Geometrically induced bound states in Dirichlet layers

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Talk overview

- Physical and mathematical motivation

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- Preliminaries: geometry of a curved layer

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- Equivalent forms of the Hamiltonian
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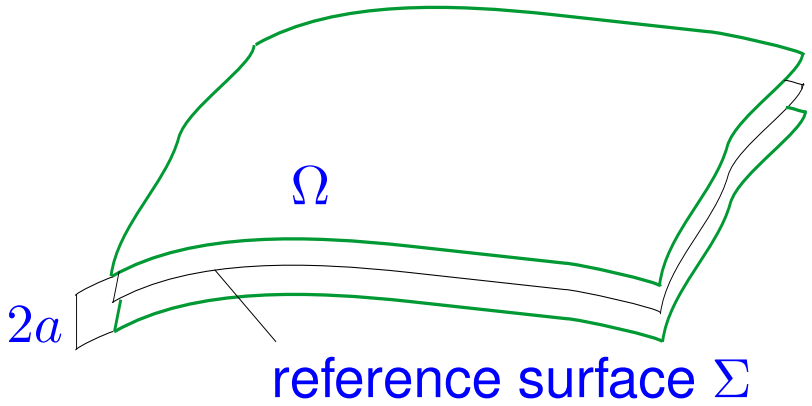
- Topologically nontrivial quantum layers
- Weak coupling: mildly curved layers
- Some open questions

Motivation



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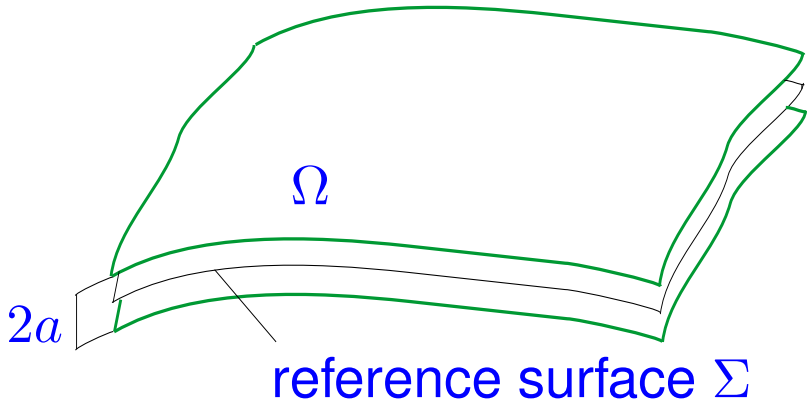

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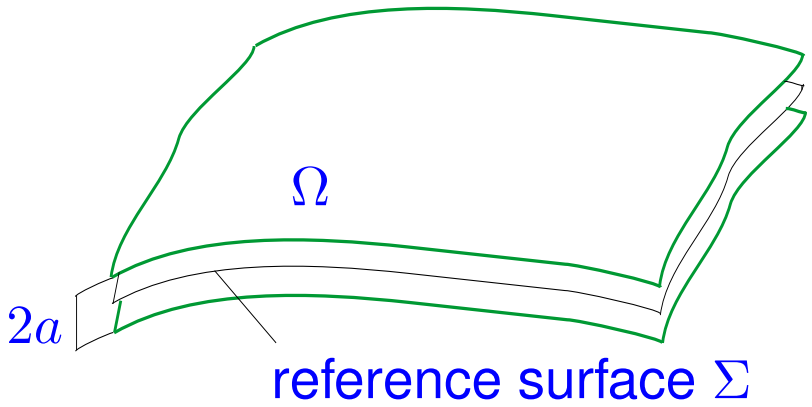

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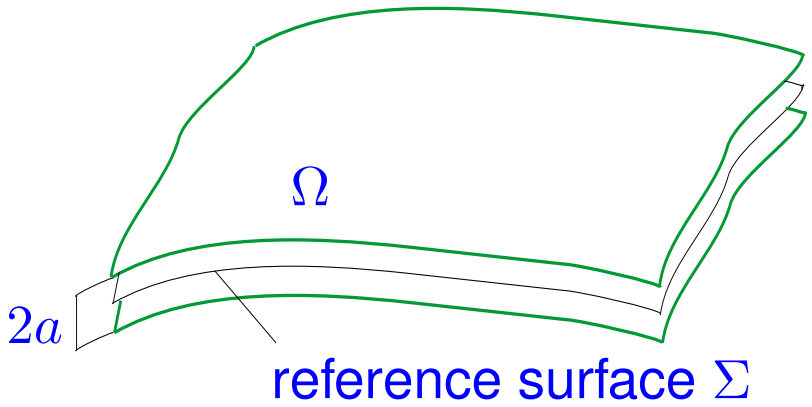

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- Recently made rigorous in [Froese-Herbst '01] with a *harmonic confinement*
- We are interested primarily in relations between *geometry* and *spectral properties*, i.e. a trademark topic of mathematical physics

Motivation: semiconductor films

A natural model for *dilute electron gas* in *semiconductor films* built on a *curved substrate*. Recall that a typical mesoscopic system has

- *small size:* submicron, down to nanometers
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One typically one assumes *hard wall (Dirichlet)* boundary conditions. It is an idealization, in reality rather a finite potential jump

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- Thin enough periodically curved waveguides have *open gaps*, etc.

Preliminaries

The surface Σ in $\mathbb{R}^3$ supposed to be C^2-*smooth* and to have at least one *pole* (i.e., exponential mapping $\exp_o : T_o\Sigma \to \Sigma$ is a diffeomorphism). Hence σ is *diffeomorphic to* $\mathbb{R}^2$, i.e. *simply connected* and *non-compact*. Using *geodesic polar coordinates* we parametrize

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The layer $\Omega := \mathcal{L}(\Omega_0)$ of width $d = 2a$ over Σ, where $\Omega_0 := \Sigma_0 \times (-a, a)$, is defined by the map

$$\mathcal{L} : \Omega_0 \to \mathbb{R}^3 : \{(q, u) \mapsto \mathcal{L}(q, u) := p(q) + un(q) \in \Omega\}$$

Motivation: surfaces with poles

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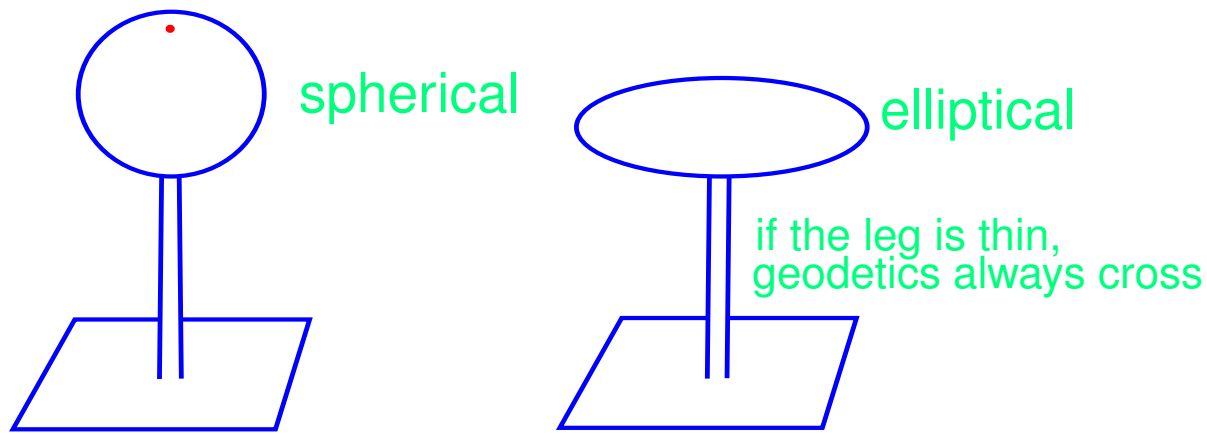
The assumption is nontrivial. *Example* [Gromol-Meyer '69]:



However, the assumption is not necessary for the spectral result we are going to derive. Later we get rid of it.

