On quantum particles that change dimension

In memoriam Vladimir Geyler

on the subject he used to like

Pavel Exner

Doppler Institute

for Mathematical Physics and Applied Mathematics

Prague

What we will speak about

In both classical and QM there are systems with constraints for which the configuration space is a nontrivivial subset of $\mathbb{R}^n$. Sometimes it happens that one can idealize as a *union of components of lower dimension*

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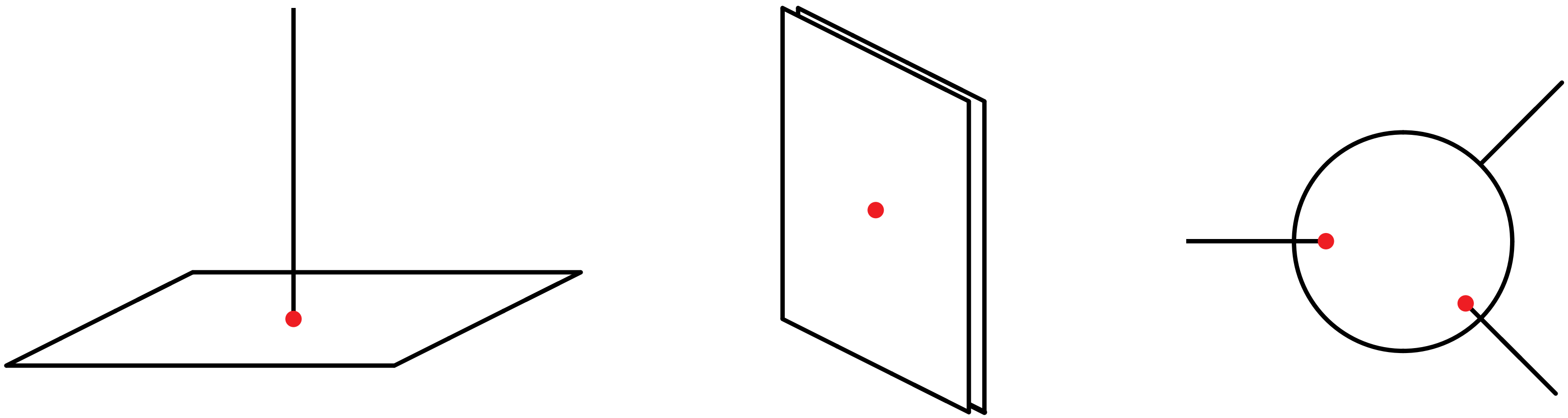

A nontrivial configuration space

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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. One can also consider some *electromagnetic systems* such as flat microwave resonators with attached antennas

Systems like these ones were for *Volodya Geyler* a source of inspiration and a way to interesting results

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 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 $\dim M_j \leq 3$ (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

Couplings to consider

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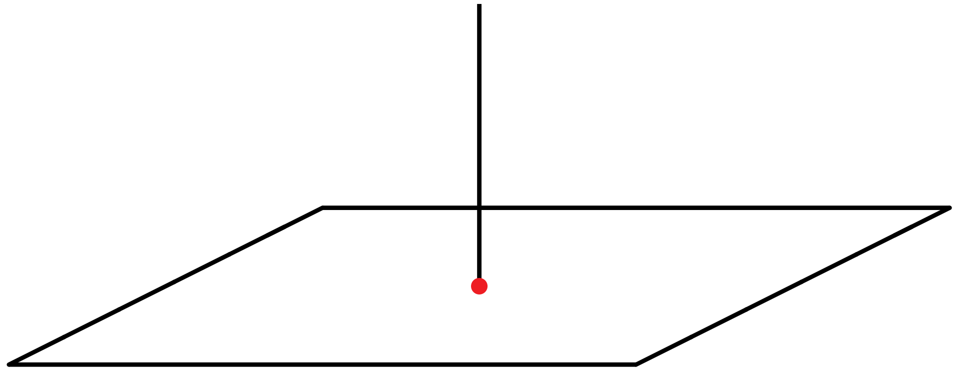
An *archetypal example*, $\mathcal{H} = L^2(\mathbb{R}_-) \oplus L^2(\mathbb{R}^2)$, so the wavefunctions are pairs $\phi := \binom{\phi_1}{\Phi_2}$ of square integrable functions



Boundary values

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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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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

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An integration by parts gives

$$(\phi, H_0^*\psi) - (H_0^*\phi, \psi) \;=\; \bar\phi_1'(0)\psi_1(0) - \bar\phi_1(0)\psi_1'(0) + \lim_{\varepsilon\to 0+} \varepsilon\left(\bar\phi_2(\varepsilon)\psi_1'(\varepsilon) - \bar\phi_2'(\varepsilon)\psi_2(\varepsilon)\right)\,,$$

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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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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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where $\gamma_E \approx 0.5772$ is Euler-Mascheroni constant

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where $\gamma_\mathrm{E} \approx 0.5772$ is Euler-Mascheroni constant

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 $\mathcal{A} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$ 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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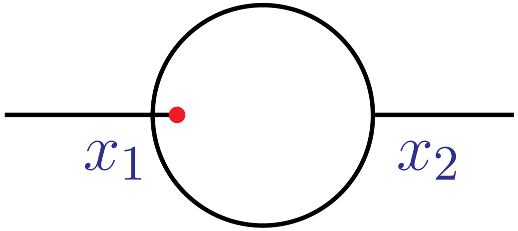
- Notice that *reflection dominates at high energies*, since $|t(k)|^2 = \mathcal{O}((\ln k)^{-2})$ holds as $k \to \infty$
- For some $\mathcal{A}$ there are also bound states decaying exponentially away of the junction, at most two

Single-mode geometric scatterers

Consider next a compact manifold with two leads attached



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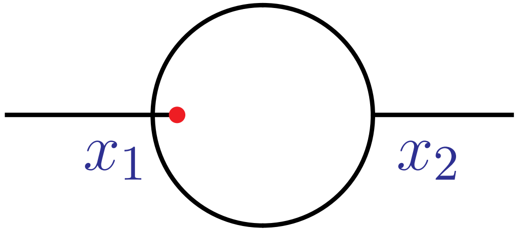

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Three one-parameter families of $\mathcal{A}$ were investigated [Kiselev, 1997; E.-Tater-Vaněk, 2001; Brüning-Geyler-Margulis-Pyataev, 2002]; it appears that scattering properties *en gross* are not very sensitive to the coupling:

- 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

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

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

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

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 $|t(k)|^2 = \mathcal{O}(k^{-2})$. One can *conjecture* that *coarse-grained* transmission through our “bubble” has the same decay as $k \to \infty$

