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Spectral properties of Schrödinger operators with strongly attractive graph-type singular perturbations

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We review some recent results about "leaky graph" models, in particular, those describing asymptotic behavior of the discrete spectrum in the strong-coupling regime.

This talk, presented at the Kyoto conference on October 27, 2003, is a survey of recent results obtained in collaboration with Sylwia Kondej and Kazushi Yoshitomi, and to lesser extent Francois Bentosela, Pierre Duclos, and Miloš Tater. Its topic is a model often dubbed "leaky quantum graph" which attracted attention in recent 2-3 years. The following items will be covered:

1. Why tunneling is important in quantum graphs?
2. Schrödinger operators to be considered, $H_{\alpha,\Gamma} = -\Delta - \alpha\delta(x-\Gamma)$
3. Geometrically induced discrete spectrum
4. Punctured manifolds: a perturbation theory
5. Strong-coupling asymptotics for a compact Γ
6. Proof technique: bracketing plus coordinate transformation
7. Extension: infinite manifolds
8. Extensions: periodic case, magnetic field, absolute continuity
9. Some open questions

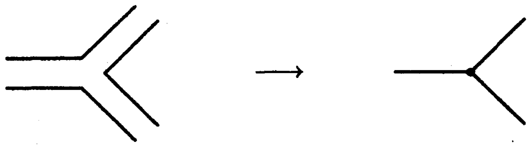
1 Motivation: why leaky graphs?

Graph models are very useful in many fields. In quantum mechanics they are used to describe in the last decade or two to describe numerous nanostructures made of semiconductor materials. Most commonly used quantum graph models employ Schrödinger operators supported by the graph itself, i.e. the Hamiltonian acts as $-\frac{\partial^2}{\partial x_j^2} + v(x_j)$ on graph edges, with the wavefunctions coupled by appropriate boundary conditions at the vertices – for a bibliography see [KS99, Ku02, Ku04].

In the same spirit one can treat also generalized graphs in which some "edges" may be manifolds of a higher dimension. Such systems are not just a mathematical whiff, they can be used to describe physical effects like scanning microscopy, structures composed of nanotubes and fullerene molecules, etc. The Hamiltonian acts in this case as $-\Delta_{\mathrm{LB}} + v(x)$ on the manifolds and the boundary condition involve generalized boundary values – see [Ki97, ETV01, BG03] and references therein.

Spectral and scattering problems in systems with such "decomposable" configuration spaces are solved using standard ODE and/or PDE techniques together with matching the solutions using boundary conditions. While being extremely useful, these models have drawbacks, in the first place:

(a) *Presence of* ad hoc *parameters* in the boundary conditions. A possible remedy would be to use a zero-width limit in a more realistic description, schematically



Unfortunately, the answer is known for Neumann boundary [KuZ01, RSch01, Sa01] and for more general situations which involves manifolds without a boundary [EP03], however, the physically most important Dirichlet case remains open (and difficult).

(b) *Neglection of tunnel effect*: a true quantum-wire boundary is a finite potential jump so the Dirichlet boundary conditions is only an approximation, even if a good one in many situations. In general, quantum

tunneling between different parts of a graph is possible and there are situations when it cannot be neglected.

2 Leaky graph Hamiltonians

This motivates us to look for a model without the said drawbacks. We shall thus consider "leaky" graphs the configuration space of which will be the whole Euclidean space; the geometry will be contained in the *attractive graph-shaped interaction*. In other words, the Hamiltonian is formally given by

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

where Γ is a smooth manifold in $\mathbb{R}^n$, or a (locally finite) union of such manifolds. We have in mind three types. In the most part of this talk, we will have is mind Γ's consisting of a simple manifold; they will be thus trivial as graphs but they will have a nontrivial geometry. In particular, we have in mind three situations: curves in $\mathbb{R}^2$, surfaces in $\mathbb{R}^3$, and finally, curves in $\mathbb{R}^3$. In the first two cases we have $\operatorname{codim}\Gamma = 1$ and the operator can be defined by means of quadratic form,