Preliminaries: surface geometry

The *surface metric* in the geodesic polar coordinates is diagonal, $(g_{\mu\nu}) = \mathrm{diag}\,(1, r^2)$, where $r^2 \equiv g := \det(g_{\mu\nu})$ is the squared Jacobian of the exponential mapping which satisfies *Jacobi equation*

$$\ddot{r}(s,\vartheta) + K(s,\vartheta)\, r(s,\vartheta) = 0\,,\ r(0,\vartheta) = 0,\ \dot{r}(0,\vartheta) = 1$$

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In addition to $g_{\mu\nu} := p_{,\mu} \cdot p_{,\nu}$ we introduce *second fundamental form* $h_{\mu\nu} := -n_{,\mu} \cdot p_{,\nu}$ with $h := \det(h_{\mu\nu})$ and *Weingärten map* $h^\mu_\nu := g^{\mu\rho} h_{\rho\nu}$ which determine

- *Gauss curvature* $K := \det(h^\mu_\nu) = h/g$
- *mean curvature* $M := \frac{1}{2}\mathrm{Tr}(h^\mu_\nu) = \frac{1}{2} g^{\mu\nu} h_{\mu\nu}$

Preliminaries: total curvatures

Using *invariant surface element*, $\mathrm{d}\Sigma := g^{1/2}\mathrm{d}^2q \equiv g^{1/2}\mathrm{d}q^1\mathrm{d}q^2$, we introduce global quantities, in particular, *total curvatures*

$$\mathcal{K} := \int_\Sigma K\mathrm{d}\Sigma \quad \text{and} \quad \mathcal{M}^2 := \int_\Sigma M^2\mathrm{d}\Sigma\,;$$

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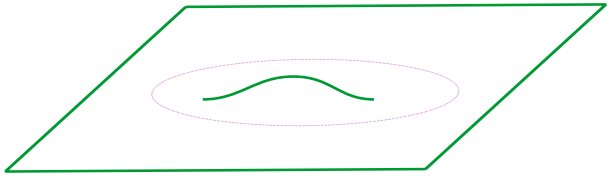
In particular, if Σ is a *locally deformed plane* we choose $\partial\mathcal{G}$ outside the deformation, so $\mathcal{K}_\mathcal{G} = \mathcal{K}_\Sigma = 0$



Preliminaries: layer geometry

Metric tensor, $G_{ij} := \mathcal{L}_{,i} \cdot \mathcal{L}_{,j}$, of the layer (regarded as a manifold with boundary in $\mathbb{R}^3$) has the block form

$$(G_{ij}) = \begin{pmatrix} (G_{\mu\nu}) & 0 \\ 0 & 1 \end{pmatrix} \quad \text{with} \quad G_{\nu\mu} = (\delta^\sigma_\nu - u h_\nu{}^\sigma)(\delta^\rho_\sigma - u h_\sigma{}^\rho) g_{\rho\mu}$$

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Then we can express the determinant, $G := \det(G_{ij})$ as

$$G = g\left[(1 - u k_1)(1 - u k_2)\right]^2 = g(1 - 2Mu + Ku^2)^2$$

In particular, the *volume element* is $\mathrm{d}\Omega := G^{1/2} \mathrm{d}^2 q \, \mathrm{d}u$

Preliminaries: assumptions

For the moment we adopt the following hypotheses:

$\langle\Sigma 0\rangle$ $K \in L^1(\Sigma_0, \mathrm{d}\Sigma)$

$\langle\Omega 0\rangle$ Ω is not self-intersecting, i.e. $\mathcal{L}$ is injective

$\langle\Omega 1\rangle$ $a < \rho_m := (\max\{\|k_1\|_\infty, \|k_2\|_\infty\})^{-1}$

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The last one ensures that $\mathcal{L}$ is a diffeomorphism, in particular, that Ω has a smooth boundary. Furthermore, $\langle\Omega 1\rangle$ also implies a useful estimate,

$$C_- g_{\mu\nu} \leq G_{\mu\nu} \leq C_+ g_{\mu\nu} \quad \text{with} \quad 0 < C_- < 1 < C_+ < 4$$

and the constants expressed in terms of the *minimal normal curvature radius* ρ_m as $C_\pm := \left(1 \pm a\rho_m^{-1}\right)^2$

Hamiltonian: curvilinear coordinates

Neglecting physical constants the Hamiltonian is identified with the Dirichlet Laplacian $-\Delta_D^\Omega$ on $L^2(\Omega)$ with the usual properties, e.g., the form domain is $W_0^{1,2}(\Omega)$.

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$$H := -G^{-1/2}\partial_i G^{1/2} G^{ij}\partial_j \quad \text{on} \quad L^2(\Omega_0, G^{1/2}\mathrm{d}^2 q\,\mathrm{d}u)\,,$$

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If Σ is not C^3-smooth, H is understood in the form sense

$$Q(\psi) := \|H^{1/2}\psi\|_G^2 = (\psi_{,i}, G^{ij}\psi_{,j})_G\,, \quad D(Q) = W_0^{1,2}(\Omega_0,\mathrm{d}\Omega)\,,$$

where "G" indicates the norm and the inner product in the above Hilbert space

Hamiltonian: decomposition

The block form of G_{ij} yields $H = H_1 + H_2$ with

$$H_1 := -G^{-1/2}\partial_\mu G^{1/2} G^{\mu\nu}\partial_\nu = -\partial_\mu G^{\mu\nu}\partial_\nu - 2F_{,\mu}G^{\mu\nu}\partial_\nu \,,$$

$$H_2 := -G^{-1/2}\partial_3 G^{1/2}\partial_3 = -\partial_3^2 - 2\,\frac{Ku - M}{1 - 2Mu + Ku^2}\,\partial_3 \,,$$

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An alternative form, with the factor $1 - 2Mu + Ku^2$ removed from the weight $G^{1/2}$, is obtained by another unitary transformation $\hat{U} : L^2(\Omega_0, \mathrm{d}\Omega) \to L^2(\Omega_0, \mathrm{d}\Sigma\,\mathrm{d}u)$,