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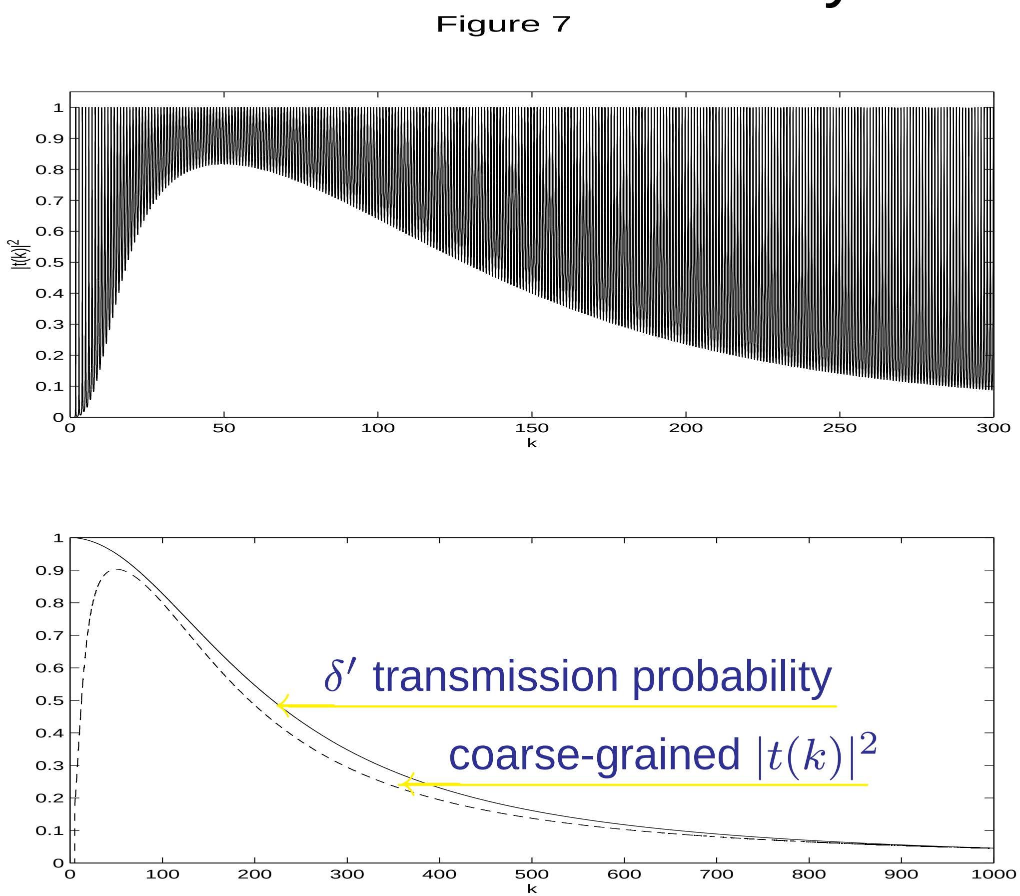

An *asymmetric* spherical scatterer

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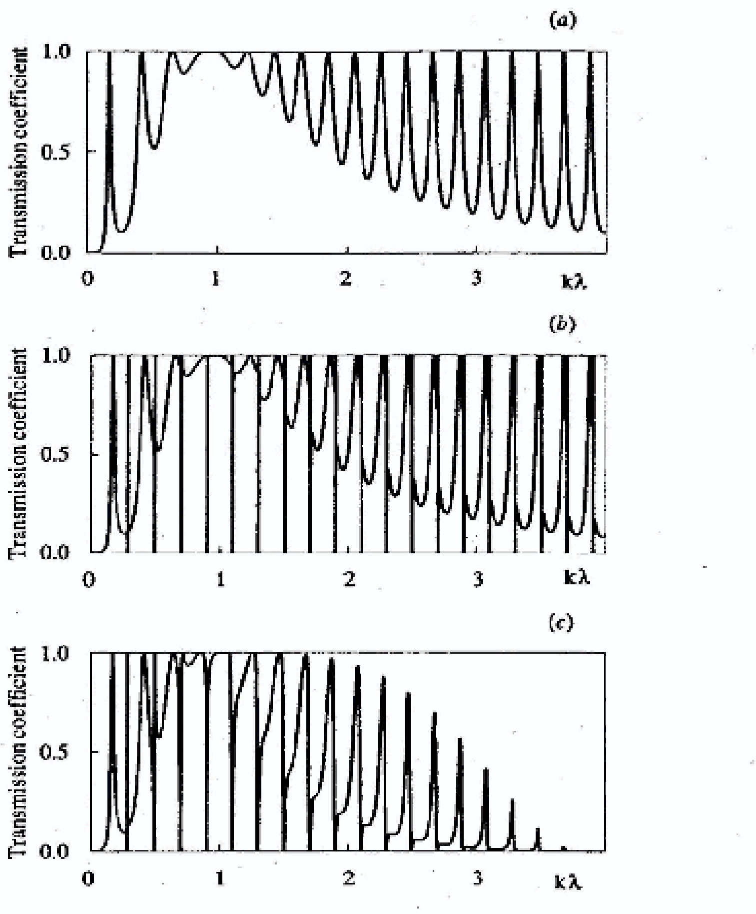

Figure 2. The transmission coefficient as a function of $k\lambda$ at $a = 10\lambda$: (*a*) $r = \pi a$; (*b*) $r = 0.98\pi a$; (*c*) $r = 0.96\pi a$.

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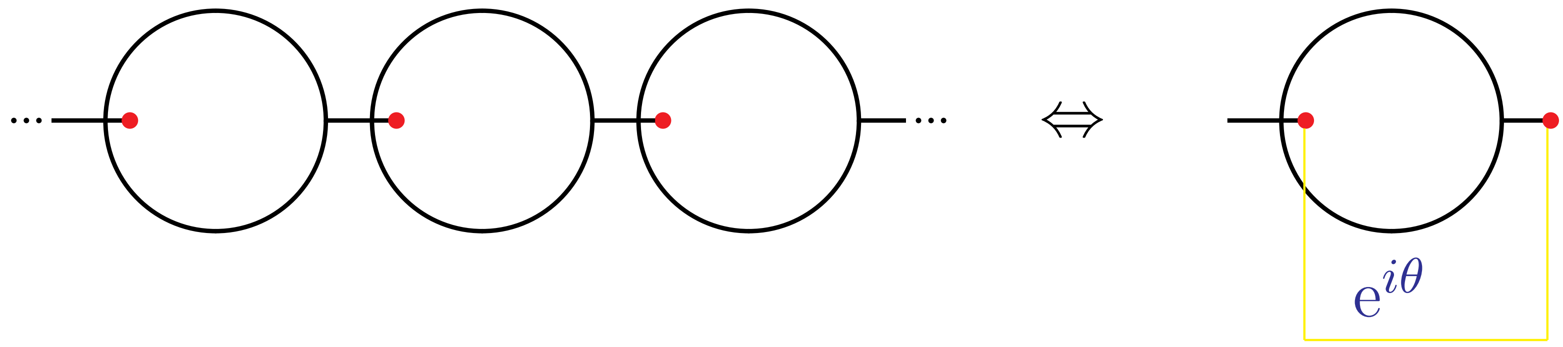
Furthermore, infinite periodic systems can be treated by Floquet-Bloch decomposition



