Strong-coupling asymptotic expansion for Schrödinger operators with a singular interaction supported by a curve in $\mathbb{R}^3$

P. Exner[a,b] and S. Kondej[c,d]

a) Nuclear Physics Institute, Academy of Sciences, 25068 Řež near Prague, Czech Republic
b) Doppler Institute, Czech Technical University, Břehová 7, 11519 Prague, Czech Republic
c) Institute of Theoretical Physics, University of Wrocław, pl. Maxa Borna 9, 50-205 Wrocław, Poland
d) Information Technology Vocational College in Gorzów Wlkp, ul. Myśliborska 34, 66-400 Gorzów Wlkp, Poland

exner@ujf.cas.cz, kondej@ift.uni.wroc.pl

Abstract. We investigate a class of generalized Schrödinger operators in $L^2(\mathbb{R}^3)$ with a singular interaction supported by a smooth curve Γ. We find a strong-coupling asymptotic expansion of the discrete spectrum in case when Γ is a loop or an infinite bent curve which is asymptotically straight. It is given in terms of an auxiliary one-dimensional Schrödinger operator with a potential determined by the curvature of Γ. In the same way we obtain an asymptotics of spectral bands for a periodic curve. In particular, the spectrum is shown to have open gaps in this case if Γ is not a straight line and the singular interaction is strong enough.

1 Introduction

The subject of this paper are asymptotic spectral properties for several classes of generalized Schrödinger operators in $L^2(\mathbb{R}^3)$ with an attractive singular interaction supported by a smooth curve or a family of such curves. On a formal level, we can write such a Hamiltonian as

$$-\Delta - \tilde{\alpha}\delta(x-\Gamma)\,, \tag{1.1}$$

however, a proper way to define the operator corresponding to the formal expression is involved and will be explained in Sec. 2.2 below[1]. A physical motivation for this model is to understand the electron behavior in "leaky" quantum wires, i.e. a model of these semiconductor structures which is realistic in the sense that it takes into account the fact that the electron as a quantum particle capable of tunelling can be found outside the wire – cf. [EI] for a more detailed discussion.

One natural question is whether in case of a strong transverse coupling properties of such a "leaky" wire will approach those of an ideal wire of zero thickness, i.e. the model in which the particle is confined to Γ alone, and how the geometry of the configuration manifold will be manifested at that. In the two-dimensional case when Γ is a planar curve this problem was analyzed in [EY1, EY2] where it was shown that apart of the divergent term which describes the energy of coupling to the curve, the spectrum coincides asymptotically with that of an auxiliary one-dimensional Schrödinger operator with a curvature-induced potential[2].

The case of a curve in $\mathbb{R}^3$ which we are going to discuss here is more complicated for several reasons. First of all, the codimension of Γ is two in this situation which means that to define the Hamiltonian we cannot use the natural quadratic form and have to employ generalized boundary conditions instead. Furthermore, while the strategy of [EY1, EY2] based on bracketing bounds combined with the use of suitable curvilinear coordinates in the vicinity of Γ can be applied again, the "straightening" transformation we have to employ is more involved here. Also the bound on the transverse part of the estimating operators are less elementary in this case.

Let us review briefly the contents of the paper. We begin by constructing a self-adjoint operator $H_{\alpha,\Gamma}$ which corresponds to the formal expression (1.1), where Γ is a curve in $\mathbb{R}^3$; this will be done in Sec. 2.2. To this aim we employ in the transverse plane to Γ the usual boundary conditions defining

[1] In particular, this is the reason why we use here a formal coupling constant different from the parameter α introduced in the condition (2.1) below.