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

giving $\hat{H} := \hat{U}H\hat{U}^{-1}$. The norm in the corresponding Hilbert space is indicated by the subscript "g"

Hamiltonian: decomposition

The operator $\hat{H}$ contains an *effective potential*; introducing $J := \frac{1}{2}\ln(1 - 2Mu + Ku^2)$ we rewrite it as follows,

$$\hat{H} = -g^{-1/2}\partial_i g^{1/2} G^{ij}\partial_j + V\,, \quad V = g^{-1/2}(g^{1/2}G^{ij}J_{,j})_{,i} + J_{,i}G^{ij}J_{,j}$$

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In analogy with the curved tube case it is illustrative to write $\hat{H} = \hat{H}_q - \partial_3^2$, where $\hat{H}_q := \hat{H}_1 + V_2$

Heuristic considerations

In thin layers, $a \ll \rho_m$, the longitudinal and transverse variables are *asymptotically decoupled*, because

$$H_q := -g^{-1/2}\partial_\mu g^{1/2} g^{\mu\nu}\partial_\nu + K - M^2 + \mathcal{O}(a\rho_m^{-1})\,;$$

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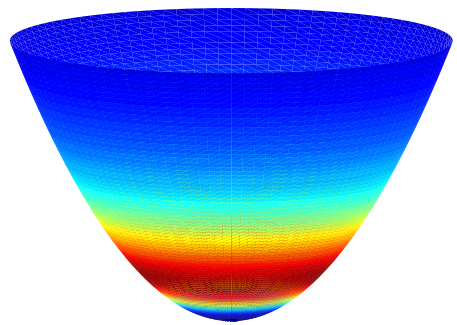
The additional potential $K - M^2$ rewrites in terms of principal curvatures as $-\frac{1}{4}(k_1 - k_2)^2$. It is *attractive* unless

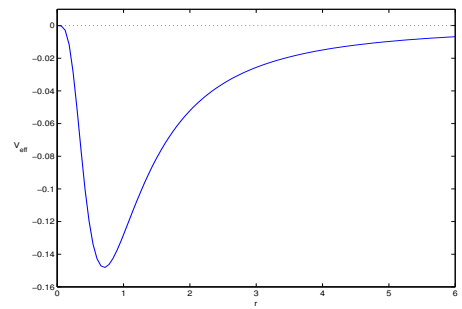
- Σ is planar, $k_1 = k_2 = 0$
- Σ is spherical, $k_1 = k_2$, however, a noncompact Σ clearly cannot be spherical globally

Examples of the effective interaction

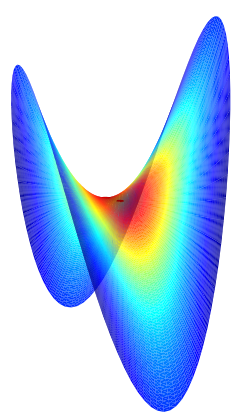
Effective Potential $V_{\text{eff}} = -\frac{1}{4}(k_+ - k_-)^2$

Paraboloid of Revolution $z = x^2 + y^2$

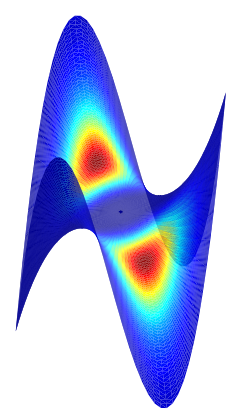




Hyperbolic Paraboloid $z = x^2 - y^2$



Monkey Saddle $z = x^3 - 3xy^2$



The minima of V_{eff} are marked by the dark red colour.

Essential spectrum threshold

Notation: we use eigenfunctions $\{\chi_n\}_{n=1}^{\infty}$ of the transverse operator $(-\partial_3^2)_D$ given by $\sqrt{\frac{2}{d}}\binom{\cos}{\sin}\kappa_n u$ for n $\binom{\text{odd}}{\text{even}}$, where $\kappa_n^2 := (\kappa_1 n)^2$ with $\kappa_1 := \pi/d$ are the corresponding ev's

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Theorem [Duclos-E.-Krejčiřík, 2001]: Assume $\langle\Omega 0\rangle$, $\langle\Omega 1\rangle$ and $\langle\Sigma 0\rangle$, then we have

$$\inf \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega}) \geq \kappa_1^2$$

$\inf \sigma_{\rm ess}$: sketch of the proof

Divide Ω into an exterior and interior by extra *Neumann b.c.* at $s = s_0$, then $H \geq H^N_{\rm int} \oplus H^N_{\rm ext}$. The interior does not contribute to $\sigma_{\rm ess}$, so by minimax principle we infer

$$\inf \sigma_{\rm ess}(H) \geq \inf \sigma_{\rm ess}(H^N_{\rm ext}) \geq \inf \sigma(H^N_{\rm ext})$$

In the exterior we have for all $\psi \in D(Q^N_{\rm ext})$ the estimate

$$\begin{aligned} Q^N_{\rm ext}(\psi) &\geq \|\psi_{,3}\|^2_{G,\rm ext} \geq \inf_{\Omega_{\rm ext}} \{1 - 2Mu + Ku^2\} \, \|\psi_{,3}\|^2_{g,\rm ext} \\ &\geq \left(1 - \sup_{\Sigma_{\rm ext}} \{2a|M| + a^2|K|\}\right) \kappa_1^2 \, \|\psi\|^2_{g,\rm ext} \\ &\geq \frac{1 - \sup_{\Sigma_{\rm ext}} \{2a|M| + a^2|K|\}}{1 - \inf_{\Sigma_{\rm ext}} \{2a|M| + a^2|K|\}} \, \kappa_1^2 \, \|\psi\|^2_{G,\rm ext} \\ &= (1 + o(s_0)) \, \kappa_1^2 \, \|\psi\|^2_{G,\rm ext} \quad \square \end{aligned}$$

Curvature-induced binding, $\mathcal{K} \leq 0$

Theorem [Duclos-E.-Krejčiřík, 2001]: Assume $\langle\Omega 0\rangle$, $\langle\Omega 1\rangle$ and $\langle\Sigma 1\rangle$, and suppose that Σ *is not planar*. If $\mathcal{K} \leq 0$, then

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Sketch of the proof: By a variational argument, seeking a trial function Ψ from $\mathcal{Q}(H)$ such that

$$\tilde{Q}(\Psi) := Q(\Psi) - \kappa_1^2 \|\Psi\|_G^2 < 0$$

It is convenient to split the Hamiltonian form, $Q = Q_1 + Q_2$ with parts associated to H_1 and H_2 introduced above. We employ *Goldstone-Jaffe trick*, choosing radially symmetric $\psi(s, \vartheta, u) := \varphi(s)\chi_1(u)$ with φ to be specified

$\mathcal{K} \leq 0$, sketch of the proof

Using the factorized form of ψ we get directly

$$Q_2(\psi) - \kappa_1^2 \|\psi\|_G^2 = (\psi, K\psi)_g$$

On the other hand, the "longitudinal kinetic part" $Q_1(\psi)$ can be estimated by the radial gradient norm of ψ as

$$Q_1(\psi) \leq C_1 \int_0^\infty |\dot{\varphi}(s)|^2 s \, \mathrm{d}s$$

with some $C_1 > 0$. To make it small we need a suitable family of radial functions such that $\psi \in \mathcal{Q}(H)$; we choose them as scaled Macdonald functions outside a circle, i.e.

