Locally curved quantum layers

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We consider a quantum particle constrained to a curved layer of a constant width built over an infinite smooth surface. We suppose that the latter is a locally deformed plane and that the layer has the hard-wall boundary. Under this assumptions we prove that the particle Hamiltonian possesses geometrically induced bound states.

1 Introduction

Relations between geometry and spectral properties are one of the trademark topic of mathematical physics, in fact, an abstraction of various acoustic problems can be found in the roots of this discipline. For a long time, however, it seemed that such questions were restricted to the area of classical physics. This was mostly because geometrical properties of quantum systems were supposed to result from their dynamics, and as such they were not accessible to experimenters choice and manipulation. Interesting results dependent on geometry existed, of course, such as chaotic behaviour of certain quantum billiards observed first in [BGS] and studied in numerous subsequent papers, but they remained to be mostly academic exercises.

The situation has changed dramatically with the advent of mesoscopic techniques which allow us to produce tiny structures of various shapes devised and reproducible in the laboratory and yet small enough to exhibit quantum effects. Moreover, the physical nature of these objects makes it possible to describe them by a simple model in which a free particle (with an effective mass) is confined to the spatial region of the structure – see [DE] and references therein – borrowing the terminology one can speak about quantum waveguides, resonators, *etc.*

Theoretical studies of such systems have brought interesting results, some of them being purely quantum, without a classical counterpart. Among the most beautiful is the binding effect of curvature due to which infinitely extended regions with hard walls and a constant width can exhibit localized states. The effect was in fact observed a long time ago – see, *e.g.*, [dC1, dC2, Tol] and references therein – in formal attempts to justify quantization on nontrivial manifolds, but only in [EŠ] it was placed into a proper quantum-waveguide context and the existence of geometrically induced discrete spectrum for a curved planar strip was rigorously proven. This was followed by numerous other studies in which the results were improved and properties of the bound states were investigated – see, *e.g.*, [DE, GJ, RB].

Much less is known about analogous system in higher dimensions starting from the physically interesting case of a curved layer. This may seem strange at a glance, since the leading term of the effective potential for a general n-dimensional manifold in $\mathbb{R}^{m+n}$ was computed more than two decades ago [Tol]. However, going beyond the formal limit of infinitely thin layer one has to be able to estimate the next terms which is not an easy task. The aim of the present paper is to stimulate an investigation of the "two-in-three" case; we will concentrate at the simplest case where the deformation of a planar layer is infinitely smooth and compactly supported.

Let us describe the contents of the paper. In the next section we will formulate the problem and introduce a technique to handle it based on a suitable change of coordinates. The main results are given in Section 3. We will show first that under our assumption the essential spectrum starts at the first transverse eigenvalue. Then we will present a variational argument showing that a local deformation of the layer pushes the bottom of the spectrum below this value inducing thus a nonempty discrete spectrum. Properties of these bound states will be discussed elsewhere.

2 Formulation of the problem

Let Σ_0 be an open set in $\mathbb{R}^2$; its points will be denoted by $q = (q^1, q^2) \in \mathbb{R}^2$. Let a regular and simple *surface* Σ of class $\boldsymbol{C}^\infty$ in the space $\mathbb{R}^3$ be given by a mapping

$$p : \Sigma_0 \to \mathbb{R}^3 : \{q \mapsto p(q) \in \Sigma\} \tag{2.1}$$

such that the vectors $p_{,\mu} \equiv \partial_\mu p := \partial p/\partial q^\mu$, $\mu = 1, 2$, are linearly independent. We have in mind in this paper surfaces diffeomorphic to the plane, but since we will use different parametrizations, it is reasonable to consider Σ_0 generally as a subset of $\mathbb{R}^2$. Under the linear independence condition a unit normal of the surface

$$n : \Sigma_0 \to \mathbb{R}^3 : \left\{ q \mapsto n(q) := \frac{p_{,1} \times p_{,2}}{|p_{,1} \times p_{,2}|} \in \mathbb{R}^3 \right\} \tag{2.2}$$

is a well-defined smooth function, which defines an orientation of Σ. Together they determine a *layer* Ω of a width $d = 2\,a > 0$ over the surface Σ by virtue of the mapping

$$\phi : \Omega_0 \to \mathbb{R}^3 : \{(q, u) \mapsto \phi(q, u) := p(q) + un(q) \in \Omega\}, \tag{2.3}$$

where $\Omega_0 := \Sigma_0 \times (-a, a)$.