Sphere array spectrum

A band spectrum example from [E.-Tater-Vaněk, 2001]:
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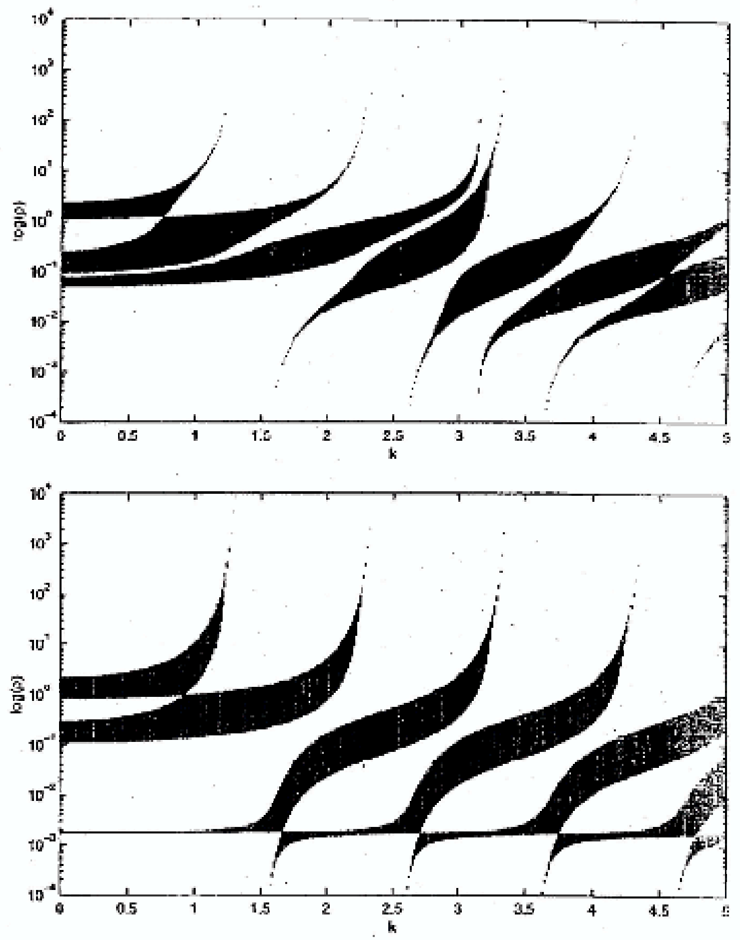

FIG. 8. Band spectrum of an infinite "bubble" array. The spheres are of unit radius, the spacing is l = 1 (upper figure) and l = 0.01 (lower figure), ρ is the contact radius.

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

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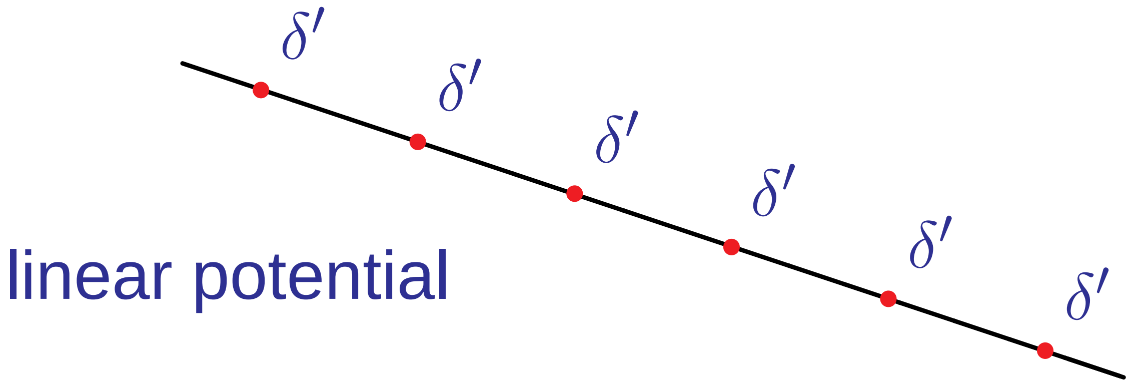
Recall properties of *singular Wannier-Stark* systems:



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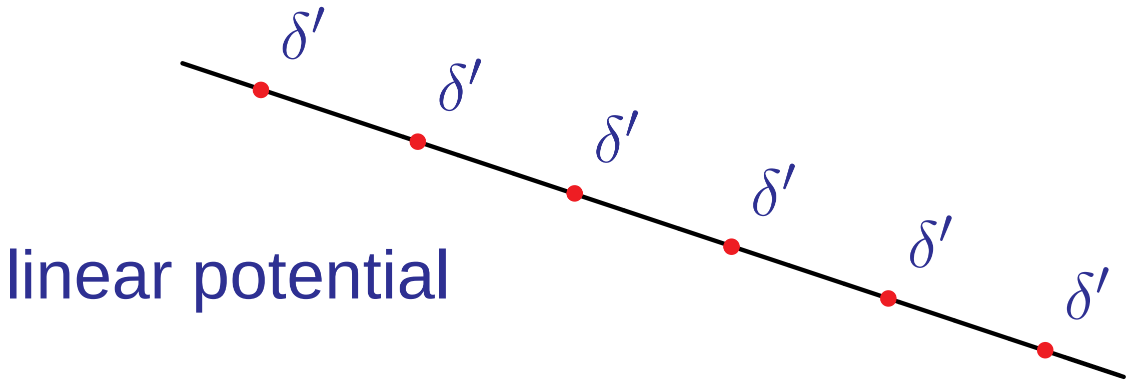
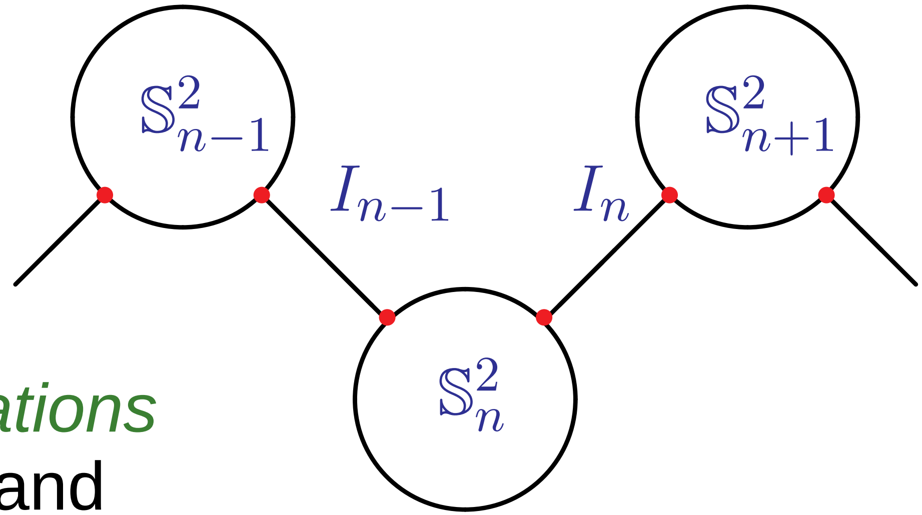


Spectrum of such systems is *purely discrete* which is proved for "most" values of the parameters [Asch-Duclos-E., 1998] and conjectured for *all* values. The reason behind are *large gaps* of δ' Kronig-Penney systems

Periodic systems – assumptions



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

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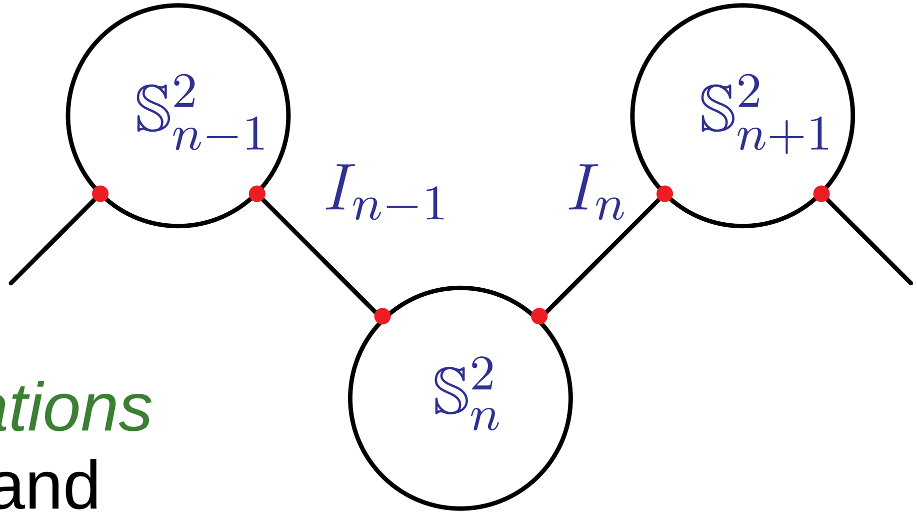