$$\varphi_\sigma(s) := \min \left\{ 1, \frac{K_0(\sigma s)}{K_0(\sigma s_0)} \right\}$$

$\mathcal{K} \leq 0$, sketch of the proof

It is straightforward to compute the integral; we get

$$\exists C_2 > 0 : \qquad \int_0^\infty |\dot\varphi_\sigma(s)|^2 s\, ds < \frac{C_2}{|\ln \sigma s_0|}\,,$$

and therefore $Q_1(\psi_\sigma) \to 0+$ as $\sigma \to 0+$. We assume $\langle \Sigma 1 \rangle$, so by dominated the first part of the shifted energy form tends to $\mathcal{K}$ as $\sigma \to 0+$; this proves the theorem if $\mathcal{K} < 0$.

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If $\mathcal{K} = 0$ we follow GJ idea choosing $\Psi_{\sigma,\varepsilon} := \psi_\sigma + \varepsilon\Theta$, where $\Theta(q,u) := j(q)^2 u \chi_1(u)$ with $j \in C_0^\infty((0,s_0)\times S^1)$; it gives

$$\tilde Q(\Psi_{\sigma,\varepsilon}) = \tilde Q(\psi_\sigma) + 2\varepsilon \tilde Q(\Theta,\psi_\sigma) + \varepsilon^2 \tilde Q(\Theta)$$

Since $\tilde Q(\Theta,\psi_\sigma) = -\frac{1}{d}(j,M)_g \neq 0$ in general, the sum of the last two terms can be made negative; then $\tilde Q(\Psi_{\sigma,\varepsilon}) < 0$ will hold for σ small enough. $\square$

$\mathcal{K} \leq 0$, examples

The theorem applies to layers built over *Cartan-Hadamard surfaces*, i.e. geodesically complete simply connected non-compact ones with $\mathcal{K} \leq 0$ (then each point is a pole)

- *Locally curved plane* has $\mathcal{K} = 0$ by Gauss-Bonnet, the same is true for surfaces with curvatures which are not compactly supported but decay fast enough

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- *Hyperbolic paraboloid:* the simple quadric given in $\mathbb{R}^3$ by the equation $z = x^2 - y^2$ is an asymptotically planar surface with $\mathcal{K} = -2\pi$
- *Monkey saddle:* another example of a saddle surface is $z = x^3 - 3xy^2$; it satisfies again $\langle \Sigma 1 \rangle$ and $\mathcal{K} = -4\pi$

Other sufficient conditions

The GJ trick – constructing a trial function starting from a factorized function $\psi(s, \vartheta, u) := \varphi(s)\chi_1(u)$ – does not work for $\mathcal{K} > 0$. However, other sufficient conditions can still be obtained variationally:

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Theorem [Duclos-E.-Krejčiřík, 2001]: Assume $\langle\Omega 0\rangle$ and $\langle\Omega 1\rangle$ and suppose that Σ is C^3-smooth and *non-planar*. In addition, let *one of the following conditions be valid:*

- the layer Ω is *thin enough*
- we have $\langle\Sigma 1\rangle$, $\mathcal{M} = \infty$, and

  $\langle\Sigma 2\rangle$ the covariant derivative $\nabla_g M \in L^2(\Sigma_0, \mathrm{d}\Sigma)$

Then $\inf\sigma(-\Delta_D^\Omega) < \kappa_1^2$, in particular, curvature-induced bound states exist under the assumption $\langle\Sigma 0\rangle$

Sketch of the proof

Trial function $\Psi_\sigma(s,\vartheta,u) := (1 + M(s,\vartheta)u)\,\psi_\sigma(s,u)$ gives

$$Q_1(\Psi_\sigma) \;\leq\; 2(C_+/C_-)^2 \Big((1 + a\|M\|_\infty)^2 \, \|\dot{\psi}_\sigma\|_g^2 + a^2 \|\psi_\sigma \nabla_g M\|_g^2 \Big)$$

$$\text{small as } \sigma \to 0 \qquad\qquad \mathcal{O}(a^2)$$

$$Q_2(\Psi_\sigma) - \kappa_1^2 \|\psi\|_G^2 \;=\; \big(\psi_\sigma, (K - M^2)\psi_\sigma\big)_g + \frac{\pi^2 - 6}{12\kappa_1^2} \big(\psi_\sigma, K M^2 \psi_\sigma\big)_g$$

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Under the second assumption, $\big(\psi_\sigma, -M^2\psi_\sigma\big)_g \to -\infty$ as $\sigma \to 0+$, while the other terms remain finite. $\square$

Cylindrically symmetric layers

Another sufficient condition can be derived for layers *invariant w.r.t. rotations around a fixed axis in* $\mathbb{R}^3$ with Σ parameterized by means of $r, z \in C^2\left((0,\infty)\right)$ as

$$p : \Sigma_0 \to \mathbb{R}^3 : \{(s,\vartheta) \mapsto (r(s)\cos\vartheta, r(s)\sin\vartheta, z(s))\}$$

It is a geodesic polar coordinate chart if we require

$$\dot{r}^2 + \dot{z}^2 = 1\,; \quad \text{then also} \quad \dot{r}\ddot{r} + \dot{z}\ddot{z} = 0$$

The Weingärten tensor is $(h_\mu{}^\nu) = \mathrm{diag}\,(k_s, k_\vartheta)$ with the principal curvatures $k_s = \dot{r}\ddot{z} - \ddot{r}\dot{z}$ and $k_\vartheta = \frac{\dot{z}}{r}$. We have

$$\mathcal{K} + 2\pi\dot{r}(\infty) = 2\pi\,, \quad \text{where} \quad \dot{r}(\infty) := \lim_{s\to\infty} \dot{r}(s)$$

by Gauss-Bonnet theorem, and since $0 \le \dot{r}(\infty) \le 1$, such a cylindrically invariant surface Σ always has $0 \le \mathcal{K} \le 2\pi$

Cylindrically symmetric layers

We exclude the case already resolved and assume $\mathcal{K} > 0$, i.e. $0 \leq \dot{r}(\infty) < 1$. Using the above parametrization we get

Lemma: Let $\mathcal{K} > 0$, then there are $\delta > 0$ and $s_0 > 0$ s.t.

$$\forall s \geq s_0 : \quad \frac{\delta}{r(s)} \leq |k_\vartheta(s)| \leq \frac{1}{r(s)}$$

and $k_\vartheta(s)$ does not change sign. It follows that k_ϑ is not integrable in $L^1(\mathbb{R}_+)$. If $\langle \Sigma 1 \rangle$ is satisfied, we have $\mathcal{M} = \infty$

