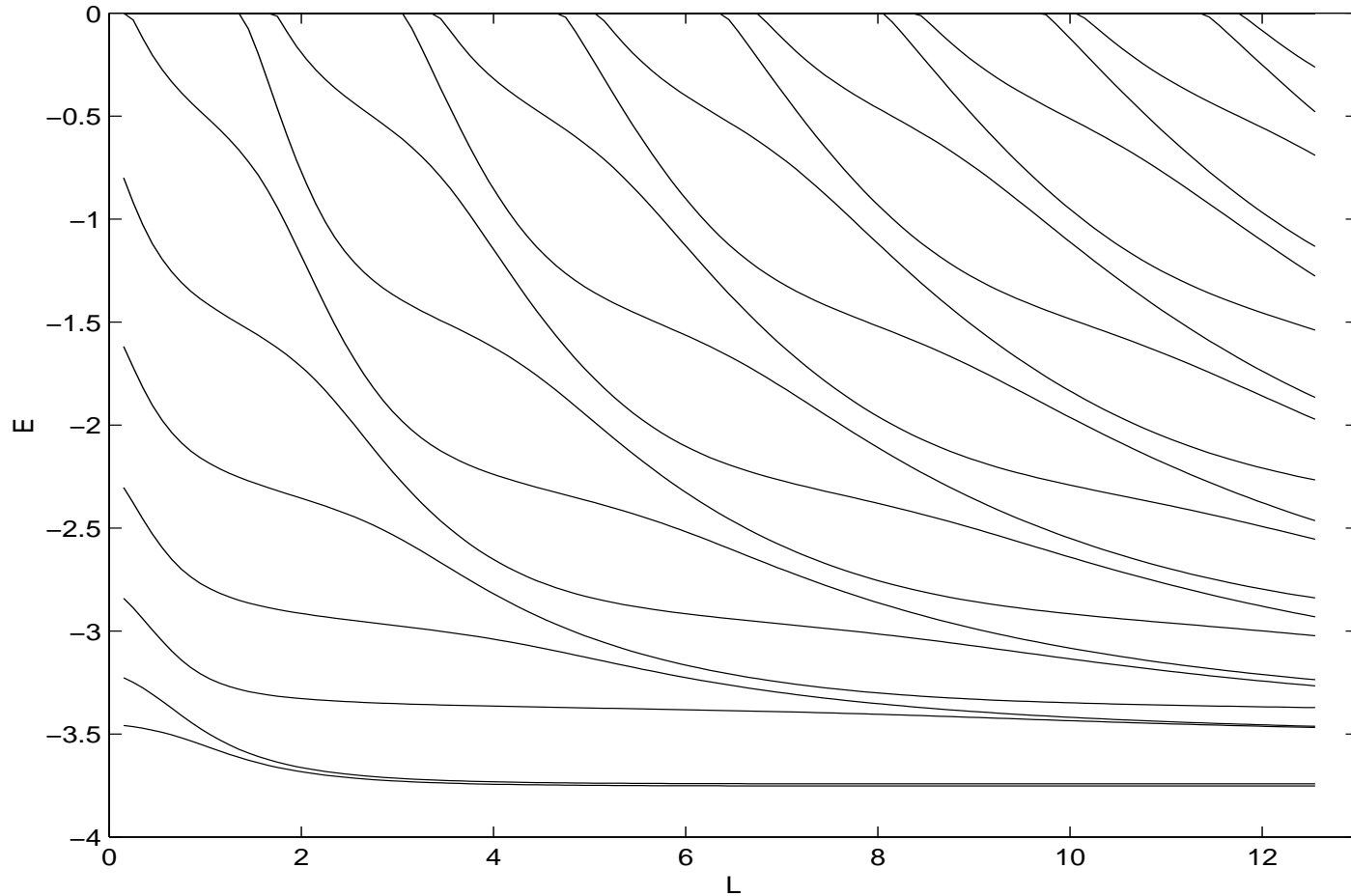


# Z shape with $\theta = \frac{\pi}{2}$

$$\left. \begin{array}{l} L_c = 10 \\ \alpha = 5 \end{array} \right\}$$

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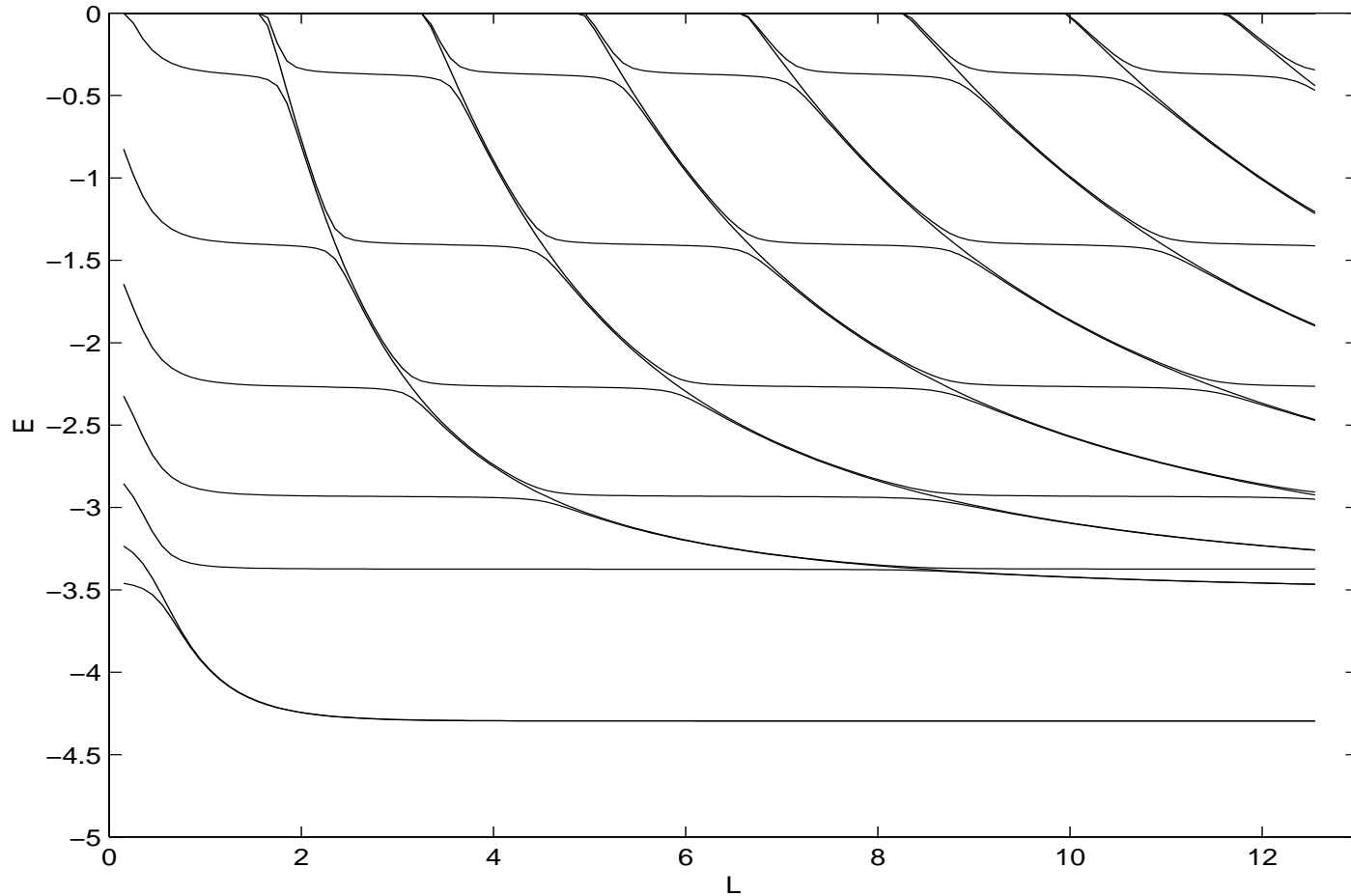


