Schrödinger operators with strongly attractive graph-type interaction

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Talk overview

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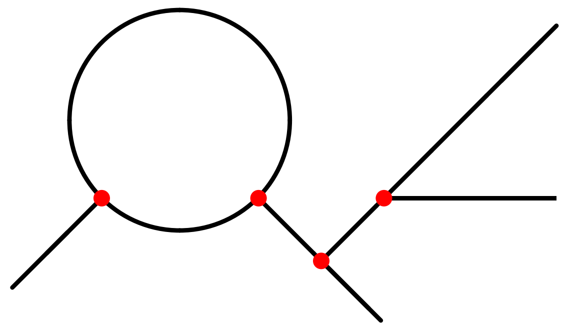
- Open questions

Leaky graphs – why are they interesting?

Recall the “standard” graph models:



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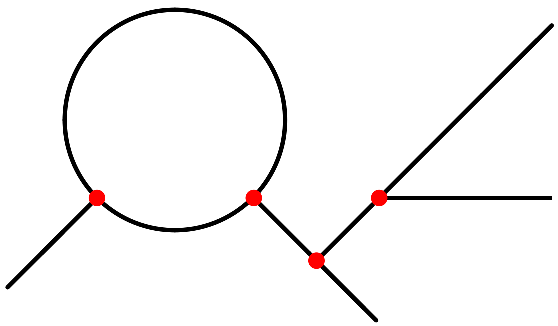

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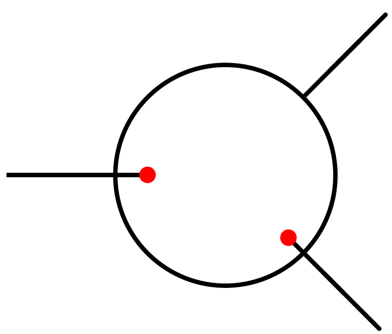
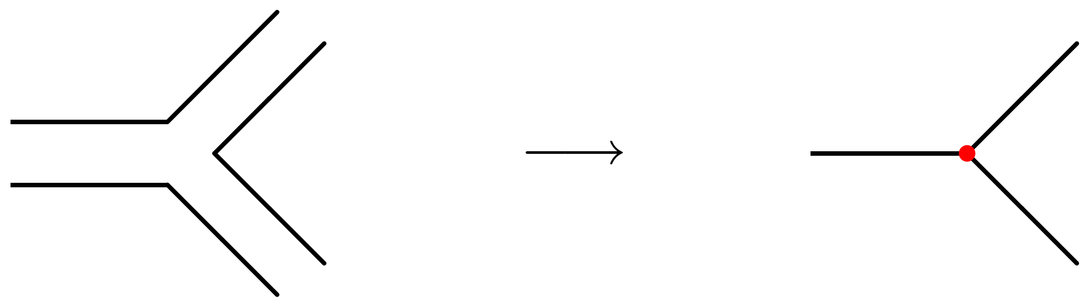
Also, generalized graphs – nanotubes + fullerenes, etc.



the edges same above,
$-\Delta_{\mathrm{LB}} + v(x)$ on the manifold
boundary conditions at vertices

Drawbacks of these models

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



However, the answer is known so far only for Neumann-type situations [Rubinstein-Schatzman, 2001; Kuchment-Zeng, 2001; E.-Post, 2003], the Dirichlet case needed here is open (and difficult)

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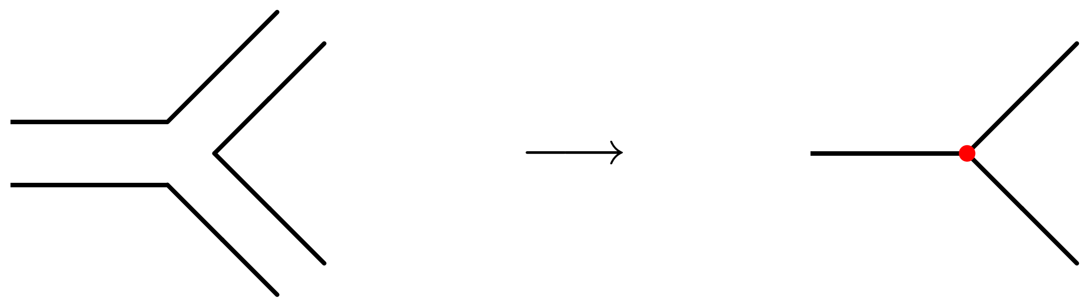

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- Quantum tunneling is neglected: recall that a true quantum-wire boundary is a finite potential jump

Leaky quantum graphs

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

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

in $L^2(\mathbb{R}^n)$, where Γ is a graph in question, or generalized graph, understood as a subset of $\mathbb{R}^n$

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In this talk we will *mostly* consider the simplest graphs, or *building blocks* or more complicated graphs, where Γ is a *smooth manifold* in $\mathbb{R}^n$. We have in mind three cases:

- curves in $\mathbb{R}^2$
- surfaces in $\mathbb{R}^3$
- curves in $\mathbb{R}^3$

Definition of the Hamiltonian

In the first two cases we have $\operatorname{codim}\Gamma = 1$ and the operator can be defined by means of quadratic form,

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

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

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

The case $\operatorname{codim} \Gamma = 2$

Boundary conditions can be used but they are more complicated. Moreover, for an infinite Γ corresponding to $\gamma : \mathbb{R} \to \mathbb{R}^3$ we have to assume in addition that there is a tubular neighbourhood of Γ which *does not intersect itself*