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Theorem [Duclos-E.-Krejčiřík, 2001]: Assume $\langle\Omega 0\rangle$, $\langle\Omega 1\rangle$ and $\langle\Sigma 1\rangle$, and suppose that Σ is a surface of revolution with $\mathcal{K} > 0$. Then $\inf \sigma(-\Delta_D^\Omega) < \kappa_1^2$, in particular, $\sigma_{\mathrm{disc}}(d - \Delta_D^\Omega) \neq \emptyset$ holds under the assumption $\langle\Sigma 0\rangle$

Sketch of the proof

By assumption M dominates over K in effective potential at large distances, hence we choose trial functions supported there. Consider sequences $\{n^i\}_{n=1}^{\infty}$, $i = 1, 2, 3$, and put

$$\varphi_n(s) := \frac{\ln(sn^{-i})}{\ln(n^{j-i})}\,, \quad \phi_n(s) := \frac{\varphi_n(s)}{s}\,, \qquad (i,j) \in \{(1,2),(3,2)\}$$

if $\min\{n^i, n^j\} < s \leq \max\{n^i, n^j\}$ and zero otherwise. We employ functions $\Psi_{n,\varepsilon}(s,u) := (\varphi_n(s) + \varepsilon\phi_n(s)u)\chi_1(u)$ which belong to form domain of H and are uniformly bounded

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By a direct computation and simple estimates we get

$$\lim_{n\to\infty} \tilde{Q}[\Psi_{n,\varepsilon}] = \lim_{n\to\infty} \left[\varepsilon^2 \|\phi_n\|_{\Sigma}^2 - 2\varepsilon(\varphi_n, M\phi_n)_{\Sigma}\right]$$

if the r.h.s. limit exists, where the norms refer to $L^2(\Sigma, \mathrm{d}\Sigma_0)$

Sketch of the proof

We choose $\varepsilon \equiv \varepsilon_n := (\varphi_n, M\phi_n)_\Sigma^{-1}$ which makes sense as the integral diverges; thus one has to compare -2 with

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Now finally we use *rotational symmetry*. Since $k_s \in L^1(\mathbb{R}_+)$ and ϕ_n is chosen to eliminate the weight r, the meridian curvature does not contribute in the denominator, while in view of the lemma $k_\vartheta r$ behaves as one at infinity. Consequently, the limit in question is

$$\frac{\int_0^\infty \phi_n(s)^2 s\, ds}{\left(\int_0^\infty \varphi_n(s)\phi_n(s) ds\right)^2} = \frac{1}{\int_0^\infty \phi_n(s)^2 s\, ds} = \frac{3}{\ln(n^2)} \to 0\,,$$

and thus $\lim_{n\to\infty} \tilde{Q}(\Psi_{n,\varepsilon}) \to -2$ as we sought to prove $\square$

Remarks

- *Partial wave decomposition:* one can decompose $-\Delta_D^{\Omega}$ to angular momentum subspaces and employ 2D methods. It is not much simpler, but one gets an insight: the trial function could be supported in the far off region where the *centrifugal term is weak*

Remarks

- *Partial wave decomposition:* one can decompose $-\Delta_D^\Omega$ to angular momentum subspaces and employ 2D methods. It is not much simpler, but one gets an insight: the trial function could be supported in the far off region where the *centrifugal term is weak*
- *Layers without bound states:* if you "close" Σ too much the discrete spectrum may be lost. *Example:* let Σ be a *cylinder with a hemispherical "cap"*, then by Neumann bracketing we check that $\sigma_{\mathrm{disc}}(-\Delta_D^\Omega) = \emptyset$. While it does not satisfy our smoothness assumptions, a counterexample is obtained using domain continuity. The reason is, of course, that such a Σ *ceases to be asymptotically planar* pushing $\inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega)$ down

Generalizations

Let Ω be built over Σ which is complete non-compact connected C^2-smooth surface, and suppose that $\langle\Omega 0\rangle$, $\langle\Omega 1\rangle$ and $\langle\Sigma 1\rangle$ are satisfied.

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- the same is true if the generating surface Σ *is not conformally equivalent to the plane*

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The upper bound: If $K \to 0$ at infinity, to any $\varepsilon > 0$ there is an infinite-dimensional $\mathcal{D}_g \subset C_0^\infty(\Sigma)$ s.t. $\|\nabla_g \varphi\|_g \le \varepsilon \|\varphi\|_g$ holds for $\varphi \in \mathcal{D}_g$. Then we employ the identity

$$\|\nabla \varphi \chi_1\|^2 = \||\nabla \varphi|\, \chi_1\|^2 - (\varphi \chi_1, \varphi \Delta \chi_1)$$

The first term is estimated by $(C_+/C_-{}^2)\, \varepsilon^2\, \|\varphi\, \chi_1\|^2$, while the one can be rewritten as

$$-\left(\varphi \Delta \chi_1, \varphi \chi_1\right) = \kappa_1^2\, \|\varphi\, \chi_1\|^2 + \left(\varphi \chi_1', 2 M_u \varphi \chi_1\right),$$

where $M_u := \frac{M - Ku}{1 - 2Mu + Ku^2}$ refers to "parallel" surface $\mathcal{L}(\Sigma \times \{u\})$

$\inf \sigma_{\mathrm{ess}}\left(-\Delta_D^{\Omega}\right)$ revisited

Integrating the last term by parts in u we conclude that for any $\varepsilon > 0$ there is $\mathcal{D} := \mathcal{D}_g \otimes \{\chi_1\} \subset C_0^\infty(\Omega)$ such that

$$\forall \psi \in \mathcal{D}: \quad \|\nabla\psi\|^2 - (\psi, K_u\psi) \leq \left(\kappa_1^2 + (C_+/C_-{}^2)\,\varepsilon^2\right)\|\psi\|^2,$$

where $K_u := \frac{K}{1-2Mu+Ku^2}$ is the Gauss curvature of the above indicated parallel surface

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This proves $\inf \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega} - K_u) \leq \kappa_1^2$. Since K_u vanishes at infinity by assumption, the operator $K_u(-\Delta_D^{\Omega} + 1)^{-1}$ is compact in $L^2(\Omega)$ and the same spectral result holds thus for the operator $-\Delta_D^{\Omega}$ we are interested in $\square$

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Remark: Notice that only $K \to 0$ at infinity is needed in order to establish the upper bound

Surfaces without poles

We needed geodetical polar coordinates to construct mollifiers in our trial functions. This can be circumvented:

Lemma [Carron-E.-Krejčiřík, 2004]: Assume $\langle\Sigma 1\rangle$, then there is a sequence $\{\varphi_n\}_{n\in\mathbb{N}}$ of smooth functions with compact supports in Σ such that

- $\forall n \in \mathbb{N}: \; 0 \leq \varphi_n \leq 1$
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Proof: Under $\langle\Sigma 1\rangle$ a classical result of [Huber '57] states that (Σ, g) is conformally equivalent to a closed surface with a finite number of points removed. However, the integral $\|\nabla_g \varphi_n\|_g$ is a conformal invariant and it is easy to find a sequence having the required properties on the "pierced" closed surface. $\square$