# Z shape with $\theta = 0.32\pi$

$$\sum_{\alpha=5} L_c = 10$$

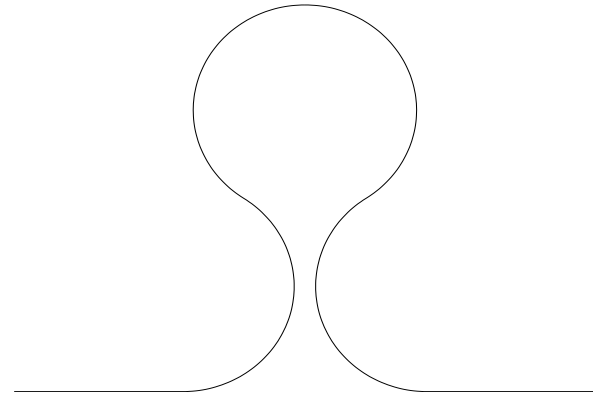
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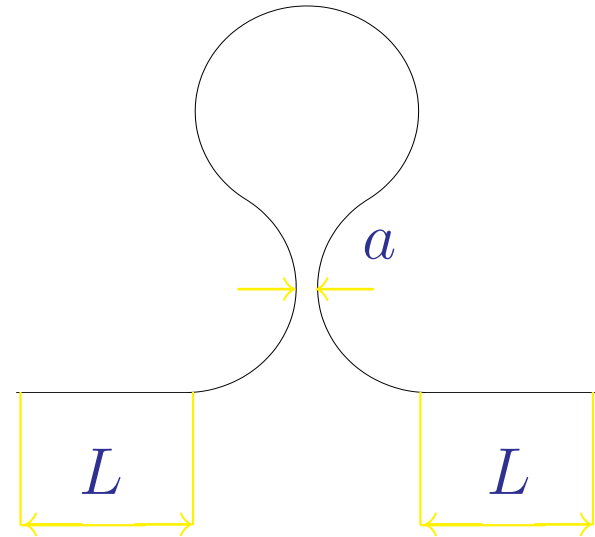
# A bottleneck curve

