Quantum Graphs
and their generalizations

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Lecture V

Leaky graphs – strong coupling, approximation of leaky graphs, eigenvalues and resonances

Lecture overview

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- *Geometrically induced spectral bound states* of leaky wires and graphs: bent edges
- *Leaky-graph resonances*: a solvable model

Strong coupling for a compact Γ

Let Γ have a single component, smooth and compact

Theorem [EY01, 02; EK03, Ex04]: *(i)* Let Γ be a C^4 smooth manifold. In the limit $(-1)^{\operatorname{codim}\Gamma-1}\alpha \to \infty$ we have

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

for $\dim\Gamma = 1$, $\operatorname{codim}\Gamma = 1$,

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$$\#\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma}(h)) = \frac{|\Gamma|\alpha^2}{16\pi^2} + \mathcal{O}(\ln\alpha)$$

for $\dim\Gamma = 2$, $\mathrm{codim}\,\Gamma = 1$, and

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for $\dim\Gamma = 2$, $\operatorname{codim}\Gamma = 1$, and

$$\#\sigma_{\text{disc}}(H_{\alpha,\Gamma}) = \frac{|\Gamma|(-\epsilon_\alpha)^{1/2}}{\pi} + \mathcal{O}(\mathrm{e}^{-\pi\alpha})$$

for $\dim\Gamma = 1$, $\operatorname{codim}\Gamma = 2$. Here $|\Gamma|$ is the curve length or surface area, respectively, and $\epsilon_\alpha = -4\,\mathrm{e}^{2(-2\pi\alpha+\psi(1))}$

Strong coupling for a compact Γ

Theorem, continued: *(ii)* In addition, suppose that Γ has *no boundary*. Then the j-th eigenvalue of $H_{\alpha,\Gamma}$ behaves as

$$\lambda_j(\alpha) = -\frac{\alpha^2}{4} + \mu_j + \mathcal{O}(\alpha^{-1}\ln\alpha)$$

for $\operatorname{codim}\Gamma = 1$ and

$$\lambda_j(\alpha) = \epsilon_\alpha + \mu_j + \mathcal{O}(\mathrm{e}^{\pi\alpha})$$

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for $\operatorname{codim}\Gamma = 2$, where μ_j is the j-th eigenvalue of

$$S_\Gamma = -\frac{\mathrm{d}}{\mathrm{d}s^2} - \frac{1}{4}k(s)^2$$

on $L^2((0,|\Gamma|))$ for $\dim\Gamma = 1$, where k is *curvature* of Γ, and

$$S_\Gamma = -\Delta_\Gamma + K - M^2$$

on $L^2(\Gamma,\mathrm{d}\Gamma)$ for $\dim\Gamma = 2$, where $-\Delta_\Gamma$ is Laplace-Beltrami operator on Γ and K, M, respectively, are the corresponding *Gauss* and *mean* curvatures

Proof technique

Consider first the $1+1$ case. Take a closed curve Γ and call $L = |\Gamma|$. We start from a *tubular neighborhood* of Γ

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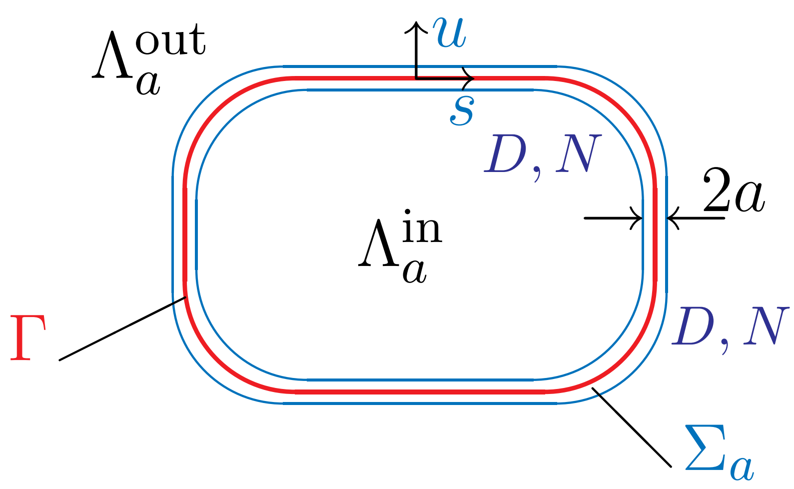
Lemma: $\Phi_a : [0,L) \times (-a,a) \to \mathbb{R}^2$ defined by

$$(s,u) \mapsto (\gamma_1(s) - u\gamma_2'(s), \gamma_2(s) + u\gamma_1'(s)).$$

is a diffeomorphism for all $a > 0$ small enough



constant-width strip,
do not take the LaTeX
drawing too literary!

DN bracketing

The idea is to apply to the operator $H_{\alpha,\Gamma}$ in question *Dirichlet-Neumann bracketing* at the boundary of $\Sigma_a := \Phi([0,L) \times (-a,a))$. This yields

$$(-\Delta_{\Lambda_a}^{\mathrm{N}}) \oplus L_{a,\alpha}^{-} \le H_{\alpha,\Gamma} \le (-\Delta_{\Lambda_a}^{\mathrm{D}}) \oplus L_{a,\alpha}^{+},$$

where $\Lambda_a = \Lambda_a^{\mathrm{in}} \cup \Lambda_a^{\mathrm{out}}$ is the exterior domain, and $L_{a,\alpha}^{\pm}$ are self-adjoint operators associated with the forms

$$q_{a,\alpha}^{\pm}[f] = \|\nabla f\|_{L^2(\Sigma_a)}^2 - \alpha \int_\Gamma |f(x)|^2 \, \mathrm{d}S$$

where $f \in W_0^{1,2}(\Sigma_a)$ and $W^{1,2}(\Sigma_a)$ for $\pm$, respectively

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where $f \in W_0^{1,2}(\Sigma_a)$ and $W^{1,2}(\Sigma_a)$ for $\pm$, respectively

Important: The exterior part does not contribute to the negative spectrum, so we may consider $L_{a,\alpha}^{\pm}$ only

Transformed interior operator

We use the curvilinear coordinates passing from $L^{\pm}_{a,\alpha}$ to unitarily equivalent operators given by quadratic forms

$$b^{+}_{a,\alpha}[f] = \int_0^L \int_{-a}^{a} (1+uk(s))^{-2} \left|\frac{\partial f}{\partial s}\right|^2 \mathrm{d}u\,\mathrm{d}s + \int_0^L \int_{-a}^{a} \left|\frac{\partial f}{\partial u}\right|^2 \mathrm{d}u\,\mathrm{d}s$$

$$+ \int_0^L \int_{-a}^{a} V(s,u)|f|^2\,\mathrm{d}s\,\mathrm{d}u - \alpha \int_0^L |f(s,0)|^2\,\mathrm{d}s$$

with $f \in W^{1,2}((0,L)\times(-a,a))$ satisfying periodic b.c. in the variable s and Dirichlet b.c. at $u = \pm a$, and

$$b^{-}_{a,\alpha}[f] = b^{+}_{a,\alpha}[f] - \sum_{j=0}^{1} \frac{1}{2}(-1)^j \int_0^L \frac{k(s)}{1+(-1)^j a k(s)} |f(s,(-1)^j a)|^2\,\mathrm{d}s$$

where V is the curvature induced potential,

$$V(s,u) = -\frac{k(s)^2}{4(1+uk(s))^2} + \frac{uk''(s)}{2(1+uk(s))^3} - \frac{5u^2k'(s)^2}{4(1+uk(s))^4}$$

Estimates with separated variables

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Here $U^{\pm}_{a}$ are s-a operators on $L^2(0,L)$

$$U^{\pm}_{a} = -(1 \mp a\|k\|_{\infty})^{-2} \frac{\mathrm{d}^2}{\mathrm{d}s^2} + V_{\pm}(s)$$

with PBC, where $V_{-}(s) \leq V(s,u) \leq V_{+}(s)$ with an $\mathcal{O}(a)$ error, and the transverse operators are associated with the forms

$$t^{+}_{a,\alpha}[f] = \int_{-a}^{a} |f'(u)|^2 \,\mathrm{d}u - \alpha|f(0)|^2$$

and

$$t^{-}_{a,\alpha}[f] = t^{-}_{a,\alpha}[f] - \|k\|_{\infty}(|f(a)|^2 + |f(-a)|^2)$$

with $f \in W^{1,2}_{0}(-a,a)$ and $W^{1,2}(-a,a)$, respectively

Concluding the planar curve case

Lemma: There are positive $c,\ c_N$ such that $T^{\pm}_{\alpha,a}$ has for α large enough a single negative eigenvalue $\kappa^{\pm}_{\alpha,a}$ satisfying

$$-\frac{\alpha^2}{4}\left(1+c_N\mathrm{e}^{-\alpha a/2}\right) < \kappa^{-}_{\alpha,a} < -\frac{\alpha^2}{4} < \kappa^{+}_{\alpha,a} < -\frac{\alpha^2}{4}\left(1-8\mathrm{e}^{-\alpha a/2}\right)$$

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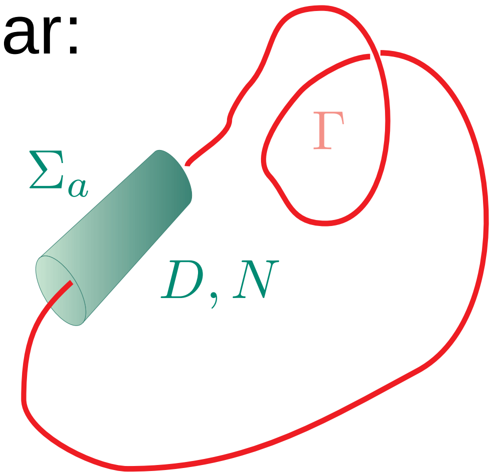
Finishing the proof:

- the eigenvalues of $U^{\pm}_a$ differ by $\mathcal{O}(a)$ from those of the comparison operator
- we choose $a = 6\alpha^{-1}\ln\alpha$ as the neighbourhood width
- putting the estimates together we get the eigenvalue asymptotics for a planar loop, i.e. the claim *(ii)*
- if Γ is not closed, the same can be done with the comparison operators $S^{\mathrm{D,N}}_{\Gamma}$ having appropriate b.c. at the endpoints of Γ. This yields the claim *(i)*

A curve in $\mathbb{R}^3$

The argument is similar:



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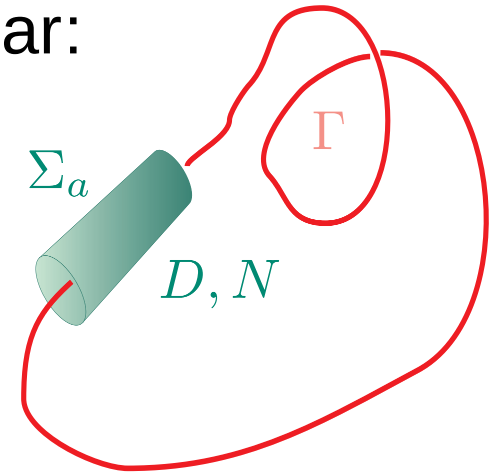

The *"straightening" transformation* Φ_a is defined by

$$\Phi_a(s,r,\theta) := \gamma(s) - r[n(s)\cos(\theta-\beta(s)) + b(s)\sin(\theta-\beta(s))]$$

To separate variables, we choose β so that $\dot{\beta}(s)$ equals the torsion $\tau(s)$ of Γ. The *effective potential* is then

$$V = -\frac{k^2}{4h^2} + \frac{h_{ss}}{2h^3} - \frac{5h_s^2}{4h^4},$$

where $h := 1 + rk\cos(\theta-\beta)$. It is important that the *leading term is* $-\frac{1}{4}k^2$ *again*, the torsion part being $\mathcal{O}(a)$

A curve in $\mathbb{R}^3$

The transverse estimate is replaced by

Lemma: There are $c_1,\, c_2 > 0$ such that $T_\alpha^\pm$ has for large enough negative α a single negative ev $\kappa_{\alpha,a}^\pm$ which satisfies

$$\epsilon_\alpha - S(\alpha) < \kappa_{\alpha,a}^- < \xi_\alpha < \kappa_{\alpha,a}^+ < \xi_\alpha + S(\alpha)$$

as $\alpha \to -\infty$, where $S(\alpha) = c_1 \mathrm{e}^{-2\pi\alpha} \exp(-c_2 \mathrm{e}^{-\pi\alpha})$

The rest of the argument is the same as above

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Remark: Notice that the result extends easily to Γ's consisting of a *finite number of connected components* (curves) which are C^4 and do not intersect. The same will be true for surfaces considered below

A surface in $\mathbb{R}^3$

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Let $\Gamma \subset \mathbb{R}^3$ be a C^4 smooth compact Riemann surface of a finite genus g. The metric tensor given in the local coordinates by $g_{\mu\nu} = p_{,\mu} \cdot p_{,\nu}$ defines the invariant surface area element $\mathrm{d}\Gamma := g^{1/2} d^2 s$, where $g := \det(g_{\mu\nu})$.

The Weingarten tensor is then obtained by raising the index in the second fundamental form, $h_\mu{}^\nu := -n_{,\mu} \cdot p_{,\sigma} g^{\sigma\nu}$; the eigenvalues $k_\pm$ of $(h_\mu{}^\nu)$ are the principal curvatures. They determine *Gauss curvature* K and *mean curvature* M by

$$K = \det(h_\mu{}^\nu) = k_+ k_- \,, \; M = \frac{1}{2} \mathrm{Tr}\,(h_\mu{}^\nu) = \frac{1}{2}(k_+ + k_-)$$

Proof sketch in the surface case

The bracketing argument proceeds as before,

$$-\Delta_{\Lambda_a}^N \oplus H_{\alpha,\Gamma}^- \le H_{\alpha,\Gamma} \le -\Delta_{\Lambda_a}^D \oplus H_{\alpha,\Gamma}^+ \,, \;\Lambda_a := \mathbb{R}^3 \setminus \overline{\Sigma}_a,$$

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Using the curvilinear coordinates: For small enough a we have the "straightening" diffeomorphism

$$\mathcal{L}_a(x,u) = x + un(x)\,, \quad (x,u) \in \mathcal{N}_a := \Gamma \times (-a,a)$$

Then we transform $H^\pm_{\alpha,\Gamma}$ by the unitary operator

$$\hat{U}\psi = \psi \circ \mathcal{L}_a :\; L^2(\Omega_a) \to L^2(\mathcal{N}_a, \mathrm{d}\Omega)$$

and estimate the operators $\hat{H}^\pm_{\alpha,\Gamma} := \hat{U} H^\pm_{\alpha,\Gamma} \hat{U}^{-1}$ in $L^2(\mathcal{N}_a, \mathrm{d}\Omega)$

Straightening transformation

Denote the pull-back metric tensor by G_{ij},

$$G_{ij} = \begin{pmatrix} (G_{\mu\nu}) & 0 \\ 0 & 1 \end{pmatrix}, \quad G_{\mu\nu} = (\delta_\mu^\sigma - u h_\mu{}^\sigma)(\delta_\sigma^\rho - u h_\sigma{}^\rho) g_{\rho\nu},$$

so $\mathrm{d}\Sigma := G^{1/2} \mathrm{d}^2 s \, \mathrm{d}u$ with $G := \det(G_{ij})$ given by

$$G = g \left[(1 - uk_+)(1 - uk_-)\right]^2 = g(1 - 2Mu + Ku^2)^2$$

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Let $(\cdot, \cdot)_G$ denote the inner product in $L^2(\mathcal{N}_a, \mathrm{d}\Omega)$. Then $\hat{H}^\pm_{\alpha,\Gamma}$ are associated with the forms

$$\eta^\pm_{\alpha,\Gamma}[\hat{U}^{-1}\psi] := (\partial_i \psi, G^{ij} \partial_j \psi)_G - \alpha \int_\Gamma |\psi(s,0)|^2 \, \mathrm{d}\Gamma \,,$$

with the domains $W_0^{1,2}(\mathcal{N}_a, \mathrm{d}\Omega)$ and $W^{1,2}(\mathcal{N}_a, \mathrm{d}\Omega)$ for the $\pm$ sign, respectively