Handles: a non-simply connected Σ

Theorem [Carron-E.-Krejčiřík, 2004]: Under the stated assumptions, one has $\inf \sigma(-\Delta_D^\Omega) < \kappa_1^2$ whenever Σ is *not* conformally equivalent to the plane

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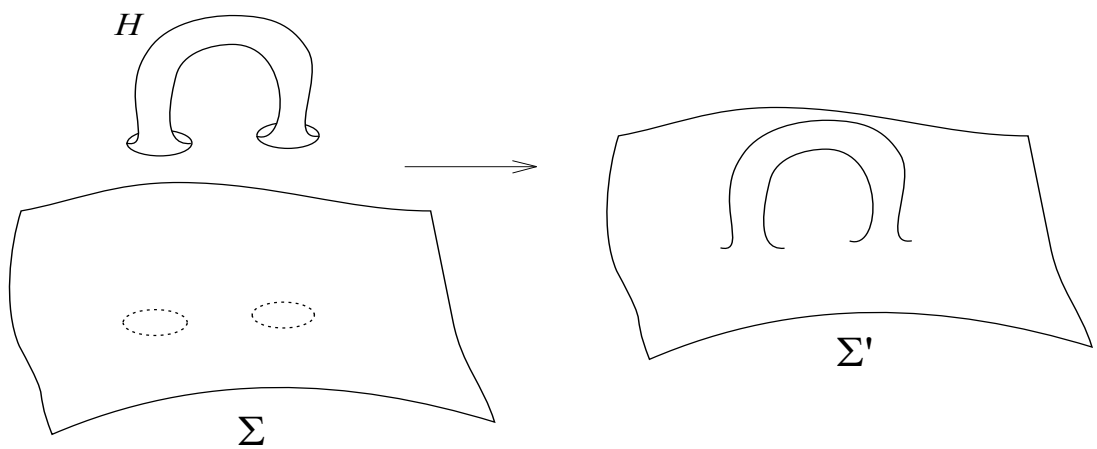
Proof: Indeed, the Cohn-Vossen inequality yields

$$\mathcal{K} \leq 2\pi\,(2 - 2h - e),$$

where h is the genus of Σ and e is the number of ends. Hence $\mathcal{K} < 0$ whenever $h \geq 1$. $\square$



Layers over Σ with cylindrical ends

Theorem [Carron-E.-Krejčiřík, 2004]: Assume $\langle\Omega 0\rangle$, $\langle\Omega 1\rangle$, $\langle\Sigma 0\rangle$ and $\langle\Sigma 1\rangle$. Let the reference surface Σ have $N \geq 1$ *cylindrically symmetric ends*, each with a positive total Gauss curvature. Let $\Omega' \subset \mathbb{R}^3$ be an unbounded, without boundary, obtained by a compact deformation of Ω. Then

- $\inf \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega'}) = \kappa_1^2$
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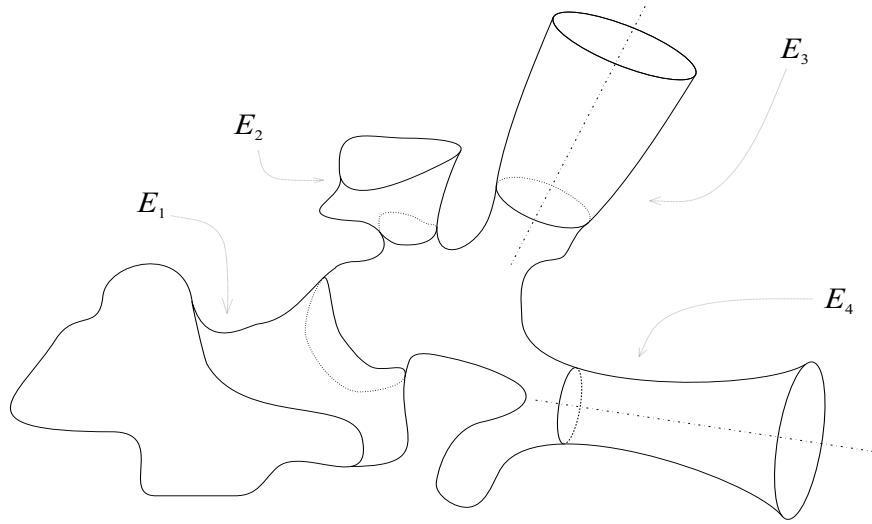
Sketch of the proof: Deriving the sufficient condition for cylindrical surfaces with $\mathcal{K} > 0$; we constructed sequences of trial functions "localised at infinity" we may use them for our Ω. Moreover, trial functions localized at different ends are orthogonal in $L^2(\Omega)$. Finally, these estimates as well as σ_{ess} are stable under compact deformations of Ω. $\square$

Layers with ends: examples

- *Layer over Σ with multiple ends:*



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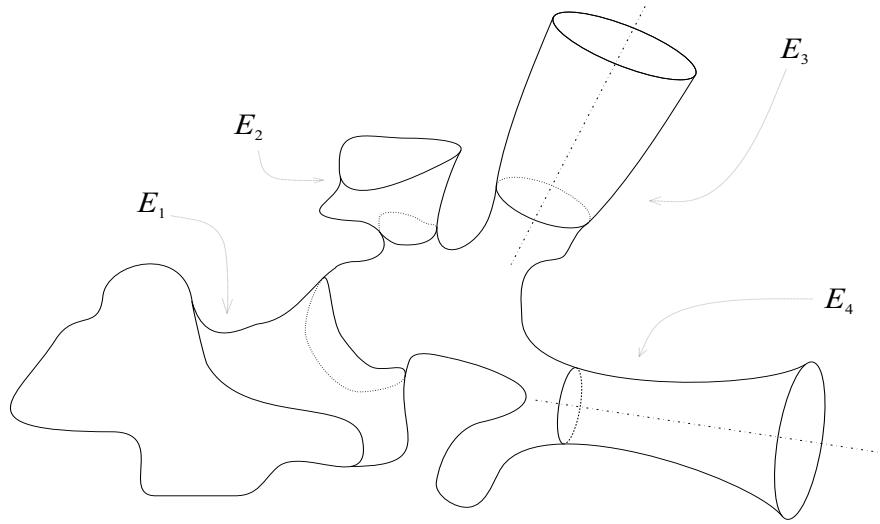
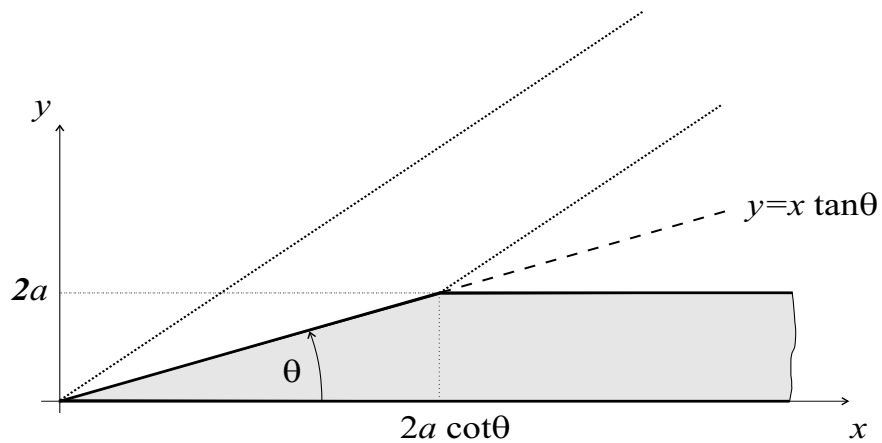