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

which is closed and below bounded in $W^{2,1}(\mathbb{R}^2)$; the second term makes sense in view of Sobolev embedding. Since Γ is regular here, we can also use an *alternative definition* by boundary conditions: $H_{\alpha,\Gamma}$ acts $-\Delta$ on functions from $W^{2,1}_{\mathrm{loc}}(\mathbb{R}^2 \setminus \Gamma)$, 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 situation changes if $\operatorname{codim}\Gamma = 2$. Boundary conditions can be again 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 to that there is a tubular neighborhood of Γ which does not intersect itself. Then one employs *Frenet's frame* $(t(s), b(s), n(s))$ for Γ. Given $\xi, \eta \in \mathbb{R}$ we denote $r = (\xi^2+\eta^2)^{1/2}$ and define the set the "shifted" curves

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

By Sobolev argument the restriction of $f \in W^{2,2}_{\mathrm{loc}}(\mathbb{R}^3 \setminus \Gamma)$ to Γ_r is well defined for r small enough. 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 the limits

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

exist a.e. in $\mathbb{R}$, are independent of the direction $\frac{1}{r}(\xi, \eta)$, and define functions from $L^2(\mathbb{R})$. Then it is straighforward to chech [EK02] that the operator $H_{\alpha,\Gamma}$ has the domain

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

and acts as follows,

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

Remarks 2.1 (i) If Γ has components of codimension one and two, one combines the above boundary conditions.
(ii) The boundary conditions are natural way to describe point interaction in the normal plane to Γ. Thus there is no way (within standard QM) to define $H_{\alpha,\Gamma}$ in the case $\operatorname{codim}\Gamma \geq 4$
(iii) 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

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

Recall simple facts about the spectrum [BT92, BEKŠ94, EI01, EK02, Ex04]:

(a) $\sigma_{\mathrm{ess}}(H_{\alpha,\Gamma}) = [0, \infty)$ if Γ is compact
(b) $\sigma_{\mathrm{ess}}(H_{\alpha,\Gamma}) = [-\frac{1}{4}\alpha^2, \infty)$ if $\operatorname{codim}\Gamma = 1$ and Γ has finite number of semi-infinite edges, which are straight and non-parallel, or at least asymptotically straight in a suitable sense
(c) for higher codimensions $-\frac{1}{4}\alpha^2$ is replaced by the appropriate point-interaction eigenvalue, e.g., by $\epsilon_\alpha = -4\,\mathrm{e}^{2(-2\pi\alpha + \psi(1))}$ when $\operatorname{codim}\Gamma = 2$ (recall that strong coupling here means $\alpha \to -\infty$)

3 Geometrically induced discrete spectrum

Nontrivial geometry, bending etc., may give rise to isolated eigenvalues of $H_{\alpha,\Gamma}$. For simplicity, consider a planar curve $\Gamma : \mathbb{R} \to \mathbb{R}^2$ parameterized by its arc length, and assume:

(i) Γ is piecewise C^1-smooth

(ii) $|\Gamma(s) - \Gamma(s')| \geq c|s - s'|$ holds for some $c \in (0, 1)$

(iii) 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 $S_\omega := \left\{(s, s') : \omega < \frac{s}{s'} < \omega^{-1}\right\}$.