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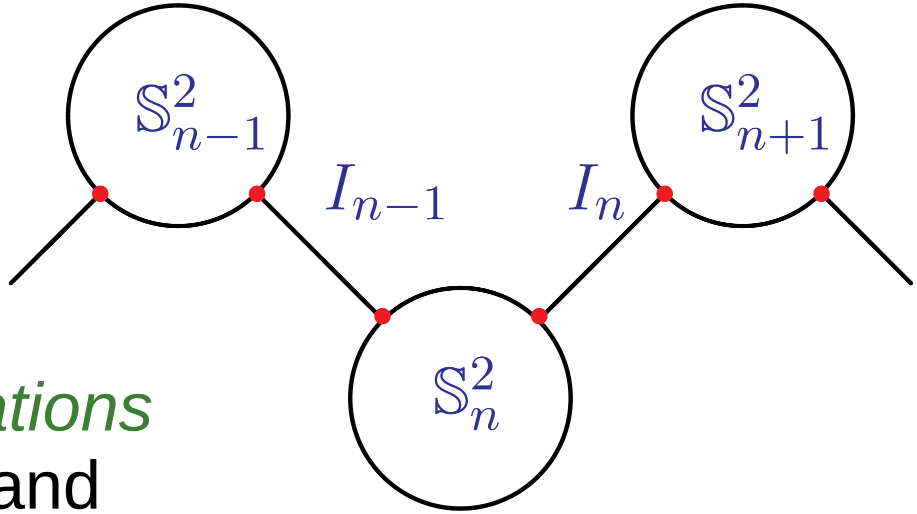

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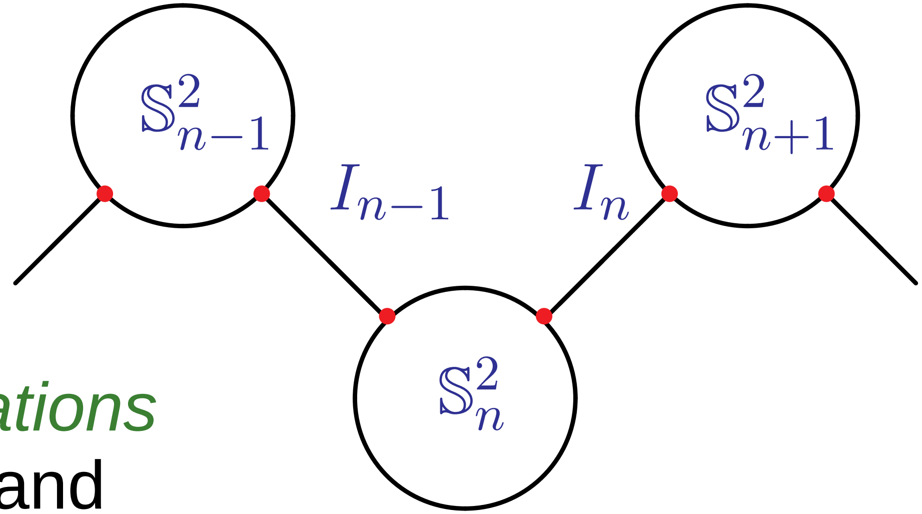

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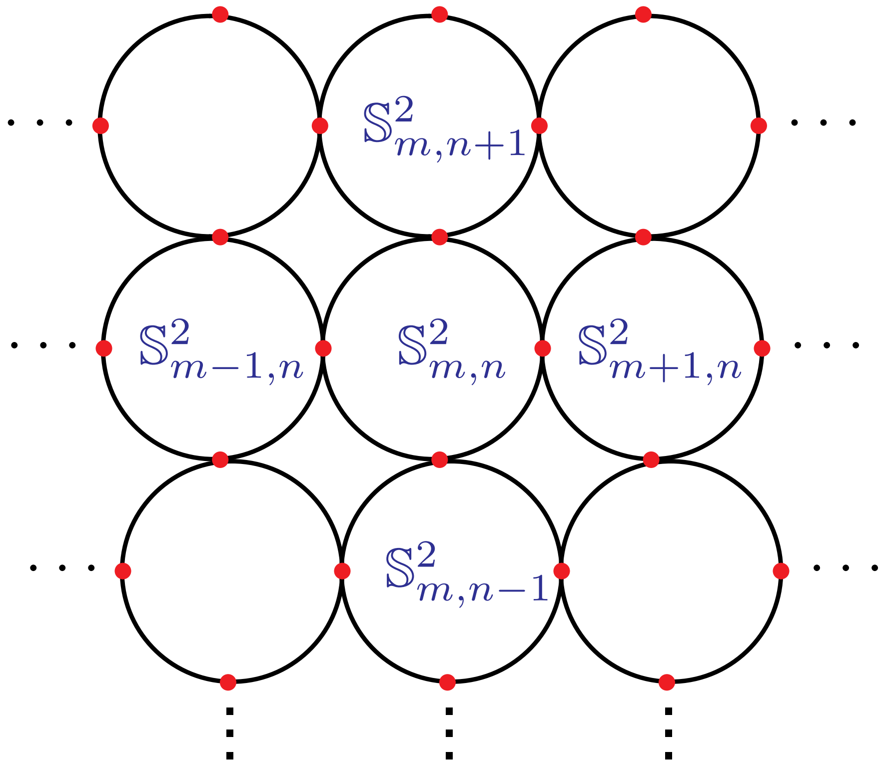
- we allow also *tight coupling* when the spheres touch

Tightly coupled spheres



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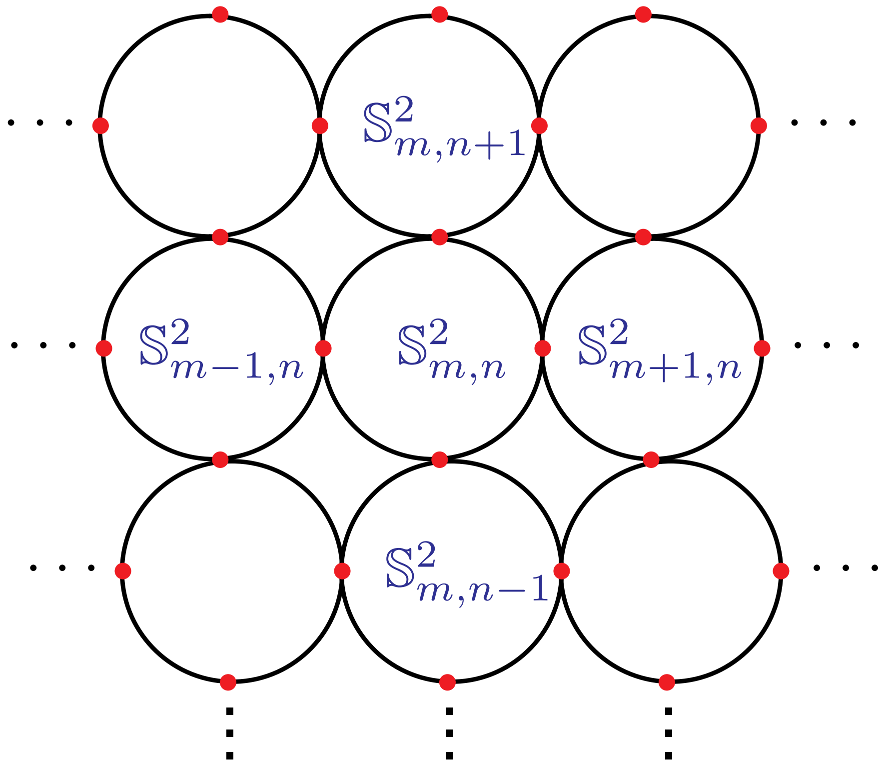