- *Conical layer:*



Weak coupling: preliminaries

Consider *mildly curved quantum layers* generated by a family of surfaces $\Sigma_\varepsilon := p\left(\mathbb{R}^2\right)$ given by a Monge patch

$$p : \mathbb{R}^2 \to \mathbb{R}^3, \quad p\left(x^1, x^2; \varepsilon\right) := \left(x^1, x^2, \varepsilon f(x^1, x^2)\right)$$

with $f \in C^4$ and ask what happens in the asymptotics $\varepsilon \to 0$

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Regularity and decay assumptions:

$\langle d1, 4\rangle$ $f_{,\mu},\ f_{,\mu\nu\rho\sigma} \in L^\infty(\mathbb{R}^2)$

$\langle d2, 3\rangle$ $f_{,\mu\nu},\ f_{,\mu\nu\rho} \to 0$ as $|x| \to \infty$

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Integral decay assumptions:

$\langle r1, 2\rangle$ $f_{,\mu\nu}\,,\ f_{,\mu\nu\rho} \in L^2\left(\mathbb{R}^2, (1 + |x|^\delta)\,\mathrm{d}x\right)$

$\langle r3\rangle$ $f_{,\mu\nu\rho\sigma} \in L^1\left(\mathbb{R}^2, (1 + |x|^\delta)\,\mathrm{d}x\right)$ for some $\delta > 0$

Weak coupling: asymptotic expansion

Theorem [E.-Krejčiřík, 2001]: Let Ω_ε be layers generated by Σ_ε with $f \in C^4(\mathbb{R}^2)$ satisfying $\langle d1\text{-}4\rangle$ and $\langle r1\text{-}3\rangle$. If Σ_1 is not planar, then for all ε small enough $-\Delta_D^{\Omega_\varepsilon}$ has exactly one isolated eigenvalue $E(\varepsilon)$ below the essential spectrum, and

$$E(\varepsilon) = \kappa_1^2 - \mathrm{e}^{2w(\varepsilon)^{-1}},$$

where $w(\varepsilon)$ has the following asymptotic expansion

$$w(\varepsilon) = -\varepsilon^2 \sum_{j=2}^{\infty} (\chi_1, u\chi_j) \left(\kappa_j^2 - \kappa_1^2\right)^2 \int_{\mathbb{R}^2} \frac{|\widehat{m_0}(\omega)|^2}{|\omega|^2 + \kappa_j^2 - \kappa_1^2} \, \mathrm{d}\omega + \mathcal{O}(\varepsilon^{2+\gamma})$$

with $\gamma := \min\{1, \delta/2\}$. Here m_0 is the lowest-order term in the expansion of the mean curvature of Σ_ε w.r.t. ε

Remarks

- The sum in the asymptotic expansion runs in fact *over even n only* because one integrates over $(-a, a)$ on which $u \mapsto \chi_1(u) u \chi_j(u)$ is odd for odd j

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- *The leading-term coefficient* w_1 in the expansion $w(\varepsilon) =: \varepsilon^2 w_1 + \mathcal{O}(\varepsilon^{2+\gamma})$ does not have a very transparent structure. For thin layers it can be rewritten as

$$w_1 = -\frac{1}{2\pi} \|m_0\|^2 + \frac{\pi^2 - 6}{24\pi^3} \|\nabla m_0\|^2 d^2 + \mathcal{O}(d^4),$$

which is instructive because the first term comes from the surface attractive potential $K - M^2$ which dominates the picture in this case

Birman-Schwinger analysis

Let $M \subset \mathbb{R}^m$, $m \geq 1$, be open connected precompact; put

$$H_\lambda = -\Delta_D + \lambda V \quad \text{with} \quad \lambda > 0 \quad \text{on} \quad \mathcal{H} := L^2(\mathbb{R}^2) \otimes L^2(M)$$

where $-\Delta_D$ is the closure of $-\Delta \otimes I_m + I_2 \otimes -\Delta_D^M$

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Assumptions:

$\langle a0 \rangle$ $\inf \sigma_{\text{ess}}(H_\lambda) \geq \kappa_1^2$

$\langle a1 \rangle$ $\exists\, a, b \geq 0 \;\; \forall \psi \in W_0^{1,2}(\Omega_0) : \;\; \|V\psi\| \leq a\|\psi\| + b\,\|H_0^{1/2}\psi\|$

$\langle a2 \rangle$ $|V|_{11} \in L^{1+\delta}\left(\mathbb{R}^2\right)$

$\langle a3 \rangle$ $|V|_{11} \in L^1\left(\mathbb{R}^2, (1+|x|^\delta)\,\mathrm{d}x\right)$

where $V_{jj'} := \int_M \bar{\chi}_j(y)\, V(\cdot, y)\, \chi_{j'}(y)\, \mathrm{d}y$ w.r.t. transverse basis of ef's χ_j, $j = 1, 2, \ldots$ with ev's $\kappa_1^2 < \kappa_2^2 \leq \ldots \leq \kappa_j^2 < \ldots$

Birman-Schwinger analysis

The free resolvent operator can be rewritten as

$$R_0(\alpha) = \sum_{j=1}^{\infty} \chi_j \left(-\Delta + k_j(\alpha)^2\right)^{-1} \bar{\chi}_j, \quad k_j(\alpha) := \sqrt{\kappa_j^2 - \alpha^2}$$

We are interested in ev's below κ_1^2, i.e. $\alpha \in [0, \kappa_1)$, when

$$R_0(x, y, x', y'; \alpha) = \frac{1}{2\pi} \sum_{j=1}^{\infty} \chi_j(y)\, K_0\left(k_j(\alpha)|x - x'|\right)\, \bar{\chi}_j(y')$$

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Define $K(\alpha) := |V|^{1/2} R_0(\alpha) V^{1/2}$, where $V^{1/2} := |V|^{1/2} \operatorname{sgn} V$.
By *Birman-Schwinger principle* $\alpha(\lambda)^2 \equiv E(\lambda)$ is an ev of H_λ *iff* $\lambda K(\alpha)$ has eigenvalue -1, in other words

$$\alpha^2 \in \sigma_{\mathrm{disc}}(H_\lambda) \Longleftrightarrow -1 \in \sigma_{\mathrm{disc}}(\lambda K(\alpha))$$

BS analysis: decomposition

One has to split the logarithmic singularity responsible for the weakly coupled ev. Put $K(\alpha) = L_\alpha + M_\alpha$, where

$$L_\alpha(x, y, x', y') := -\frac{1}{2\pi} |V(x, y)|^{1/2} \chi_1(y) \ln k_1(\alpha) \chi_1(y') V(x', y')^{1/2}$$

contains the singularity and M_α splits into two parts again, $M_\alpha = A_\alpha + B_\alpha$ with B_α being the projection of resolvent onto higher transverse modes, $j \geq 2$