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



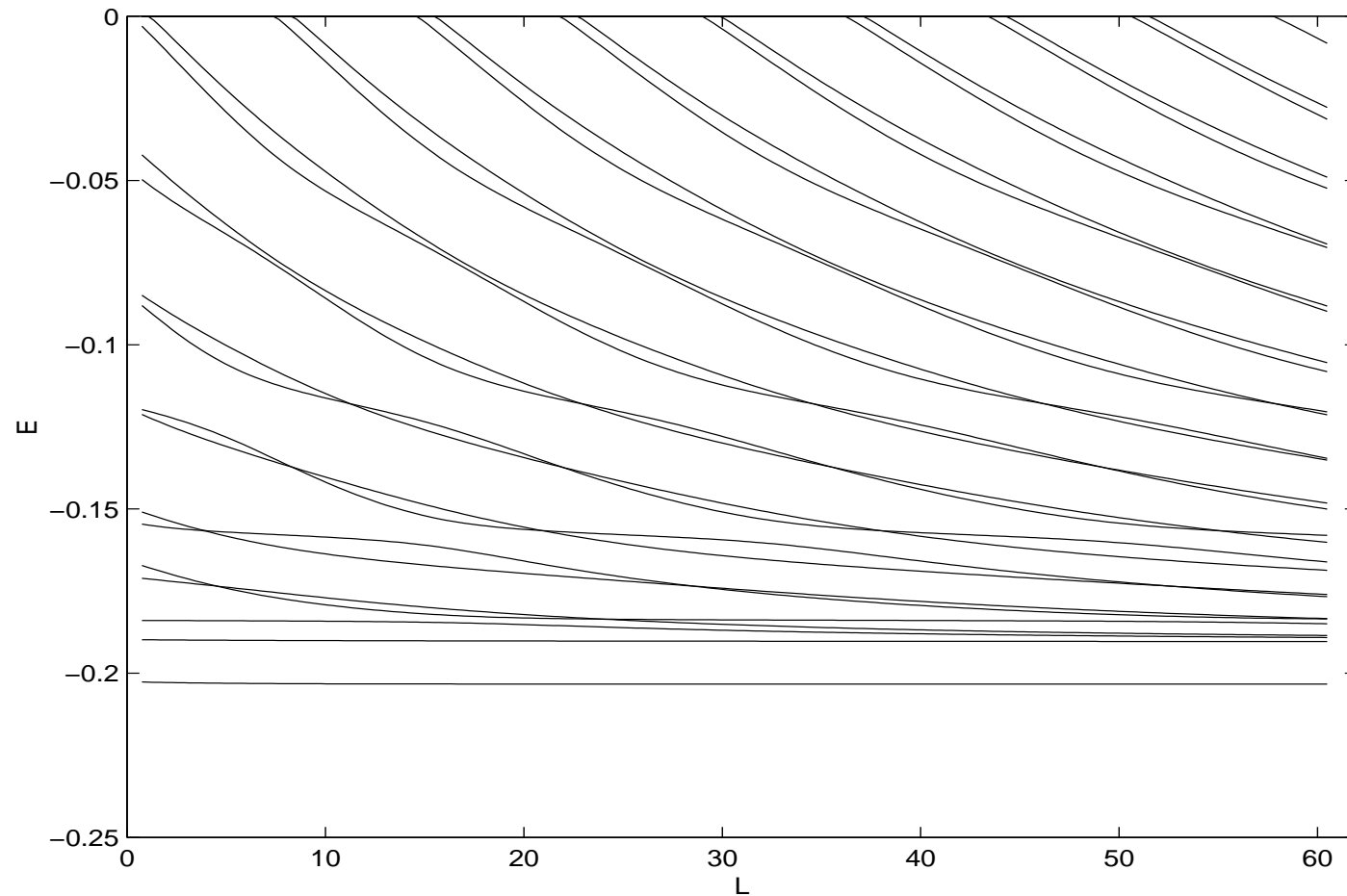
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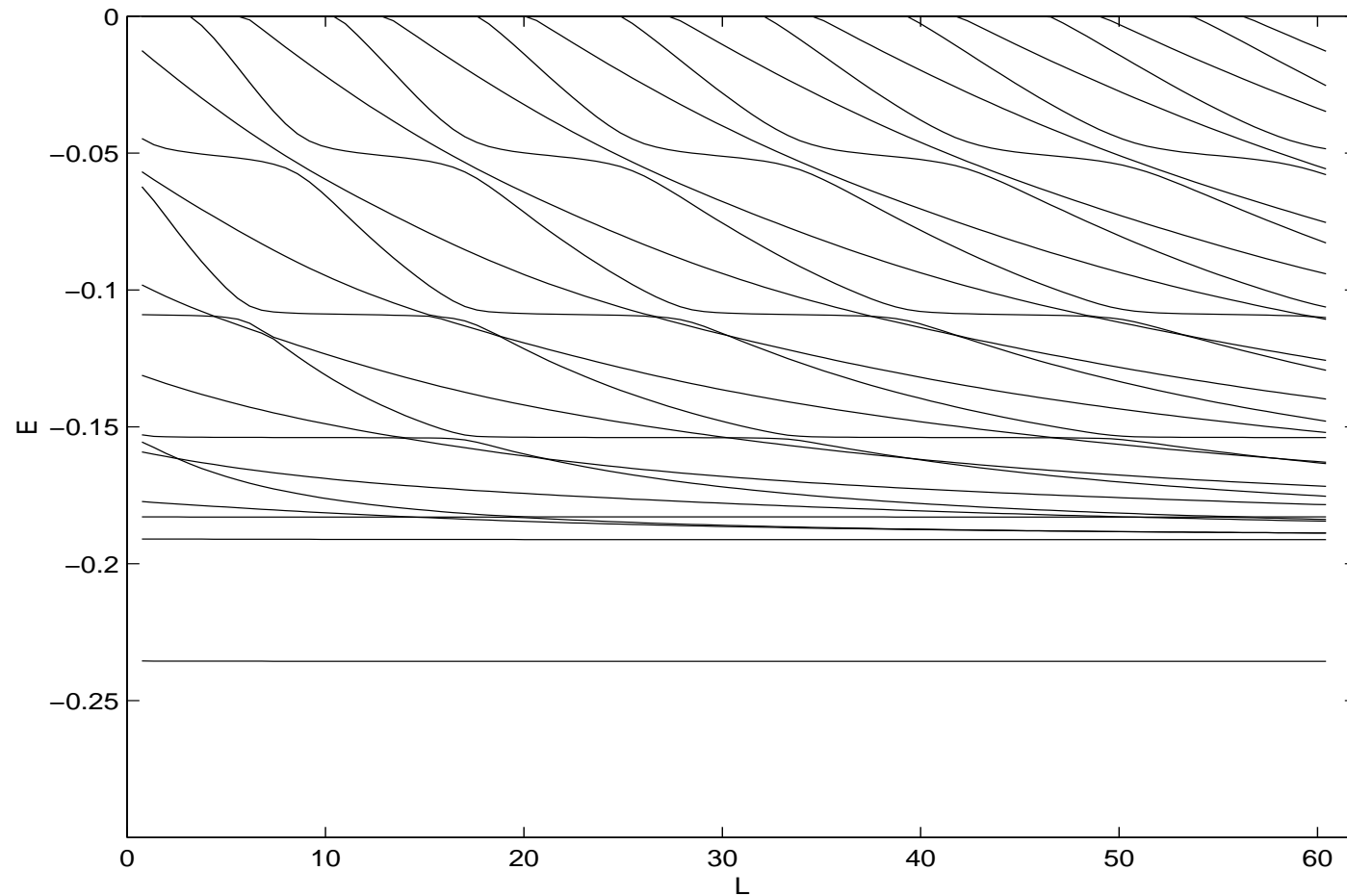


If  $\Gamma$  is a straight line, the transverse eigenfunction is  $e^{-\alpha|y|/2}$ , hence the distance at which tunneling becomes significant is  $\approx 4\alpha^{-1}$ . In the example, we choose  $\alpha = 1$