(iv) straight line is excluded, $|\Gamma(s) - \Gamma(s')| < |s - s'|$ for some $s, s' \in \mathbb{R}$

Theorem 3.1 [EI01]: *Under the stated assumptions, the operator $H_{\alpha,\Gamma}$ has at least one (isolated) eigenvalue in $(-\infty, -\frac{1}{4}\alpha^2)$.*

Before sketching the proof, let us mention several possible extensions:

(a) A similar result holds for a curve in $\mathbb{R}^3$ under stronger regularity requirements: global C^1-smoothness and piecewise C^2 – cf. [EK02]

(b) for a C^2 smooth curve the asymptotic straightness condition holds if its curvature decays fast enough, $|k(s)| \leq C\langle s\rangle^{-5/4-\varepsilon}$ – which is probably not optimal, one conjectures that $\leq C\langle s\rangle^{-1-\varepsilon}$ would be natural

(c) For a curved surface $\Gamma \subset \mathbb{R}^3$ such a result is proved in the strong coupling asymptotic regime, $\alpha \to \infty$, see below and [EK03a]. Existence of a discrete spectrum without this assumption is an *open problem*

(d) these results can be used to prove bound-state existence for more complicated (generalized) graphs. Suppose that $\tilde{\Gamma} \supset \Gamma$ holds in the set sense, then we have
$$H_{\alpha,\tilde{\Gamma}} \leq H_{\alpha,\Gamma}\,.$$
If the essential spectrum threshold is the same for both graphs and Γ fits the above assumptions, we infer that $\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma}) \neq \emptyset$ holds by minimax principle

(e) similar results hold for non-straight equidistant arrays of point interactions and more complicated graph-shaped sets – cf. [Ex01] and [EN03]

Let us describe briefly the main steps in the demonstration of Theorem 3.1:

1. The classical Birman-Schwinger principle based on the identity

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

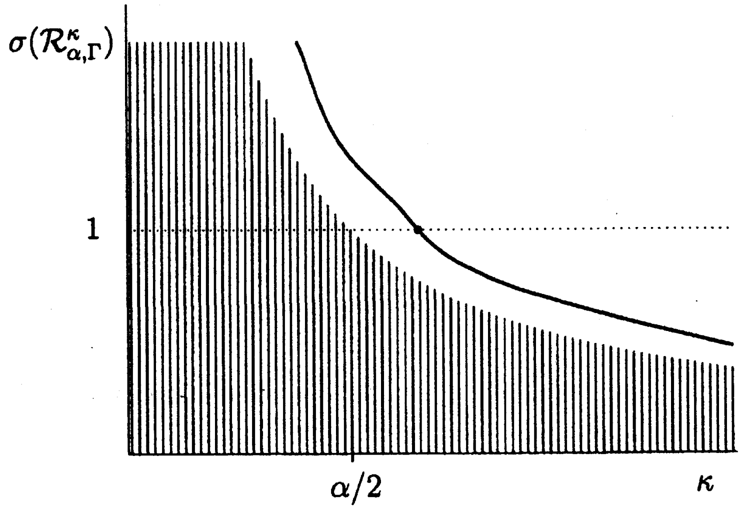
can be extended to generalized Schrödinger operators $H_{\alpha,\Gamma}$ – see [BEKŠ94] – the multiplication by $(H_0 - z)^{-1}V^{1/2}$ etc. is replaced by suitable trace maps. In this way we find that $-\kappa^2$ is an eigenvalue of $H_{\alpha,\Gamma}$ iff the integral operator $\mathcal{R}^\kappa_{\alpha,\Gamma}$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

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

3. The curvature-induced perturbation is sign-definite, specifically 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 check that $\sup \sigma(\mathcal{R}^\kappa_{\alpha,\Gamma}) > \frac{\alpha}{2\kappa}$

4. Due to the asymptotic straightness of Γ the perturbation $\mathcal{R}^\kappa_{\alpha,\Gamma} - \mathcal{R}^\kappa_{\alpha,\Gamma_0}$ is Hilbert-Schmidt, hence the spectrum of $\mathcal{R}^\kappa_{\alpha,\Gamma}$ in $(\alpha/2\kappa, \infty)$ is discrete

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



4 Perturbation theory for punctured manifolds

A natural question is what happens with $\sigma_{\text{disc}}(H_{\alpha,\Gamma})$ if Γ has a small "hole". We will give the answer for a compact, $(n-1)$-dimensional, $C^{1+[n/2]}$-smooth manifold. Consider a family $\{S_\varepsilon\}_{0\le\varepsilon<\eta}$ of subsets of Γ such that

(i) each S_ε is measurable w.r.t. $(n-1)$-dimensional Lebesgue measure on Γ,

(ii) they shrink to origin, $\sup_{x\in S_\varepsilon}|x| = \mathcal{O}(\varepsilon)$ as $\varepsilon \to 0$,

(iii) $\sigma_{\text{disc}}(H_{\alpha,\Gamma}) \neq \emptyset$, nontrivial for $n \geq 3$.

