Quantum systems coupling manifolds of different dimensionality

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Talk overview

- Motivation – a nontrivial configuration space

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- Coupling by means of s-a extensions

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- And something else: spin conductance oscillations

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- An illustration on microwave experiments
- And something else: spin conductance oscillations
- Finally, some open questions

A nontrivial configuration space

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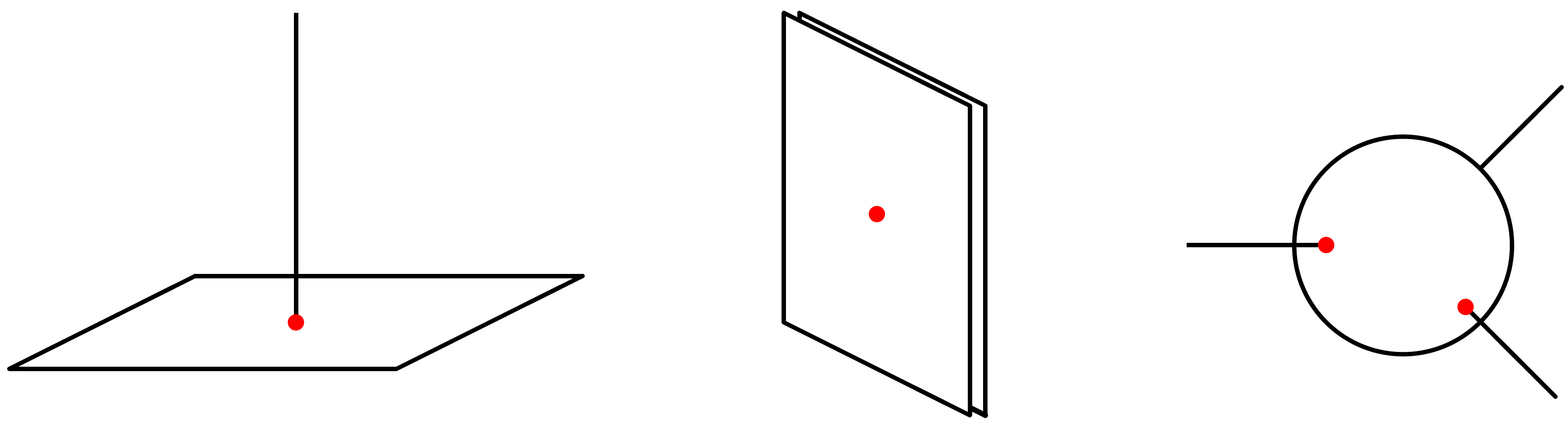

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In contrast, QM offers interesting examples, e.g.

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

etc. Similarly one can consider some *electromagnetic systems* such as flat microwave resonators with attached antennas

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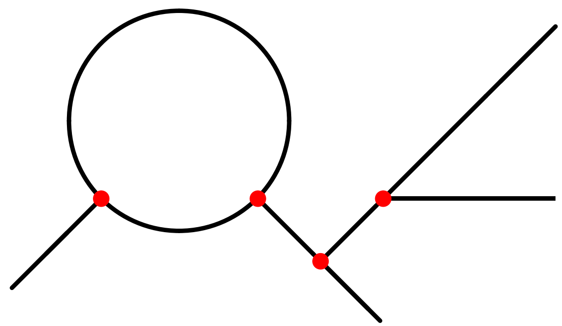
Physical meaning: The construction guarantees that the *probability current is conserved* at the junction

Quantum graphs

Most known example is represented by *quantum graphs* where the components M_j are line segments,



Hamiltonian: $-\frac{\partial^2}{\partial x_j^2} + v(x_j)$
on graph edges,
boundary conditions at vertices

and the parameters classify the b.c. at graph vertices – for a review see [Kostrykin-Schrader, 1999; Kuchment, 2004] and other papers

Different dimensions

Here 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

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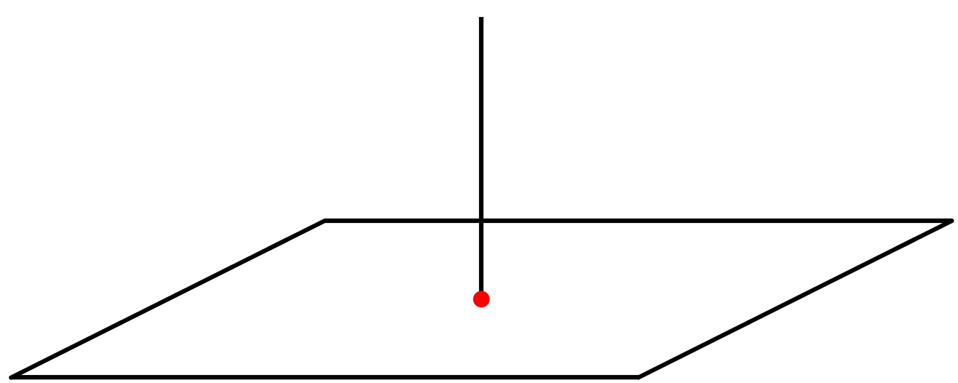
An archetypal example, $\mathcal{H} = L^2(\mathbb{R}_-) \oplus L^2(\mathbb{R}^2)$, so the wavefunctions are pairs $\phi := \binom{\phi_1}{\Phi_2}$ of square integrable functions



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

$$\begin{aligned} \phi_1'(0-) &= A\phi_1(0-) + BL_0(\Phi_2)\,, \\ L_1(\Phi_2) &= C\phi_1(0-) + DL_0(\Phi_2)\,, \end{aligned}$$

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where

$$A,\ D \in \mathbb{R} \quad \text{and} \quad B = 2\pi\bar{C}$$

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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, $\Phi_2(r,\varphi) = (2\pi)^{-1/2}\phi_2(r)$ can be coupled nontrivially to the halfline

$2+1$ point-contact coupling

An integration by parts gives

$$
\begin{aligned}
(\phi, H_0^*\psi) - (H_0^*\phi, \psi) \;=\; & \bar{\phi}_1'(0)\psi_1(0) - \bar{\phi}_1(0)\psi_1'(0) \\
& + \lim_{\varepsilon\to 0+} \varepsilon \left(\bar{\phi}_2(\varepsilon)\psi_1'(\varepsilon) - \bar{\phi}_2'(\varepsilon)\psi_2(\varepsilon) \right) \,,
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and using the asymptotic behaviour

$$\phi_2(\varepsilon) = \sqrt{2\pi}\,\left[L_0(\Phi_2)\ln\varepsilon + L_1(\Phi_2) + \mathcal{O}(\varepsilon)\right]\,,$$