Straightening continued

Next we remove $1 - 2Mu + Ku^2$ from the weight $G^{1/2}$ in the inner product of $L^2(\mathcal{N}_a, \mathrm{d}\Omega)$ by the unitary transformation $U:\ L^2(\mathcal{N}_a, \mathrm{d}\Omega) \to L^2(\mathcal{N}_a, \mathrm{d}\Gamma \mathrm{d}u)$,

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Denote the inner product in $L^2(\mathcal{N}_a, \mathrm{d}\Gamma du)$ by $(\cdot,\cdot)_g$. The operators $B^\pm_{\alpha,\Gamma} := U\hat{H}^\pm_{\alpha,\Gamma}U^{-1}$ are associated with the forms

$$\begin{aligned} b^+_{\alpha,\Gamma}[\psi] &= (\partial_\mu\psi, G^{\mu\nu}\partial_\nu\psi)_g + (\psi, (V_1+V_2)\psi)_g \\ &\quad + \|\partial_u\psi\|^2_g - \alpha\int_\Gamma |\psi(s,0)|^2 \mathrm{d}\Gamma\,, \\ b^-_{\alpha,\Gamma}[\psi] &= b^+_{\alpha,\Gamma}[\psi] + \sum_{j=0}^{1}(-1)^j\int_\Gamma M_{(-1)^j a}(s)|\psi(s,(-1)^j a)|^2 \mathrm{d}\Gamma \end{aligned}$$

for ψ from $W_0^{2,1}(\Omega_a, \mathrm{d}\Gamma du)$ and $W^{2,1}(\Omega_a, d\Gamma\mathrm{d}u)$, respectively

Effective potential

Here $M_u := (M-Ku)(1-2Mu+Ku^2)^{-1}$ is the mean curvature of the parallel surface to Γ and

$$V_1 = g^{-1/2}(g^{1/2}G^{\mu\nu}J_{,\nu})_{,\mu} + J_{,\mu}G^{\mu\nu}J_{,\nu}\,, \quad V_2 = \frac{K-M^2}{(1-2Mu+Ku^2)^2}$$

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A rougher estimate with separated variables: squeeze $1-2Mu+Ku^2$ between $C_\pm(a) := (1 \pm a\varrho^{-1})^2$, where $\varrho := \max(\{\|k_+\|_\infty, \|k_-\|_\infty\})^{-1}$. Consequently, the matrix inequality $C_-(a)g_{\mu\nu} \le G_{\mu\nu} \le C_+(a)g_{\mu\nu}$ is valid

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V_1 behaves as $\mathcal{O}(a)$ for $a \to 0$, while V_2 can be squeezed between the functions $C_\pm^{-2}(a)(K - M^2)$, both uniformly in the surface variables

Concluding the estimate

Hence we estimate $B^{\pm}_{\alpha,\Gamma}$ by

$$\tilde{B}^{\pm}_{\alpha,a} := S^{\pm}_{a} \otimes I + I \otimes T^{\pm}_{\alpha,a}$$

with $S^{\pm}_{a} := -C_{\pm}(a)\Delta_{\Gamma} + C^{-2}_{\pm}(a)(K - M^2) \pm va$ in the space $L^2(\Gamma, \mathrm{d}\Gamma) \otimes L^2(-a, a)$ for a $v > 0$, where $T^{\pm}_{\alpha,a}$ are the same as in the $1+1$ case (the same lemma applies)

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As above the eigenvalues of the operators $S^{\pm}_{a}$ coincide up to an $\mathcal{O}(a)$ error with those of S_{Γ}, and therefore choosing $a := 6\alpha^{-1}\ln\alpha$, we find

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To get *(ii)* we employ Weyl asymptotics for S_Γ. Extension to Γ's having a finite $\#$ of connected components is easy

Infinite manifolds

Bound states may exist also if Γ is *noncompact*. The comparison operator S_Γ has an attractive potential, so $\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma}) \neq \emptyset$ can be expected in the strong coupling regime, *even if a direct proof is missing* as for surfaces

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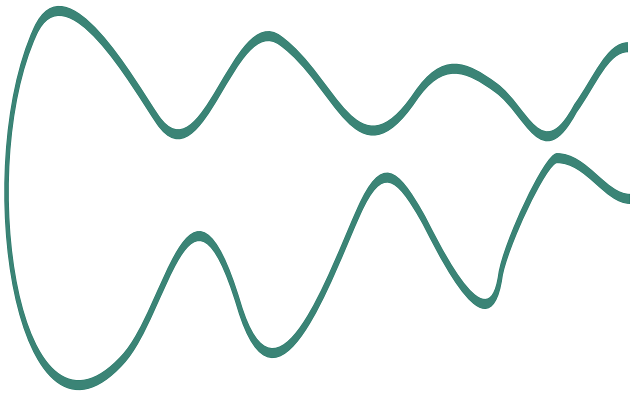
It is needed that $\sigma_{\rm ess}$ does not feel curvature, not only for $H_{\alpha,\Gamma}$ but for the estimating operators as well. *Sufficient conditions:*

- $k(s), k'(s)$ and $k''(s)^{1/2}$ are $\mathcal{O}(|s|^{-1-\varepsilon})$ as $|s| \to \infty$ for a planar curve
- in addition, the torsion bounded for a curve in $\mathbb{R}^3$
- a surface Γ admits a global normal parametrization with a uniformly elliptic metric, $K, M \to 0$ as the geodesic radius $r \to \infty$

Infinite manifolds

We must also *assume* that there is a tubular neighborhood Σ_a without self-intersections for small a, i.e. to avoid



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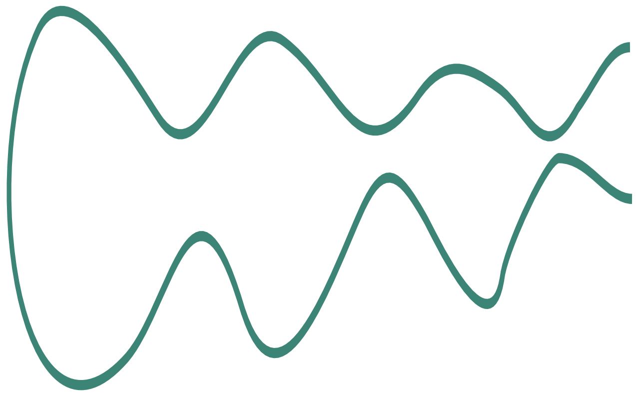
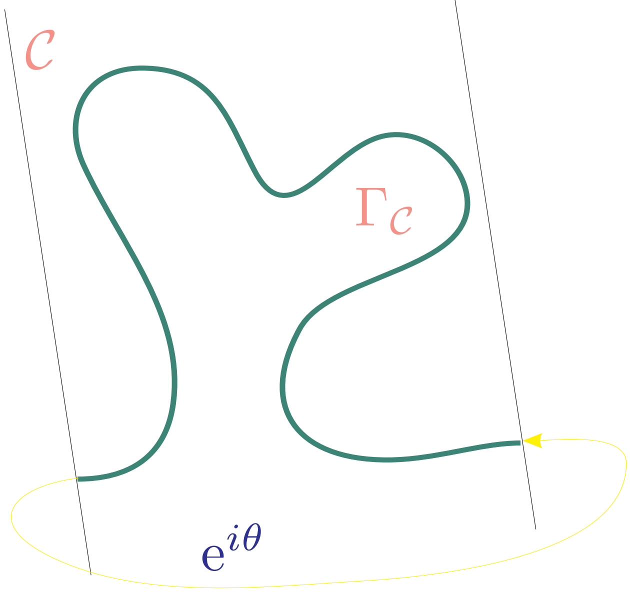


Theorem [EY02; EK03, Ex04]: With the above listed assumptions, the asymptotic expansions *(ii)* for the eigenvalues derived in the compact case hold again

Periodic manifolds

One uses Floquet expansion. It is important to choose the periodic cells $\mathcal{C}$ of the space and $\Gamma_{\mathcal{C}}$ of the manifold consistently, $\Gamma_{\mathcal{C}} = \Gamma \cap \mathcal{C}$; we assume that $\Gamma_{\mathcal{C}}$ is *connected*



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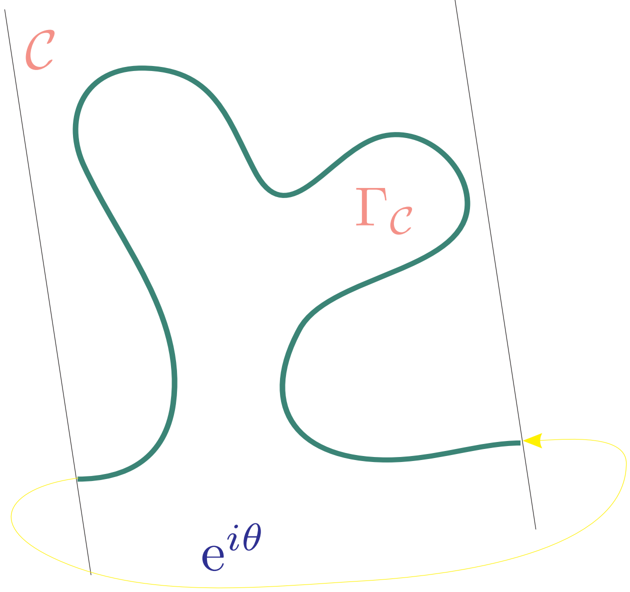

Lemma: $\exists$ unitary $\mathcal{U} :\ L^2(\mathbb{R}^3) \to \int_{[0,2\pi)^r}^{\oplus} L^2(\mathcal{C})\, \mathrm{d}\theta$ s.t.

$$\mathcal{U} H_{\alpha,\Gamma} \mathcal{U}^{-1} = \int_{[0,2\pi)^r}^{\oplus} H_{\alpha,\theta}\, \mathrm{d}\theta \quad \text{and} \quad \sigma(H_{\alpha,\Gamma}) = \bigcup_{[0,2\pi)^r} \sigma(H_{\alpha,\theta})$$

Comparison operators

The fibre comparison operators are

$$S_\theta = -\frac{\mathrm{d}}{\mathrm{d}s^2} - \frac{1}{4}k(s)^2$$

on $L^2(\Gamma_\mathcal{C})$ parameterized by arc length for $\dim\Gamma = 1$, with Floquet b.c., and

$$S_\theta = g^{-1/2}(-i\partial_\mu + \theta_\mu)g^{1/2}g^{\mu\nu}(-i\partial_\nu + \theta_\nu) + K - M^2$$

with periodic b.c. for $\dim\Gamma = 2$, where $\theta_\mu,\ \mu = 1,\dots,r$, are *quasimomentum components*; recall that $r = 1,2,3$ depending on the manifold type

Periodic manifold asymptotics

Theorem [EY01; EK03, Ex04]: Let Γ be a C^4-smooth r-periodic manifold without boundary. The strong coupling asymptotic behavior of the j-th Floquet eigenvalue is

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

for $\operatorname{codim}\Gamma = 1$ and

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Corollary: If $\dim\Gamma = 1$ and coupling is strong enough, $H_{\alpha,\Gamma}$ has *open spectral gaps*

Large gaps in the disconnected case

If Γ is not connected and each connected component is contained in a translate of $\Gamma_{\mathcal{C}}$, the comparison operator is independent of θ and asymptotic formula reads

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

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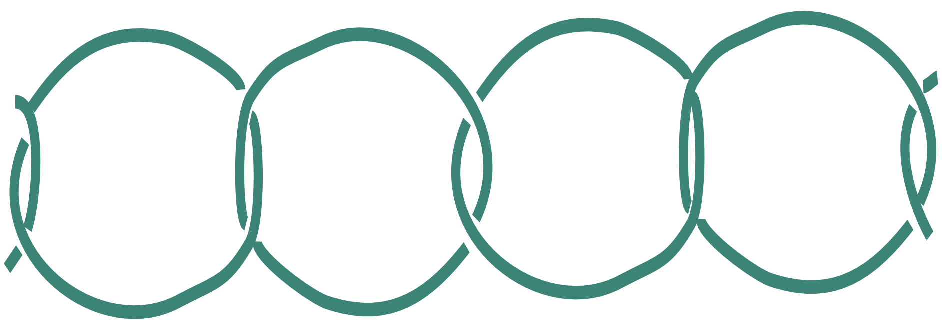
Moreover, the assumptions can be weakened



Soft graphs with magnetic field

Add a homogeneous magnetic field with the vector potential $A = \frac{1}{2}B(-x_2, x_1)$. We ask about existence of *persistent currents*, i.e. nonzero probability flux along a closed loop

$$\frac{\partial \lambda_n(\varphi)}{\partial \varphi} = -\frac{1}{c} I_n \,,$$

where $\lambda_n(\varphi)$ is the n-th eigenvalue of the Hamiltonian

$$H_{\alpha,\Gamma}(B) := (-i\nabla - A)^2 - \alpha\delta(x-\Gamma)$$

and φ is the magnetic flux through the loop (in standard units its quantum equals $2\pi\hbar c|e|^{-1}$)

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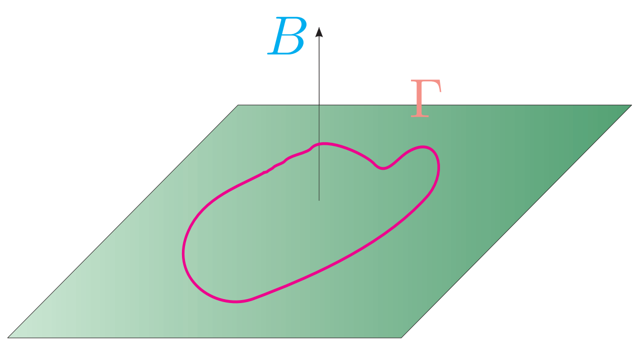

Persistent currents

The same technique, different comparison operator, namely

$$S_\Gamma(B) = -\frac{\mathrm{d}}{\mathrm{d}s^2} - \frac{1}{4}k(s)^2$$

on $L^2(0,L)$ with $\psi(L-) = \mathrm{e}^{iB|\Omega|}\psi(0+)$, $\psi'(L-) = \mathrm{e}^{iB|\Omega|}\psi'(0+)$, where Ω is the area encircled by Γ

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Remark: [Honnouvo-Hounkonnou'04] proved the same for AB flux

Absolute continuity

One is also interested in the nature of the spectrum of $H_{\alpha,\Gamma}$ with a periodic Γ. By [Birman-Suslina-Shterenberg'00,01] the spectrum is *absolutely continuous* if $\operatorname{codim}\Gamma = 1$ and the period cell is compact. This tells us nothing, e.g., about a single periodic curve in $\mathbb{R}^d$, $d = 2, 3$.