[2] A similar analysis was performed in [Ex] for smooth surfaces in $\mathbb{R}^3$ where the asymptotic form of the spectrum is given by a suitable "two-dimensional" operator supported by the surface Γ.

a two-dimensional point interaction [AGHH, Sec. I.5]. Recall that the latter is known to have for any $\alpha \in \mathbb{R}$ a single negative eigenvalue which equals $\xi_\alpha = -4\mathrm{e}^{2(-2\pi\alpha+\psi(1))}$. The main topic of this paper are spectral properties of $H_{\alpha,\Gamma}$ in the strong-coupling asymptotic regime which means here that $-\alpha$ is large. The auxiliary operator mentioned above is given by

$$S := -\Delta - \frac{1}{4}\kappa^2,$$

where Δ is the one-dimensional Laplace operator on the segment parameterizing Γ and κ is the curvature of Γ. Its discrete spectrum is non-empty unless Γ is a straight line; we denote the j-th eigenvalue as μ_j. Our main results can be then characterized briefly as follows:

Discrete spectrum: If Γ is a loop, we show in Sec. 3 that the j-th eigenvalue $\lambda_j(\alpha)$ of $H_{\alpha,\Gamma}$ admits an asymptotic expansion of the following form,

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

and the counting function $\alpha \mapsto \#\sigma_d(H_{\alpha,\Gamma})$ satisfies in this limit the relation

$$\#\sigma_d(H_\alpha) = \frac{L}{2\pi}(-\xi_a)^{1/2}(1+\mathcal{O}(e^{\pi\alpha})).$$

In addition, the last formula does not require Γ to be a closed curve as we shall show in Sec. 3.5. Moreover, if Γ is infinite with $\kappa \neq 0$ and at the same time asymptotically straight in an appropriate sense then the above expansion for $\lambda_j(\alpha)$ holds again – cf. Sec. 4.

Periodic curves are discussed in Sec. 5; we perform Bloch decomposition and use the same technique as above to estimate the discrete spectrum of the fiber operators. In particular, we find that if Γ is periodic curve and $\kappa(\cdot)$ is nonconstant then $\sigma(H_{\alpha,\Gamma})$ contains open gaps for $-\alpha$ sufficiently large. In the closing section we will show that the problem can be rephrased in terms of a semiclassical approximation and list some open problems.

2 Hamiltonians with curve-supported perturbations

2.1 The curve geometry

Let Γ be a curve in $\mathbb{R}^3$ (either infinite or a closed loop) which is assumed to be C^k, $k \geq 4$. Without loss of generality we may assume that it is parameterized by its arc length, i.e. to identify Γ with the graph of a function $\gamma:\, I \to \mathbb{R}^3$, where $I = [0, L]$ (with the periodic boundary conditions, $\gamma(0) = \gamma(L)$ and the same for the derivatives) if Γ is finite and $I = \mathbb{R}$ otherwise. In view of the smoothness assumption we can introduce the Frenet's frame for the curve, i.e. the triple $(t(s), b(s), n(s))$ of tangent, binormal, and normal vectors which are C^{k-2} smooth functions of $s \in I$.

With a later purpose on mind we impose additional restrictions on Γ which allow us to work in certain neighbourhoods of the curve. Given $d > 0$ we denote $B_d := \{r \in [0, d),\, \theta \in [0, 2\pi)\}$ and call Ω_d the tube built around Γ defined by the map $\phi_d :\, \mathcal{D}_d \to \mathbb{R}^3$,

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

where $\mathcal{D}_d := I \times B_d$ and the function β will be specified further. For convenience we will denote the curvilinear coordinates (s, r, θ) also as q with the coordinate indices $(1, 2, 3) \leftrightarrow (s, r, \theta)$. We will employ tubular neighbourhoods $\Omega_d := \phi_d(\mathcal{D}_d) \subset \mathbb{R}^3$ of Γ; the indicated restriction means that we exclude self-intersections and "near-intersections" of the curve assuming that

(aΓ) there exists $d > 0$ such that the map $\phi_d : \mathcal{D}_d \to \Omega_d$ is injective.