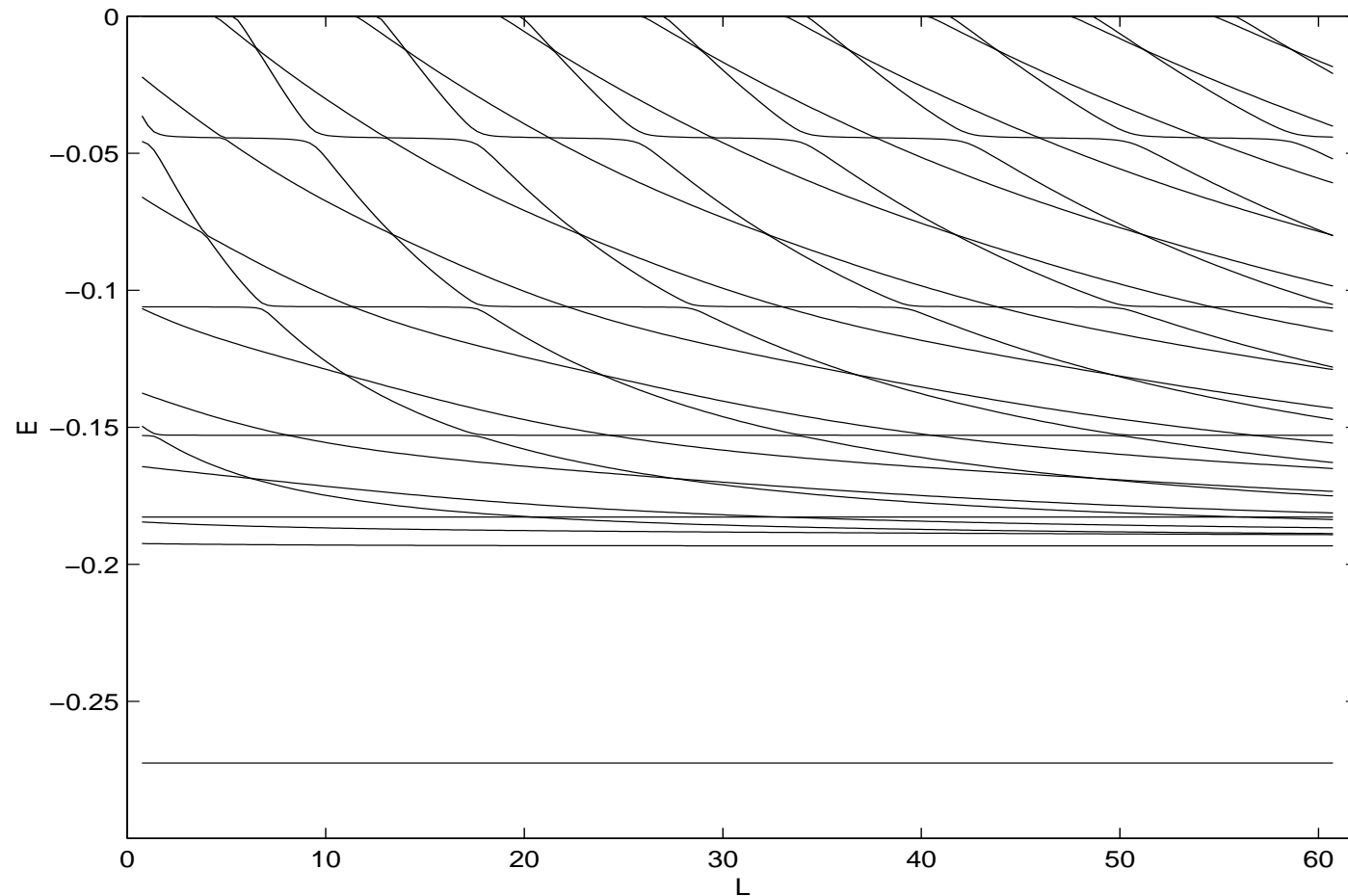
# Bottleneck with $a = 5.2$



# Bottleneck with $a = 2.9$



# Bottleneck with $a = 1.9$



# Open questions

- *Scattering on leaky graphs*: existence and completeness beyond the local deformation case; one has to use suitable identification operator



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- etc., 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  $\delta$  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  $\delta$  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), 4865–4874.
- [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  $\delta$ -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  $\delta$ -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  $\delta$ -interaction on a loop, *J. Phys.* **A35** (2002), 3479-3487.



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