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$$\phi_2(\varepsilon) = \sqrt{2\pi}\;[L_0(\Phi_2)\ln\varepsilon + L_1(\Phi_2) + \mathcal{O}(\varepsilon)\,]\;,$$

we can express the above limit term as

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

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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$$\mathcal{D}_\pm := (A \pm ik)\left[1 + \frac{2i}{\pi}\left(\gamma_{\mathrm{E}} - D + \ln\frac{k}{2}\right)\right] + \frac{2i}{\pi}BC\,,$$

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Remark: More general coupling, $\mathcal{A}\binom{\phi_1}{L_0} + \mathcal{B}\binom{\phi_1'}{L_1} = 0$, 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 in *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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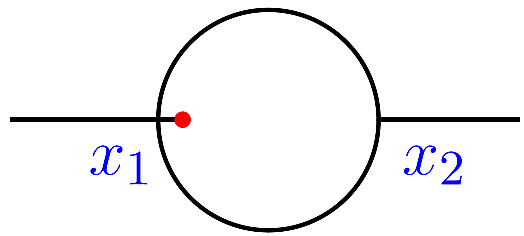
- Notice that *reflection dominates at high energies*, since $|t(k)|^2 = \mathcal{O}((\ln k)^{-2})$ holds as $k \to \infty$
- For some $\mathcal{A}$ there are also bound states decaying exponentially away of the junction, at most two

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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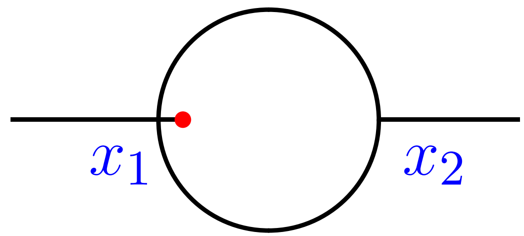

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Three one-parameter families of $\mathcal{A}$ were investigated [Kiselev, 1997; E.-Tater-Vaněk, 2001; Brüning-Geyler-Margulis-Pyataev, 2002]; it appears that scattering properties *en gross* are not very sensitive to the coupling:

- 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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where $G(\cdot, \cdot; k)$ is Green's function of Δ_{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 $\{\phi(x)_n\}_{n=1}^{\infty}$. Then we find easily

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

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and

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

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

A *symmetric spherical* scatterer

Theorem [Kiselev, 1997, E.-Tater-Vaněk, 2001]: 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 $K_\varepsilon := \setminus \bigcup_{l=2}^{\infty} \left(\mu_l - \varepsilon(l)(\ln l)^{-2}, \mu_l + \varepsilon(l)(\ln l)^{-2}\right)$.

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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 at 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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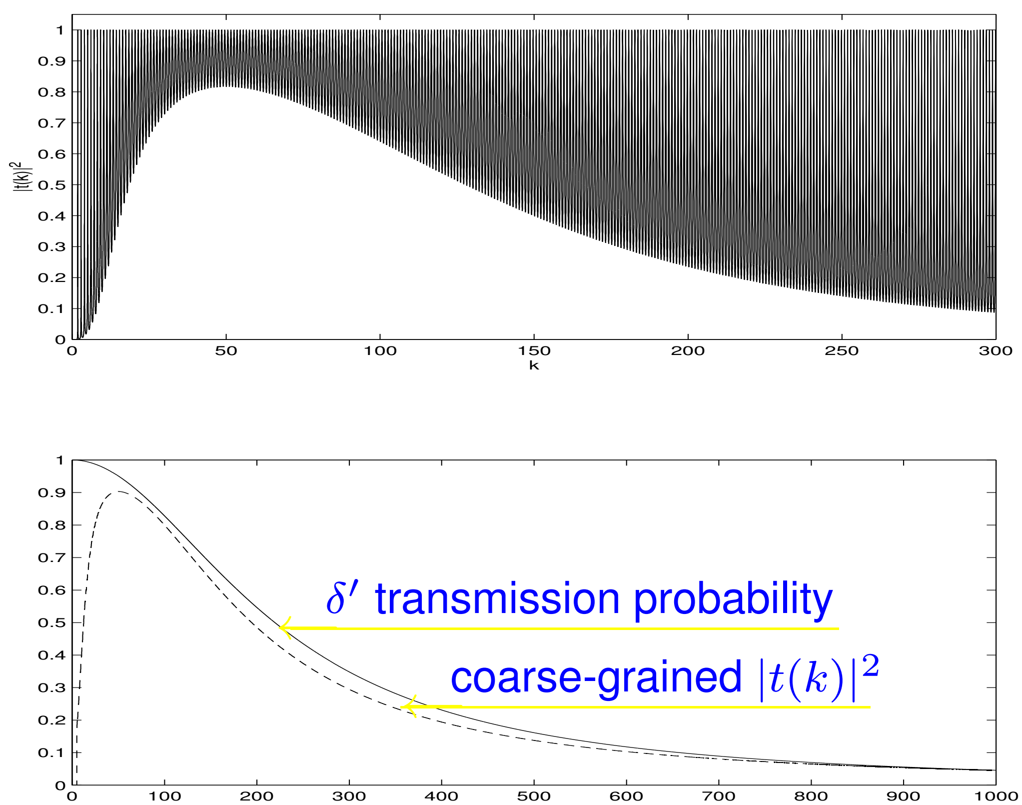
Figure 7



An *asymmetric* spherical scatterer

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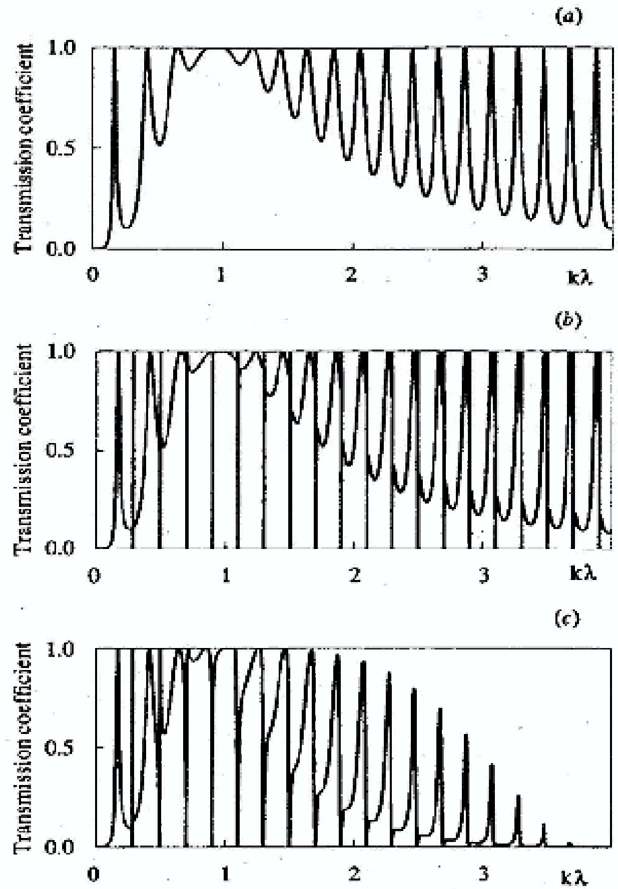