Since it can hardly lead to a confusion we use the same notation ϕ_d for the mappings with target spaces $\mathbb{R}^3$ and Ω_d. The geometry of Ω_d is naturally described in terms of its metric tensor (g_{ij}); the latter is according to [DE] expressed by means of the curvature κ and torsion τ of Γ in the following way

$$g_{ij} = \begin{pmatrix} h^2 + r^2\varsigma^2 & 0 & r^2\varsigma \\ 0 & 1 & 0 \\ r^2\varsigma & 0 & r^2 \end{pmatrix},$$

where

$$\varsigma := \tau - \beta_{,s} \quad \text{and} \quad h := 1 + r\kappa\cos(\theta-\beta)\,. \tag{2.1}$$

We use the standard convention $g^{ij} = (g_{ij})^{-1}$. In particular, the volume element of Ω_d is given by $d\Omega = g^{1/2}dq$ where $g := \det(g_{ij})$. The simplest situation occurs if we choose

$$\beta_{,s} = \tau\,,$$

because then the tensor g_{ij} takes the diagonal form $g_{ij} = \mathrm{diag}(h^2, 1, r^2)$. In what follows we shall employ this special rotating system which is sometimes called Tang system of coordinates.

Remarks 2.1 (a) It is well known that compact manifolds in $\mathbb{R}^n$ have the tubular neighbourhood property. Thus if Γ is a finite C^4 curve then the assumption (aΓ) is satisfied iff Γ has no self-intersections.
(b) Combining the explicit formula for g_{ij} with the inverse function theorem it easy to see that the inequality $d\|\kappa\|_\infty < 1$ is sufficient for ϕ_d to be locally diffeomorphic.

2.2 Singularly perturbed Schrödiger operators

The Hamiltonians we want to study are Schrödinger operators with s-independent perturbations supported by the curve Γ. Such operators can be understood as the Laplacian with specific boundary conditions on Γ and the aim of this section is to make this conditions precise.

Given $\rho > 0$ and $\theta_0 \in [0, 2\pi)$ denote by Γ_{ρ,θ_0} the "shifted" curve located in the distance ρ from Γ which is defined as the ϕ_d image of the set $I \times \{\rho, \theta_0\} \subset \mathcal{D}_d$. Let $\mathcal{M}$ be an open set in $\mathbb{R}^3$ containing Γ. Consider the Sobolev space $W^{2,2}_{\text{loc}}(\mathcal{M} \setminus \Gamma)$. Since its elements are continuous on $\mathcal{M}$ away of Γ, the restriction of a function $f \in W^{2,2}_{\text{loc}}(\mathcal{M} \setminus \Gamma)$ to the "shifted" curve located sufficiently close to Γ is well defined; we will denote it as $f\restriction_{\Gamma_{\rho,\theta_0}}(\cdot)$. In fact, we can regard $f\restriction_{\Gamma_{\rho,\theta_0}}$ as a distribution from $D'(0, L)$ parameterized by the distance ρ and the angle θ_0. We shall say that a function $f \in W^{2,2}_{\text{loc}}(\mathcal{M} \setminus \Gamma) \cap L^2(\mathcal{M})$ belongs to $\Upsilon_{\mathcal{M}}$ if the following limits,

$$
\begin{aligned}
\Xi(f)(s) &:= -\lim_{\rho\to 0} \frac{1}{\ln \rho} f\restriction_{\Gamma_{\rho,\theta_0}}(s)\,, \\
\Omega(f)(s) &:= \lim_{\rho\to 0} \left[f\restriction_{\Gamma_{\rho,\theta_0}}(s) + \Xi(f)(s) \ln \rho \right]\,,
\end{aligned}
$$

exist a.e. in $[0, L]$, are independent of θ_0, and define a pair functions belonging to $L^2(0, L)$. The limits here are understood in the sense of the $D'(0, L)$ topology; for an infinite curve $[0, L]$ is replaced by $\mathbb{R}$. We should also stress here that the elements of $W^{2,2}_{\text{loc}}(\mathcal{M} \setminus \Gamma)$ are in fact distributions from $D'(\mathbb{R}^3)$, however, in the definition of $\Upsilon_{\mathcal{M}}$ we can naturally identify them with their canonical imbeddings into $L^2(\mathcal{M})$.