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

Theorem 4.1 [EY03]: *With the stated assumptions, we have*

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

Remarks 4.2 (a) Formally a small-hole perturbation acts as a repulsive δ interaction with the coupling constant equal to $\alpha m_\Gamma(S_\varepsilon)$.

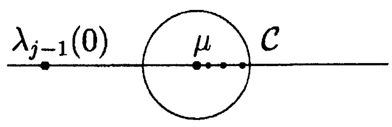
(b) Notice that no self-similarity of S_ε is required

(c) If $n = 2$, i.e. Γ is a curve, $m_\Gamma(S_\varepsilon)$ is the length of the hiatus; then the same asymptotic formula holds for bound states of an infinite curved Γ

(d) Asymptotic perturbation theory for quadratic forms does not apply in this situation, because $C_0^\infty(\mathbb{R}^n) \ni u \mapsto |u(0)|^2 \in \mathbb{R}$ does not extend to a bounded form in $H^1(\mathbb{R}^n)$.

Let us now describe briefly the scheme of the proof:

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



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

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

3. Next, $H^1(\mathbb{R}^n) \ni f \mapsto f|_\Gamma \in L^2(\Gamma)$ is compact, using a factorization and an abstract result from [LM]. It implies

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

4. Let P_ε be spectral projection to these eigenvalues, then

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

holds in $H^1(\mathbb{R}^n)$ as $\varepsilon \to 0$. 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 $(P_\varepsilon\varphi_i, P_\varepsilon\varphi_k) = \delta_{ik} + o(\varepsilon^{n-1})$. The above result then gives

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

and the claim of the theorem follows.

5 Strong coupling asymptotics for a compact Γ

Suppose that Γ has a single component, which is smooth and compact.

Theorem 5.1 [EY02a, EK02, EK03a]: *(i) Let Γ be a C^4 smooth manifold. In the strong-coupling limit, $(-1)^{\operatorname{codim}\Gamma-1}\alpha \to \infty$, we have*

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

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

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

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

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

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

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

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

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

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

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

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

on $L^2((0,|\Gamma|))$ *for* $\dim\Gamma = 1$, *where* k *is the 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 the Laplace-Beltrami operator on* Γ *and* K, M, *respectively, are the corresponding Gauss and mean curvatures.*

Remark 5.2 We have mentioned that this also determines the semiclassical asymptotics of the operator $-h^2\Delta - \alpha\delta(x-\Gamma)$, however, in case $\operatorname{codim}\Gamma = 2$ the choice of the effective coupling $\alpha(h)$ is arbitrary to some extent.

6 Proof technique

Let us sketch the proof of the theorem in the $1+1$ case. Take a closed curve Γ and call $L = |\Gamma|$. We start from a tubular neighbourhood of Γ.