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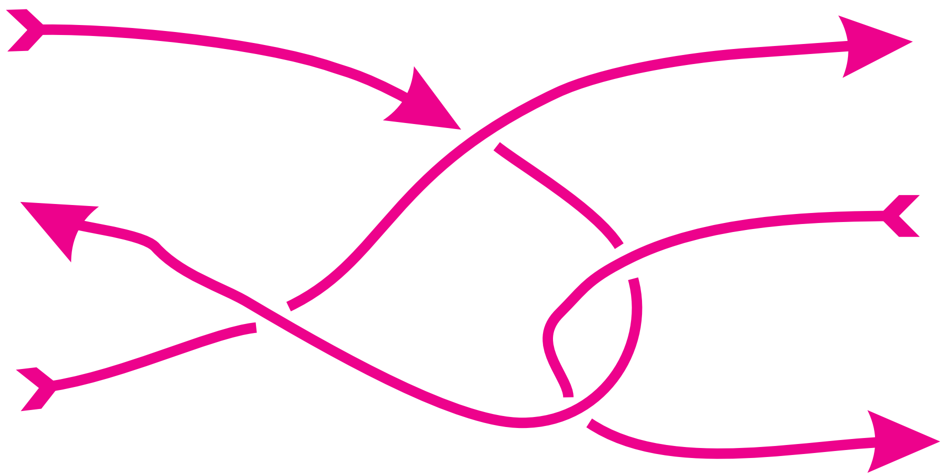
The assumption about connectedness of $\Gamma_{\mathcal{C}}$ can be always satisfied if $d = 2$ but not for $d = 3$; recall the *crochet curve*



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Theorem [Bentosela-Duclos-E'03]: To any $E > 0$ there is an $\alpha_E > 0$ such that the spectrum of $H_{\alpha,\Gamma}$ is absolutely continuous in $(-\infty, \xi(\alpha) + E)$ as long as $(-1)^d \alpha > \alpha_E$, where $\xi(\alpha) = -\frac{1}{4}\alpha^2$ and ϵ_α for $d = 2, 3$, respectively

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Proof: The fiber operators $H_{\alpha,\Gamma}(\theta)$ form a type A analytic family. In a finite interval each of them has a finite number of ev's , so one has just to check non-constancy of the functions $\lambda_j(\alpha, \cdot)$ as in the case of persistent currents $\square$

How can one find the spectrum?

The above general results do not tell us how to find the spectrum for a particular Γ. There are various possibilities:

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

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

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

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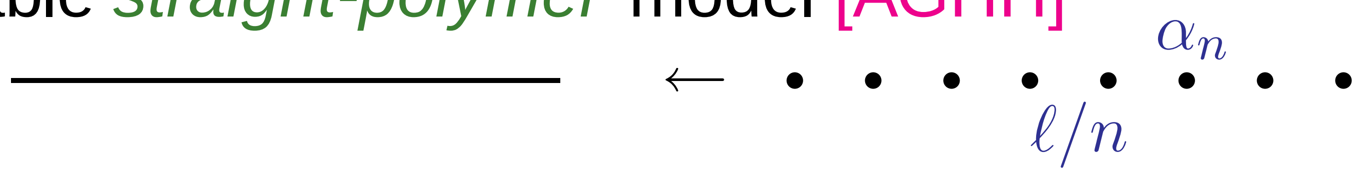
For our purpose, the coupling should depend on the set Y approximating Γ. To see how compare a line Γ with the solvable *straight-polymer* model [AGHH]



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; also a magnetic field can be added [Ožanová'06] *(=Němcová)*

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- *A uniform resolvent convergence* can be achieved in this scheme if the term $-\varepsilon^2\Delta^2$ is added to the Hamiltonian [Brasche-Ožanová'07]

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

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

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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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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

An interlude: scattering on leaky graphs

Let Γ be a graph with *semi-infinite "leads"*, e.g. an infinite asymptotically straight curve. What we know about scattering in such systems? Not much.

- *First question:* What is the "free" operator? $-\Delta$ is not a good candidate, rather $H_{\alpha,\Gamma}$ for a straight line Γ. Recall that we are particularly interested in energy interval $(-\frac{1}{4}\alpha^2, 0)$, i.e. 1D transport of states laterally bound to Γ

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- On the other hand, in general, the global geometry of Γ is expected to determine the S-matrix

Something more on 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'00]. Try the same here:

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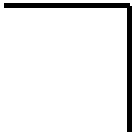
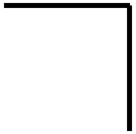
- *Broken line:* absence of "intrinsic" resonances due lack of higher transverse thresholds
- *Z-shaped Γ:* if a single bend has a significant reflection, a double band should exhibit resonances
- *Bottleneck curve:* a good candidate to demonstrate tunneling resonances

Broken line



$\alpha = 1$

Broken line



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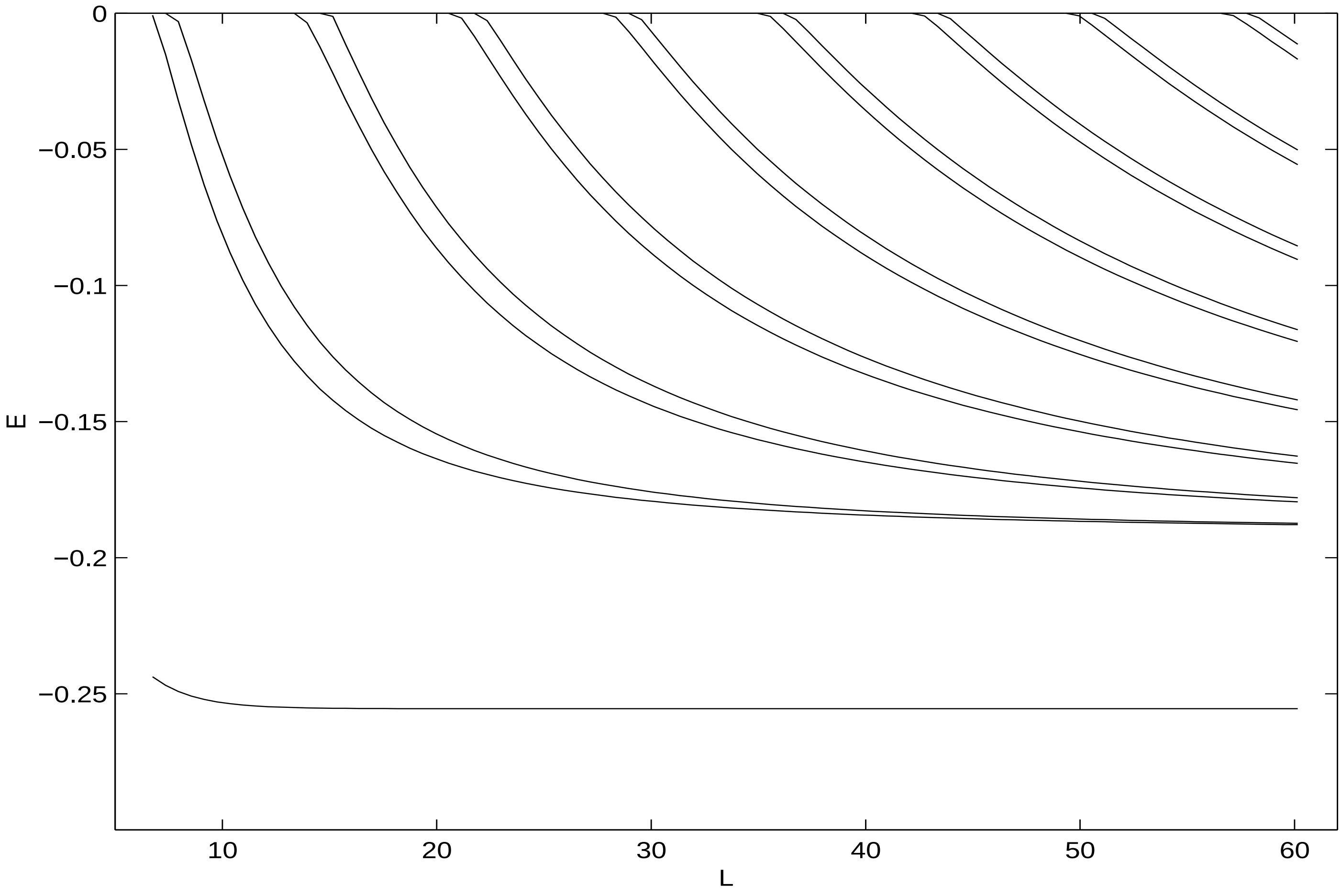
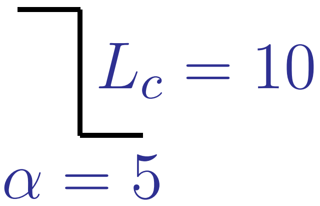


Z shape with $\theta = \frac{\pi}{2}$



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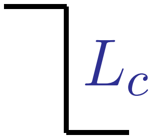
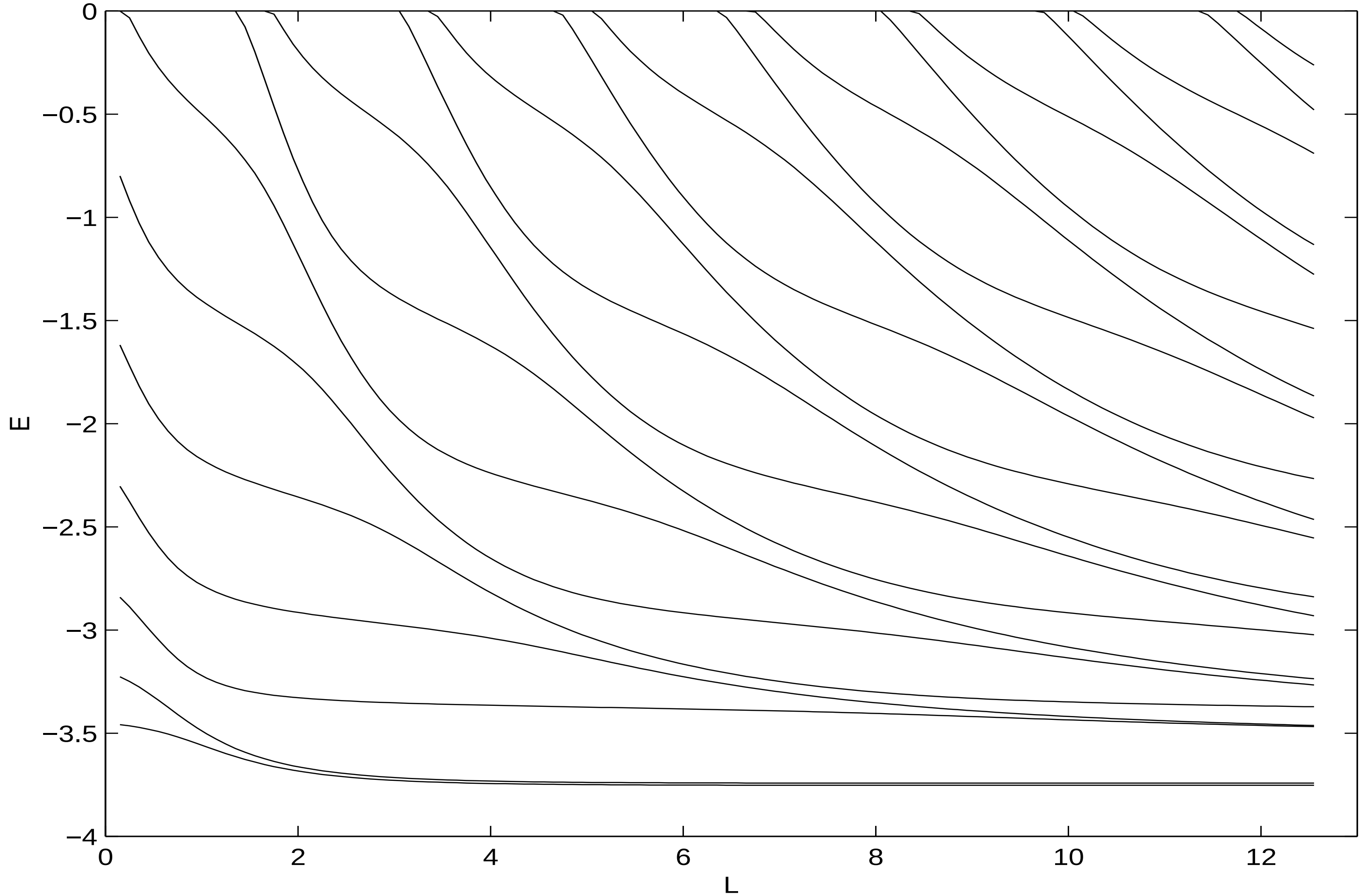
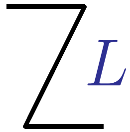


$L_c = 10$

$\alpha = 5$



Z shape with $\theta = 0.32\pi$



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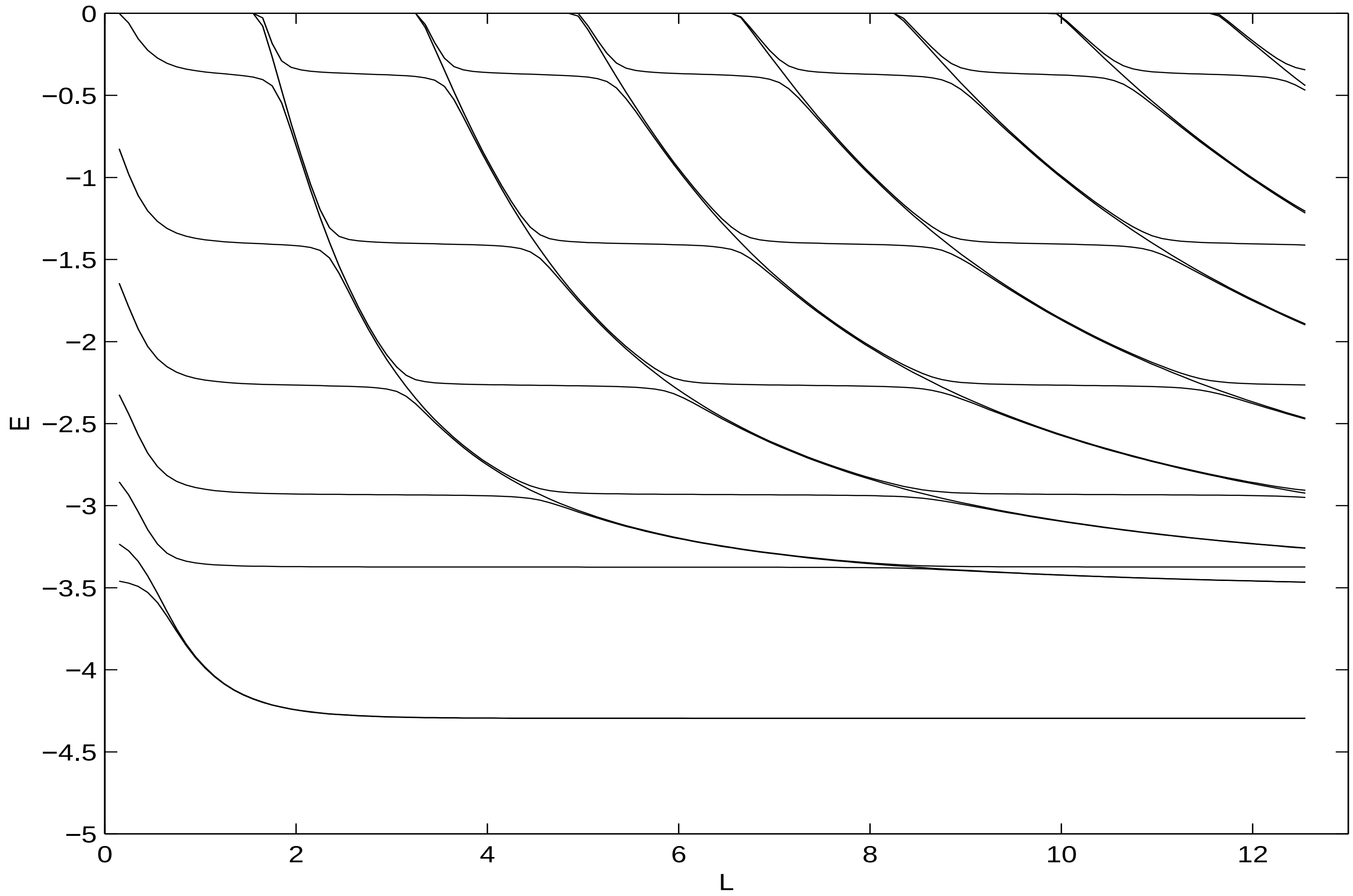
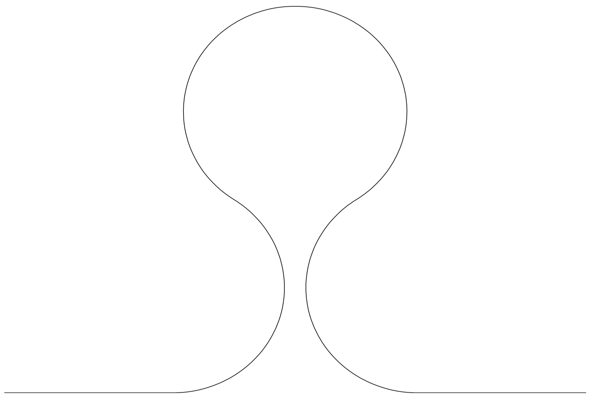
Z shape with $\theta = 0.32\pi$