Figure 2. The transmission coefficient as a function of $k\lambda$ at $a = 10\lambda$: (a) $r = \pi a$; (b) $r = 0.98\pi a$; (c) $r = 0.96\pi a$.

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, 2003]

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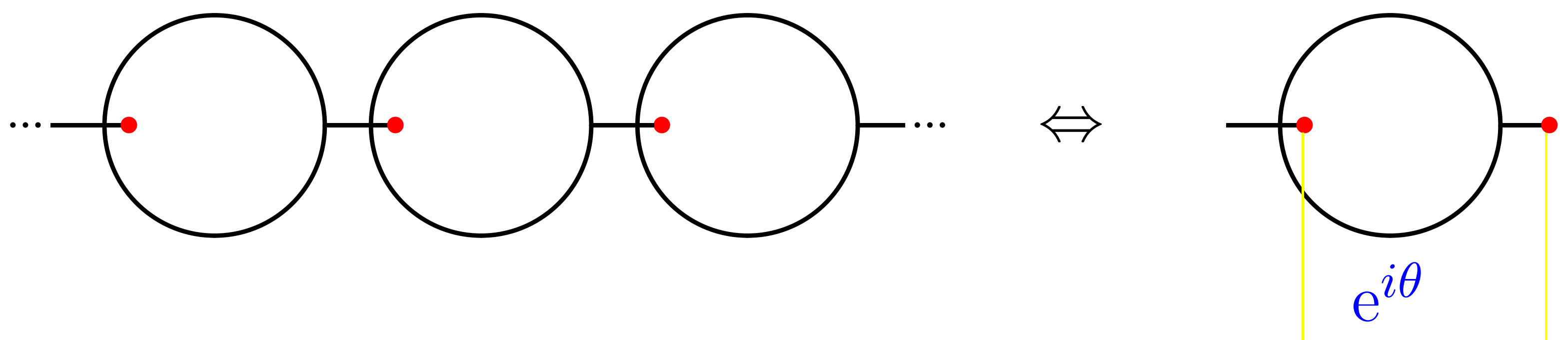
Furthermore, infinite periodic systems can be treated by Floquet-Bloch decomposition



Sphere array spectrum

A band spectrum example from [E.-Tater-Vaněk, 2001]: radius $R = 1$, segment length $\ell = 1, 0.01$ and coupling ρ

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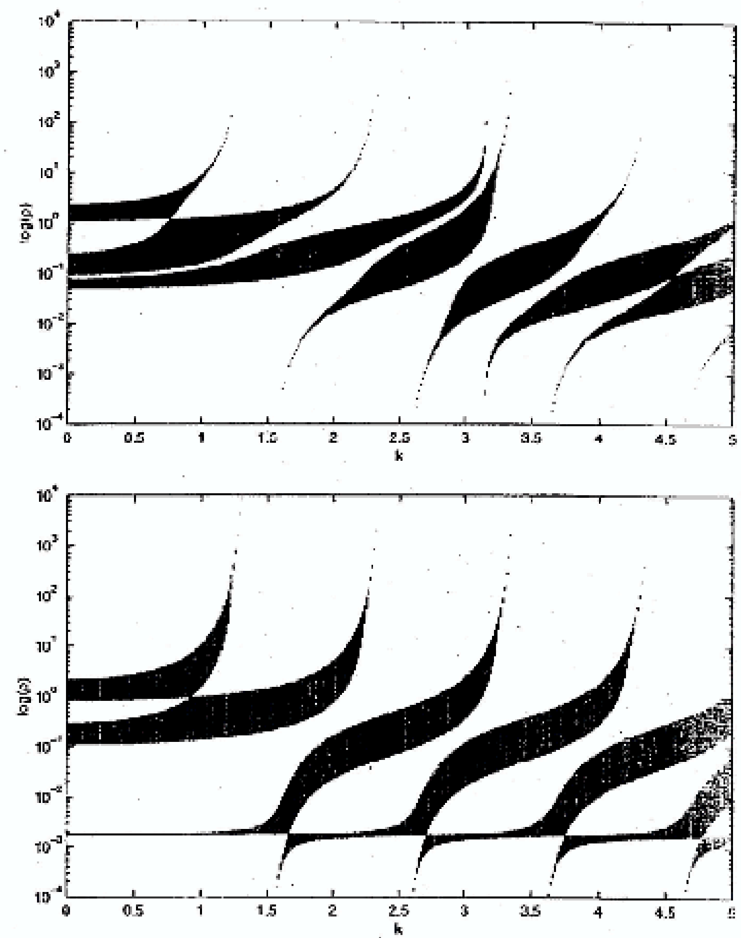

FIG. 8. Band spectrum of an infinite "bubble" array. The spheres are of unit radius, the spacing is l = 1 (upper figure) and l = 0.01 (lower figure), ρ is the contact radius.