Lemma 6.1 [EY02a]: *The map* $\Phi_a : [0, L) \times (-a, a) \to \mathbb{R}^2$ *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.*

The idea is to apply to the operator $H_\alpha \equiv H_{\alpha(h),\Gamma}(1)$ Dirichlet-Neumann bracketing at the boundary of $\Sigma_a := \Phi([0, L) \times (-a, a))$. This yields

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

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

It is important to notice that the exterior part does not contribute to the negative spectrum. In the interior we use the curvilinear coordinates passing from $L^\pm_{a,\alpha}$ to unitarily equivalent operators corresponding to quadratic forms

$$\begin{aligned} b^+_{a,\alpha}[f] &= \int_0^L \int_{-a}^a (1 + uk(s))^{-2} \left|\frac{\partial f}{\partial s}\right|^2 \mathrm{d}u\, \mathrm{d}s \\ &+ \int_0^L \int_{-a}^a \left|\frac{\partial f}{\partial u}\right|^2 \mathrm{d}u\, \mathrm{d}s + \int_0^L \int_{-a}^a V(s, u)|f|^2 \,\mathrm{d}s\, \mathrm{d}u \\ &- \alpha \int_0^L |f(s, 0)|^2 \,\mathrm{d}s \end{aligned}$$

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

$$\begin{aligned} b^-_{a,\alpha}[f] &= b^+_{a,\alpha}[f] - \frac{1}{2} \int_0^L \frac{k(s)}{1 + ak(s)} |f(s, a)|^2 \,\mathrm{d}s \\ &+ \frac{1}{2} \int_0^L \frac{k(s)}{1 - ak(s)} |f(s, -a)|^2 \,\mathrm{d}s \end{aligned}$$

with periodic boundary conditions in the longitudinal variable. Here V is the curvature induced potential,

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

In the next step we use estimate with separated variables, squeezing the operator between

$$\tilde{H}^{\pm}_{a,\alpha} = U^{\pm}_{a} \otimes 1 + 1 \otimes T^{\pm}_{a,\alpha}\,.$$

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

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

with periodic boundary conditions, 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. They can be estimated as follows:

Lemma 6.2 [EY02a]: *There are positive c, c_N such that $T^{\pm}_{\alpha,a}$ has a single negative eigenvalue $\kappa^{\pm}_{\alpha,a}$ satisfying the inequalities*

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

for α large enough.

To finish the proof, we observe that the eigenvalues of $U^{\pm}_{a}$ differ by $\mathcal{O}(a)$ from those of the comparison operator. Then we choose $a = 6\alpha^{-1}\ln\alpha$ as the neighborhood width; putting the estimates together we get

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

which is by the above lemma equivalent to the claim (ii) for planar loops.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).

Notice that the argument naturally extends to Γ consisting of a finite number of connected components.

Let us comment on the other dimensions. For a curve in $\mathbb{R}^3$ the argument is similar: we take a tubular neighborhood and employ D-N bracketing. 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 the longitudinal and transverse 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 $\mathcal{O}(a)$. Up to this error, we get an upper and lower bound by operators with separated variables. The transverse estimate is replaced by

Lemma 6.3 [EK03b]: *There are $c_1,\, c_2 > 0$ such that $T_\alpha^\pm$ has for large enough negative α a single negative eigenvalue $\kappa_{\alpha,a}^\pm$ which satisfies*

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

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

The rest of the argument is the same as above. It again extends to Γ consisting of a finite number of connected components.

For 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. 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 $d\Gamma := g^{1/2} d^2 s$, 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 the *Gauss curvature* K and *mean curvature* M by

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

The bracketing argument proceeds as before,

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

the interior only contributing to the negative spectrum. Next we use again the *curvilinear coordinates*: for small enough a we have the "straightening" diffeomorphism

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

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

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

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

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

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

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

Let $(\cdot,\cdot)_G$ denote the inner product in $L^2(\mathcal{N}_a, d\Omega)$. Then $\hat{H}^{\pm}_{\alpha,\Gamma} := \hat{U}H^{\pm}_{\alpha,\Gamma}\hat{U}^{-1}$ in $L^2(\mathcal{N}_a, d\Omega)$ are associated with the forms