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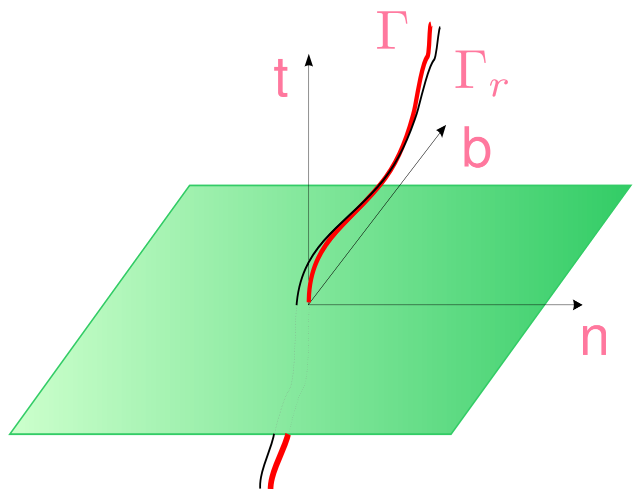
Employ *Frenet's frame* $(t(s), b(s), n(s))$ for Γ. Given $\xi, \eta \in \mathbb{R}$ we set $r = (\xi^2 + \eta^2)^{1/2}$ and define family of "shifted" curves



$$\Gamma_r \equiv \Gamma_r^{\xi\eta} := \{\, \gamma_r(s) \equiv \gamma_r^{\xi\eta}(s) := \gamma(s) + \xi b(s) + \eta n(s) \,\}$$

The case $\operatorname{codim}\Gamma = 2$

The restriction of $f \in W^{2,2}_{\mathrm{loc}}(\mathbb{R}^3 \setminus \Gamma)$ to Γ_r is well defined for small r; we say that $f \in W^{2,2}_{\mathrm{loc}}(\mathbb{R}^3 \setminus \Gamma) \cap L^2(\mathbb{R}^3)$ belongs to Υ if

$$\begin{aligned} \Xi(f)(s) &:= -\lim_{r\to 0} \frac{1}{\ln r} f\restriction_{\Gamma_r}(s)\,, \\ \Omega(f)(s) &:= \lim_{r\to 0} \left[f\restriction_{\Gamma_r}(s) + \Xi(f)(s) \ln r \right]\,, \end{aligned}$$

exist a.e. in $\mathbb{R}$, are independent of the direction $\frac{1}{r}(\xi,\eta)$, and define functions from $L^2(\mathbb{R})$

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Then the operator $H_{\alpha,\Gamma}$ has the domain

$$\{\, g \in \Upsilon :\ 2\pi\alpha\Xi(g)(s) = \Omega(g)(s) \,\}$$

and acts as

$$-H_{\alpha,\Gamma} f = -\Delta f \quad \text{for} \quad x \in \mathbb{R}^3 \setminus \Gamma$$

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- The b.c. are natural describing point interaction in the normal plane to Γ. Thus there is *no way* (at least within standard QM) to define $H_{\alpha,\Gamma}$ in the case $\operatorname{codim}\Gamma \geq 4$
- Strong coupling considered below is closely related to *semiclassical behaviour* of the operator

$$H_{\alpha,\Gamma}(h) = -h^2\Delta - \alpha\delta(x-\Gamma)\,, \quad \alpha > 0\,,$$

which can be regarded as $h^2 H_{\alpha(h),\Gamma}$, where the effective coupling constant is $\alpha(h) := \alpha h^{-2}$ for $\operatorname{codim}\Gamma = 1$, and

$$\alpha(h) := \alpha + \frac{1}{2\pi}\ln h \quad \text{if} \quad \operatorname{codim}\Gamma = 2$$

Geometrically induced spectrum

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

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

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

  in the sector $S_\omega:=\left\{(s,s'):\;\omega<\frac{s}{s'}<\omega^{-1}\right\}$
- straight line is excluded, i.e. $|\Gamma(s)-\Gamma(s')|<|s-s'|$ holds for some $s,s'\in\mathbb{R}$

Bending means binding

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

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

Proof: generalized BS principle

Classical Birman-Schwinger principle based on the identity

$$(H_0 - V - z)^{-1} = (H_0 - z)^{-1} + (H_0 - z)^{-1} V^{1/2} \times \left\{ I - |V|^{1/2} (H_0 - z)^{-1} V^{1/2} \right\}^{-1} |V|^{1/2} (H_0 - z)^{-1}$$

can be extended to generalized Schrödinger operators $H_{\alpha,\Gamma}$ [BEKŠ94]: the multiplication by $(H_0 - z)^{-1} V^{1/2}$ etc. is replaced by suitable trace maps. In this way we find that $-\kappa^2$ is an eigenvalue of $H_{\alpha,\Gamma}$ *iff* the integral operator $\mathcal{R}^{\kappa}_{\alpha,\Gamma}$ on $L^2(\mathbb{R})$ with the kernel

$$(s, s') \mapsto \frac{\alpha}{2\pi} K_0 \left(\kappa |\Gamma(s) - \Gamma(s')| \right)$$

has an eigenvalue equal to one

Sketch of the proof

We treat $\mathcal{R}^{\kappa}_{\alpha,\Gamma}$ as a *perturbation* of the operator $\mathcal{R}^{\kappa}_{\alpha,\Gamma_0}$ referring to a *straight line*. The spectrum of the latter is found easily: it is *purely ac* and equal to $[0, \alpha/2\kappa)$