Given a function $f \in \Upsilon_{\mathcal{M}}$ we write $f\,\tilde{}\,\alpha.bc(\Gamma)$ if the limits $\Xi(f)(\cdot)$, $\Omega(f)(\cdot)$, characterizing the behaviour of f close to Γ satisfy the following relation

$$
2\pi\alpha\Xi(f)(s) = \Omega(f)(s)\,. \tag{2.1}
$$

With these prerequisites we can define the singularly perturbed Schrödinger operator in question through the set

$$D(H_{\alpha,\Gamma}) = \{f \in \Upsilon_{\mathbb{R}^3} : f \tilde{\ } \alpha.bc(\Gamma)\}$$

on which the operator $H_{\alpha,\Gamma} : D(H_{\alpha,\Gamma}) \to L^2(\mathbb{R}^3)$ acts as

$$H_{\alpha,\Gamma} f(x) = -\Delta f(x)\,, \quad x \in \mathbb{R}^3 \setminus \Gamma\,. \tag{2.2}$$

To show that $H_{\alpha,\Gamma}$ makes sense as a quantum mechanical Hamiltonian we will assume here that Γ finite or infinite periodic. Another interesting case, that of an infinite non-periodic curve which is asymptotically straight, needs additional assumptions and will be discussed separately in Sec. 4.

Theorem 2.2 *Under the stated assumptions $H_{\alpha,\Gamma}$ is self-adjoint.*

Proof. One check using integration by parts and passing to the curvilinear system of coordinates $q = (s, r, \theta)$ in a sufficiently small tubular neighbourhood of Γ that the following boundary form,

$$\upsilon : \ \upsilon(f, g) = (H_{\alpha,\Gamma} f, g) - (f, H_{\alpha,\Gamma} g)$$

vanishes for all $f,\, g \in D(H_{\alpha,\Gamma})$, i.e. that the operator $H_{\alpha,\Gamma}$ is symmetric. To check its self-adjointness we can proceed in analogy with [EK, Thm. 4.1]. Repeating the argument presented there step by step we derive the resolvent of $H_{\alpha,\Gamma}$ and the sought result then follows from [Po, Theorem 2.1]. An alternative way is to note that $H_{\alpha,\Gamma}$ is one of the self-adjoint extensions discussed in [Ku]. It is true that in this paper stronger smoothness conditions for Γ were adopted, however, the results remain valid for the C^4 class. ∎

The operator $H_{\alpha,\Gamma}$ will be a central object of our interest. It is natural to regard it as a Schrödinger operator with the singular perturbation supported by the curve Γ.

Remarks 2.3 (a) The choice of boundary conditions (2.1) which we used in the construction had a natural motivation. If Γ is a line in $\mathbb{R}^3$ one can separate variables; in the cross plane we then have the two dimensional Laplace operator with a single-centre point interaction $-\Delta_{\alpha,\{0\}}$ which is a well studied object – cf. [AGHH, Sec. I.5]. To define it, one considers for a function $f \in W^{2,2}_{\mathrm{loc}}(\mathbb{R}^2 \setminus \{0\}) \cap L^2(\mathbb{R}^2)$ the following limits

$$\tilde{\Xi}(f) := -\lim_{r\to 0} \frac{1}{\ln r} f\,, \quad \tilde{\Omega}(f) := \lim_{r\to 0}(f + \tilde{\Xi}(f) \ln r)\,;$$

if they are finite and satisfy the relation

$$2\pi\alpha\tilde{\Xi}_s(f) = \tilde{\Omega}(f)\,, \tag{2.3}$$

the function f belongs to the domain of $-\Delta_{\alpha,\{0\}}$. Using the explicit form of its resolvent it is easy to see that such an operator has for any $\alpha \in \mathbb{R}$ exactly one negative eigenvalue which is given by

$$\xi_\alpha = -4e^{2(-2\pi\alpha+\psi(1))}\,, \quad \psi(1) = -0.577... \tag{2.4}$$

Obviously, it coincides with the bottom of the essential spectrum of $H_{\alpha,\Gamma}$ for a straight Γ. We know from [EK] that this property is preserved if Γ is curved but asymptotically straight in a suitable sense; in that case the operator has a non-empty discrete spectrum – cf. Sec. 4. It is also clear from the relation (2.4) and the corresponding eigenfunction [AGHH, Sec. I.5] that a strong coupling corresponds to large negative values of α.