The tight-coupling boundary conditions will be

$$\begin{aligned} L_1(\Phi_1) &= AL_0(\Phi_1) + CL_0(\Phi_2)\,, \\ L_1(\Phi_2) &= \bar{C}L_0(\Phi_1) + DL_0(\Phi_2) \end{aligned}$$

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

holds as $n\to\infty$ for *loosely connected* systems, where $\epsilon=\frac12$ for arrays and $\epsilon=\frac14$ 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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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 $n \to \infty$

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

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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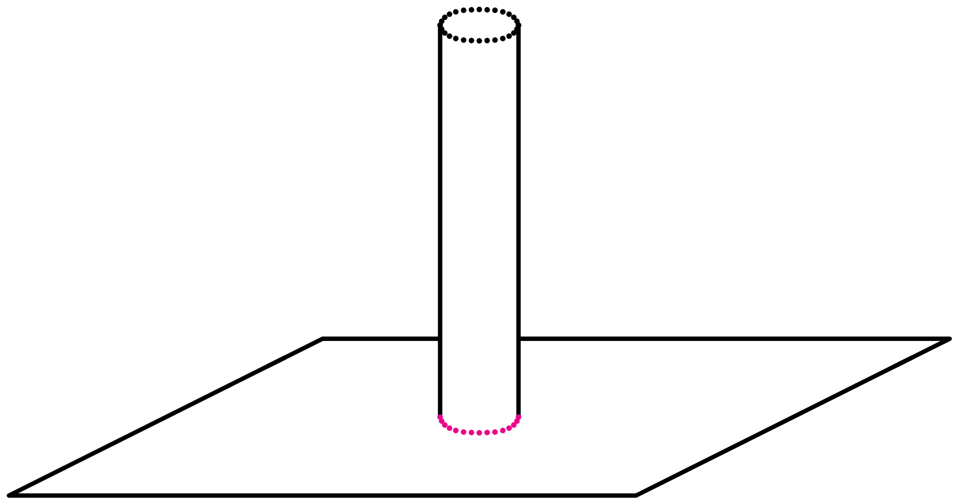

Plane plus tube scattering

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

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

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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- Let a *rectangular resonator* be equipped with an *antenna* which serves a source. Such a system has many resonances; we ask about distribution of their spacings
- 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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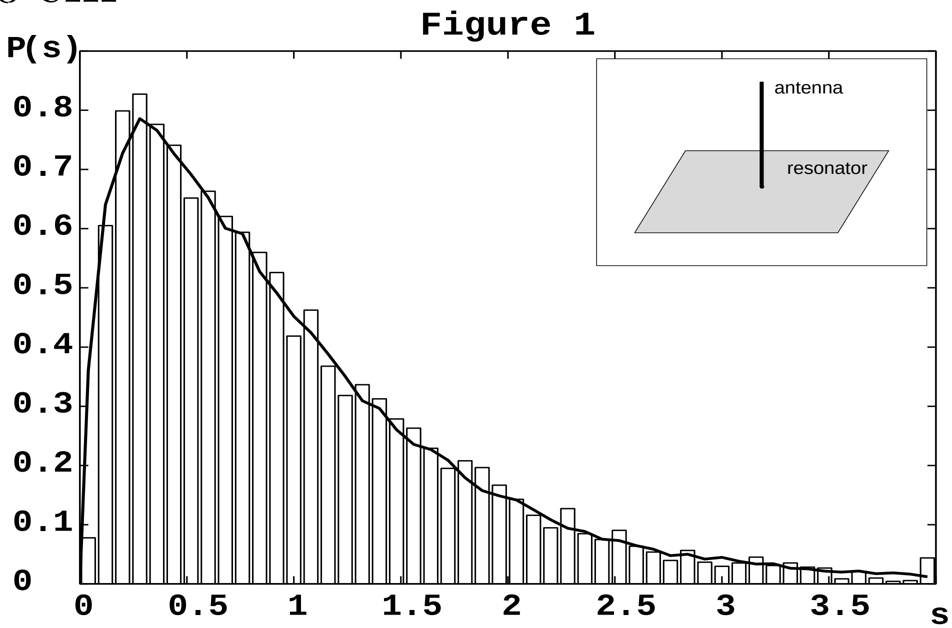

Important: An agreement is achieved with the *lower third* of measured frequencies – confirming thus validity of our approximation, since shorter wavelengths are comparable with the antenna radius a and $ka \ll 1$ is no longer valid

Spin conductance oscillations

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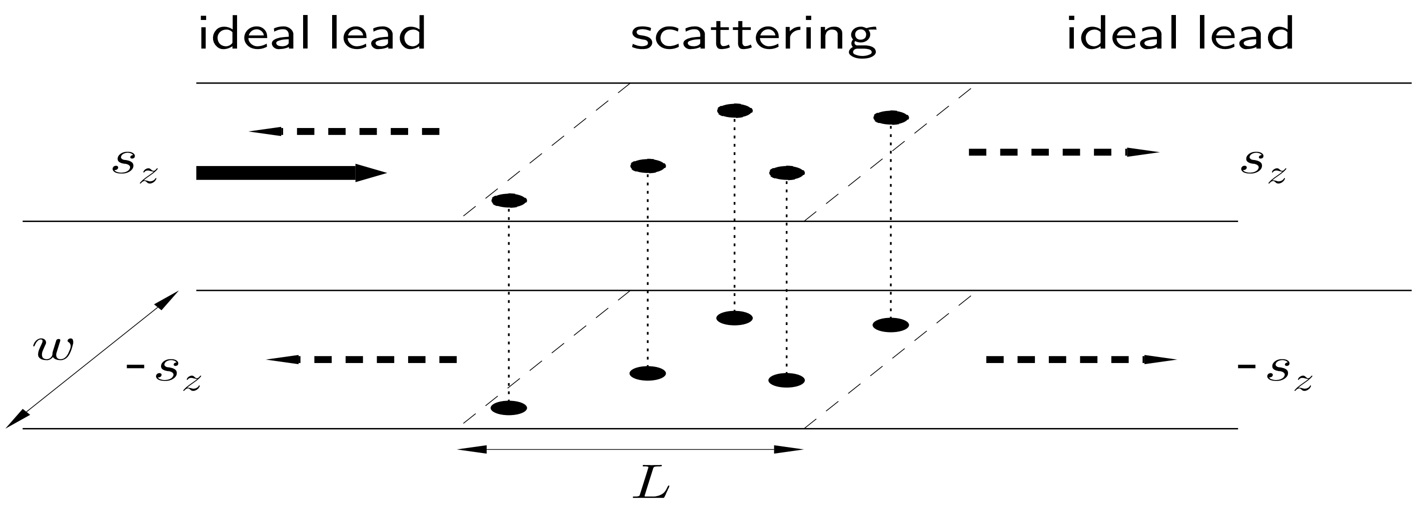
We construct a *model* in which spin-flipping interaction has a *point character*. Semiconductor bar is described as *two strips coupled at the impurity sites* by the boundary condition described above