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The curvature-induced perturbation is *sign-definite*: we have $\left(\mathcal{R}^\kappa_{\alpha,\Gamma} - \mathcal{R}^\kappa_{\alpha,\Gamma_0}\right)(s,s') \geq 0$, and the inequality is sharp somewhere unless Γ is a straight line. Using a *variational argument* with a suitable trial function we can check the inequality $\sup \sigma(\mathcal{R}^\kappa_{\alpha,\Gamma}) > \frac{\alpha}{2\kappa}$

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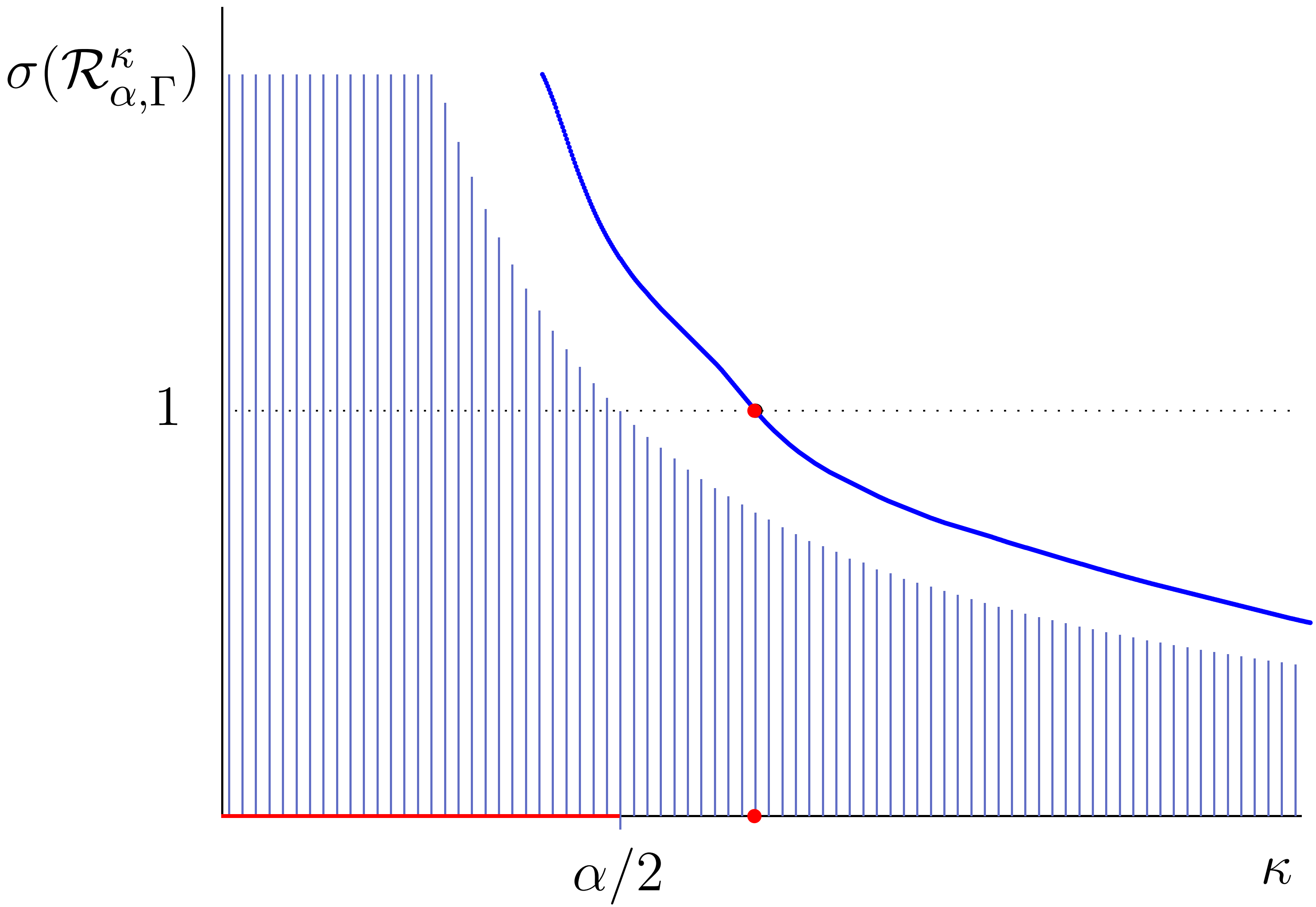
To conclude we employ continuity and $\lim_{\kappa\to\infty} \|\mathcal{R}^\kappa_{\alpha,\Gamma}\| = 0$. The argument can be pictorially expressed as follows:

Pictorial sketch of the proof



Punctured manifolds

A natural question is what happens with $\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma})$ if Γ has a small *"hole"*. We will give the answer for a compact, $(n-1)$-dimensional, $C^{1+[n/2]}$-smooth manifold in $\mathbb{R}^n$

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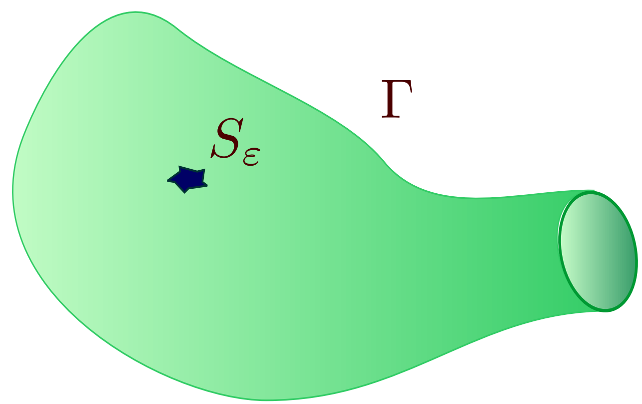