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



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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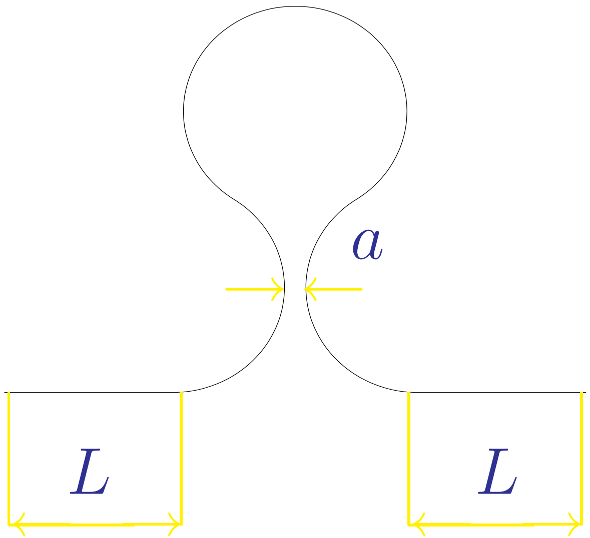
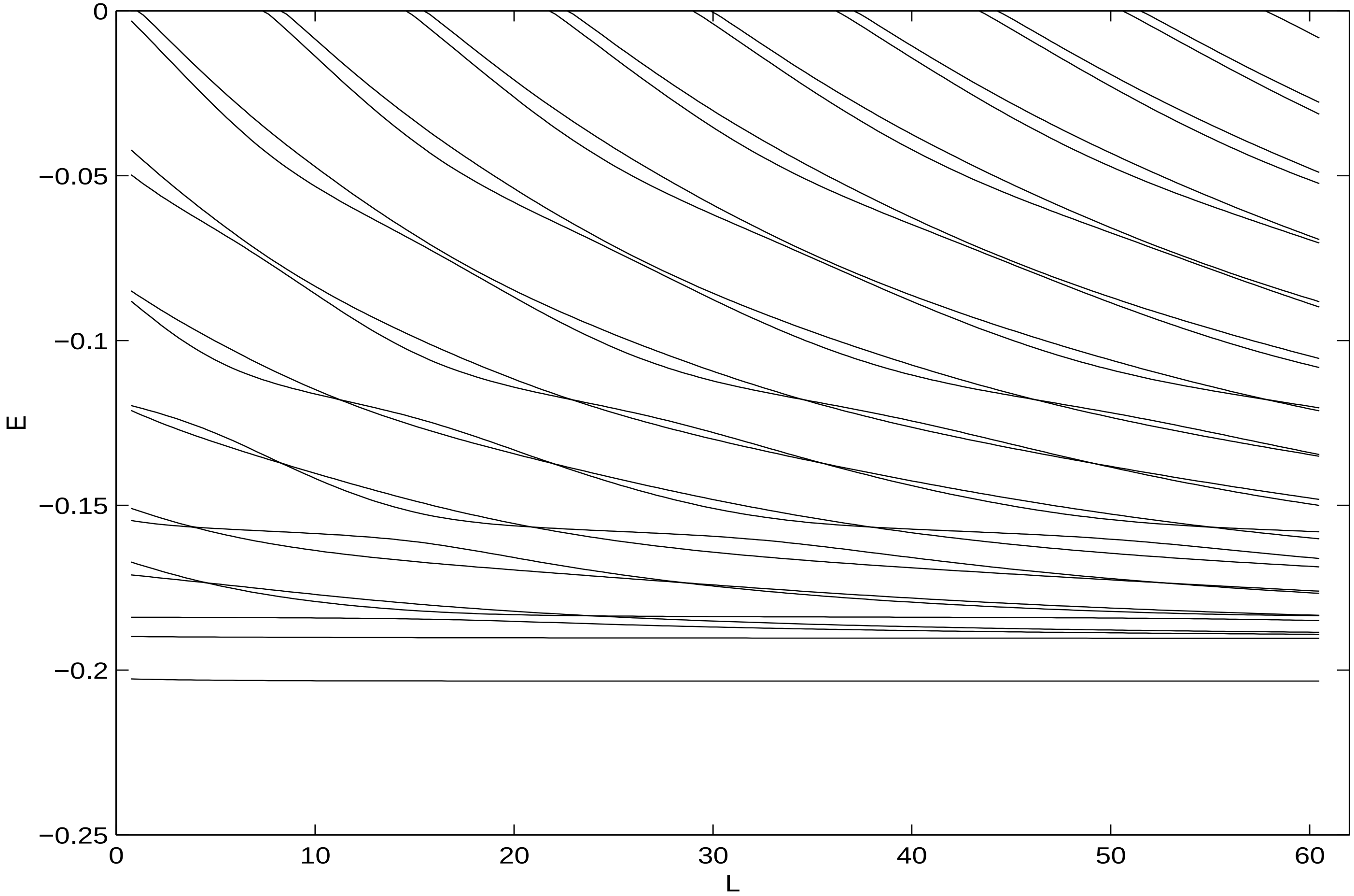
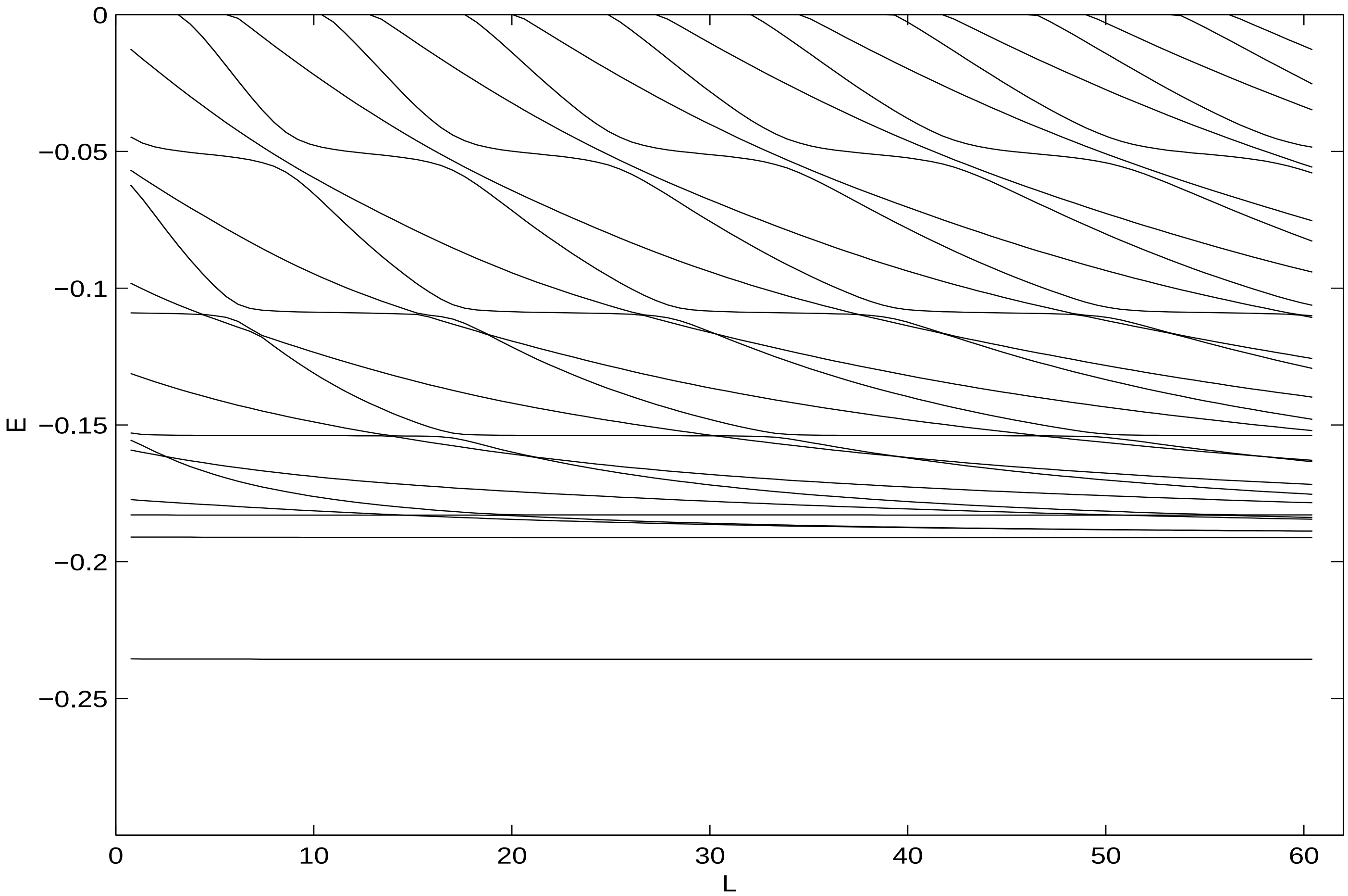


If Γ is a straight line, the transverse eigenfunction is $\mathrm{e}^{-\alpha|y|/2}$, hence the distance at which tunneling becomes significant is $\approx 4\alpha^{-1}$. In the example, we choose $\alpha = 1$

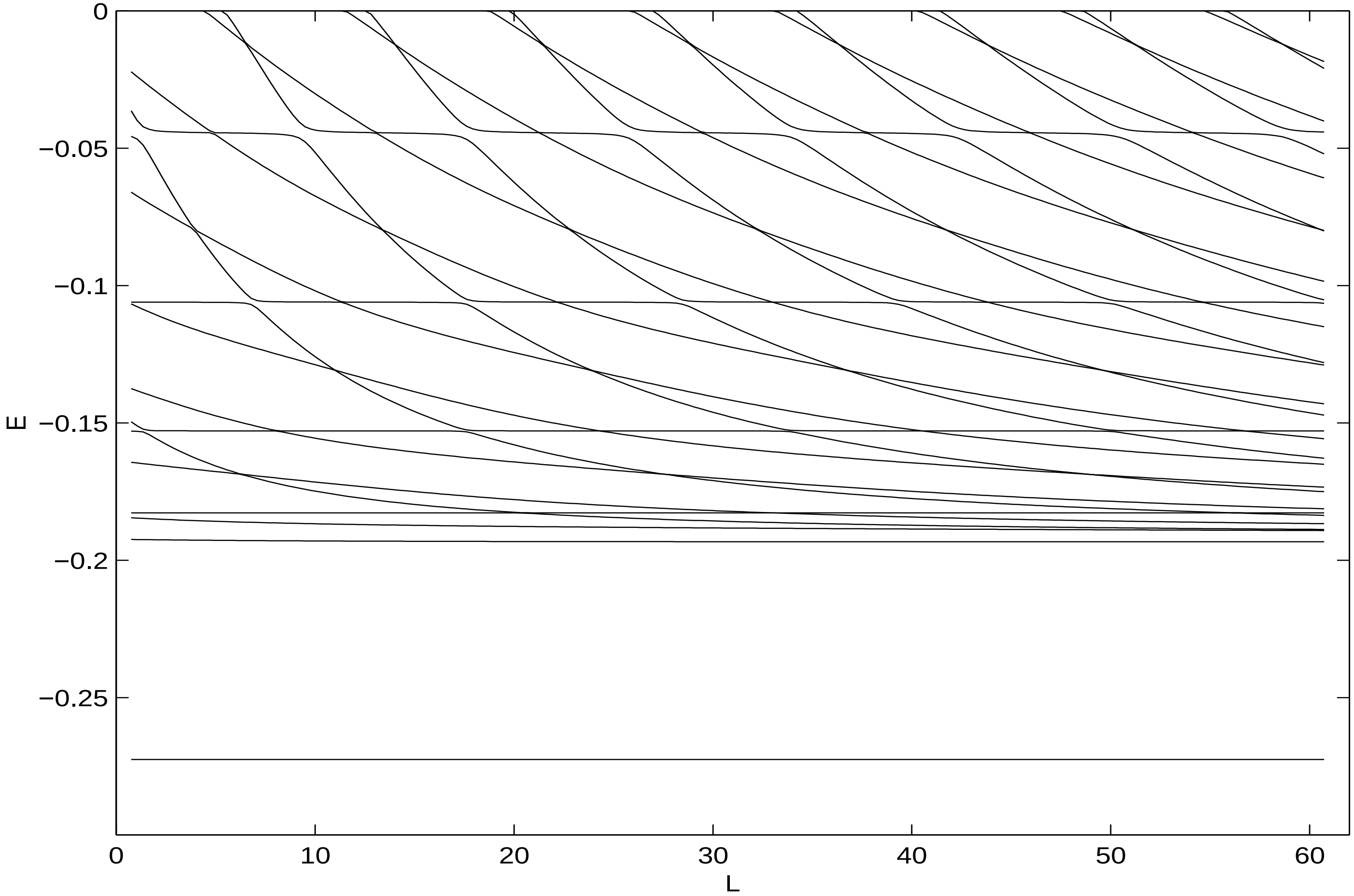
Bottleneck with $a = 5.2$



Bottleneck with $a = 2.9$



Bottleneck with $a = 1.9$



A caricature but solvable model

Let us pass to a simple model in which existence of resonances can be proved: a straight *leaky wire* and a family of *leaky dots*.

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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 $\tau_0 f := f \restriction_\Sigma$ and $\tau_1 f := f \restriction_\Pi$,

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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"

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

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

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

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'04]: 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

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

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

$$\dim\ker\Gamma(z) \;=\; \dim\ker R_{\alpha,\beta}(z)\,,$$

$$H_{\alpha,\beta}\varphi_z = z\varphi_z \;\Leftrightarrow\; \varphi_z = \sum_{i=0}^{1} \mathbf{R}_{L,i}(z)\eta_{i,z}\,,$$

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

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

where $\epsilon_\beta := -4\mathrm{e}^{2(-2\pi\beta+\psi(1))}$, while $\lim_{a\to 0}(-\kappa_a^2)$ is finite.