Spin-orbit coupled strips



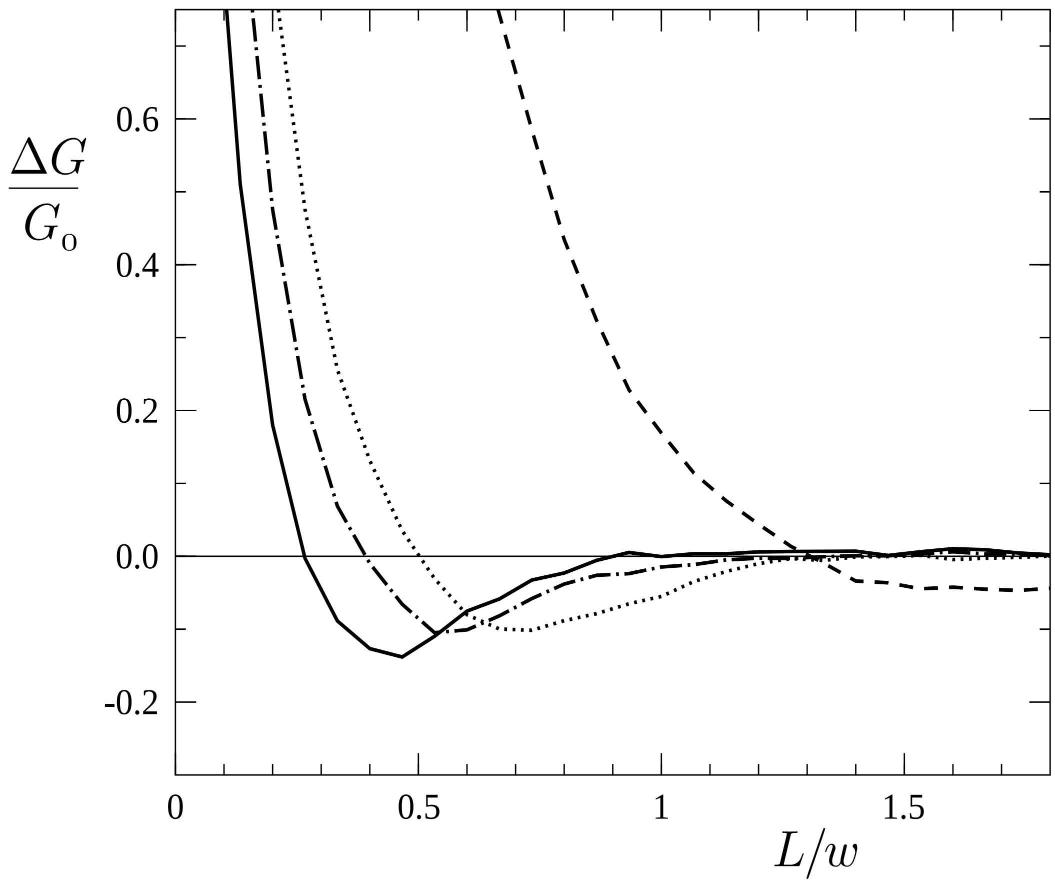
We assume that impurities are randomly distributed with the same coupling, $A = D$ and $C \in \mathbb{R}$. Then we can instead study a pair of decoupled strips,

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

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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As the last part of this talk let me therefore attempt to reconstruct, without going to details, what he might want to say in that lecture which never occurred

Spin-orbit interaction

Let us thus return to our first example and see how it changes when the particle is an *electron with spin* which is subject to *spin-orbit interaction*. Recall first a few facts:

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Consider the state Hilbert space is $\mathcal{H}_{\mathrm{plane}} = L^2(\mathbb{R}^2, \mathbb{C}^2)$ with the free Hamiltonian $\hat{H}_0 = \frac{1}{2m^*}\mathbf{p}^2\sigma_0$, where $p_j = -i\hbar\partial_j$ and σ_0 is the 2×2 unit matrix. One uses conventionally either the *Rashba Hamiltonian*

$$\hat{H}_{\mathrm{R}} := \hat{H}_0 + \frac{\alpha_{\mathrm{R}}}{\hbar}\hat{U}_{\mathrm{R}}\,, \qquad \hat{U}_{\mathrm{R}} := \sigma_1 p_2 - \sigma_2 p_1\,,$$

where $\alpha_{\mathrm{R}} \in$ is the Rashba constant and σ_j are the usual Pauli matrices, or the *Dresselhaus Hamiltonian*

$$\hat{H}_{\mathrm{D}} := \hat{H}_0 + \frac{\alpha_{\mathrm{D}}}{\hbar}\hat{U}_{\mathrm{D}}\,, \qquad \hat{U}_{\mathrm{D}} := \sigma_2 p_2 - \sigma_1 p_1\,.$$

Getting rid of the constants

Since the choice of the units is again unimportant we get rid of the constants in the usual way introducing $\mathbf{k} := \hbar^{-1}\mathbf{p}$ and $\varkappa_j := \hbar^{-2} m^* \alpha_{\mathrm{J}},\; \mathrm{J} = \mathrm{R}, \mathrm{D}$. Up to the multiplicative factor, $\hat{H}_{\mathrm{J}} = \frac{\hbar^2}{2m^*} H_{\mathrm{J}},\; \mathrm{J} = \mathrm{R}, \mathrm{D},$ the both versions of the Hamiltonian acquire then the simple form

$$H_{\mathrm{J}} = H_0 + 2\varkappa_{\mathrm{J}} U_{\mathrm{J}}\,, \quad U_{\mathrm{R}} := \sigma_1 k_2 - \sigma_2 k_1\,, \quad U_{\mathrm{D}} := \sigma_2 k_2 - \sigma_1 k_1$$

with $H_0 := \mathbf{p}^2 \sigma_0$, which we shall use in the following

Green's function of $H_{\rm J}$

It was derived in [Brüning-Geyler-Pankrashkin'07]. By a nice algebraic trick, so characteristic for the work of Volodya Geyler, the problem is reformulated as a scalar one which involves the kernel $G_0(\mathbf{x},\mathbf{x}';z) = \frac{1}{2\pi}K_0(\sqrt{-z}|\mathbf{x}-\mathbf{x}'|)$ of the Laplacian in $L^2(\mathbb{R}^2)$, leading to

$$G_{\rm J}(\mathbf{x},\mathbf{x}';z) = \begin{pmatrix} G_{\rm J}^{11}(\mathbf{x},\mathbf{x}';z) & G_{\rm J}^{12}(\mathbf{x},\mathbf{x}';z) \\ G_{\rm J}^{21}(\mathbf{x},\mathbf{x}';z) & G_{\rm J}^{22}(\mathbf{x},\mathbf{x}';z) \end{pmatrix}$$

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Here the diagonal elements are

$$G_\mathrm{J}^{11}(\mathbf{x},\mathbf{x}';z) = G_\mathrm{J}^{22}(\mathbf{x},\mathbf{x}';z) = \frac{1}{4\pi}\Big[-\frac{\varkappa_\mathrm{J}}{\mathrm{i}\sqrt{-(z+\varkappa_\mathrm{J}^2)}}$$

$$\times\big(K_0(\zeta_\mathrm{J}^+|\mathbf{x}-\mathbf{x}'|) - K_0(\zeta_\mathrm{J}^-|\mathbf{x}-\mathbf{x}'|)\big) + K_0(\zeta_\mathrm{J}^+|\mathbf{x}-\mathbf{x}'|) + K_0(\zeta_\mathrm{J}^-|\mathbf{x}-\mathbf{x}'|)\Big]$$

for both the $\mathrm{J}=\mathrm{R},\mathrm{D}$.