Consider a family $\{S_\varepsilon\}_{0\le\varepsilon<\eta}$ of subsets of Γ such that

- each S_ε is *Lebesgue measurable* on Γ
- they shrink to origin, $\sup_{x\in S_\varepsilon}|x| = \mathcal{O}(\varepsilon)$ as $\varepsilon\to 0$
- $\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma}) \ne \emptyset$, nontrivial for $n\ge 3$

Punctured manifolds: ev asymptotics

Call $H_\varepsilon := H_{\alpha,\Gamma\setminus S_\varepsilon}$. For small enough ε these operators have the same finite number of eigenvalues, naturally ordered, which satisfy $\lambda_j(\varepsilon) \to \lambda_j(0)$ as $\varepsilon \to 0$

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Let φ_j be the eigenfunctions of H_0. By Sobolev trace thm $\varphi_j(0)$ makes sense. Put $s_j := |\varphi_j(0)|^2$ if $\lambda_j(0)$ is simple, otherwise they are ev's of $C := \left(\overline{\varphi_i(0)}\varphi_j(0)\right)$ corresponding to a degenerate eigenvalue

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Theorem [E.-Yoshitomi, 2003]: Under the assumptions made about the family $\{S_\varepsilon\}$, we have

$$\lambda_j(\varepsilon) = \lambda_j(0) + \alpha s_j m_\Gamma(S_\varepsilon) + o(\varepsilon^{n-1}) \quad \text{as} \quad \varepsilon \to 0$$

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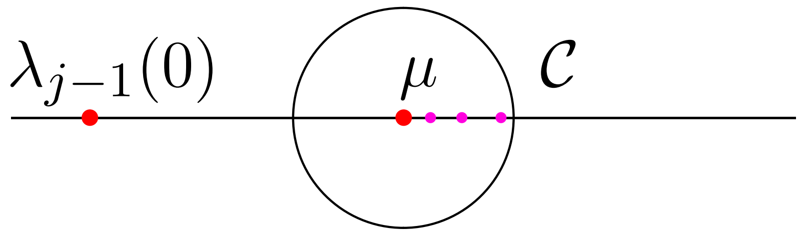
- If $n=2$, i.e. Γ is a curve, $m_\Gamma(S_\varepsilon)$ is the length of the hiatus. In this case the same asymptotic formula holds for bound states of an infinite curved Γ
- Asymptotic perturbation theory for quadratic forms does not apply, because $C_0^\infty(\mathbb{R}^n) \ni u \mapsto |u(0)|^2 \in \mathbb{R}$ does not extend to a bounded form in $W^{1,2}(\mathbb{R}^n)$

Sketch of the proof

Take an eigenvalue $\mu \equiv \lambda_j(0)$ of multiplicity m. It splits in general, for small enough ε one has m eigenvalues inside $\mathcal{C} := \{z :\ |z-\mu| < \frac{3}{4}\kappa\}$, where $\kappa := \frac{1}{2}\mathrm{dist}\,(\{\mu\},\, \sigma(H_0) \setminus \{\mu\})$



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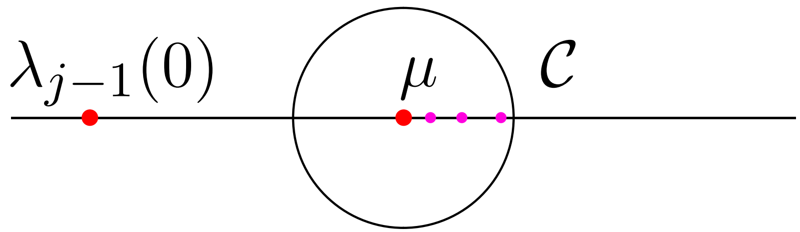

Set $w_k(\zeta, \varepsilon) := (H_\varepsilon - \zeta)^{-1}\varphi_k - (H_0 - \zeta)^{-1}\varphi_k$ for $\zeta \in \mathcal{C}$ and $k = j, j+1, \dots, j+m-1$. Using the choice of $\mathcal{C}$ and Sobolev imbedding thm, one proves

$$\|w_k(\zeta, \varepsilon)\|_{W^{1,2}(\mathbb{R}^n)} = \mathcal{O}(\varepsilon^{(n-1)/2}) \quad \text{as} \quad \varepsilon \to 0$$

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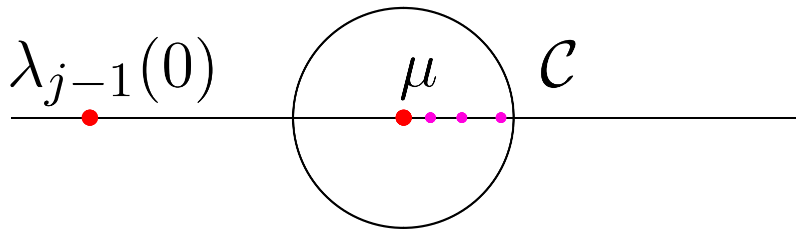