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(b) For any $\alpha > 0,\ \beta \in \mathbb{R}^n$, and $n \in \mathbb{N}_+$ the operator $H_{\alpha,\beta}$ has N isolated eigenvalues, $1 \le N \le n$. If all the point interactions are strong enough, we have $N = n$

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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

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

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

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

$$\begin{aligned} \varphi_a^0(\lambda) &= I(\lambda) + g_{\alpha,a}(\lambda) \quad \text{for} \quad \lambda \in \left(-\frac{1}{4}\alpha^2, 0\right)\,, \\ \varphi_a^-(z) &= -\int_0^\infty \frac{\mu(z,t)}{t - z - \frac{1}{4}\alpha^2}\, \mathrm{d}t - 2g_{\alpha,a}(z)\,,\ z \in \Omega_- \end{aligned}$$

Analytic continuation

Proof: By a direct computation one checks

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

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 $M = \{z : \mathrm{Im}\, z > 0\} \cup (-\frac{1}{4}\alpha^2, 0) \cup \Omega_-$, acting as

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

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

Resonance for $n = 1$

Theorem [E-Kondej'04]: 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 $a \to \infty$,

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

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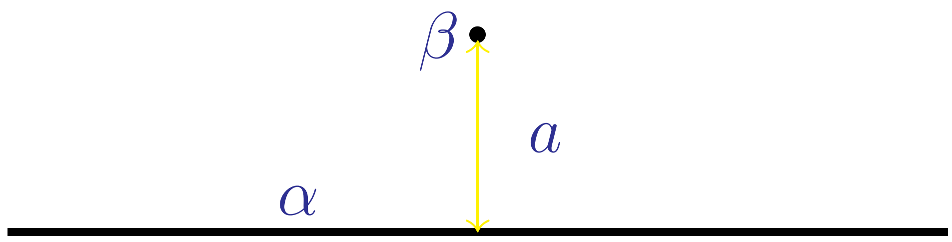
Remark: We have $|\varphi_a^-(z)| \to 0$ uniformly in a and $|s_\beta(z)| \to \infty$ as $\operatorname{Im} z \to -\infty$. Hence the imaginary part $z(a)$ is bounded as a function of a, in particular, *the resonance pole survives* as $a \to 0$.

Scattering for $n = 1$

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



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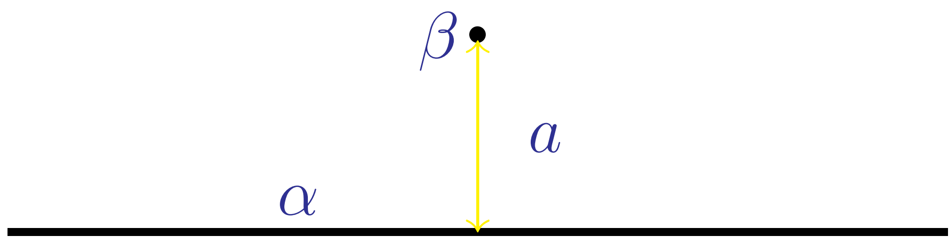

Existence and completeness by Birman-Kuroda theorem; we seek on-shell S-matrix in $(-\frac{1}{4}\alpha^2, 0)$. By Krein formula, resolvent for $\mathrm{Im}\, z > 0$ expresses as

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

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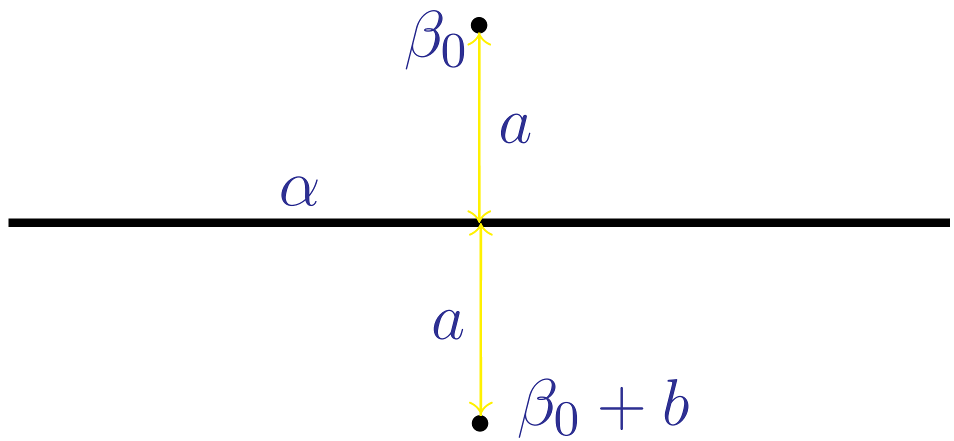
Proposition: For any $\lambda \in (-\frac{1}{4}\alpha^2, 0)$ the reflection and transmission amplitudes are

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

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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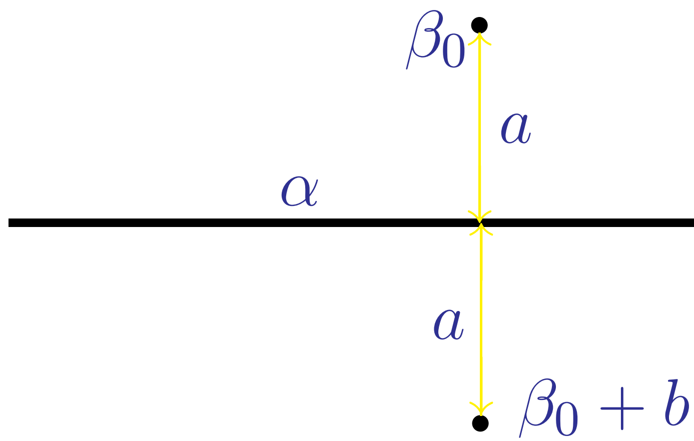

Let $\sigma_{\mathrm{disc}}(H_{0,\beta_0}) \cap \left(-\frac{1}{4}\alpha^2, 0\right) \neq \emptyset$, so that Hamiltonian H_{0,β_0} has two eigenvalues, the larger of which, ϵ_2, exceeds $-\frac{1}{4}\alpha^2$. Then H_{α,β_0} has the same eigenvalue ϵ_2 embedded in the negative part of continuous spectrum

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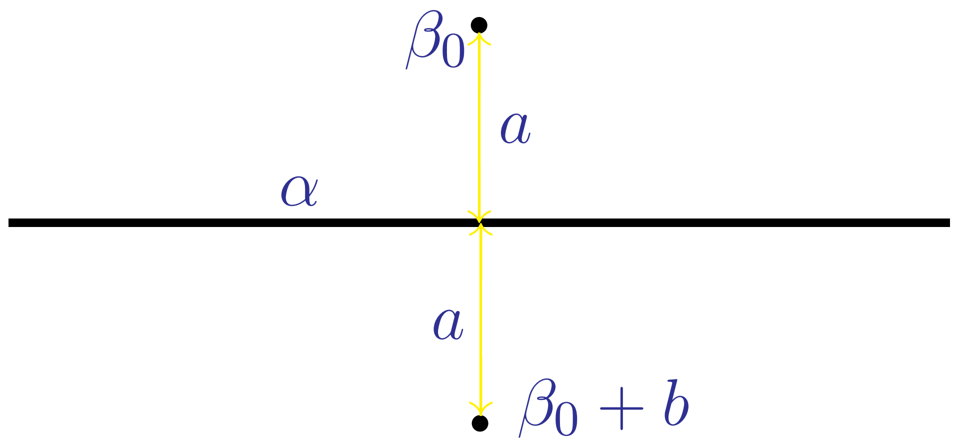

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One has now to continue analytically the 2×2 matrix function $D(\cdot)$. Put $\kappa_2 := \sqrt{-\epsilon_2}$ and $\breve{s}_\beta(\kappa) := s_\beta(-\kappa^2)$

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

$$\mu_2(b) \;=\; \epsilon_2 + \frac{\kappa_2 b}{\breve{s}'_\beta(\kappa_2) + K'_0(2a\kappa_2)} + \mathcal{O}(b^2)\,,$$

$$\nu_2(b) \;=\; -\frac{\kappa_2 \tilde{g}(\epsilon_2) b^2}{2(\breve{s}'_\beta(\kappa_2) + K'_0(2a\kappa_2))|\breve{s}'_\beta(\kappa_2) - \varphi^0_a(\epsilon_2)|} + \mathcal{O}(b^3)$$

Unstable state decay, $n = 1$

Complementary point of view: investigate decay of unstable state associated with the resonance; assume again $n = 1$. We found that if the "unperturbed" ev ϵ_β of H_β is embedded in $(-\frac{1}{4}\alpha^2, 0)$ and a is large, the corresponding resonance has a long halflife. In analogy with *Friedrichs model* [Demuth, 1976] one conjectures that in weak coupling case, the resonance state would be similar up to normalization to the eigenvector $\xi_0 := K_0(\sqrt{-\epsilon_\beta}\,\cdot)$ of H_β, with the *decay law being dominated by the exponential term*

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At the same time, $H_{\alpha,\beta}$ has always an isolated ev with ef which is *not* orthogonal to ξ_0 for any a (recall that both functions are positive). Consequently, the decay law $|(\xi_0, U(t)\xi_0)|^2 \|\xi_0\|^{-2}$ *has always a nonzero limit as* $t \to \infty$

Summarizing Lecture V

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Summarizing Lecture V

- A *strong coupling* turns leaky wires into essentially one-dimensional objects as far as the discrete spectrum is concerned
- The analogous problem for *scattering* remains open
- *Approximation by point interaction arrays* is an efficient method to determine spectra of leaky graphs
- *Rigorous results* on spectra and scattering are available so far in simple situations only, and a number of problems remains open

Some literature to Lecture V

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Lecture VI

Generalized graphs – or what happens

if a quantum particle has to change its dimension

Lecture overview

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- Large gaps in periodic systems
- A heuristic way to choose the coupling
- An illustration on microwave experiments
- And something else: spin conductance oscillations

A nontrivial configuration space

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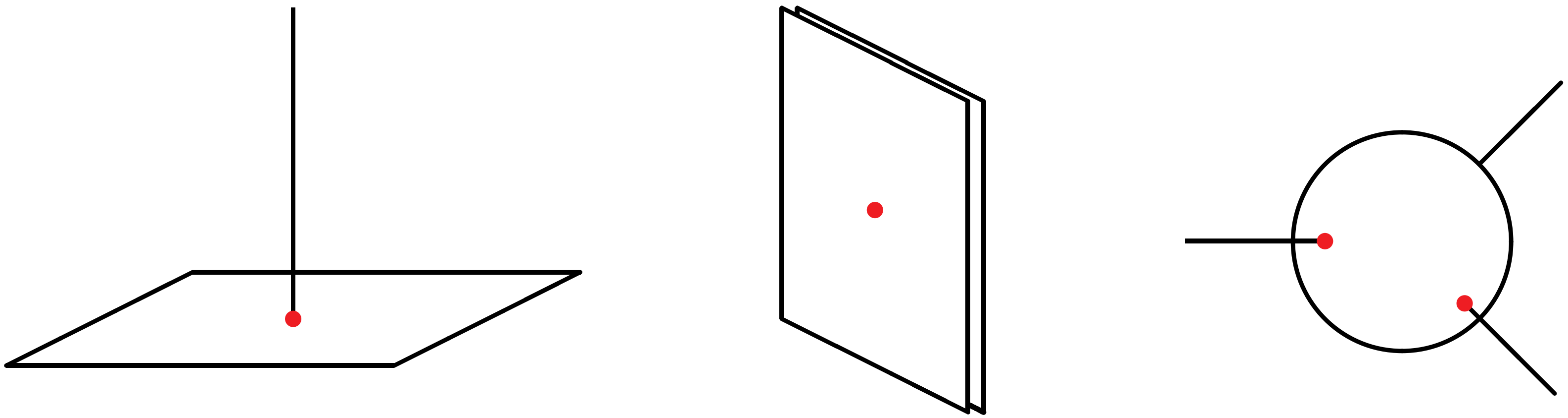

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In contrast, QM offers interesting examples, e.g.

- *point-contact* spectroscopy,
- *STEM-type devices*,
- compositions of *nanotubes* with *fulleren* molecules,

etc. Similarly one can consider some *electromagnetic systems* such as flat microwave resonators with attached antennas; we will comment on that later in the lecture

Coupling by means of s-a extensions

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The idea: Quantum dynamics on $M_1 \cup M_2$ coupled by a point contact $x_0 \in M_1 \cap M_2$. Take Hamiltonians H_j on the *isolated* manifold M_j and restrict them to functions vanishing in the vicinity of x_0

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The operator $H_0 := H_{1,0} \oplus H_{2,0}$ is symmetric, in general not s-a. We seek admissible Hamiltonians of the coupled system among *its self-adjoint extensions*

Coupling by means of s-a extensions

Limitations: In nonrelativistic QM considered here, where H_j is a *second-order operator* the method works for $\dim M_j \le 3$ (more generally, codimension of the contact should not exceed *three*), since otherwise the restriction is *e.s.a.* [similarly for Dirac operators we require the codimension to be at most *one*]

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Non-uniqueness: Apart of the trivial case, there are many s-a extensions. A junction where n configuration-space components meet contributes typically by n to deficiency indices of H_0, and thus adds n^2 parameters to the resulting Hamiltonian class; recall a similar situation in *Lecture I*

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Physical meaning: The construction guarantees that the *probability current is conserved* at the junction

Different dimensions

In distinction to quantum graphs "$1+1$" situation, we will be mostly concerned with cases "*2*+*1*" and "*2*+*2*", i.e. manifolds of these dimensions coupled through *point contacts*. Other combinations are similar

We use "rational" units, in particular, the Hamiltonian acts at each configuration component as $-\Delta$ (or Laplace-Beltrami operator if M_j has a nontrivial metric)

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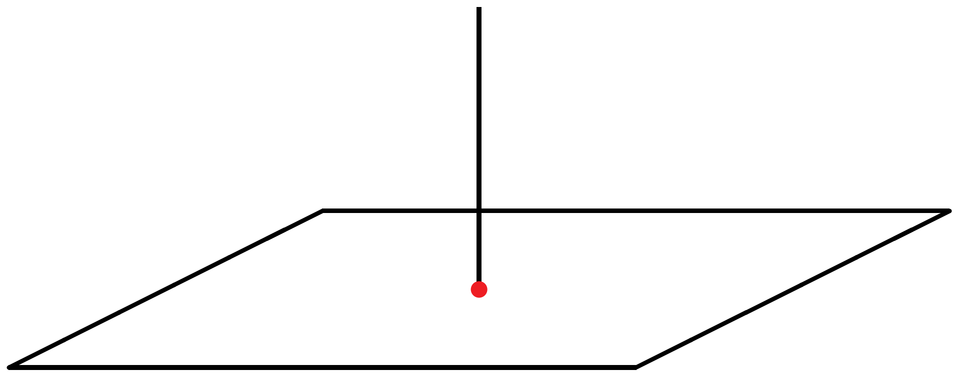
An archetypal example, $\mathcal{H} = L^2(\mathbb{R}_-) \oplus L^2(\mathbb{R}^2)$, so the wavefunctions are pairs $\varphi := \binom{\varphi_1}{\Phi_2}$ of square integrable functions



A model: *point-contact spectroscopy*

Restricting $\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)_{\mathrm{D}} \oplus -\Delta$ to functions vanishing in the vicinity of the junction gives symmetric operator with deficiency indices $(2,2)$.

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von Neumann theory gives a general prescription to construct the s-a extensions, however, it is practical to characterize the by means of *boundary conditions*. We need *generalized boundary values*

$$L_0(\Phi) := \lim_{r\to 0} \frac{\Phi(\vec{x})}{\ln r}\,, \;\; L_1(\Phi) := \lim_{r\to 0} \left[\, \Phi(\vec{x}) - L_0(\Phi) \ln r \,\right]$$

(in view of the 2D character, in three dimensions L_0 would be the coefficient at the pole singularity)

$2+1$ point-contact coupling

Typical b.c. determining a s-a extension

$$\begin{aligned} \varphi_1'(0-) &= A\varphi_1(0-) + BL_0(\Phi_2)\,, \\ L_1(\Phi_2) &= C\varphi_1(0-) + DL_0(\Phi_2)\,, \end{aligned}$$

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The easiest way to see that is to compute the boundary form to H_0^*, recall that the latter is given by the same differential expression.