2.1 Properties of the reference surface

Recall first basic facts about the three fundamental forms of Σ. The coefficients of the first fundamental form $\mathbf{I}$ of the surface can be identified with the covariant components of its *metric tensor*

$$g_{\mu\nu} := p_{,\mu} \cdot p_{,\nu} \qquad g := \det(g_{\mu\nu}) \tag{2.4}$$

while for the second one, $\mathbf{II}$, we use the common notation

$$h_{\mu\nu} := -n_{,\mu} \cdot p_{,\nu} \qquad h := \det(h_{\mu\nu}). \tag{2.5}$$

The Weingarten map h_μ^ν (*cf.* [Kli, Def. 3.3.4 & Prop. 3.5.5]) determines the *Gauss curvature* of Σ, $K := \det(h_\mu^\nu) = \frac{h}{g}$, and its *mean curvature*, $M := \frac{1}{2}\operatorname{Tr}(h_\mu^\nu) = \frac{1}{2} g^{\mu\nu} h_{\mu\nu}$. The third fundamental form $\mathbf{III} := (n_{,\mu} \,.\, n_{,\nu})$ may be expressed by means of the first and second fundamental forms as follows:

Proposition 2.1 $n_{,\mu} \cdot n_{,\nu} = -K g_{\mu\nu} + 2M h_{\mu\nu} = h_{\mu\rho}\, g^{\rho\sigma}\, h_{\sigma\nu}$

PROOF: The first relation is equivalent to the identity $\mathbf{III} - 2M\mathbf{II} + K\mathbf{I} = 0$ – *cf.* [Kli, Prop. 3.5.6] or [LR, Problem 7.53] for a general dimension. To prove the second one, we use the fact that K, M are determined by the characteristic equation

$$k_\pm^2 - 2Mk_\pm + K = 0, \tag{2.6}$$

where k_+, k_- are the *principal curvatures*, *i.e.* the eigenvalues of h_μ^σ. Let $T_\sigma^\pm$ be the principal direction, *i.e.* the eigenvector of h_μ^σ, corresponding to $k_\pm$. Multiplying (2.6) by this vector we get $h_\mu^\rho h_\rho^\sigma T_\sigma^\pm - 2M h_\mu^\sigma T_\sigma^\pm + K\delta_\mu^\sigma T_\sigma^\pm = 0$. Since the principal directions forms locally an orthogonal basis in $\mathbb{R}^2$, the same must hold in the matrix sense, $h_\mu^\rho h_\rho^\sigma - 2M h_\mu^\sigma + K\delta_\mu^\sigma = 0$. The desired equality is then obtained by multiplication with $g_{\sigma\nu}$. ∎

Remark 2.2 We use the standard *summation convention* about repeated indices; the Greek and Latin ones run through $1, 2$ and $1, 2, 3$, respectively. The indices are associated with the above coordinates by $(1, 2, 3) \leftrightarrow (q^1, q^2, u)$. Furthermore, upper and lower index denote components of contravariant and covariant tensors, respectively. Indices are raised and lowered by the corresponding metric tensor. For instance, the matrix of the Weingerten map is given by $h_\mu^\nu = h_{\mu\rho}\, g^{\rho\nu}$. The same applies to the metric tensor $G_{\mu\nu}$ in the layer Ω which we shall introduce below.

Next we use the Jacobian $g^{\frac{1}{2}}$ to write down the invariant surface element

$$d\Sigma := g^{\frac{1}{2}} d^2 q \equiv g^{\frac{1}{2}} dq^1 dq^2.$$

It makes it possible define a global quantity characterizing Σ, namely the *total curvature* of our surface as

$$\mathsf{Tot}(\Sigma) := \int_\Sigma K d\Sigma.$$

Suppose that $\mathcal{G} \subset \Sigma$ is a region encircled by a simple closed curve $\mathcal{C}$ of class $\boldsymbol{C}^2$, then the Gauss-Bonnet theorem [LR, 7.6.45] claims that

$$\mathsf{Tot}(\mathcal{G}) + \oint_\mathcal{C} k_g d\ell = 2\pi, \tag{2.7}$$

where k_g is the geodesic curvature of $\mathcal{C}$ (traversed in the positive sense) and ℓ denotes its arc length. For the purpose of this paper it is important that the geodesic curvature of a circle in the plane is equal to its reciprocal radius. Consequently, an infinite surface obtained by a compactly supported deformation of a plane has $\mathsf{Tot}(\Sigma) = 0$.