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Next, $W^{1,2}(\mathbb{R}^n) \ni f \mapsto f|_\Gamma \in L^2(\Gamma)$ is compact; it implies

$$\sup_{\zeta\in\mathcal{C}} \|w_k(\zeta,\varepsilon)\|_{W^{1,2}(\mathbb{R}^n)} = o(\varepsilon^{(n-1)/2}) \quad \text{as} \quad \varepsilon \to 0$$

Sketch of the proof

Let P_ε be spectral projection to these eigenvalues,

$$P_\varepsilon \varphi_k - \varphi_k = \frac{1}{2\pi i} \oint_{\mathcal{C}} w_k(\zeta, \varepsilon)\, d\zeta = o(\varepsilon^{(n-1)/2})$$

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Take $m \times m$ matrices $L(\varepsilon) := ((H_\varepsilon P_\varepsilon\varphi_i, P_\varepsilon\varphi_k))$ and $M(\varepsilon) := ((P_\varepsilon\varphi_i, P_\varepsilon\varphi_k))$. We find that

$$((H_\varepsilon P_\varepsilon\varphi_i, P_\varepsilon\varphi_k)) - \mu\delta_{ik} - \alpha\overline{\varphi_i(0)}\varphi_k(0)m_\Gamma(S_\varepsilon)$$

is $o(\varepsilon^{n-1})$ and $(P_\varepsilon\varphi_i, P_\varepsilon\varphi_k) = \delta_{ik} + o(\varepsilon^{n-1})$

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$$P_\varepsilon\varphi_k - \varphi_k = \frac{1}{2\pi i}\oint_{\mathcal{C}} w_k(\zeta,\varepsilon)\, d\zeta = o(\varepsilon^{(n-1)/2})$$

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Take $m \times m$ matrices $L(\varepsilon) := ((H_\varepsilon P_\varepsilon\varphi_i, P_\varepsilon\varphi_k))$ and $M(\varepsilon) := ((P_\varepsilon\varphi_i, P_\varepsilon\varphi_k))$. We find that

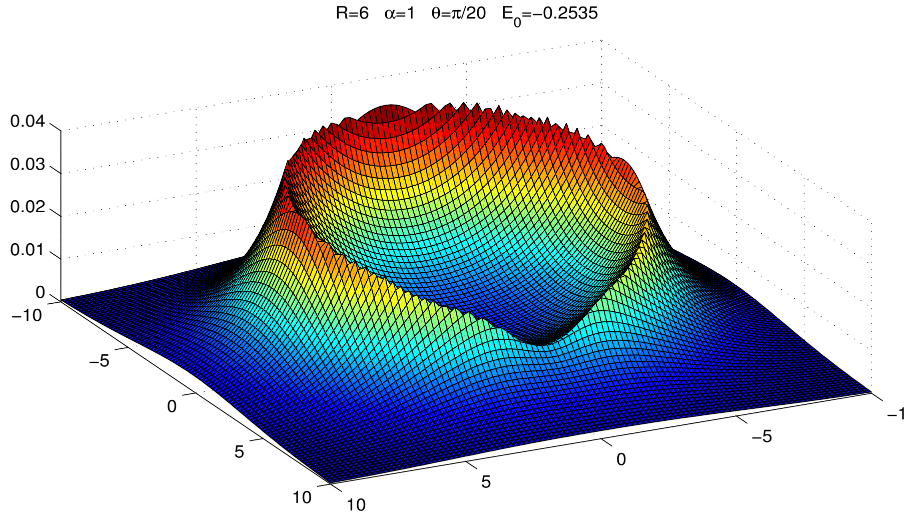
$$((H_\varepsilon P_\varepsilon\varphi_i, P_\varepsilon\varphi_k)) - \mu\delta_{ik} - \alpha\overline{\varphi_i(0)}\varphi_k(0)m_\Gamma(S_\varepsilon)$$

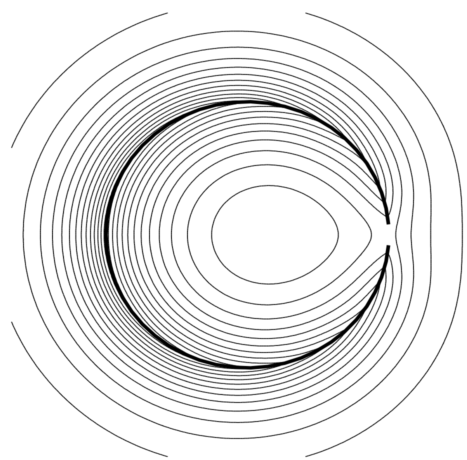
is $o(\varepsilon^{n-1})$ and $(P_\varepsilon\varphi_i, P_\varepsilon\varphi_k) = \delta_{ik} + o(\varepsilon^{n-1})$. Then

$$L(\varepsilon)M(\varepsilon)^{-1} = \mu I + \alpha C m_\Gamma(S_\varepsilon) + o(\varepsilon^{n-1})$$