Notice that *only the s-wave part* of Φ in the plane, $\Phi_2(r,\varphi) = (2\pi)^{-1/2}\varphi_2(r)$ can be coupled nontrivially to the halfline

$2+1$ **point-contact coupling**

An integration by parts gives

$$\begin{aligned}(\varphi, H_0^*\psi) - (H_0^*\varphi, \psi) \;=\; & \bar\varphi_1'(0)\psi_1(0) - \bar\varphi_1(0)\psi_1'(0) \\ & + \lim_{\varepsilon\to 0+} \varepsilon\left(\bar\varphi_2(\varepsilon)\psi_1'(\varepsilon) - \bar\varphi_2'(\varepsilon)\psi_2(\varepsilon)\right)\,,\end{aligned}$$

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and using the asymptotic behaviour

$$\varphi_2(\varepsilon) = \sqrt{2\pi}\;\left[L_0(\Phi_2)\ln\varepsilon + L_1(\Phi_2) + \mathcal{O}(\varepsilon)\right]\,,$$

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we can express the above limit term as

$$2\pi \left[L_1(\Phi_2)L_0(\Psi_2) - L_0(\Phi_2)L_1(\Psi_2)\right] \, ,$$

so the form vanishes under the stated boundary conditions

Transport through point contact

Using the b.c. we match plane wave solution $\mathrm{e}^{ikx} + r(k)\mathrm{e}^{-ikx}$ on the halfline with $t(k)(\pi kr/2)^{1/2} H_0^{(1)}(kr)$ in the plane obtaining

$$r(k) = -\frac{\mathcal{D}_-}{\mathcal{D}_+}\,, \quad t(k) = \frac{2iCk}{\mathcal{D}_+}$$

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Remark: More general coupling, $\mathcal{A}\binom{\varphi_1}{L_0} + \mathcal{B}\binom{\varphi_1'}{L_1} = 0$, gives rise to similar formulae (an invertible $\mathcal{B}$ can be put to one)

Transport through point contact

Let us finish discussion of this *“point contact spectroscopy”* model by a few remarks:

- Scattering is *nontrivial* if $\mathcal{A} = \left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right)$ is not diagonal. For any choice of s-a extension, the on-shell S-matrix is *unitary*, in particular, we have $|r(k)|^2 + |t(k)|^2 = 1$

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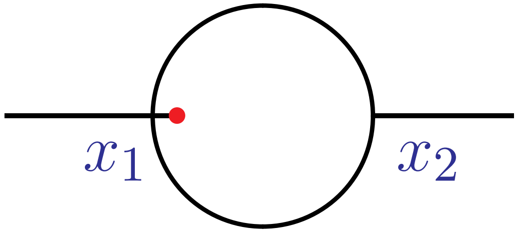
- For some $\mathcal{A}$ there are also *bound states* decaying exponentially away of the junction, at most two
- a similar analysis can be done also in a more general model where the electron is subject to *spin-orbit coupling* and *mg field*, cf. [E-Šeba'07, Carlone-E'11]

Single-mode geometric scatterers

Consider a sphere with two leads attached



with the coupling at both vertices given by the same $\mathcal{A}$

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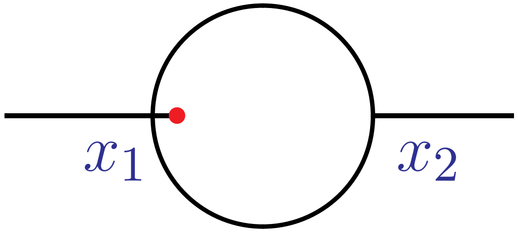

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Three one-parameter families of $\mathcal{A}$ were investigated [Kiselev'97; E-Tater-Vaněk'01; Brüning-Geyler-Margulis-Pyataev'02]; it appears that scattering properties *en gross* are not very sensitive to the coupling:

- there numerous resonances
- in the background reflection dominates as $k \to \infty$

Geometric scatterer transport

Let us describe the argument in more details: construction of generalized eigenfunctions means to couple plane-wave solution at leads with

$$u(x) = a_1 G(x, x_1; k) + a_2 G(x, x_2; k)\,,$$

where $G(\cdot, \cdot; k)$ is Green's function of Δ_{LB} on the sphere

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$$u(x) = a_1 G(x, x_1; k) + a_2 G(x, x_2; k)\,,$$

where $G(\cdot, \cdot; k)$ is Green's function of $\Delta_{\rm LB}$ on the sphere The latter has a logarithmic singularity so $L_j(u)$ express in terms of $g := G(x_1, x_2; k)$ and

$$\xi_j \equiv \xi(x_j; k) := \lim_{x \to x_j} \left[G(x, x_j; k) + \frac{\ln |x - x_j|}{2\pi} \right]$$

Geometric scatterer transport

Introduce $Z_j := \frac{D_j}{2\pi} + \xi_j$ and $\Delta := g^2 - Z_1 Z_2$, and consider, e.g., $\mathcal{A}_j = \begin{pmatrix} (2a)^{-1} & (2\pi/a)^{1/2} \\ (2\pi a)^{-1/2} & -\ln a \end{pmatrix}$ with $a > 0$. Then the solution of the matching condition is given by

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$$r(k) = -\frac{\pi\Delta + Z_1 + Z_2 - \pi^{-1} + 2ika(Z_2 - Z_1) + 4\pi k^2 a^2 \Delta}{\pi\Delta + Z_1 + Z_2 - \pi^{-1} + 2ika(Z_1 + Z_2 + 2\pi\Delta) - 4\pi k^2 a^2 \Delta},$$

$$t(k) = -\frac{4ikag}{\pi\Delta + Z_1 + Z_2 - \pi^{-1} + 2ika(Z_1 + Z_2 + 2\pi\Delta) - 4\pi k^2 a^2 \Delta}.$$

Geometric scatterers: needed quantities

So far formulae are valid for any compact manifold G. To make use of them we need to know $g,\ Z_1,\ Z_2,\ \Delta$. The spectrum $\{\lambda_n\}_{n=1}^{\infty}$ of Δ_{LB} on G is purely discrete with eigenfunctions $\{\varphi(x)_n\}_{n=1}^{\infty}$. Then we find easily

$$g(k) = \sum_{n=1}^{\infty} \frac{\varphi_n(x_1)\overline{\varphi_n(x_2)}}{\lambda_n - k^2}$$

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and

$$\xi(x_j,k) = \sum_{n=1}^{\infty} \left(\frac{|\varphi_n(x_j)|^2}{\lambda_n - k^2} - \frac{1}{4\pi n} \right) + c(G)\,,$$

where $c(G)$ depends of the manifold only (changing it is equivalent to a coupling constant renormalization)

A *symmetric* spherical scatterer

Theorem [Kiselev'97, E-Tater-Vaněk'01]: For any l large enough the interval $(l(l-1), l(l+1))$ contains a point μ_l such that $\Delta(\sqrt{\mu_l}) = 0$. Let $\varepsilon(\cdot)$ be a positive, strictly increasing function which tends to ∞ and obeys the inequality $|\varepsilon(x)| \le x \ln x$ for $x > 1$. Furthermore, denote $K_\varepsilon := \mathbb{R} \setminus \bigcup_{l=2}^{\infty} \left(\mu_l - \varepsilon(l)(\ln l)^{-2}, \mu_l + \varepsilon(l)(\ln l)^{-2}\right)$.

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$$|t(k)|^2 \le c\varepsilon(l)^{-2}$$

in the *background*, i.e. for $k^2 \in K_\varepsilon \cap (l(l-1), l(l+1))$ and any l large enough. On the other hand, there are *resonance peaks* localized outside K_ε with the property

$$|t(\sqrt{\mu_l})|^2 = 1 + \mathcal{O}\left((\ln l)^{-1}\right) \quad \text{as} \quad l \to \infty$$

A *symmetric* spherical scatterer

The high-energy behavior shares features with strongly singular interaction such as δ', for which $|t(k)|^2 = \mathcal{O}(k^{-2})$. *We conjecture* that *coarse-grained* transmission through our “bubble” has the same decay as $k \to \infty$

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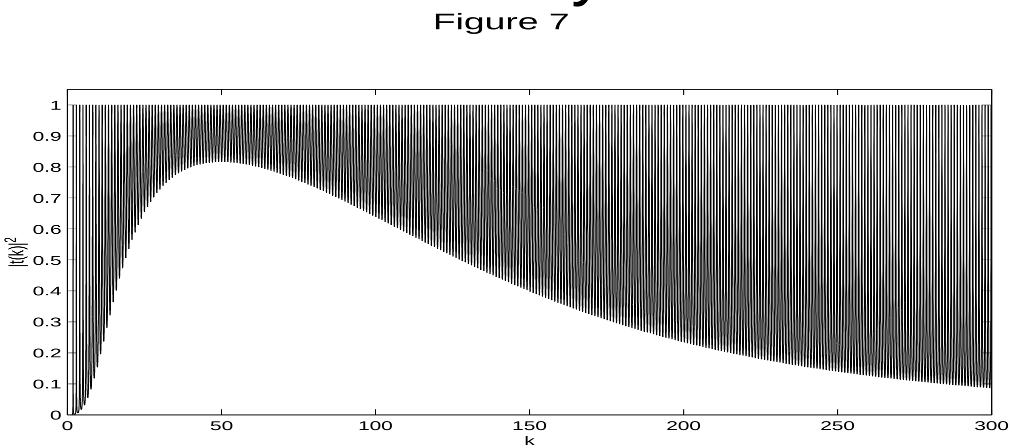

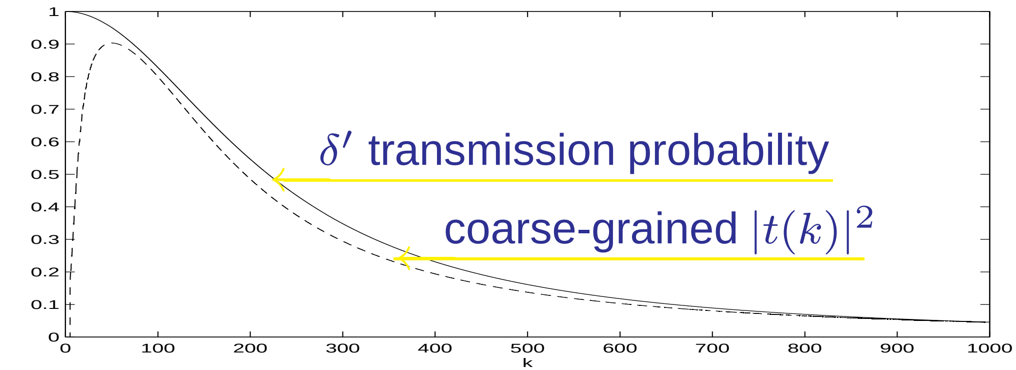

An *asymmetric* spherical scatterer

While the above general features are expected to be the same if the angular distance of junctions is less than π, the detailed transmission plot changes [Brüning et al'02]:

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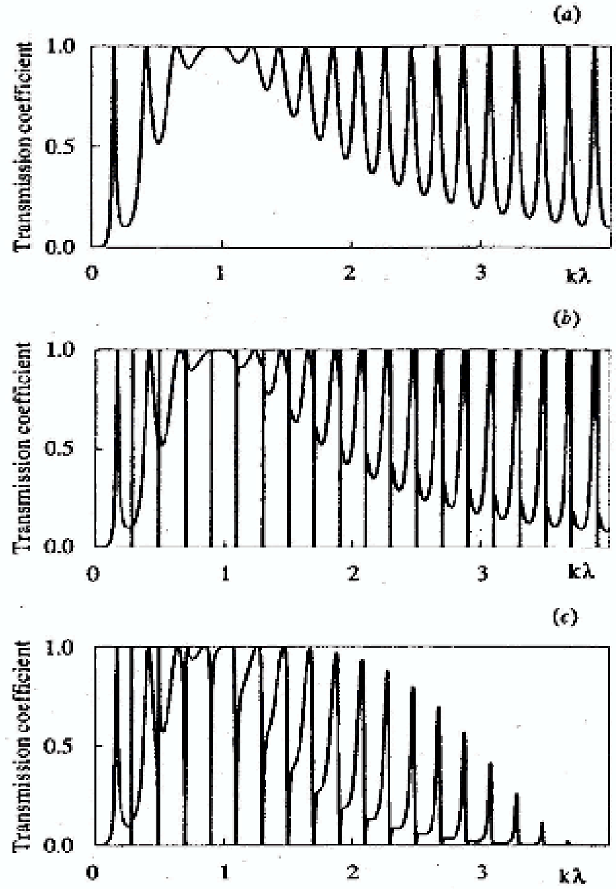

Figure 2. The transmission coefficient as a function of $k\lambda$ at $a = 10\lambda$: (*a*) $r = \pi a$; (*b*) $r = 0.98\pi a$; (*c*) $r = 0.96\pi a$.

Arrays of geometric scatterers

In a similar way one can construct *general scattering theory* on such “hedgehog” manifolds composed of compact scatterers, connecting edges and external leads [Brüning-Geyler’03]

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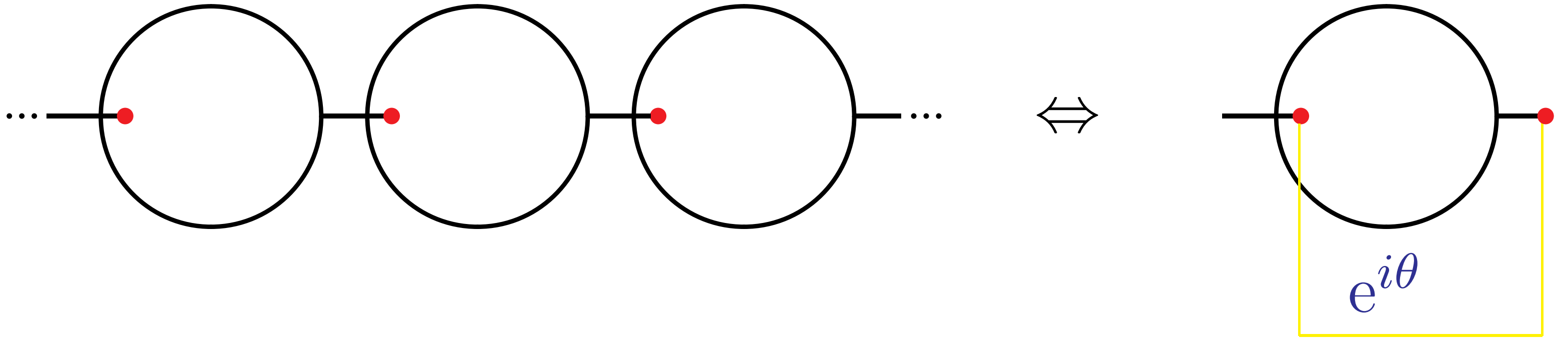
Furthermore, infinite periodic systems can be treated by Floquet-Bloch decomposition



Sphere array spectrum

A band spectrum example from [E-Tater-Vaněk'01]: radius $R = 1$, segment length $\ell = 1,\ 0.01$ and coupling ρ

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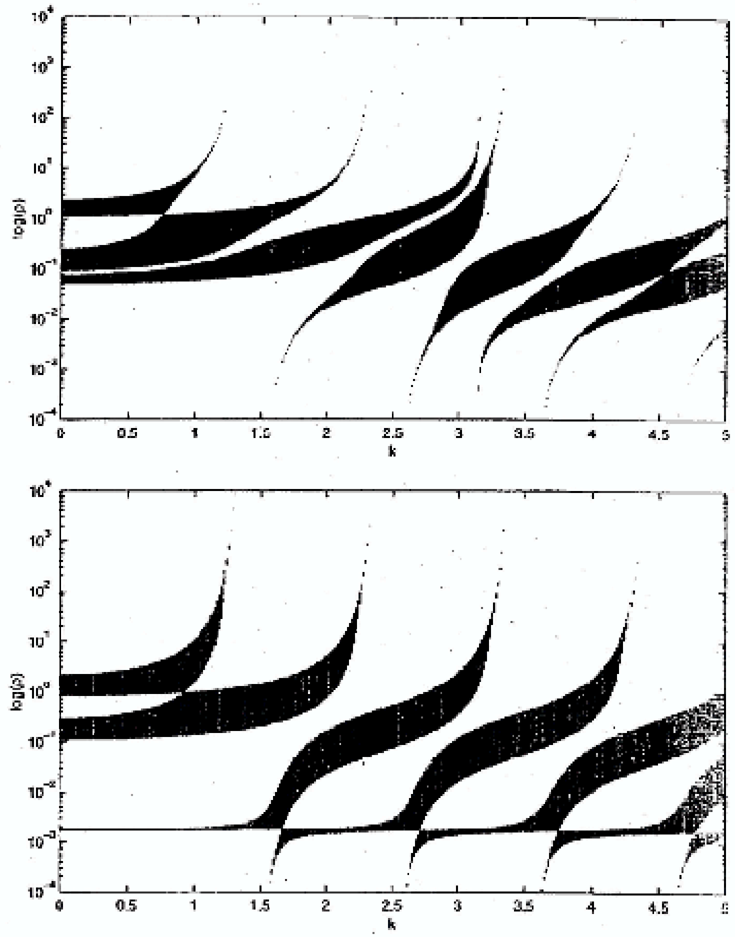

FIG. 8. Band spectrum of an infinite "bubble" array. The spheres are of unit radius, the spacing is l = 1 (upper figure) and l = 0.01 (lower figure), ρ is the contact radius.