2.2 Metric properties of the layer

It is clear from the definition (2.3) that the metric tensor of the layer (as a manifold with a boundary in $\mathbb{R}^3$) is of the following form

$$G_{ij} := \phi_{,i} \,.\, \phi_{,j} \qquad (G_{ij}) = \begin{pmatrix} G_{11} & G_{12} & 0 \\ G_{12} & G_{22} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{2.8}$$

where $G_{\mu\nu} = g_{\mu\nu} - 2\,u\,h_{\mu\nu} + u^2\,n_{,\mu}\,.\,n_{,\nu}$. In view of Proposition 2.1 we can rewrite the last expression as

$$G_{\mu\nu} = g_{\mu\rho}(\delta^\rho_\sigma - uh^\rho_\sigma)(\delta^\sigma_\nu - uh^\sigma_\nu), \tag{2.9}$$

which makes it easy to compute the determinant because the matrix of the Weingarten map h^ν_μ has the principal curvatures k_+, k_- as eigenvalues. Hence

$$G := \det(G_{\mu\nu}) = g\,[(1-uk_+)(1-uk_-)]^2 = g(1-2Mu+Ku^2)^2, \tag{2.10}$$

where in the second step we employed the relations $K = k_+k_-$ and $M = \frac{1}{2}(k_+ + k_-)$. As above,

$$d\Omega := G^{\frac{1}{2}} d\Omega_0 \equiv G^{\frac{1}{2}} d^2q\,du$$

defines the volume element of the layer.

The "straightening" transformation employed below requires that the mapping ϕ defining the layer is a diffeomorphism. In view of the regularity assumptions imposed on Σ and the inverse function theorem it is sufficient that $G_{\mu\nu}$ has an inverse bounded uniformly in Ω. This imposes a restriction of the layer thickness d. Define $\rho_m := \left(\max\{\|k_\nu(q)\|_\infty :\ \nu = \pm,\ q \in \Sigma_0\}\right)^{-1}$. It follows from (2.9) that $G_{\mu\nu}$ can be estimated by the surface metric,

$$C_- g_{\mu\nu} \le G_{\mu\nu} \le C_+ g_{\mu\nu}, \tag{2.11}$$

where the constants $C_\pm := \left(1 \pm a\rho_m^{-1}\right)^2$ are well defined since $\rho_m > 0$ by definition. Hence for a smooth surface Σ the bijectivity of ϕ is ensured as long as $a < \rho_m$.

2.3 Various expressions of the Hamiltonian

After these preliminaries let us define the Hamiltonian $\tilde{H}$ of our model. As we have said, the particle is supposed to be free within Ω and the boundary of the layer is a hard wall, *i.e.*, the wavefunctions should satisfy the Dirichlet boundary condition there. For the sake of simplicity we set the Planck's constant $\hbar = 1$ and the effective mass of the electron $m_* = 1/2$; then $\tilde{H}$ can be identified with the Dirichlet Laplacian

$$\tilde{H} := -\Delta_D^\Omega \quad \text{on} \quad \boldsymbol{L}^2(\Omega), \tag{2.12}$$

which is defined for an open set $\Omega \subset \mathbb{R}^3$ as the Friedrichs extension of the operator $-\Delta$ with the domain $\boldsymbol{C}_0^\infty(\Omega)$ – *cf.* [RS, Sec. XIII.15].

A natural way to investigate the operator (2.12) is to pass to the intrinsic coordinates (q, u) in which it acquires the Laplace-Beltrami form,

$$\hat{H} := -G^{-\frac{1}{2}} \partial_i G^{\frac{1}{2}} G^{ij} \partial_j \quad \text{on} \quad \boldsymbol{L}^2(\Omega_0, G^{\frac{1}{2}} d^2q\, du). \tag{2.13}$$

To find its action explicitly, we employ (2.8) together with the expression of the determinant (2.10). Then $\hat{H}$ splits into a sum of two parts,

$$\hat{H} = \hat{H}_1 + \hat{H}_2,$$

given by

$$\hat{H}_1 = -G^{-\frac{1}{2}} \partial_\mu G^{\frac{1}{2}} G^{\mu\nu} \partial_\nu = -\partial_\mu G^{\mu\nu} \partial_\nu - \frac{1}{2} G^{-1} G_{,\mu}\, G^{\mu\nu} \partial_\nu \tag{2.14}$$

$$\hat{H}_2 = -G^{-\frac{1}{2}} \partial_3 G^{\frac{1}{2}} \partial_3 = -\partial_3^2 - 2\, \frac{Ku - M}{1 - 2Mu + Ku^2}\, \partial_3\,. \tag{2.15}$$

The above coordinate change is nothing else than the unitary transformation

$$\hat{U} : \boldsymbol{L}^2(\Omega) \to \boldsymbol{L}^2(\Omega_0, G^{\frac{1}{2}} d^2q\, du) : \{\psi \mapsto \hat{U}\psi := \psi \circ \phi\}$$

which relates the two operators by $\hat{H} = \hat{U} \tilde{H} \hat{U}^{-1}$.