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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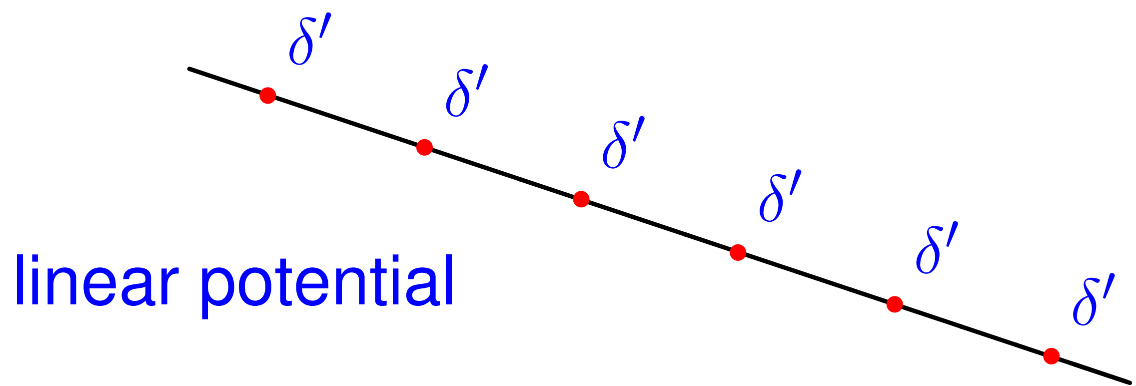
Recall properties of *singular Wannier-Stark* systems:



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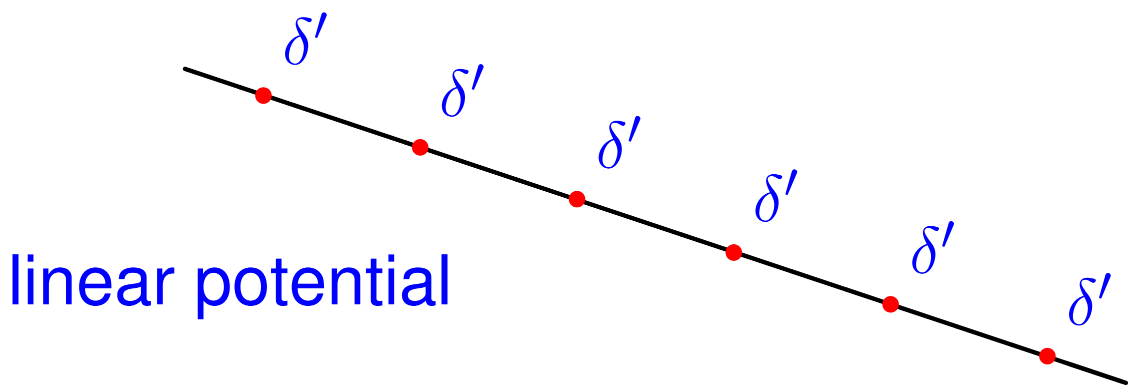
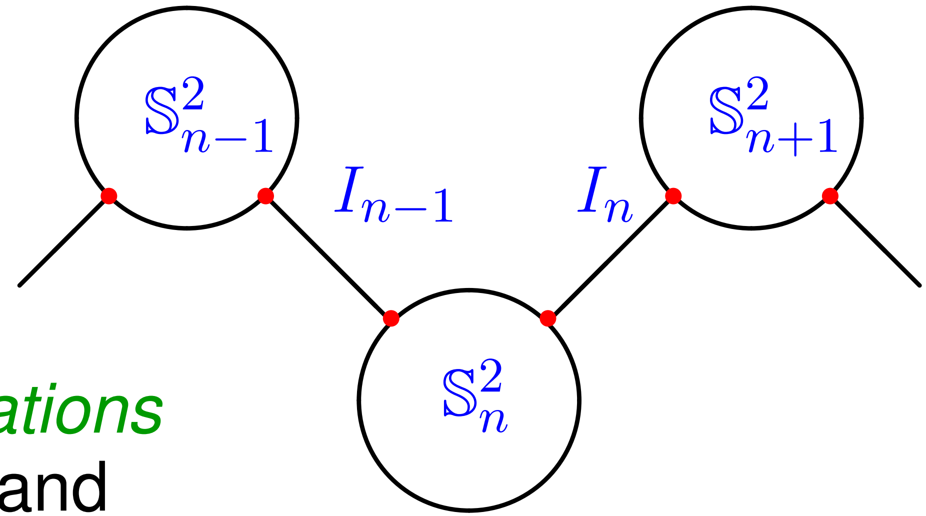


Spectrum of such systems is *purely discrete* which is proved for “most” values of the parameters [Asch-Duclos-E., 1998] and conjectured for *all* values. The reason behind are *large gaps* of δ' Kronig-Penney systems

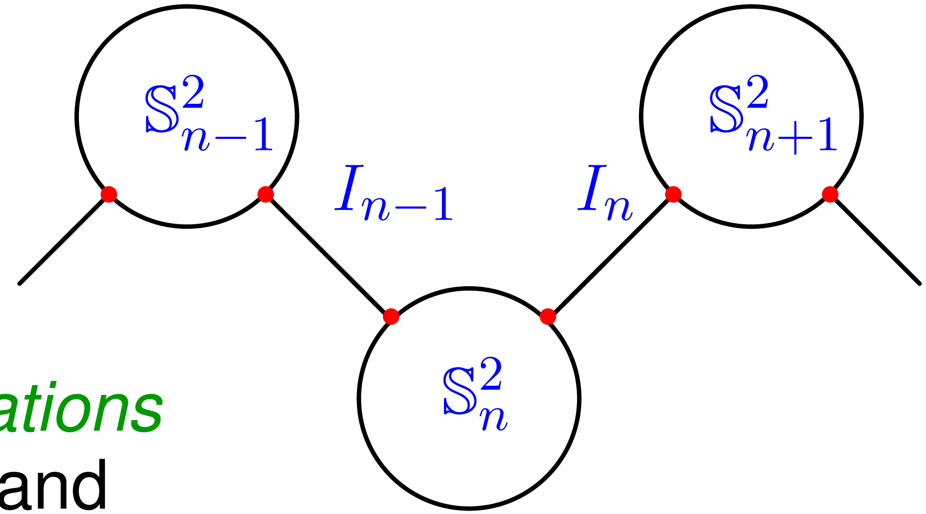
Periodic systems – assumptions



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")

Periodic systems – assumptions



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

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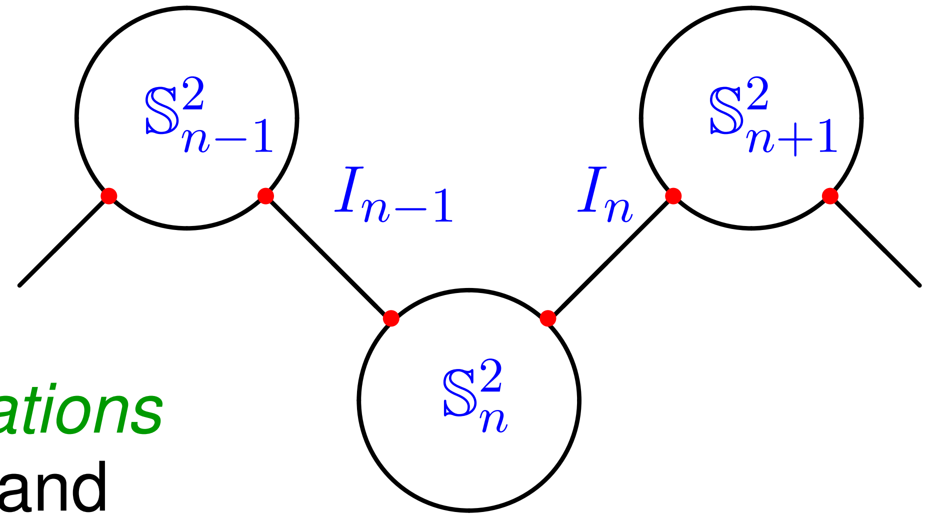