Green's function of H_J, continued

On the other hand, the off-diagonal ones are

$$G_\mathrm{R}^{12}(\mathbf{x},\mathbf{x}';z) = \frac{\mathrm{i}(x_2-x_2')-(x_1-x_1')}{4\pi\,\mathrm{i}\sqrt{-(z+\varkappa_\mathrm{R}^2)}\,|\mathbf{x}-\mathbf{x}'|}\sum_{\nu=\pm}\nu\,\zeta_\mathrm{R}^\nu K_1\big(\zeta_\mathrm{R}^\nu|\mathbf{x}-\mathbf{x}'|\big)\,,$$

$$G_\mathrm{D}^{12}(\mathbf{x},\mathbf{x}';z) = \frac{(x_2-x_2')-\mathrm{i}(x_1-x_1')}{4\pi\,\mathrm{i}\sqrt{-(z+\varkappa_\mathrm{D}^2)}\,|\mathbf{x}-\mathbf{x}'|}\sum_{\nu=\pm}\nu\,\zeta_\mathrm{D}^\nu K_1\big(\zeta_\mathrm{D}^\nu|\mathbf{x}-\mathbf{x}'|\big)\,,$$

and $G_\mathrm{J}^{21}(\mathbf{x},\mathbf{x}';z)=\overline{G_\mathrm{J}^{12}(\mathbf{x}',\mathbf{x};\bar z)}$; the effective momenta appearing in these expressions are defined as

$$\zeta_\mathrm{J}^\pm := \sqrt{-(z+\varkappa_\mathrm{J}^2)}\pm\mathrm{i}\varkappa_\mathrm{J}$$

Renormalized Green's function

Subtracting the divergence of the diagonal we get

$$G_{\mathrm{J}}^{\mathrm{ren}}(z) := \lim_{\mathbf{x}'\to\mathbf{x}} \left[G_{\mathrm{J}}(\mathbf{x},\mathbf{x}';z) + \frac{1}{2\pi} \ln|\mathbf{x}-\mathbf{x}'|\sigma_0 \right];$$

the limit is independent of the position $\mathbf{x}$ in view of the translational invariance of H_{J}. By a direct computation the off-diagonal elements vanish in the limit while

$$G_{\mathrm{J}}^{\mathrm{ren};jj}(z) = -\frac{\varkappa_{\mathrm{J}}}{2\mathrm{i}\sqrt{-(z+\varkappa_{\mathrm{J}}^2)}}(Q(\zeta^+)-Q(\zeta^-))+\frac{1}{2}(Q(\zeta^+)+Q(\zeta^-))$$

with $Q(z) := \frac{1}{2\pi}(\psi(1) - \frac{1}{2}\ln(-z) + \ln 2)$.

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$$G_{\mathrm{J}}^{\mathrm{ren}}(z) = \frac{1}{2\pi}\left[\psi(1)-\frac{1}{2}\ln\left(-\frac{z}{4}\right)+\frac{\varkappa_{\mathrm{J}}}{2\mathrm{i}\sqrt{-(z+\varkappa_{\mathrm{J}}^2)}}\ln\frac{\sqrt{-(z+\varkappa_{\mathrm{J}}^2)}+i\varkappa_{\mathrm{J}}}{\sqrt{-(z+\varkappa_{\mathrm{J}}^2)}-\mathrm{i}\varkappa_{\mathrm{J}}}\right]\sigma_0,$$

where $-\psi(1) \approx 0.577$ is the Euler-Mascheroni constant

A remark on the magnetic case

The case when a homogeneous magnetic field $B = \frac{\hbar c}{e} b$ perpendicular to the plane is applied is treated in an analogous manner

The momentum $\mathbf{k}$ in the Hamiltonian has to be replaced with $\mathbf{K} = \mathbf{k} - \mathbf{a}$ where $\mathbf{A} = \frac{\hbar c}{e}\mathbf{a}$ is the vector potential associated with the field, and the *Zeeman term* $\gamma b \sigma_3$ with $\gamma := \frac{1}{2} g_* \frac{m_*}{m_e}$ has to be added.

The the reduction to the scalar case works again and yields explicit expression for Green's functions in terms of confluent hypergeometric instead of Bessel functions – see [Brüning-Geyler-Pankrashkin'07]

“Hybrid plane” with SO interaction

Since the lead carries the same spin $\frac{1}{2}$ particle its component Hilbert space is $\mathcal{H}_{\mathrm{lead}} = L^2(\mathbb{R}_+, \mathbb{C}^2)$, and the whole state space of the system is the consequently the orthogonal sum $\mathcal{H} := \mathcal{H}_{\mathrm{lead}} \oplus \mathcal{H}_{\mathrm{plane}}$.

The wave functions are thus of the form $\Psi = \{\psi_{\mathrm{lead}}, \psi_{\mathrm{plane}}\}^{\mathrm{T}}$ where each of the components is a 2×1 column.

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We start from the decoupled operator $H^0 := H_{\mathrm{lead}} \oplus H_J$ where the first component acts as $H_{\mathrm{lead}}\psi_{\mathrm{lead}} = -\psi''_{\mathrm{lead}}$ with *Neumann boundary condition* at the endpoint. We restrict H^0 to functions which vanish in the vicinity of the junction, obtaining thus a symmetric operator of *deficiency indices* $(4, 4)$, and after that we seek admissible Hamiltonians among its self-adjoint extensions.

The self-adjoint extensions

We need the boundary values. Those on the halfline are the columns $\psi_{\mathrm{lead}}(0+)$ and $\psi'_{\mathrm{lead}}(0+)$; in the plane they are coefficients in the expansion

$$\psi_{\mathrm{plane}}(\mathbf{x}) = -\frac{1}{2\pi} L_0(\psi_{\mathrm{plane}}) \ln|\mathbf{x}| + L_1(\psi_{\mathrm{plane}}) + o(|\mathbf{x}|) \,.$$

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Now we can write the sought boundary conditions as

$$\begin{aligned} \psi'_{\mathrm{lead}}(0+) &= A\psi_{\mathrm{lead}}(0+) + C^* L_0(\psi_{\mathrm{plane}})\,, \\ L_1(\psi_{\mathrm{plane}}) &= C\psi_{\mathrm{lead}}(0+) + D L_0(\psi_{\mathrm{plane}})\,, \end{aligned}$$

where A, C, D are 2×2 *matrices*, the first and the third Hermitian, so $\mathcal{A} := \left(\begin{smallmatrix} A & C^* \\ C & D \end{smallmatrix}\right)$ depends of 16 real parameters

The analogous b.c. apply also to the magnetic case in view of the same character of the singularity.