At the same time, it is useful to have an alternative form of the Hamiltonian which is symmetric w.r.t. G and has the Jacobian removed from the inner product. It is obtained by another unitary transformation,

$$U : \boldsymbol{L}^2(\Omega) \to \boldsymbol{L}^2(\Omega_0) : \{\psi \mapsto U\psi := G^{\frac{1}{4}} \psi \circ \phi\}.$$

which leads to the unitarily equivalent operator

$$H := U\tilde{H}U^{-1} = -G^{-\frac{1}{4}}\partial_\mu G^{\frac{1}{2}}G^{\mu\nu}\partial_\nu G^{-\frac{1}{4}} - G^{-\frac{1}{4}}\partial_3 G^{\frac{1}{2}}\partial_3 G^{-\frac{1}{4}} \tag{2.16}$$

with the domain

$$D(H) := \{\psi \in \boldsymbol{W}_2^2(\Omega_0)|\ \forall q \in \Sigma_0 : \psi(q,-a) = \psi(q,a) = 0\},, \tag{2.17}$$

where $\boldsymbol{W}_2^2(\Omega_0)$ is the appropriate local Sobolev space in the sense of [RS, Sec. XIII.14]. Commuting $G^{-\frac{1}{4}}$ with the gradient components we cast the operator (2.16) into a form which has a simpler kinetic part but contains an effective potential,

$$H = -\partial_\mu G^{\mu\nu}\partial_\nu - \partial_3^2 + V, \tag{2.18}$$

with

$$V = F^i_{,i} + F_i F^i\,, \quad F_i := (\ln G^{\frac{1}{4}})_{,i}.$$

This expression of the potential is valid for any smooth metric G_{ij}. If we employ the particular form (2.8) of the metric tensor, we can write again (2.18) as a sum of two parts, $H \equiv H_1 + H_2$ with $V = V_1 + V_2$, where

$$\begin{aligned}
H_1 &= -\partial_\mu G^{\mu\nu}\partial_\nu + V_1 && (2.19)\\
V_1 &:= \frac{1}{4}\partial_\mu G^{-1}G^{\mu\nu}G_{,\nu} + \frac{1}{16}G^{-2}G_{,\mu}G^{\mu\nu}G_{,\nu} &&\\
&= -\frac{3}{16}G^{-2}G_{,\mu}G^{\mu\nu}G_{,\nu} + \frac{1}{4}G^{-1}G^{\mu\nu}G_{,\mu\nu} + \frac{1}{4}G^{-1}G_{,\mu}G^{\mu\nu}{}_{,\nu} && (2.20)\\
H_2 &= -\partial_3^2 + V_2 && (2.21)\\
V_2 &:= \frac{K - M^2}{(1 - 2Mu + Ku^2)^2} && (2.22)
\end{aligned}$$

2.4 Coordinate decoupling

While the operator $H_1 + V_2$ depends on all the three coordinates, in thin layers its "leading term" depend on the longitudinal coordinates q only. The transverse coordinate $u = q_3$ is isolated in $H_2 - V_2 = -\partial_3^2$, so up to higher-order terms in a the Hamiltonian decouples into a sum of the operators

$$\begin{aligned}
H_q &= -g^{-\frac{1}{4}}\partial_\mu g^{\frac{1}{2}}g^{\mu\nu}\partial_\nu g^{-\frac{1}{4}} + K - M^2, && (2.23)\\
H_u &= -\partial_3^2. && (2.24)
\end{aligned}$$

This observation is behind the formal limit $a \to 0+$ mentioned in the introduction [dC1, dC2, Tol] in which the transverse part is thrown away and the thin-layer Hamiltonian is replaced by the surface operator H_q, with the energy appropriately renormalized. This procedure can be given meaning in the perturbation-theory framework, in analogy with [DE], as we shall discuss elsewhere.