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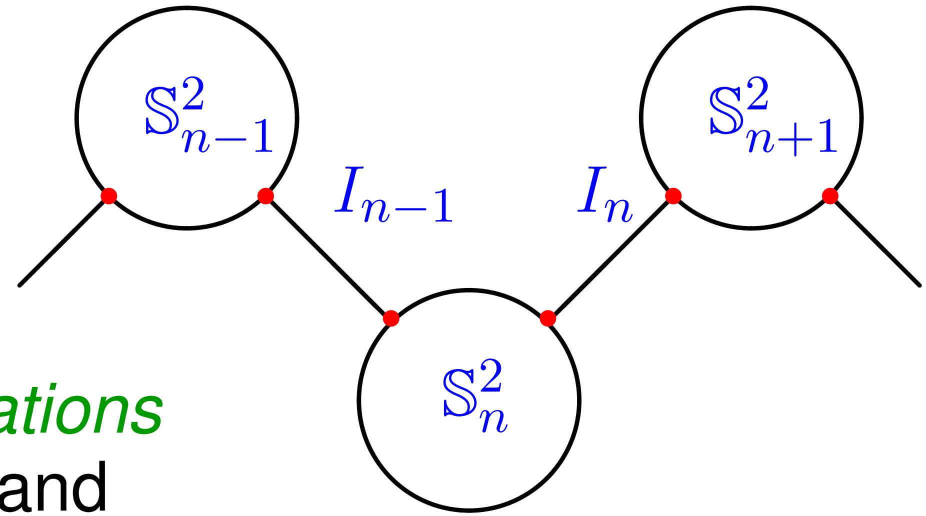

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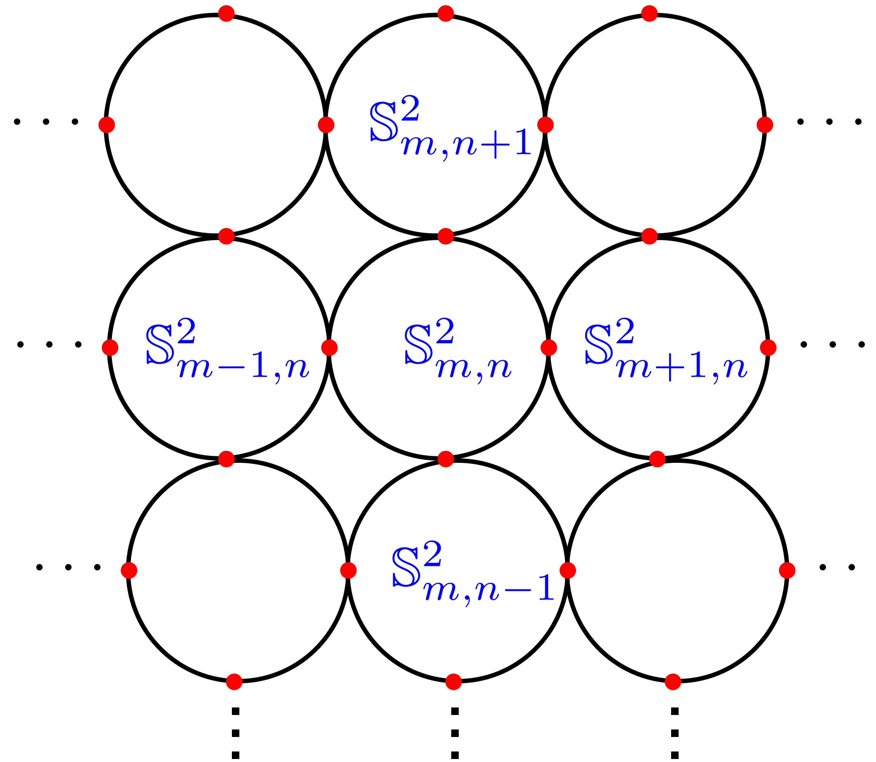
- we allow also *tight coupling* when the spheres touch

Tightly coupled spheres



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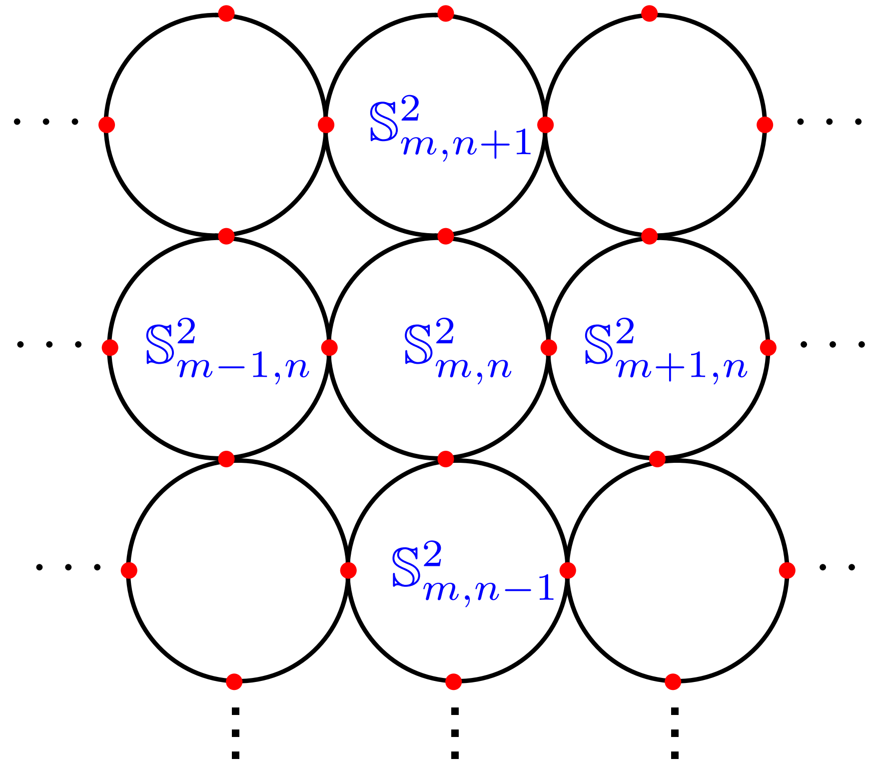