and the claim of the theorem follows $\square$

Illustration: a ring with $\frac{\pi}{20}$ cut





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

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

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

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

for $\dim\Gamma = 1$, $\mathrm{codim}\,\Gamma = 2$. 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 $\mathrm{codim}\,\Gamma = 1$ 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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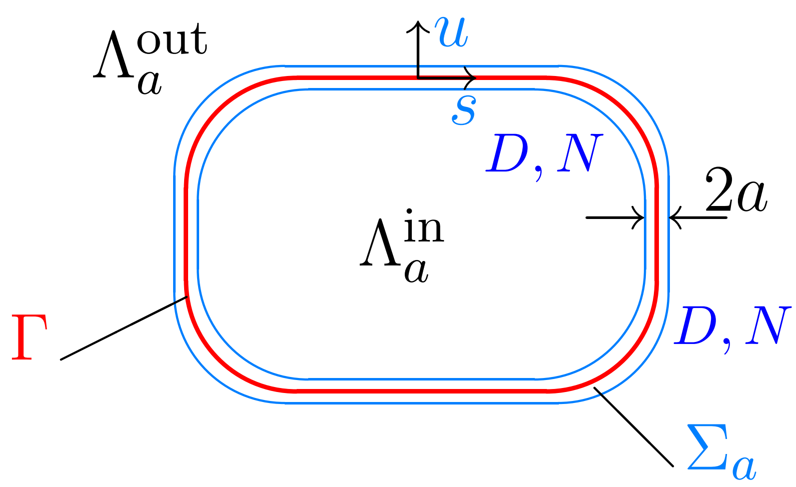
Lemma: $\Phi_a :\ [0,L) \times (-a,a) \to \mathbb{R}^2$ defined by

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

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

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

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

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

where $f \in W^{1,2}_0(\Sigma_a)$ 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 $L^{\pm}_{a,\alpha}$ 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

We pass to rougher bounds squeezing $H_{\alpha,\Gamma}$ between

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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 $V_-(s) \le V(s,u) \le V_+(s)$ 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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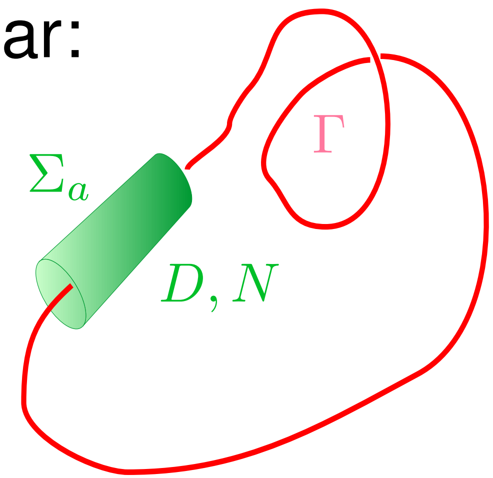
Finishing the proof:

- 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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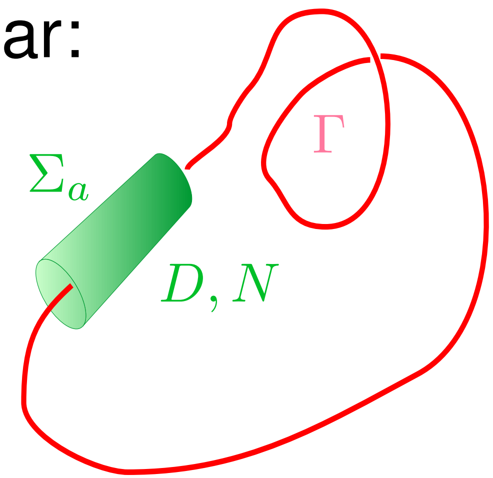

The *"straightening" transformation* Φ_a is defined by

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

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 $T^\pm_\alpha$ has for large enough negative α a single negative ev $\kappa^\pm_{\alpha,a}$ 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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The rest of the argument is the same as above

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 $\mathbb{R}^3$

The argument modifies easily; Σ_a is now a *layer neighborhood*. However, the intrinsic geometry of Γ can no longer be neglected

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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

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

Proof sketch in the surface case

The bracketing argument proceeds as before,

$$-\Delta^N_{\Lambda_a} \oplus H^-_{\alpha,\Gamma} \le H_{\alpha,\Gamma} \le -\Delta^D_{\Lambda_a} \oplus H^+_{\alpha,\Gamma}\,, \;\Lambda_a := \mathbb{R}^3 \setminus \overline{\Sigma}_a,$$

the interior only contributing to the negative spectrum

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the interior only contributing to the negative spectrum

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 $H_{\alpha,\Gamma}^\pm$ 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 $\hat{H}_{\alpha,\Gamma}^\pm := \hat{U} H_{\alpha,\Gamma}^\pm \hat{U}^{-1}$ in $L^2(\mathcal{N}_a, \mathrm{d}\Omega)$

Straightening transformation

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

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

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 $\hat{H}_{\alpha,\Gamma}^{\pm}$ are associated with the forms

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

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 $W^{2,1}_0(\Omega_a, \mathrm{d}\Gamma du)$ 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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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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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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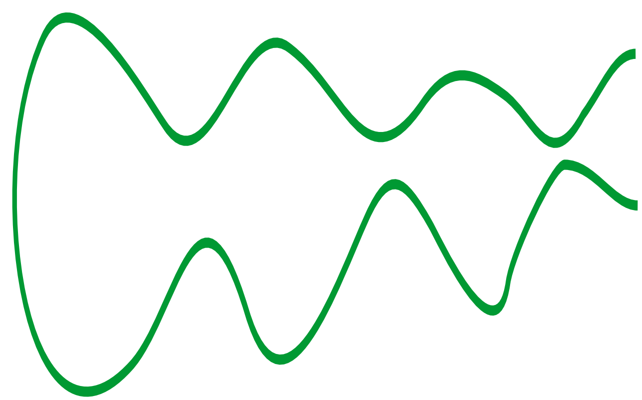
It is needed that σ_{ess} does not feel curvature, not only for $H_{\alpha,\Gamma}$ but for the estimating operators as well. *Sufficient conditions:*