How do gaps behave as $k \to \infty$?

Question: Are the scattering properties of such junctions reflected in *gap behaviour* of periodic families of geometric scatterers *at high energies?* And if we ask so, why it should be interesting?

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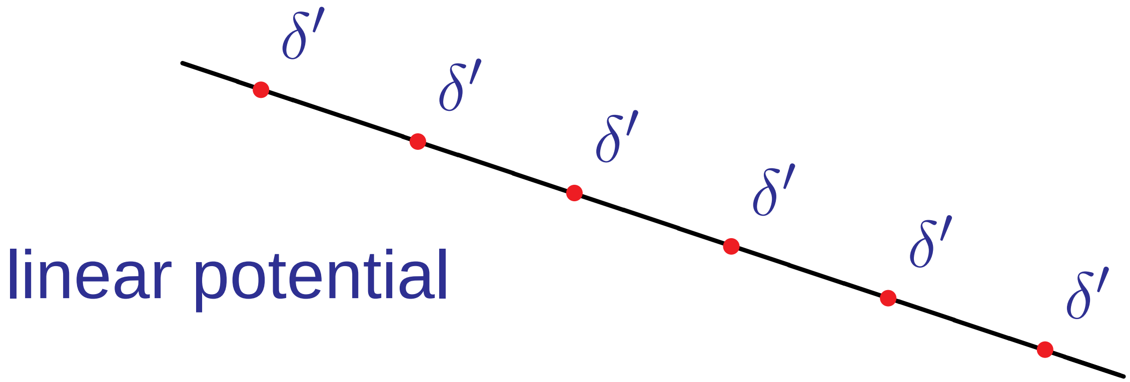
Recall properties of *singular Wannier-Stark* systems:



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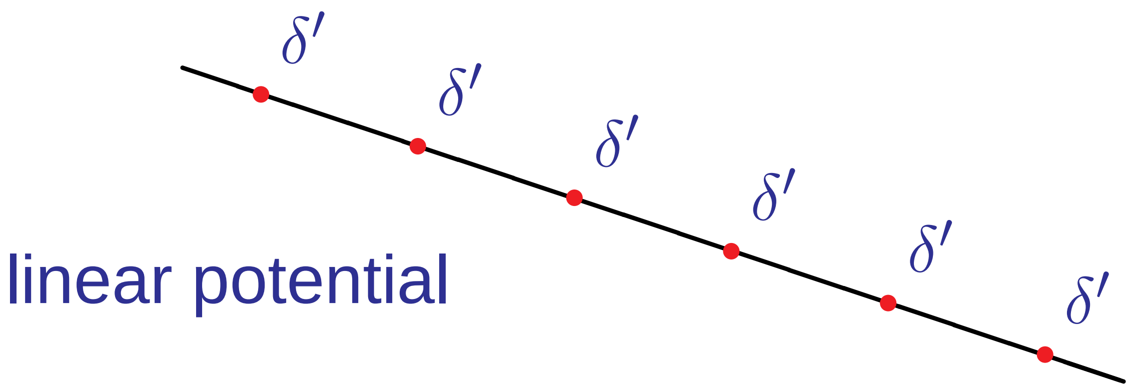
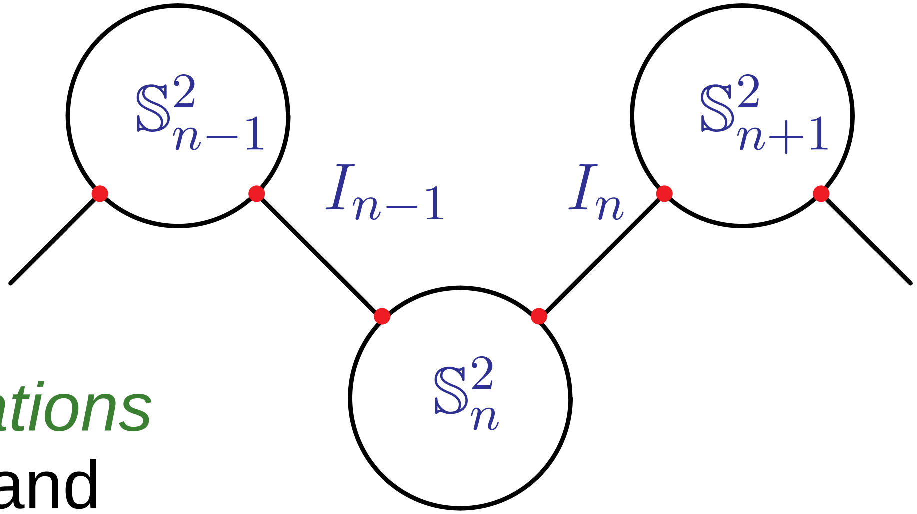


Spectrum of such systems is *purely discrete* which is proved for “most” values of the parameters [Asch-Duclos-E’98] and conjectured for *all* values. The reason behind are *large gaps* of δ' Kronig-Penney systems

Periodic systems – assumptions



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- periodicity in one or two directions (one can speak about "bead arrays" and "bead carpets")

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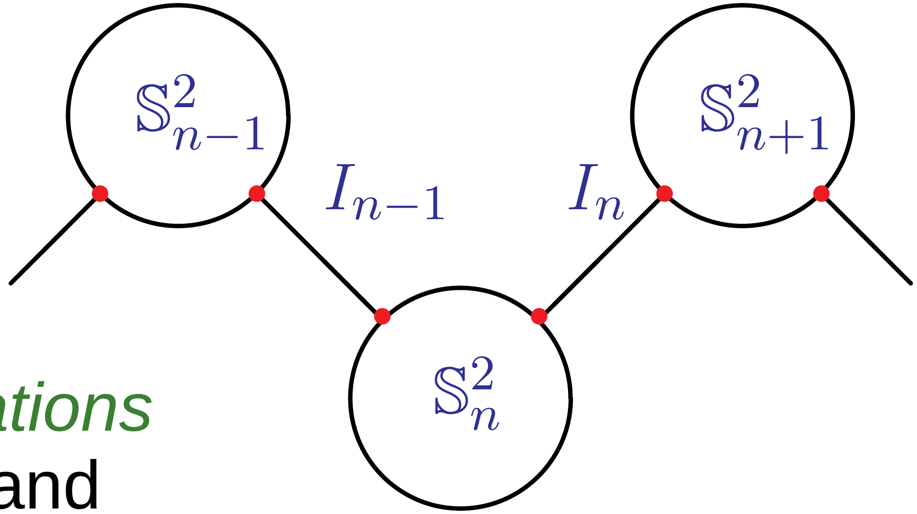

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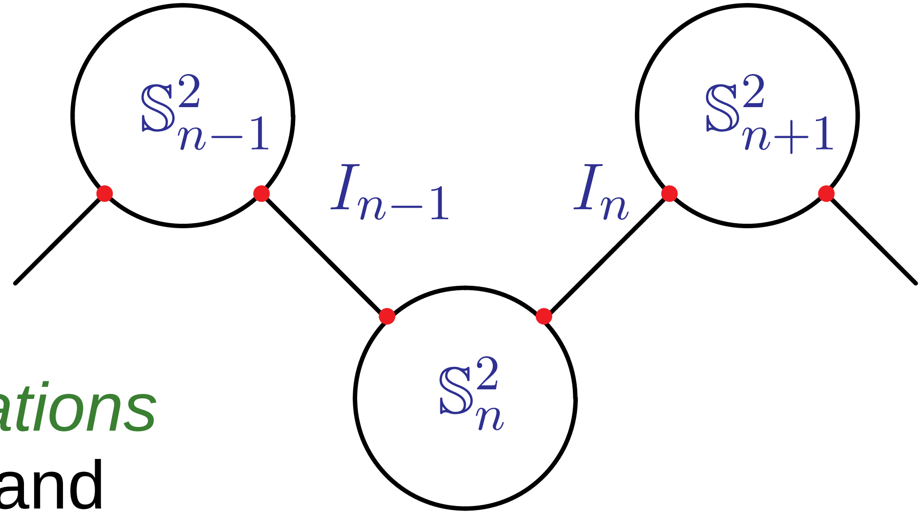

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- sphere-segment coupling $\mathcal{A} = \begin{pmatrix} 0 & 2\pi\alpha^{-1} \\ \bar{\alpha}^{-1} & 0 \end{pmatrix}$

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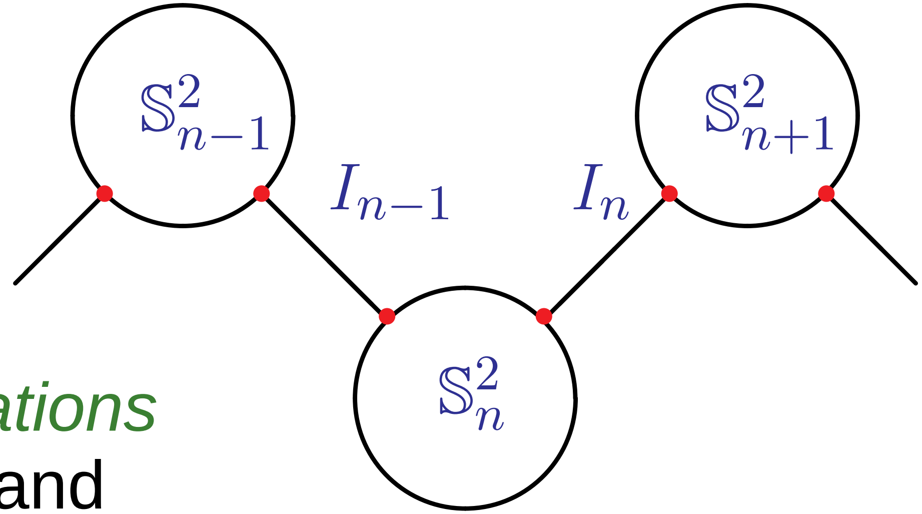
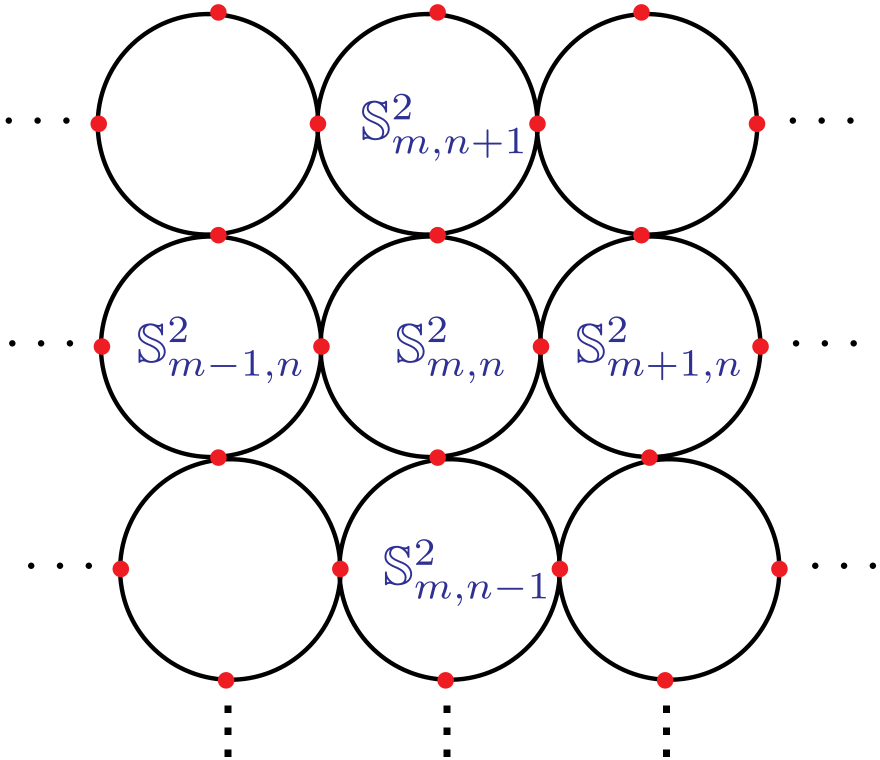


Consider *periodic combinations of spheres and segments* and adopt the following assumptions:

- periodicity in one or two directions (one can speak about “bead arrays” and “bead carpets”)
- angular distance between contacts equals π or $\pi/2$
- sphere-segment coupling $\mathcal{A} = \begin{pmatrix} 0 & 2\pi\alpha^{-1} \\ \bar{\alpha}^{-1} & 0 \end{pmatrix}$
- we allow also *tight coupling* when the spheres touch

Tightly coupled spheres



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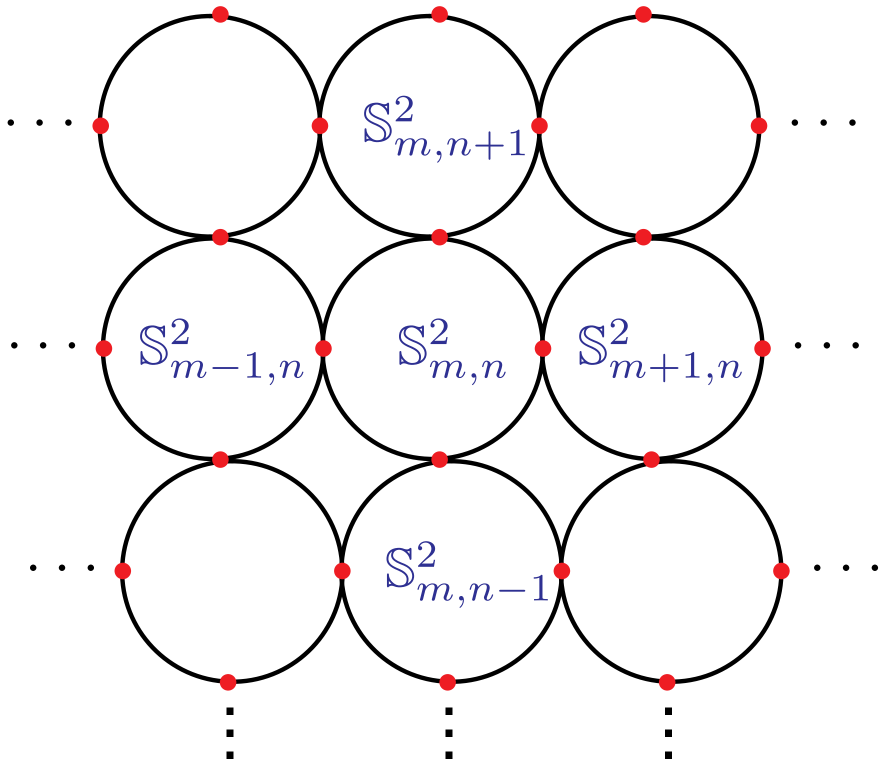