The tight-coupling boundary conditions will be

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

with $A, D \in$, $C \in \mathbb{C}$. 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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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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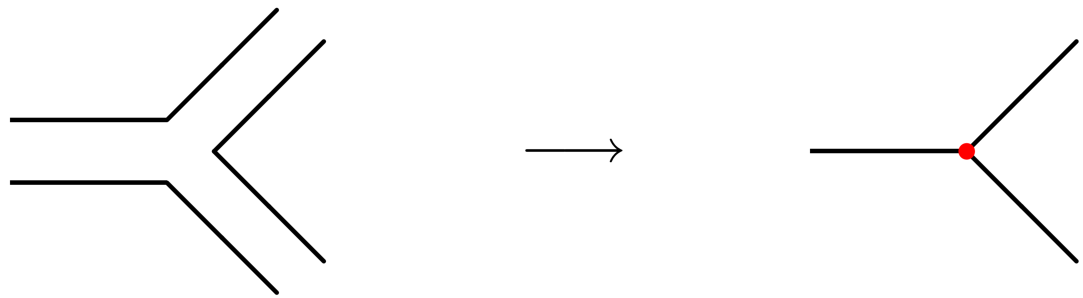
Conjecture: Similar results hold for other couplings and angular distances of the junctions. The problem is just technical; the dispersion curves are less in general

Justification? Shrinking manifolds

Inspiration in *fat-graph limit* [Kuchment-Zeng, 2001]



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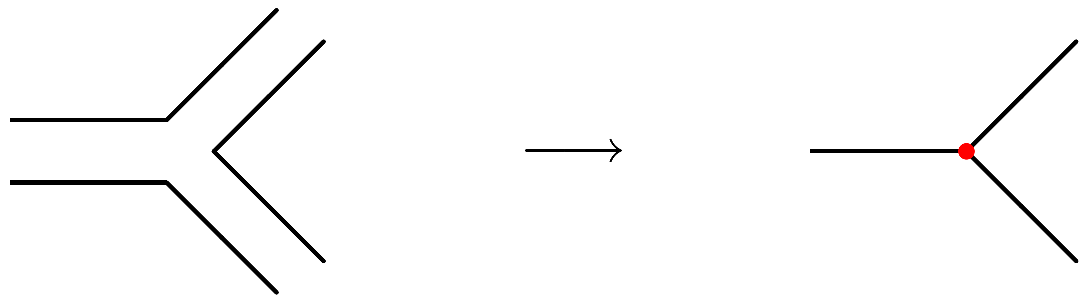

If the graph is *compact* and the fat graph supports Laplacian with *Neumann* boundary conditions, then in the shrinking limit "most" ev's diverge as width $\to 0$ and a finite number of them tend to ev's of the graph Laplacian with *Kirchhoff b.c.*, i.e. continuity and

$$\sum_{\text{edges meeting at } v_k} u_j'(v_k) = 0\,;$$

one uses minimax and suitable embedding operators

Shrinking “sleeved” manifolds

An analogous results holds more general “graph-shaped” manifolds, for instance *graph-type sleeves*, not necessarily embedded in $\mathbb{R}^d$ [E.-Post, 2003]

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For a compact graph, one compares Schrödinger operators supported by the following structures

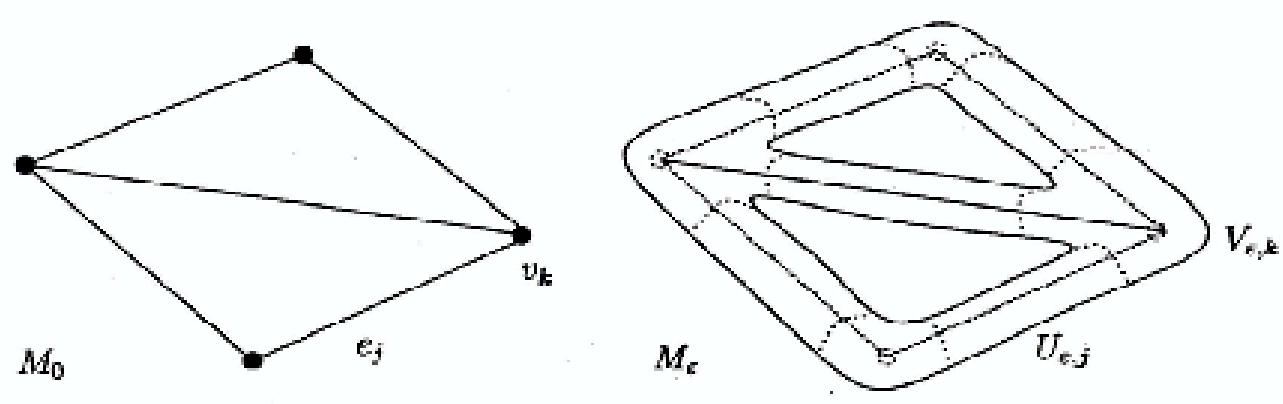
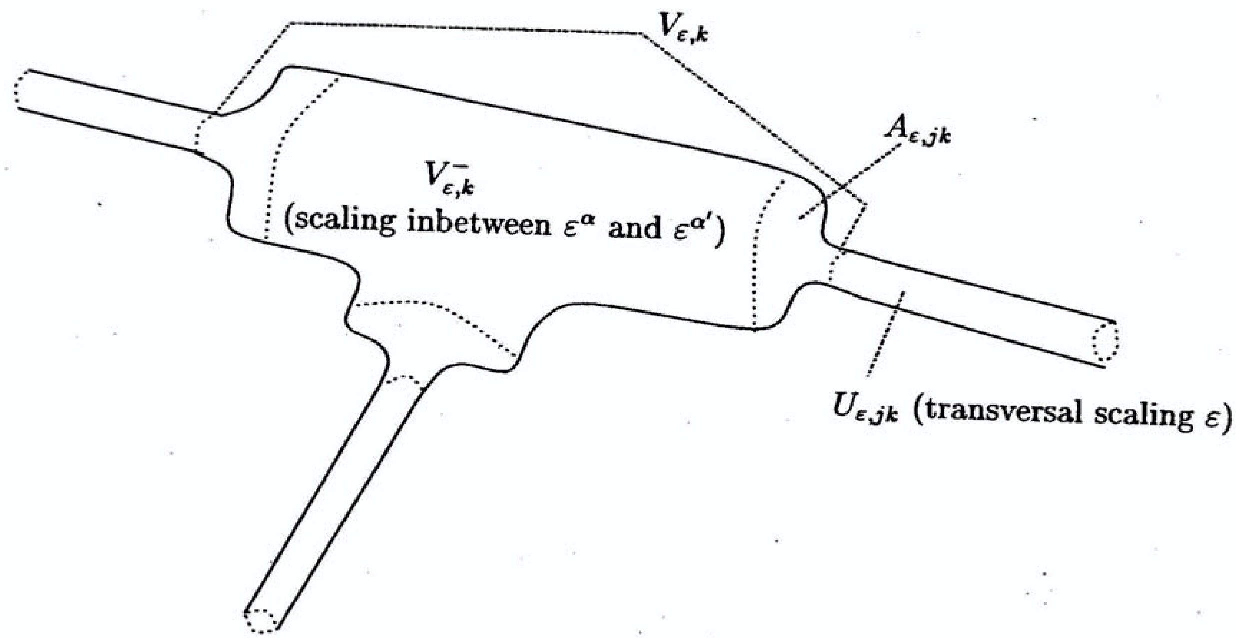