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On the other hand, the operator A_α has the kernel

$$\frac{1}{2\pi} |V(x, y)|^{1/2} \chi_1(y) \Big(K_0(k_1(\alpha)|x - x'|) + \ln k_1(\alpha) \Big) \chi_1(y') V(x', y')^{1/2}$$

Note that M_α is well defined for $\alpha = \kappa_1$

BS analysis: eliminating regular part

Using asymptotic behaviour of K_0 we deduce

Lemma [E.-Krejčiřík, 2001]: Assume $\langle a1\text{-}3\rangle$, then there are positive C_2, C_3 and C_4 such that

- $\forall \alpha \in [0, \kappa_1]: \quad \|M_\alpha\| < C_2$
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Next we employ the factorization

$$(I + \lambda K(\alpha))^{-1} = \left[I + \lambda (I + \lambda M_\alpha)^{-1} L_\alpha\right]^{-1} (I + \lambda M_\alpha)^{-1}$$

By the lemma we have $\|\lambda M_\alpha\| < 1$ for small λ, the second factor is invertible and the singularities are determined by the first one

BS analysis: eliminating regular part

Observe that $\lambda(I+\lambda M_\alpha)^{-1}L_\alpha$ is rank-one operator of the form $(\psi,\cdot)\varphi$, where

$$\begin{aligned}\psi(x,y) &:= -\frac{\lambda}{2\pi}\ln k_1(\alpha)\,V(x,y)^{1/2}\,\chi_1(y),\\ \varphi(x,y) &:= [(I+\lambda M_\alpha)^{-1}|V|^{1/2}\chi_1](x,y),\end{aligned}$$

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If the latter should equal -1 we get the implicit equation

$$w = F(\lambda,w),\quad F(\lambda,w) := \frac{\lambda}{2\pi}\left(V^{1/2}\chi_1, \left(I+\lambda M_{\alpha(w)}\right)^{-1}|V|^{1/2}\chi_1\right)$$

with variable w related to the energy via $\alpha^2 = \kappa_1^2 - \mathrm{e}^{2w^{-1}}$

BS analysis: main result

Theorem [E.-Krejčiřík, 2001]: Assume $\langle a0\text{-}3\rangle$ and $V \neq 0$, then H_λ has for small enough $\lambda > 0$ exactly one ev $E(\lambda)$ *iff*

$$\int_{\mathbb{R}^2} V_{11}(x)\,\mathrm{d}x \leq 0$$

and in this case we can have $E(\lambda) = \kappa_1^2 - \mathrm{e}^{2w(\lambda)^{-1}}$, where

$$\begin{aligned} w(\lambda) = {} & \frac{\lambda}{2\pi}\int_{\mathbb{R}^2} V_{11}(x)\,\mathrm{d}x \\ & + \left(\frac{\lambda}{2\pi}\right)^2 \left\{ \int_{\mathbb{R}^2\times\mathbb{R}^2} V_{11}(x)\left(\gamma_{\mathrm{E}} + \ln\frac{|x-x'|}{2}\right) V_{11}(x')\,\mathrm{d}x\,\mathrm{d}x' \right. \\ & \left. - \sum_{j=2}^{\infty}\int_{\mathbb{R}^2\times\mathbb{R}^2} V_{1j}(x)\,K_0(k_j(\kappa_1)|x-x'|)\,V_{j1}(x')\,\mathrm{d}x\,\mathrm{d}x' \right\} + \mathcal{O}(\lambda^{2+\gamma}) \end{aligned}$$

with $\gamma := \min\{1, \delta/2\}$

Application to mildly curved layers

For the family of surfaces under consideration we have

$$
\begin{aligned}
g_{\mu\nu}(\varepsilon) &= \delta_{\mu\nu} + \varepsilon^2 \eta_{\mu\nu}\,, \quad (\eta_{\mu\nu}) := \begin{pmatrix} {f_{,1}}^2 & f_{,1} f_{,2} \\ f_{,1} f_{,2} & {f_{,2}}^2 \end{pmatrix} \\
g(\varepsilon) &:= \det(g_{\mu\nu}) = 1 + \varepsilon^2 \mathrm{tr}\,(\eta_{\mu\nu}) = 1 + \varepsilon^2 ({f_{,1}}^2 + {f_{,2}}^2) \\
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This gives, in particular, the curvatures

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K(\varepsilon) &= \delta_{\mu\nu} \varepsilon^2 g(\varepsilon)^{-2} k_0\,, \quad k_0 := \det(\theta_{\mu\nu}) = f_{,11} f_{,22} - {f_{,12}}^2 \\
M(\varepsilon) &= \varepsilon g(\varepsilon)^{-\frac{3}{2}} \left(m_0 + \varepsilon^2 m_1\right)\,, \quad m_0 := \frac{1}{2} \mathrm{tr}\,(\theta_{\mu\nu}) = \frac{1}{2}\left(f_{,11} + f_{,22}\right) \\
& \qquad m_1 := \frac{1}{2} \mathrm{tr}\,(\theta_{\mu\rho} \tilde{\eta}^{\rho\nu}) = \frac{1}{2}\left({f_{,1}}^2 f_{,22} + {f_{,2}}^2 f_{,11} - 2 f_{,1} f_{,2} f_{,12}\right)
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Now we apply the BS result, estimating the Hamiltonian by

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where

$$V_\pm(x,u) := \frac{1}{\varepsilon}\left(\frac{C_\pm}{C_\mp^2}\, v_1 + V_2\right)(x/\sigma_\pm, u)$$

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Furthermore, $V_2 = \frac{K-M^2}{(1-2Mu+Ku^2)^2}$ is as before and

$$v_1 := -\frac{|u^2\nabla_g K - 2u\nabla_g M|_g^2}{4(1-2Mu+Ku^2)^2} + \frac{u^2\Delta_g K - 2u\Delta_g M}{2(1-2Mu+Ku^2)}$$

Since v_1 and V_2 are ε-dependent, $V_\pm$ are well defined even for $\varepsilon = 0$. Expansion in ε yields the announced result.

Weak coupling: main result again

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Open questions

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- *More questions:* layers with magnetic fields, regular and singular potential perturbations, etc.

The talk was based on

[DEK00] P. Duclos, P.E., D. Krejčiřík: Locally curved quantum layers, *Ukrainian J. Phys.* **45** (2000), 595-601.

[DEK01] P. Duclos, P.E., D. Krejčiřík: Bound states in curved quantum layers, *Commun. Math. Phys.* **223** (2001), 13-28.

[EK01] P.E., D. Krejčiřík: Bound states in mildly curved layers, *J. Phys.* **A34** (2001), 5969-5985.

[CEK04] G. Carron, P.E., D. Krejčiřík: Topologically non-trivial quantum layers, *J. Math. Phys.* **45** (2004), 774-784.

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