Here we use it for motivation purposes. The effective "surface potential" $K-M^2$ can be rewritten by means of the principal curvatures of Σ as follows

$$K - M^2 = -\frac{1}{4}(k_+ - k_-)^2. \tag{2.25}$$

If the curvature vanishes at large distances, we get a potential well which could imply existence of bound states that would persist in layers of a finite thickness. In distinction to the "one-in-two" case of a curved planar strip the effective potential may vanish if the surface is locally spherical, $k_+ = k_-$, however, this cannot happen everywhere at a locally deformed plane. Let us also remark that similar Laplace-Beltrami operators penalized by a quadratic function of the curvature lead on compact surfaces to interesting isoperimetric problems [Ha, HL, EHL].

In the next section we shall also need the eigenfunctions $\{\chi_n\}_{n=1}^{\infty}$ of the transverse operator H_u. They are given by

$$\chi_n(u) = \begin{cases} \sqrt{\frac{2}{d}} \cos \kappa_n u & \text{if} \quad n \text{ is } \mathit{odd} \\ \\ \sqrt{\frac{2}{d}} \sin \kappa_n u & \text{if} \quad n \text{ is } \mathit{even} \end{cases} \tag{2.26}$$

and the corresponding eigenvalues are $\kappa_n^2 = (\kappa_1 n)^2$ with $\kappa_1 = \frac{\pi}{d}$.

3 Spectrum of locally deformed planar layers

In what follows we shall consider a class of layers over surfaces which are smooth local deformations of a plane. More specifically, suppose that the deformed part of the surface is $\mathcal{A} \subset \Sigma$ and denote $\operatorname{supp} K \cup \operatorname{supp} M = p^{-1}(\mathcal{A}) =: \mathcal{A}_0$; it is clear that $\Sigma \setminus \mathcal{A}$ is a plane with a "hole", not necessarily a simply connected one.

Let $(X, \delta_{\mu\nu})$ be a natural representation of $\Sigma \setminus \mathcal{A}$ in Cartesian coordinates $(x^1, x^2) \in X \subset \mathbb{R}^2$ given by an isometry

$$\mathcal{C} : \Sigma_0 \setminus \mathcal{A}_0 \to X : \{q \mapsto (x^1, x^2) =: \mathcal{C}(q)\}.$$

In view of the compact-support assumption we can choose $r_0 > 0$ in such a way that $\mathcal{B}_{r_0} := \{w \in \Sigma : |\mathcal{C} \circ p^{-1}(w)| \le r_0\}$ contains $\mathcal{A}$ and thus $\Sigma_{r_0} := \Sigma \backslash \mathcal{B}_{r_0}$ is the undeformed plane with the disc of radius r_0 removed. It is useful to introduce a polar-coordinate parametrization of Σ_{r_0} given by the isometry

$$\mathcal{P} : (r_0, \infty) \times S^1 \to X : \{(r, \vartheta) \mapsto (x^1, x^2) =: (r \cos\vartheta, r \sin\vartheta)\}; \tag{3.1}$$

the corresponding metric tensor acquires then the form $\mathrm{diag}(1, r^2)$.

3.1 The essential spectrum

In a planar layer the essential spectrum starts from the lowest transverse eigenvalue. We will use the standard bracketing argument [RS, Sec. XIII.15] in combination with the minimax principle to prove that the same remains true after a compactly supported deformation.

Proposition 3.1 $\sigma_{\mathrm{ess}}(\tilde{H}) = [\kappa_1^2, \infty)$.

Proof: We cut the layer Ω perpendicularly at the boundary of $\mathcal{B}_{r_0}$ and impose there the Neumann or Dirichlet condition respectively; this enables us to squeeze H between a pair of operators

$$H_{int}^N \oplus H_{ext}^N \le H \le H_{int}^D \oplus H_{ext}^D, \tag{3.2}$$

which have both the form of an orthogonal sum. The spectrum of the interior parts is purely discrete, so the essential components are determined by the exterior part only, $\sigma_{\mathrm{ess}}(H_{int}^\beta \oplus H_{ext}^\beta) = \sigma_{\mathrm{ess}}(H_{ext}^\beta) = \sigma(H_{ext}^\beta)$, $\beta = N, D$. The latter can be simply localized employing the polar-coordinate parametrization (3.1) of Σ_{r_0}. In particular, let

$$U_{\mathcal{P}} : \ \boldsymbol{L}^2\left(\Omega_0 \setminus p^{-1}(\Sigma_{r_0}) \times (-a, a)\right) \to \boldsymbol{L}^2\left((r_0, \infty) \times S^1 \times (-a, a)\right)$$