- $k(s), k'(s)$ 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



Infinite manifolds

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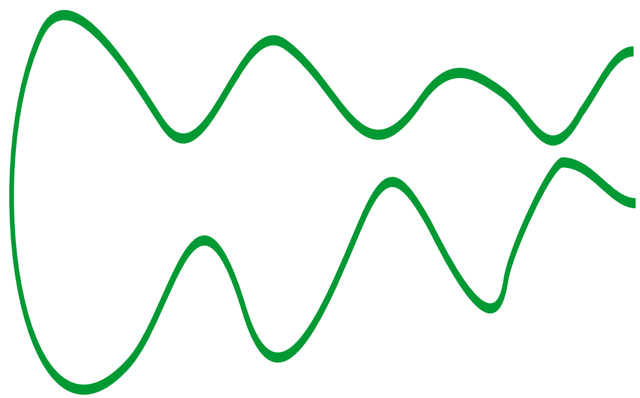
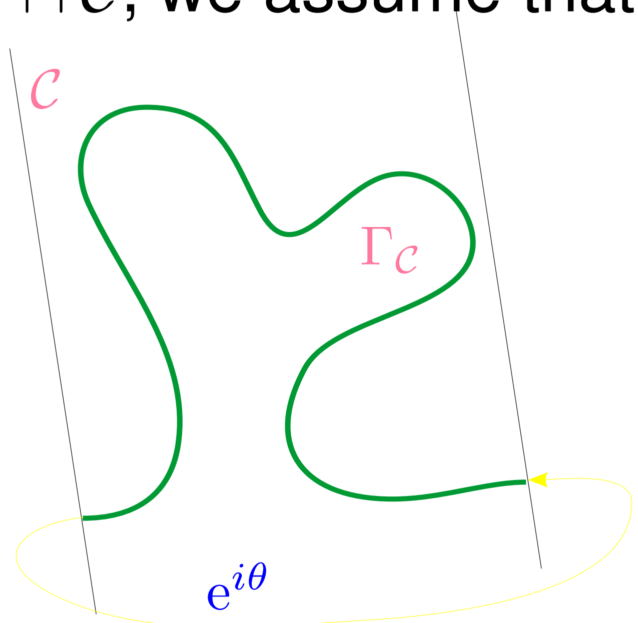


Theorem [EY02; EK03, Ex04]: With the above listed assumptions, the asymptotic expansions *(ii)* for the eigenvalues derived in the compact case hold again

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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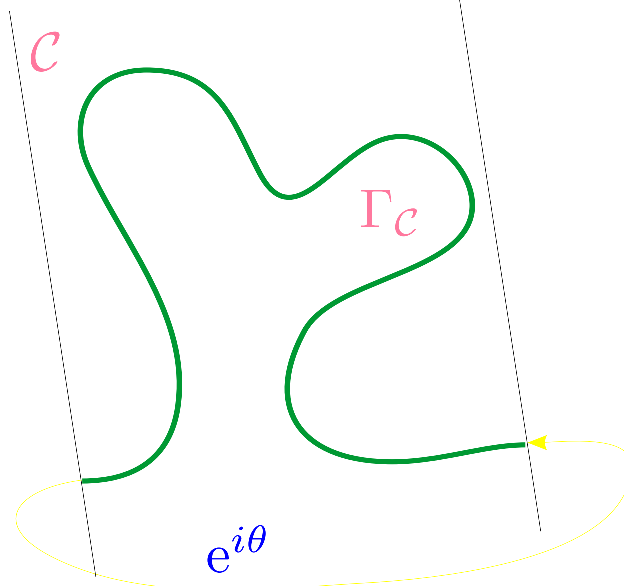

Lemma: $\exists$ unitary $\mathcal{U} : L^2(\mathbb{R}^3) \to \int_{[0,2\pi)^r}^{\oplus} L^2(\mathcal{C})\,d\theta$ s.t.

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

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

$$\lambda_j(\alpha,\theta) = \epsilon_\alpha + \mu_j(\theta) + \mathcal{O}(\mathrm{e}^{\pi\alpha}) \quad \text{as} \quad \alpha\to-\infty$$

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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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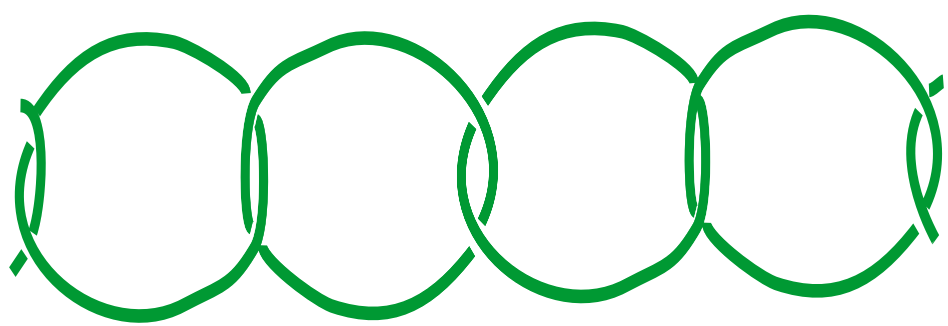
Moreover, the assumptions can be weakened