Boundary conditions, continued

The above b.c. are generic but do not cover the cases of a singular $\mathcal{A}$. More generally, we can take

$$\mathcal{A}\begin{pmatrix}\psi_{\text{lead}}(0+)\\ L_0(\psi_{\text{plane}})\end{pmatrix}+\mathcal{B}\begin{pmatrix}\psi'_{\text{lead}}(0+)\\ L_1(\psi_{\text{plane}})\end{pmatrix}=0\,,$$

where $(\mathcal{A}|\mathcal{B})$ has rank four and $\mathcal{A}\mathcal{B}^*$ is Hermitean

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Sixteen parameters may be too many. Some simplifications:

- the contact does not couple the spin states, A, C, D diagonal
- the coupling is spin-independent, the matrices are scalar
- the "natural" conditions similar to the above,

$$A=\frac{1}{2\rho}\,\sigma_0\,,\quad C=\frac{1}{\sqrt{2\pi\rho}}\,\sigma_0\,,\quad D=-\sigma_0\,\ln\rho\,.$$

Full Green's function

We employ Krein's formula. The starting point is Green function of the decoupled system which is block-diagonal,

$$G^0(x,x';\mathbf{x},\mathbf{x}';z) = \begin{pmatrix} G_{\mathrm{lead}}(x,x';z) & 0 \\ 0 & G_{\mathrm{J}}(\mathbf{x},\mathbf{x}';z) \end{pmatrix},$$

where $G_{\mathrm{lead}}(x,x';z) = \frac{\mathrm{i}}{\sqrt{z}} \cos\sqrt{z}x_< \, \mathrm{e}^{-\mathrm{i}\sqrt{z}x_>} \, \sigma_0$ corresponding to *Neumann b.c.*, and $G_{\mathrm{J}}(\mathbf{x},\mathbf{x}';z)$ was given above

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The Krein function $Q(z)$, which is an analytic 4×4-matrix valued function of the spectral parameter z, is defined through diagonal values of the kernel, with renormalization,

$$Q(z) := \begin{pmatrix} \frac{\mathrm{i}}{\sqrt{z}}\,\sigma_0 & 0 \\ 0 & G_{\mathrm{J}}^{\mathrm{ren}}(z) \end{pmatrix}$$

Full Green's function, continued

Put $\tilde{\Gamma}_1\psi := \binom{-\psi'_{\mathrm{lead}}(0+)}{L_0(\psi_{\mathrm{plane}})}$ and $\tilde{\Gamma}_2\psi := \binom{\psi_{\mathrm{lead}}(0+)}{L_1(\psi_{\mathrm{plane}})}$, then the b.c. can be rewritten as $\tilde{\mathcal{A}}\tilde{\Gamma}_1\psi + \tilde{\mathcal{B}}\tilde{\Gamma}_2\psi = 0$ with $\tilde{\mathcal{B}} = -I$ and

$$\tilde{\mathcal{A}} := \begin{pmatrix} -A^{-1} & -A^{-1}C^* \\ -CA^{-1} & D - CA^{-1}C^* \end{pmatrix};$$

the comparison operator H^0 is characterized by $\tilde{\Gamma}_1\psi = 0$.

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Even if the coupling is spin-independent, $\mathcal{A} = \begin{pmatrix} a & \bar c \\ c & d \end{pmatrix} \otimes \sigma_0$, the Green function *does not decompose* because spin states are coupled by the spin-orbit interaction in the plane.

Properties of $H_{\mathcal{A}}$

We suppose that the coupling is nontrivial, i.e. $\mathcal{A}$ is not block-diagonal. Moreover, we suppose that the coupling is spin-independent, $\mathcal{A} = \left(\begin{smallmatrix} a & \bar{c} \\ c & d \end{smallmatrix}\right) \otimes \sigma_0$ with $c \neq 0$, so

$$Q(z) = \begin{pmatrix} \frac{\mathrm{i}}{\sqrt{z}} - \tilde{a} & -\tilde{\bar{c}} \\ -\tilde{c} & G_{\mathrm{J}}^{\mathrm{ren}}(z) - \tilde{d} \end{pmatrix} \otimes \sigma_0 \, .$$

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Note first that *the junction can bind*: to any $-\kappa^2 \in (-\varkappa_{\mathrm{J}}^2, 0)$ one can find $H_{\mathcal{A}}$ for which it is an eigenvalue. Indeed, $Q(z)$ is singular if the relation $(\kappa^{-1} - \tilde{a})(G_{\mathrm{J}}^{\mathrm{ren}}(-\kappa^2) - \tilde{d}) = |\tilde{c}|^2$ is valid, or in the original parameters

$$(\kappa - a)(G_{\mathrm{J}}^{\mathrm{ren}}(-\kappa^2) - d) = |c|^2 \,.$$

Since $G_{\mathrm{J}}^{\mathrm{ren}}(-\kappa^2)$ is real-valued for $\kappa^2 < \varkappa_{\mathrm{J}}^2$, it is easy to pick a, d in such a way that the condition is satisfied.

The scattering problem

Let us pass to the transport through the junction. Using Krein's formula and the fact that any vector of $\mathcal{H}$ can be written as $(H^0 - z)^{-1}\psi^0$ for $\psi^0 \in D(H^0)$ and $\operatorname{Im} z \neq 0$, we get

$$\psi = \psi^0 - \gamma_z [Q(z) - \mathcal{A}]^{-1} \gamma_{\bar{z}}^* (H^0 - z)^{-1} \psi^0 \,,$$

where $\gamma_z :\, \mathbb{C}^4 \to \mathcal{H}$ is the trace operator given by the kernel $G^0(x, 0; \mathbf{x}, \mathbf{0}; z)$ and γ_z^* is its adjoint.

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Note that $\gamma_{\bar{z}}^*(H^0 - z)^{-1}\psi^0$ is just the vector of the values at the junction and $Q(z) - \mathcal{A}$ is position-independent, so the second term at the RHS is easy to compute.

We employ the usual trick letting z to approach a real value k^2. The resulting function ceases to be L^2 but it still satisfies locally the boundary conditions at the junction yielding a *generalized eigenfunction* associated with the scattering.

Reflection amplitude

In particular, let us choose the vector ψ^0 with the "upper" component only, $\psi^0_{\text{plane}} = 0$ and $\psi^0_{\text{lead}} = \cos kx$ (recall the Neumann b.c. at the origin!). It is straightforward to invert $Q(z)$ and to compute ψ ; it yields the *reflection amplitude* at momentum k,

$$\mathcal{R}(k) = \frac{\left(-\frac{\mathrm{i}}{k} - \tilde{a}\right)\left(G_{\mathrm{J}}^{\mathrm{ren}}(k^2) - \tilde{d}\right) - |\tilde{c}|^2}{\left(\frac{\mathrm{i}}{k} - \tilde{a}\right)\left(G_{\mathrm{J}}^{\mathrm{ren}}(k^2) - \tilde{d}\right) - |\tilde{c}|^2},$$

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naturally independent of the particle spin state, or in terms of the original parameters

$$\mathcal{R}(k) = -\frac{(a + \mathrm{i}k)(G^{\mathrm{ren}}_{\mathrm{J}}(k^2) - d) + |c|^2}{(a - \mathrm{i}k)(G^{\mathrm{ren}}_{\mathrm{J}}(k^2) - d) + |c|^2}.$$

Observations

- Since $G_{\mathrm{J}}^{\mathrm{ren}}(k^2)$ is generally complex $|\mathcal{R}(k)|^2 \neq 1$ for $|c| \neq 0$ which is natural because the coupling allows the particle to pass from the lead to the plane

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- Various ways from here are open and inviting

Coda

Time came to fall silent, recall what the old ones were saying

Curae leves loquuntur, ingentes stupent

Slight griefs talk, great ones are speechless