be the substitution-type unitary operator $(U_{\mathcal{P}}\psi)(r, \vartheta, u) := \psi(\mathcal{P}^{-1} \circ \mathcal{C}(q), u)$. It is clear that the spectrum of the corresponding exterior Hamiltonians

$$U_{\mathcal{P}} H_{\mathrm{ext}}^\beta U_{\mathcal{P}}^{-1} = -\partial_r^2 - \frac{1}{r^2}\partial_\vartheta^2 - \partial_u^2 - \frac{1}{4r^2}$$

contains all points $\kappa_1^2 + \epsilon_\beta$, where ϵ_β belongs to the spectrum of the s-wave radial part, $h^\beta := -\partial_r^2 - (4r^2)^{-1}$ in $\boldsymbol{L}^2(r_0, \infty)$ with the appropriate b.c. at $r = r_0$. We have

$$-(\partial_r^2)_N - \frac{1}{4r_0^2} \le h^N \quad \text{and} \quad h^D \le -(\partial_r^2)_D$$

in the sense of quadratic forms and $\inf \sigma_{\text{ess}}(-(\partial_r^2)_\beta) = 0$. Since r_0 can be chosen arbitrary large, the claim follows from (3.2) by the minimax principle. ∎

3.2 Existence of Bound States

Now comes the main result of this paper. We are going to show that the conjecture about existence of a discrete spectrum in locally curved layers formulated in Sec. 2.4 is true, even for layers which may not be thin. The variational proof of the following results is based on the idea adapted from [GJ], see also [DE, Thm. 2.1].

Theorem 3.2 *Suppose that the layer is not planar and the deformation satisfies the smoothness and compact support assumptions. Then* $\inf \sigma(\tilde{H}) < \kappa_1^2$.

PROOF: Denote the norm in $\boldsymbol{L}^2(\Omega_0, G^{\frac{1}{2}} d^2q\, du)$ as $\|\cdot\|_G$; then it follows from (2.13) that the quadratic form associated with our Hamiltonian $\hat{H}$ is given by

$$q[\psi] := \|\hat{H}^{\frac{1}{2}}\psi\|_G^2 = q_1[\psi] + q_2[\psi]$$

where

$$\begin{aligned} q_1[\psi] := \|\hat{H}_1^{\frac{1}{2}}\psi\|_G^2 &= (\psi_{,\mu}, G^{\frac{1}{2}} G^{\mu\nu} \psi_{,\nu}) && (3.3)\\ q_2[\psi] := \|\hat{H}_2^{\frac{1}{2}}\psi\|_G^2 &= \|G^{\frac{1}{4}}\psi_{,3}\|^2. && (3.4) \end{aligned}$$

It acts on $Q(\hat{H})$, the quadratic form domain of $\hat{H}$. In order to prove the claim it is sufficient to find a trial function $\psi \in Q(\hat{H})$ such that

$$t[\psi] := q[\psi] - \kappa_1^2\, \|\psi\|_G^2 < 0.$$

(a) We begin the construction of a trial function with $\psi(q,u) := \varphi(q)\chi_1(u)$, where χ_1 is the lowest transverse-mode function (2.26) and φ is a function from the Schwartz space $\mathcal{S}(\mathbb{R}^2)$, arbitrary for a moment. It yields

$$\begin{aligned} q_1[\psi] &= \Big(\varphi_{,\mu}, \langle G^{\frac{1}{2}} G^{\mu\nu} |\chi_1|^2\rangle_u\, \varphi_{,\nu}\Big)_q && (3.5)\\ q_2[\psi] &= \Big(\varphi, \langle G^{\frac{1}{2}} |\chi_1'|^2\rangle_u\, \varphi\Big)_q && (3.6)\\ \|\psi\|_G^2 &= \Big(\varphi, \langle G^{\frac{1}{2}} |\chi_1|^2\rangle_u\, \varphi\Big)_q && (3.7) \end{aligned}$$

where $\langle\cdot\rangle_u$ means a "transverse" expectation and the subscripts q, u mark the fact that we integrate w.r.t. the corresponding coordinate only.