FIGURE 1. On the left, we have the graph M_0, on the right, the associated graph-like manifold (in this case, $F = \mathbb{S}^1$ and M_ε is a 2-dimensional manifold).

More general scaling

Furthermore, one can try to do the same using *different scaling* of the *edge* and *vertex* regions. Some technical assumptions needed, e.g., the bottlenecks must be "simple"



Scaling limit of a sleeved manifold

Let vertices scale as ε^{α}. We find that

- if $\alpha \in (1-d^{-1}, 1]$ the result is as in [Kuchment-Zeng, 2001]: the ev's at the spectrum bottom converge the graph Laplacian with *Kirchhoff b.c.*, i.e. continuity and

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- if $\alpha \in (0, 1-d^{-1})$ the "limiting" Hilbert space is $L^2(M_0) \oplus \mathbb{C}^K$, where K is $\#$ of vertices, and the "limiting" operator acts as Dirichlet Laplacian at each edge and as zero on $\mathbb{C}^K$

Scaling limit of a sleeved manifold

- if $\alpha = 1-d^{-1}$, Hilbert space is the same but the limiting operator is given by quadratic form $q_0(u) := \sum_j \|u_j'\|^2_{I_j}$, the domain of which consists of $u = \{\{u_j\}_{j\in J}, \{u_k\}_{k\in K}\}$ such that $u \in H^1(M_0) \oplus \mathbb{C}^K$ and the *edge and vertex parts are coupled* by $(\mathrm{vol}\,(V_k^-))^{1/2} u_j(v_k) = u_k$

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- finally, if vertex regions do not scale at all, $\alpha = 0$, the manifold components decouple in the limit again,

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- Hence such a straightforward limiting procedure *does not help* us to justify choice of appropriate s-a extension

A heuristic way to choose the coupling

Try something else: 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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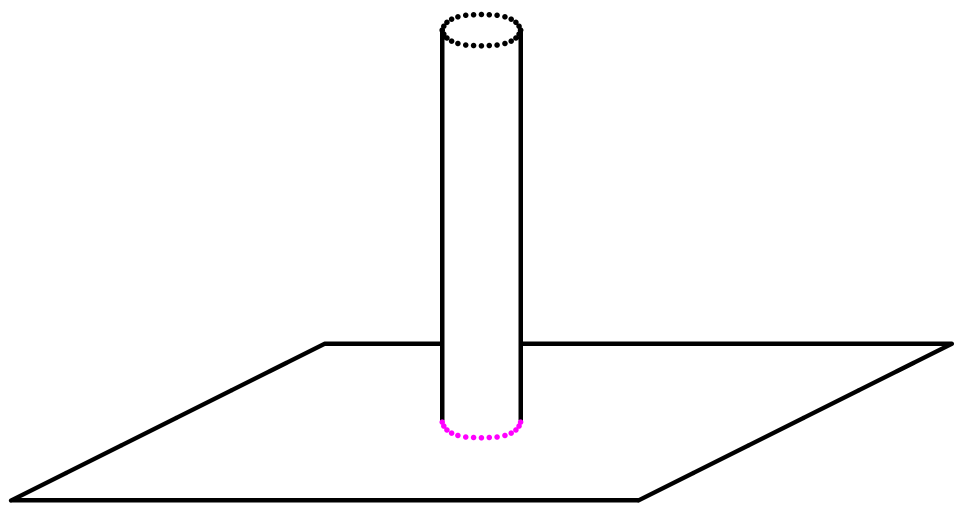

Plane plus tube scattering

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

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

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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

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

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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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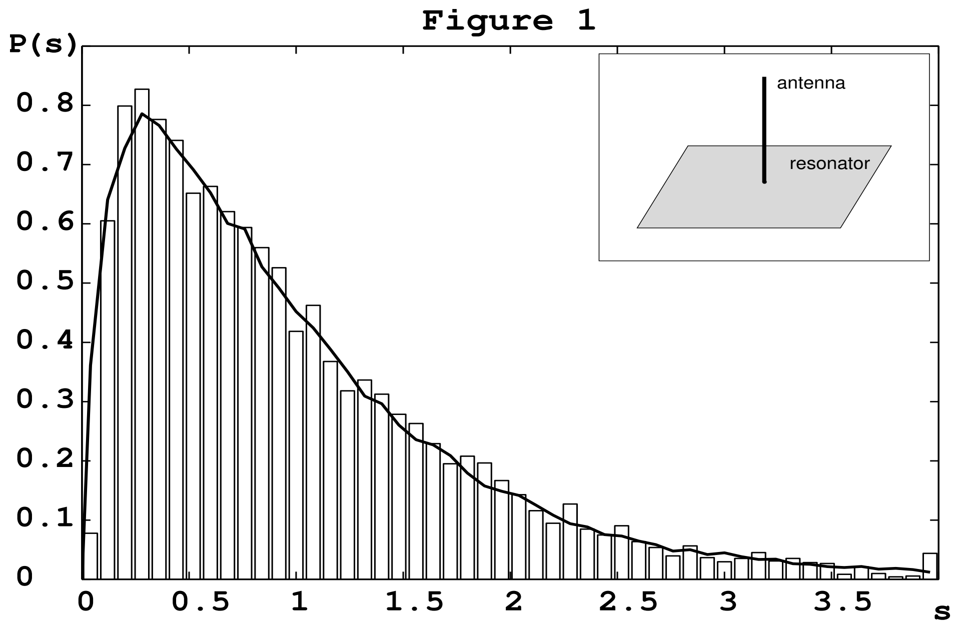