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

with the domains $W^{2,1}_0(\mathcal{N}_a, d\Omega)$ and $W^{2,1}(\mathcal{N}_a, d\Omega)$ for the $\pm$ sign, respectively. Next we remove $1-2Mu+Ku^2$ from the weight $G^{1/2}$ in the inner product of $L^2(\mathcal{N}_a, d\Omega)$ by the unitary transformation $U :\; L^2(\mathcal{N}_a, d\Omega) \to L^2(\mathcal{N}_a, d\Gamma du)$,

$$U\psi := (1-2Mu+Ku^2)^{1/2}\psi.$$

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

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

for ψ from $W_0^{2,1}(\Omega_a, d\Gamma du)$ and $W^{2,1}(\Omega_a, d\Gamma du)$, respectively. Here $M_u := (M - Ku)(1 - 2Mu + Ku^2)^{-1}$ is the mean curvature of the parallel surface to Γ and

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

with $J := \frac{1}{2}\ln(1 - 2Mu + Ku^2)$. We employ a rougher estimate with separated variables squeezing $1 - 2Mu + Ku^2$ between $C_\pm(a) := (1 \pm a\varrho^{-1})^2$, where $\varrho := \max(\{\|k_+\|_\infty, \|k_-\|_\infty\})^{-1}$. Consequently, the matrix inequality $C_-(a)g_{\mu\nu} \leq G_{\mu\nu} \leq C_+(a)g_{\mu\nu}$ is valid. We observe that V_1 behaves as $\mathcal{O}(a)$ for $a \to 0$, while V_2 can be squeezed between the functions $C_\mp^{-2}(a)(K - M^2)$, both uniformly in the surface variables. Hence we estimate $B_{\alpha,\Gamma}^\pm$ by

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

with

$$S_a^\pm := -C_\pm(a)\Delta_\Gamma + C_\mp^{-2}(a)(K - M^2) \pm va$$

in $L^2(\Gamma, d\Gamma) \otimes L^2(-a, a)$ for a $v > 0$, where $T_{\alpha,a}^\pm$ are the same as in the $1+1$ case (the same Lemma 6.2 applies).

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

$$\lambda_j(\alpha) = -\frac{1}{4}\alpha^2 + \mu_j + \mathcal{O}(\alpha^{-1}\ln\alpha) \tag{6.1}$$

as $a \to 0$ which is equivalent to the claim (i). To get (ii) we employ the Weyl asymptotics for S_Γ. The extension to Γ having a finite number of connected components is straightforward.

7 Infinite manifolds

Bound states may exist also if Γ is noncompact as we have already mentioned [EI01]. The present discussion shows another aspect of the problem: the comparison operator S_Γ has an attractive potential, so non-empty $\sigma_{\rm disc}(H_{\alpha,\Gamma})$ can be expected in the strong coupling regime.

It is needed, of course, that $\sigma_{\rm ess}$ does not feel the curvature, not only for $H_{\alpha,\Gamma}$ but for the estimating operators as well. This is ensured, e.g., if *(i)* $k(s), k'(s)$ and $k''(s)^{1/2}$ are $\mathcal{O}(|s|^{-1-\epsilon})$ as $|s| \to \infty$ for a planar curve

(ii) in addition, the torsion bounded for a curve in $\mathbb{R}^3$

(iii) a surface Γ admits a global normal parametrization with a uniformly elliptic metric, $K, M \to 0$ as the geodesic radius $r \to \infty$

In addition, we have also to *assume* that there is a tubular neighborhood Σ_a without self-intersections for small a, thus avoiding the situation where there is a sequence of pair points, far from each other in the manifold metric, with distances tending to zero.

Theorem 7.1 [EY02a, EK02, EK03a]: *With the above assumption, the asymptotic expansions derived in the compact case hold again.*

8 Periodic manifolds

In this case one combines the described technique with Floquet expansion. It is important to choose the periodic cells C of the space and Γ_C of the manifold consistently, $\Gamma_C = \Gamma \cap C$.

Lemma 8.1 [EY01, Ex04, EK03b]: *There is a unitary map* $\mathcal{U} : L^2(\mathbb{R}^3) \to \int_{[0,2\pi)^r}^{\oplus} L^2(C)\, d\theta$ *such that*

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

The fibre comparison operators are

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

on $L^2(\Gamma_C)$ 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 boundary conditions for $\dim \Gamma = 2$.