Taking into account the explicit expression (2.10) for G and using the trivial fact that $|\chi_1|$, $|\chi_1'|$ are *even* functions and that we integrate over a symmetric interval $(-a,a)$, and consequently, that we can consider just the *even* powers of u in $\langle\cdot\rangle$, we get

$$\langle G^{\frac{1}{2}}|\chi_1'|^2\rangle_u - \kappa_1^2\,\langle G^{\frac{1}{2}}|\chi_1|^2\rangle_u = K g^{\frac{1}{2}};$$

we have employed at that the identity $\langle u^2(|\chi_1'|^2 - \kappa_1^2|\chi_1|^2)\rangle_u = 1$. By virtue of (2.11), we can estimate the remaining term as

$$q_1[\psi] \le C_+ \left(\varphi_{,\mu}, g^{\frac{1}{2}} g^{\mu\nu}\varphi_{,\nu}\right)_q . \tag{3.8}$$

Suppose now that $\varphi(q) = 1$ on $p^{-1}(\mathcal{B}_{r_0})$ and that the function is radially symmetric in the sense $\tilde\varphi(r,\vartheta) = \tilde\varphi(r)$, where $\tilde\varphi := \varphi\circ\mathcal{C}^{-1}\circ\mathcal{P}$. Passing then to the polar coordinates ($g^{\frac{1}{2}}d^2q = r dr d\vartheta$) in (3.8) we arrive at

$$q_1[\psi] \le C_+ \int_{\mathbb{R}^+\times S^1} |\dot{\tilde\varphi}|^2 r\, dr d\vartheta =: C_+\, \|\dot{\tilde\varphi}\|_{\mathcal{P}},$$

where the dot denotes the derivative w.r.t. r. The *r.h.s.* of this inequality depends on the surface geometry through the constant C_+ only. Summing up the results we have

$$t[\psi] \le C_+\, \|\dot{\tilde\varphi}\|_{\mathcal{P}}^2 + (\varphi, K g^{\frac{1}{2}}\,\varphi)_q . \tag{3.9}$$

(b) In the next step we shall specify further the function $\tilde\varphi$ in a way which allows us to make the *r.h.s.* of (3.9) arbitrary small. Let us define the family $\{\tilde\varphi_\sigma : \sigma\in(0,1]\}$ by an external scaling (in the region $r > r_0$) of a suitable function. The idea is analogous to [GJ] or [DE, Thm. 2.1], however, since we deal with a two-dimensional integral we have to be more careful about the decay properties. We can adopt for this purpose the mollifier employed in [EV, BCEZ], which is expressed in terms of Macdonald functions (or modified Bessel functions in the terminology of [AS]) as

$$\tilde\varphi_\sigma(r) := \min\left\{1, \frac{K_0(\sigma r)}{K_0(\sigma r_0)}\right\}$$

Since K_0 is strictly decreasing, the corresponding $\psi_\sigma := \varphi_\sigma \chi_1$ will not be smooth at $r = r_0$ but it remains continuous, hence it is an admissible trial function as an element of $Q(\hat{H})$.

To estimate the first term at the *r.h.s.* of (3.9), let us compute the norm of the scaled function using [AS, Sec. 9.6] and [GR, 5.54]:

$$\begin{aligned}
\|\dot{\tilde{\varphi}}_\sigma\|^2_{\mathcal{P}} &= \frac{2\pi}{K_0(\sigma r_0)^2} \int_{r_0}^{\infty} \dot{K}_0(\sigma r)^2\, r\, dr = \frac{2\pi}{K_0(\sigma r_0)^2} \int_{\sigma r_0}^{\infty} K_1(t)^2\, t\, dt \\
&= \frac{\pi\, (\sigma r_0)^2}{K_0(\sigma r_0)^2} \left[K_0(\sigma r_0) K_2(\sigma r_0) - K_1(\sigma r_0)^2 \right] \\
&= \frac{\pi\, (\sigma r_0)^2}{K_0(\sigma r_0)^2} \left[K_0(\sigma r_0)^2 + \frac{2}{\sigma r_0} K_0(\sigma r_0) K_1(\sigma r_0) - K_1(\sigma r_0)^2 \right] \\
&= -\frac{\pi}{\ln \sigma r_0} \Bigg[-(\sigma r_0)^2 \ln \sigma r_0 - 2\sigma r_0 \ln \sigma r_0\, \frac{K_1(\sigma r_0)}{K_0(\sigma r_0)} \\
&\qquad\qquad + (\sigma r_0)^2 \ln \sigma r_0 \left(\frac{K_1(\sigma r_0)}{K_0(\sigma r_0)} \right)^2 \Bigg]
\end{aligned}$$

Next we use the small-argument asymptotic expressions [AS, Sec. 9.6]

$$\begin{aligned}
K_0(x) &= -\ln x + \mathcal{O}(1) \\
K_1(x) &= \frac{1}{x} + \mathcal{O}(\ln x)
\end{aligned}$$

which imply that $x \ln x\, \frac{K_1(x)}{K_0(x)}$ remains bounded as $x \to 0+$, hence

$$\|\dot{\tilde{\varphi}}_\sigma\|^2_{\mathcal{P}} < \frac{b}{|\ln \sigma r_0|} \tag{3.10}$$

holds for a positive constant b and σr_0 small enough.