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

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

where $\lambda_n(\phi)$ 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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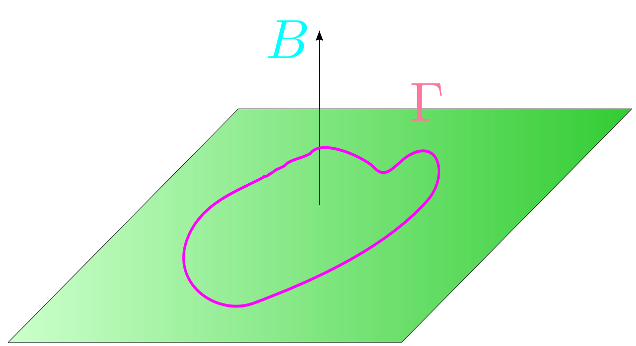

Persistent currents

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, 2004] 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 $\mathrm{codim}\,\Gamma = 1$ 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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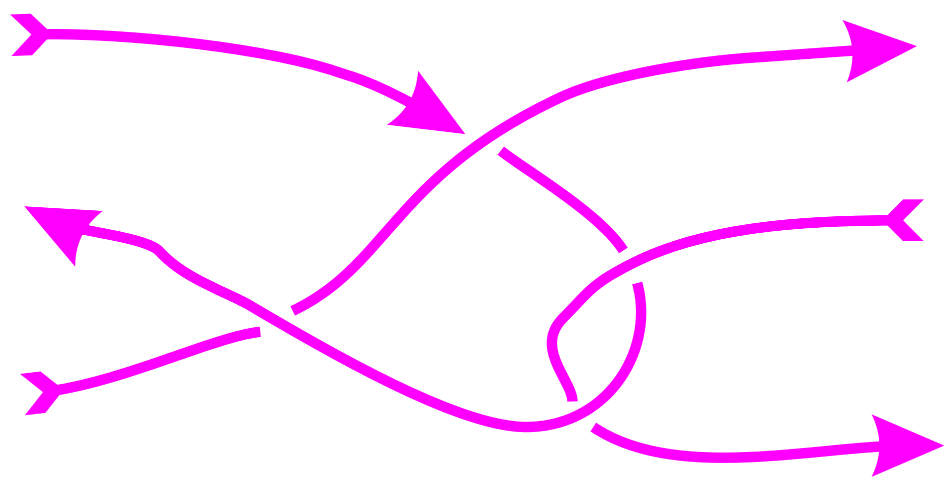
The assumption about connectedness of $\Gamma_{\mathcal{C}}$ can be always satisfied if $d = 2$ but not for $d = 3$; recall the *crotchet curve*



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Theorem [Bentosela-Duclos-E., 2003]: 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 $\square$

Open questions

- *Strong coupling, manifolds with boundary:* If Γ has a boundary, we have a strong-coupling asymptotics for the bound state number but not for ev's themselves. We *conjecture* that the latter is given again by

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  etc., where μ_j refers to S_Γ with *Dirichlet* b.c.

- *Strong coupling, less regularity:* Examples show that the above relation is not valid for a non-smooth Γ, rather μ_j is replaced by a term proportional to α^2. How does the asymptotic expansion look in this case and how it depends on dimension and codimension of Γ? The analogous question can be asked more generally for graphs with branching points and generalized graphs

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  - asymptotic behavior of S-matrix in strong-coupling regime, including relations between S-matrices of leaky and "ideal" graphs
  - *prove* existence of resonances, at least within particular models
- *Periodic* Γ*:* one expects that the *whole* spectrum is absolutely continuous, independently of α, but it remains to be proved. Also strong-coupling asymptotic properties of spectral gaps are not known

Open questions

- *Random graphs*, either by their shape or by a random coupling $\alpha : \Gamma \to \mathbb{R}_+$. Is it true that the whole negative part of $\sigma_{\mathrm{ess}}(H_{\alpha,\Gamma})$ is always *p.p.* once a disorder is present?

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- *etc, etc*

The talk was based on

[BDE03] F. Bentosela, P. Duclos, P.E.: Absolute continuity in periodic thin tubes and strongly coupled leaky wires, *Lett. Math. Phys.* **65** (2003), 75-82.

[BEKŠ94] J.F. Brasche, P.E., Yu.A. Kuperin, P. Šeba: Schrödinger operators with singular interactions, *J. Math. Anal. Appl.* **184** (1994), 112–139.

[Ex01] P.E.: Bound states of infinite curved polymer chains, *Lett. Math. Phys.* **57** (2001), 87-96.

[Ex04] P.E.: Spectral properties of Schrödinger operators with a strongly attractive δ interaction supported by a surface, to appear in *Proceedings of the NSF Summer Research Conference (Mt. Holyoke 2002)*; AMS “Contemporary Mathematics" Series, Providence, R.I., 2004

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

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

[EK03a] P.E., S. Kondej: Bound states due to a strong δ interaction supported by a curved surface, *J. Phys.* **A36** (2003), 443-457.

[EK03b] P.E., S. Kondej: Strong-coupling asymptotic expansion for Schrödinger operators with a singular interaction supported by a curve in $\mathbb{R}^3$, *Rev. math. Phys., to appear;* *math-ph/0303033*

And it is not all, see also

[EK03c] P.E., S. Kondej: Schrödinger operators with singular interactions: a model of tunneling resonances, `math-ph/0312055`

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

[ET04] P.E., M. Tater: Spectra of soft ring graphs, Waves in Random Media **13** (2003), S47-S60.

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

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

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

[EY03] P.E., K. Yoshitomi: Eigenvalue asymptotics for the Schrödinger operator with a δ-interaction on a punctured surface, *Lett. Math. Phys.* **65** (2003), 19-26.

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