Theorem 8.2 [EY01, Ex04, EK03b]: *Let Γ be a C^4-smooth r-periodic manifold without boundary, then 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*

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

for $\operatorname{codim}\Gamma = 2$. *The error terms are uniform w.r.t. θ.*

Corollary 8.3 *If* $\dim\Gamma = 1$ *and coupling is strong enough, the operator $H_{\alpha,\Gamma}$ has open spectral gaps.*

Remarks 8.4 *(a) Large gaps for disconnected manifolds:* if Γ is not connected and each connected component is contained in a translate of Γ_C, the comparison operator is independent of θ and asymptotic formula reads

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

for $\operatorname{codim}\Gamma = 1$ and similarly for for $\operatorname{codim}\Gamma = 2$. Moreover, the assumptions can be weakened to include chain-like disconnected manifolds, etc.

(b) Soft graphs with magnetic field: let Γ be a planar loop and the system is placed into a magnetic field. Thus formally the Hamiltonian has the form

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

In the asymptotic regime of large α the eigenvalues behave as in Theorem 3.1, however, the comparison operator S_Γ now refers to Floquet boundary condition: circling once around the curve Γ the function acquires the phase $(2\pi)^{-1}B\Sigma_\Gamma$, where Σ_Γ is the region inside Γ – see [EY02b]. In particular, the eigenvalues μ_j depend on a parameter – as in Theorem 8.2 – which is now the magnetic field B. A consequence is that for large enough α the eigenvalues $\lambda_j(\alpha,B)$ of $H_{\alpha,\Gamma}(B)$ are non-constant as functions of B. In physical terms it means that such a system exhibits *persistent currents.*

(c) Absolute continuity: An analogous argument combined with the analyticity of the functions $\lambda_j(\alpha,\cdot)$ in Theorem 8.2 shows that for in a fixed interval

and for α large enough the spectrum of $H_{\alpha,\Gamma}(B)$ with a periodic Γ is absolutely continuous – see [BDE03]. Recall that while for Γ periodic in two directions the absolute continuity is proved in [BSS00] and the result is extended to higher dimensions in [SŠ01], the *global* absolute continuity for a single periodic curve remains an open problem.

9 Open questions

1) Strong coupling, manifolds with boundary: If Γ has a boundary, we have a strong-coupling asymptotics for the bound state number given in Theorems 3.1 and 7.1 but not for eigenvalues themselves. We *conjecture* that the latter is given again by

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

etc., where μ_j refer to operator with *the same symbol* and *Dirichlet* boundary conditions (with natural modifications in other dimensions).

2) Strong coupling, less regularity: Examples show that the above relation is not valid for a non-smooth Γ, rather μ_j can be replaced by a term proportional to α^2, for instance if Γ has an angle. 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

3) Scattering theory on non-compact "leaky" curves, manifolds, graphs, and generalized graphs is absent. Some open questions:

- existence and completeness w.r.t. motion in asymptotic geometry of Γ, including absolute continuity of the spectrum in $(-\frac{1}{4}\alpha^2, 0)$
- asymptotics of the S-matrix in the strong-coupling regime, including relations between S-matrices of the leaky and "ideal" graphs
- to prove existence of resonances, at least within particular models. So far the result is known in a very simple situations only [EK03c]

4) Periodic Γ***:*** one conjectures 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.

5) 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 $\sigma_{\rm ess}(H_{\alpha,\Gamma})$ is always *pure point* once a disorder is present?

6) Adding magnetic field: Will the curvature-induced discrete spectrum survive under any magnetic field? On the other hand, will (at least a part of) the absolutely spectrum of $(-i\nabla - A)^2 - \alpha\delta(x-\Gamma)$ survive a randomization of a straight Γ?

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