(c) To handle the second term at the *r.h.s.* of (3.9) for $\varphi = \varphi_\sigma$ we employ the dominated convergence theorem: since $|\varphi_\sigma| \le 1$ and $\varphi_\sigma \to 1$ pointwise as $\sigma \to 0+$, we have

$$(\varphi_\sigma, K g^{\frac{1}{2}}\, \varphi_\sigma)_q \to (1, K g^{\frac{1}{2}})_q \equiv \mathsf{Tot}(\Sigma)$$

by definition. Notice that the total curvature integral is well defined because the Gauss curvature K of a surface obtained by a smooth compactly supported deformation of a plane belongs to $\boldsymbol{L}^1(\Sigma_0, g^{\frac{1}{2}} d^2 q)$. In view of (3.9), (3.10) and the last formula we have therefore

$$t[\psi_\sigma] \to \mathsf{Tot}(\Sigma) \tag{3.11}$$

as $\sigma \to 0+$. Recall that in Sec. 2.1 we have used the Gauss-Bonnet theorem (2.7) to show that $\mathsf{Tot}(\Sigma) = 0$ holds for surfaces obtained by a smooth local deformation of a plane. Thus $t[\psi_\sigma]$ can be made arbitrarily small by choosing σ small enough. Since we want to make the form negative, we have to modify the trial function ψ_σ further in analogy with [GJ].

(d) To this aim we pick $j \in \boldsymbol{C}_0^\infty(\mathcal{A}_0 \times (-a,a))$ and set $\Theta := j^2(\hat{H} - \kappa_1^2)\psi_\sigma$. From (2.14)–(2.15) and the fact that the scaling acts out of the support of the localization function j, we immediately get the following explicit expression

$$\begin{aligned}\Theta(q,u) &= j(q,u)^2\, \pi \left(\frac{2}{d}\right)^{\frac{3}{2}} \frac{Ku - M}{Ku^2 - 2Mu + 1} \sin \kappa_1 u \\ &= j(q,u)^2\, \pi \left(\frac{2}{d}\right)^{\frac{3}{2}} (\ln G^{\frac{1}{4}})_{,3} \sin \kappa_1 u \,.\end{aligned}$$

Notice that by construction the function Θ does not depend on σ. It is non-zero as an element of $\boldsymbol{L}^2(\Omega_0, G^{\frac{1}{2}} d^2q\, du)$ for a non-zero j unless G is independent of u. In view of (2.10), however, the last named situation occurs only if K, M are zero identically on the whole surface which is impossible because Σ is not a plane by assumption.

Since both ψ_σ and Θ belong to $Q(\hat{H})$, we have

$$t[\psi_\sigma + \varepsilon\, \Theta] = t[\psi_\sigma] + 2\,\varepsilon\, \|j(\hat{H} - \kappa_1^2)\psi_\sigma\|^2 + \varepsilon^2\, t[\Theta] \,.$$

For all sufficiently small *negative* ε the sum of the last two terms is negative, and the above arguments shows that we can choose σ so that $t[\psi_\sigma + \varepsilon\, \Theta] < 0$; recall that the second term on the right side is independent of σ. ∎

Remark 3.3 Notice that the choice of the Macdonald function $K_0(r)$ for the mollifier $\tilde{\varphi}$ in the part **(b)** is not indispensable. One can modify this part of the proof, *e.g.*, by using $e^{-r} \ln r$. However, the choice we made is the most natural in a sense, because it employs the Green's function kernel at zero energy.

The obtained conclusion about the bottom of the spectrum can be combined with Proposition 3.1 to get the result announced at the beginning of Sec. 3.2.

Corollary 3.4 *Let Ω be a curved layer built over Σ which is a nontrivial, local, and smooth deformation of a plane, with the half-thickness strictly smaller than the minimum curvature radius of Σ – cf.(2.11). Then $\tilde{H}$ has at least one bound state with energy below κ_1^2.*

Acknowledgment

The research has been partially supported by GAAS and the Czech Ministry of Education under the contracts #1048801 and ME099.

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