The tight-coupling boundary conditions will be

$$\begin{aligned} L_1(\Phi_1) &= A L_0(\Phi_1) + C L_0(\Phi_2)\,, \\ L_1(\Phi_2) &= \bar{C} L_0(\Phi_1) + D L_0(\Phi_2) \end{aligned}$$

with $A, D \in \mathbb{R}$, $C \in \mathbb{C}$. For simplicity we put $A = D = 0$

Large gaps in periodic manifolds

We analyze how spectra of the fibre operators depend on quasimomentum θ. Denote by $B_n,\ G_n$ the widths ot the nth band and gap, respectively; then we have

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$$\frac{B_n}{G_n} \le c\, n^{-\varepsilon}$$

holds as $n \to \infty$ for *loosely connected* systems, where $\epsilon = \frac{1}{2}$ for arrays and $\epsilon = \frac{1}{4}$ for carpets. For *tightly coupled* systems to any $\epsilon \in (0,1)$ there is a $\tilde{c} > 0$ such that the inequality $B_n/G_n \le \tilde{c}\,(\ln n)^{-\epsilon}$ holds as $n \to \infty$

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Conjecture: Similar results hold for other couplings and angular distances of the junctions. The problem is just technical; the dispersion curves are less regular in general

A heuristic way to choose the coupling

Let us return to the *plane+halfline* model and compare *low-energy scattering* to situation when the halfline is replaced by *tube of radius* a (we disregard effect of the sharp edge at interface of the two parts)

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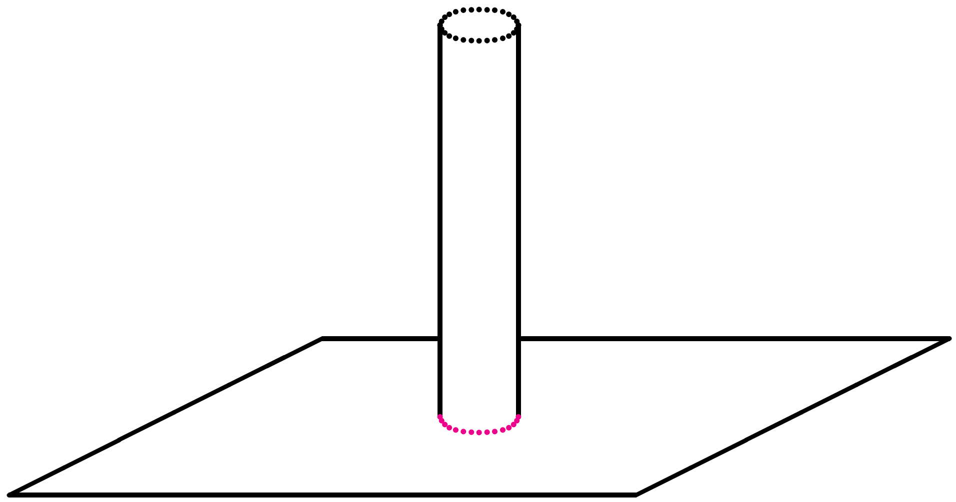

Plane plus tube scattering

Rotational symmetry allows us again to treat each partial wave separately. Given orbital quantum number ℓ one has to match smoothly the corresponding solutions

$$\psi(x) := \begin{cases} e^{ikx} + r_a^{(\ell)}(t)e^{-ikx} & \ldots & x \le 0 \\ \sqrt{\frac{\pi kr}{2}}\, t_a^{(\ell)}(k) H_\ell^{(1)}(kr) & \ldots & r \ge a \end{cases}$$

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This yields

$$r_a^{(\ell)}(k) = -\frac{\mathcal{D}_-^a}{\mathcal{D}_+^a}, \quad t_a^{(\ell)}(k) = 4i\sqrt{\frac{2ka}{\pi}}\,\left(\mathcal{D}_+^a\right)^{-1}$$

with

$$\mathcal{D}_\pm^a := (1 \pm 2ika) H_\ell^{(1)}(ka) + 2ka\left(H_\ell^{(1)}\right)'(ka)$$

Plane plus point: low energy behavior

Wronskian relation $W(J_\nu(z), Y_\nu(z)) = 2/\pi z$ implies scattering unitarity, in particular, it shows that

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Using asymptotic properties of Bessel functions with for small values of the argument we get

$$|t_a^{(\ell)}(k)|^2 \approx \frac{4\pi}{((\ell-1)!)^2} \left(\frac{ka}{2}\right)^{2\ell-1}$$

for $\ell \neq 0$, so the *transmission probability vanishes fast* as $k \to 0$ for higher partial waves

Heuristic choice of coupling parameters

The situation is different for $\ell = 0$ where

$$H_0^{(1)}(z) = 1 + \frac{2i}{\pi}\left(\gamma + \ln\frac{ka}{2}\right) + \mathcal{O}(z^2 \ln z)$$

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Notice that the “right” s-a extensions depend on a *single parameter*, namely radius of the “thin” component

Illustration on *microwave experiments*

Our models do not apply to QM only. Consider an *electromagnetic resonator*. If it is *very flat*, Maxwell equations simplify: TE modes effectively decouple from TM ones and one can describe them by Helmholz equation

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The reflection amplitude for a compact manifold with one lead attached at x_0 is found as above: we have

$$r(k) = -\frac{\pi Z(k)(1-2ika)-1}{\pi Z(k)(1+2ika)-1},$$

where $Z(k) := \xi(\vec{x}_0;k) - \frac{\ln a}{2\pi}$

Finding the resonances

To evaluate regularized Green's function we use ev's and ef's of Dirichlet Laplacian in $M = [0, c_1] \times [0, c_2]$, namely

$$\varphi_{nm}(x,y) = \frac{2}{\sqrt{c_1 c_2}} \sin(n\frac{\pi}{c_1}x)\sin(m\frac{\pi}{c_2}y)\,,$$

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Resonances are given by complex zeros of the denominator of $r(k)$, i.e. by solutions of the algebraic equation

$$\xi(\vec{x}_0, k) = \frac{\ln(a)}{2\pi} + \frac{1}{\pi(1 + ika)}$$

Comparison with experiment

Compare now *experimental results* obtained at University of Marburg with the model for $a = 1\,\mathrm{mm}$, averaging over x_0 and $c_1, c_2 = 20 \sim 50\,\mathrm{cm}$

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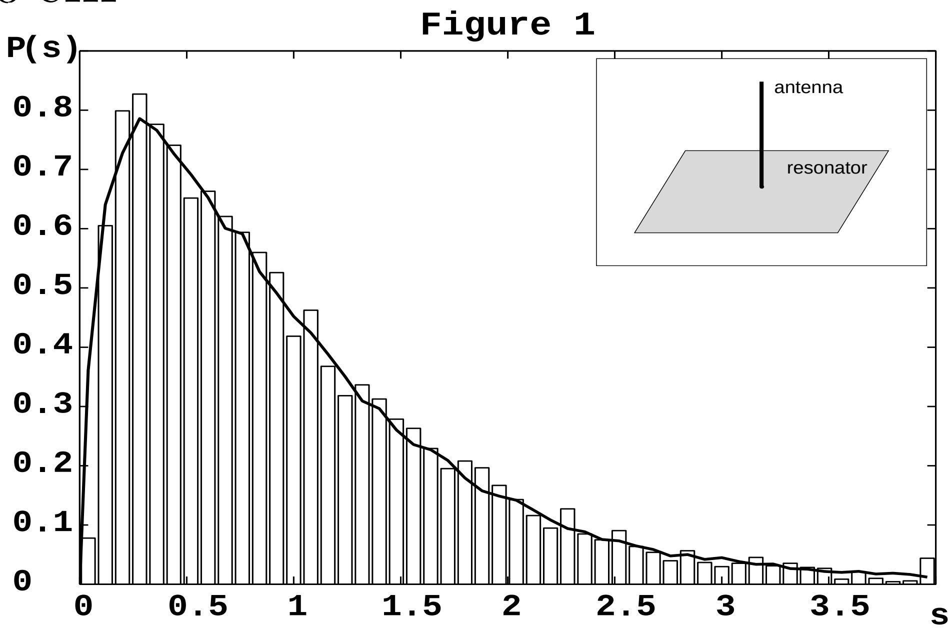

Important: An agreement is achieved with the *lower third* of measured frequencies – confirming thus validity of our approximation, since shorter wavelengths are comparable with the antenna radius a and $ka \ll 1$ is no longer valid

Spin conductance oscillations

Finally, manifolds we consider need not be separate spatial entities. Illustration: a spin conductance problem:

[Hu et al'01] measured conductance of polarized electrons through an InAs sample; the results *depended on length* L of the semiconductor "bar", in particular, that for some L *spin-flip processes dominated*

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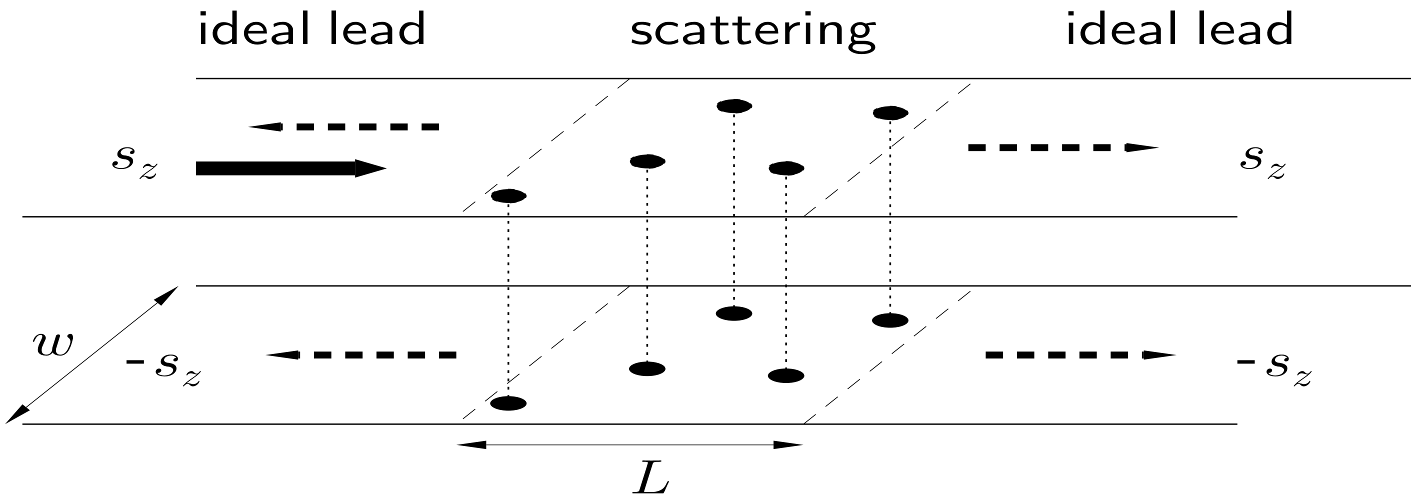
Physical mechanism of the spin flip is the *spin-orbit interaction with impurity atoms.* It is complicated and no realistic transport theory of that type was constructed

We construct a *model* in which spin-flipping interaction has a *point character*. Semiconductor bar is described as *two strips coupled at the impurity sites* by the boundary condition described above

Spin-orbit coupled strips



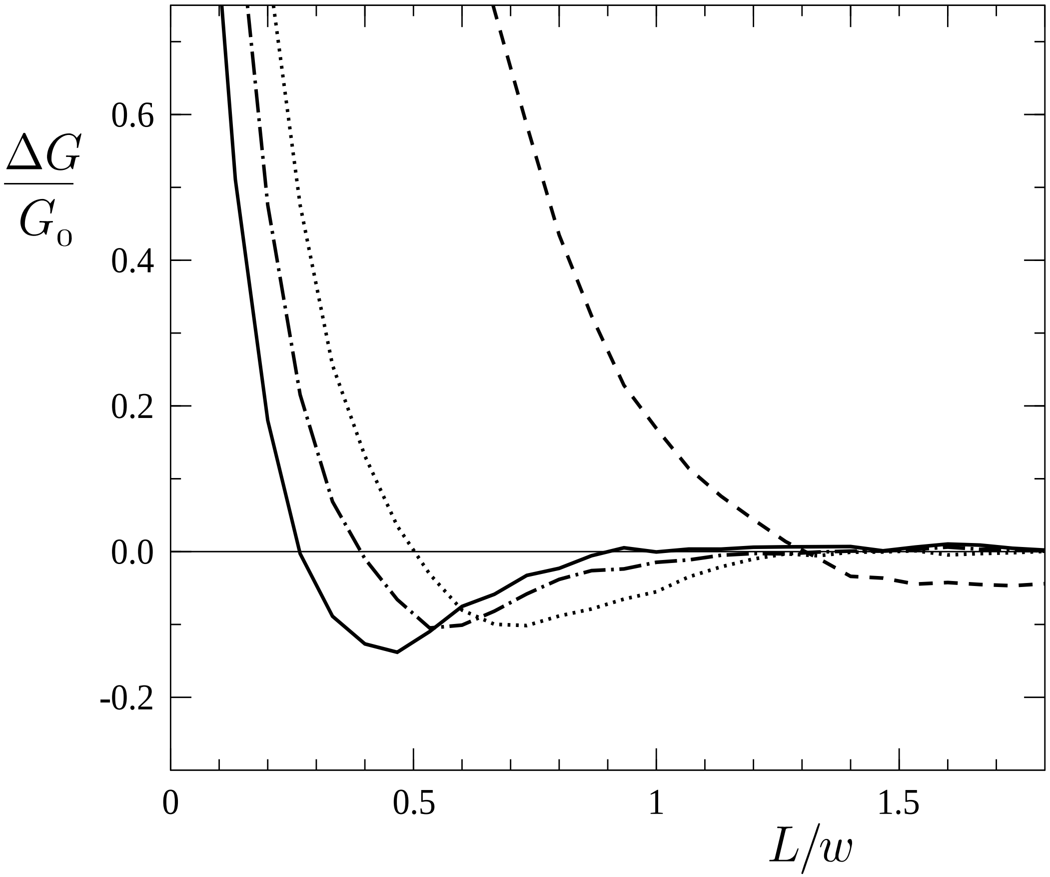
We assume that impurities are randomly distributed with the same coupling, $A = D$ and $C \in \mathbb{R}$. Then we can instead study a pair of decoupled strips,

$$L_1(\Phi_1 \pm \Phi_2) = (A \pm C)L_0(\Phi_1 \pm \Phi_2)\,,$$

which have naturally different localizations lengths

Compare with measured conductance

Returning to original functions Φ_j, *spin conductance oscillations* are expected. This is indeed what we see if the parameters assume realistic values:



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- A typical feature of such systems is a *suppression of transport at high energies*
- This has consequences for spectral properties of *periodic and WS-type systems*
- Finally, concerning the *justification of coupling choice* a lot of work remains to be done; the situation is less understood than for quantum graphs of *Lectures I-III*

Some literature to Lecture VI

- [ADE98] J. Asch, P. Duclos, P.E.: Stability of driven systems with growing gaps. Quantum rings and Wannier ladders, *J. Stat. Phys.* **92** (1998), 1053-1069
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- They describe numerous systems *of physical importance*, both of quantum and classical nature
- The field offers many *open questions*, some of them difficult, presenting thus a challenge for ambitious young people

Thank you for your attention!