Important: An agreement is achieved with the *lower third* of measured frequencies – confirming thus validity of our approximation, since shorter wavelengths are comparable with the antenna radius a and $ka \ll 1$ is no longer valid

Spin conductance oscillations

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

[Hu et al., 2001] 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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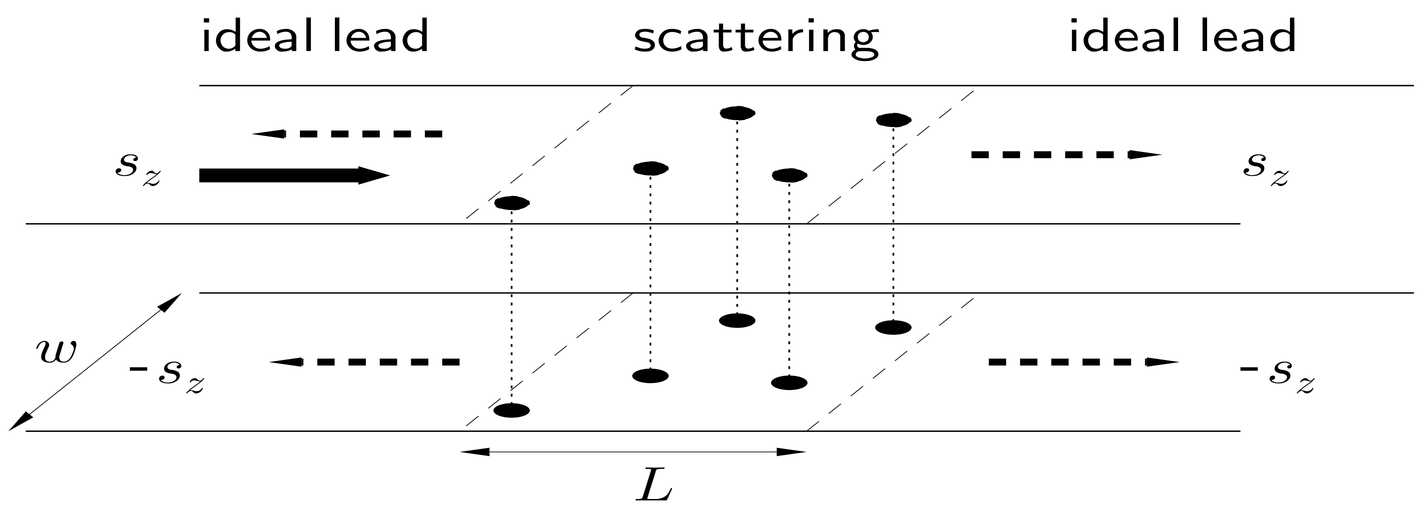
We construct a *model* in which spin-flipping interaction has a *point character*. Semiconductor bar is described as *two strips coupled at the impurity sites* by the boundary condition described above

Spin-orbit coupled strips



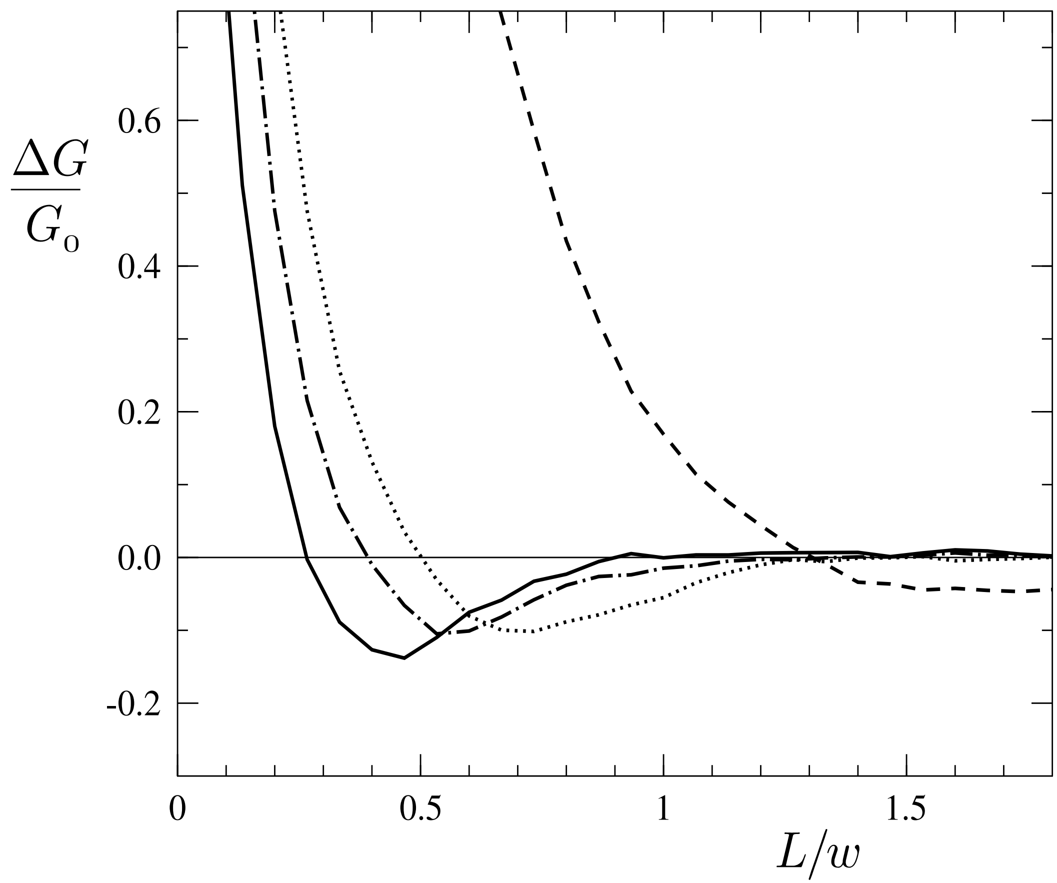
We assume that impurities are randomly distributed with the same coupling, $A = D$ and $C \in \mathbb{R}$. Then we can instead study a pair of decoupled strips,

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

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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- Coupling parameter choice: can one formulate the presented heuristic argument rigorously?

The talk was based on

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for more information see *http://www.ujf.cas.cz/˜exner*