(b) For the sake of brevity we use in analogy with (2.1) for the boundary conditions (2.3) the abbreviation $f\tilde{\ }\alpha.bc(0)$, later we employ similar self-explanatory symbols for other conditions, Dirichlet, Neumann, periodic, etc.

3 Strong coupling asymptotics for a loop

In this section we will discuss in detail the strong-coupling asymptotic behaviour of the discrete spectrum in the simplest case when Γ is a finite closed curve satisfying the regularity assumptions stated above; by Remark 2.1(a) it means that Γ is C^4 and does not intersect itself.

Since Γ is compact it does not influence the essential spectrum of $H_{\alpha,\Gamma}$. This can be seen by writing explicitly the resolvent [Po] and checking that it differs from the free one by a compact operator in analogy with the argument used in [BEKŠ] for $\operatorname{codim}\Gamma = 1$. However, there is a simpler way.

Proposition 3.1 *With the stated assumptions we have*

$$\sigma_{\text{ess}}(H_{\alpha,\Gamma}) = \sigma_{\text{ess}}(-\Delta) = [0,\infty)\,.$$

Proof. By Neumann bracketing we can check that $\inf \sigma_{\text{ess}}(H_{\alpha,\Gamma}) = 0$. Indeed, choose a ball $\mathcal{B}$ such that Γ is contained in its interior and call H_N the operator with the additional Neumann condition at $\partial\mathcal{B}$. We have $H_{\alpha,\Gamma} \geq H_N$

and the spectrum of the latter is the union of the interior and the exterior component. The first named one is discrete and the spectrum of the other is the non-negative halfline, so the claim follows from the minimax principle. To show that every positive number belongs to $\sigma(H_{\alpha,\Gamma})$ it is sufficient to construct a suitable Weyl sequence; one can use a Weyl sequence for $-\Delta$ chosen in such a way that its elements have supports disjoint from $\mathcal{B}$. ■

Let us turn to the main subject of this section. To describe how the discrete spectrum of H_α behaves asymptotically for $\alpha \to -\infty$ we employ the comparison operator defined by

$$S = -\frac{d^2}{ds^2} - \frac{\kappa(s)^2}{4} :\ D(S) \to L^2(0,L)\,, \tag{3.1}$$

with the domain $D(S) = \{\phi \in W^{2,2}(0,L); \phi\tilde{\ } p.bc(0,L)\}$, i.e. determined by periodic boundary conditions, $\phi(0) = \phi(L), \phi'(0) = \phi'(L)$. Furthermore, $\kappa(\cdot)$ is the curvature of Γ. It is worth to stress that S acts in a different Hilbert space than $H_{\alpha,\Gamma}$. We denote by μ_j the j-th eigenvalue of S. With this notations our main result looks as follows:

Theorem 3.2 *(a) To any fixed $n \in \mathbb{N}$ there exists an $\alpha(n) \in \mathbb{R}$ such that*

$$\#\sigma_d(H_{\alpha,\Gamma}) \geq n \quad for \quad \alpha \leq \alpha(n)\,.$$

The j-th eigenvalue $\lambda_j(\alpha)$ of $H_{\alpha,\Gamma}$ admits an asymptotic expansion of the following form,

$$\lambda_j(\alpha) = \xi_\alpha + \mu_j + \mathcal{O}(e^{\pi\alpha}) \quad as \quad \alpha \to -\infty\,.$$

(b) The counting function $\alpha \mapsto \#\sigma_d(H_{\alpha,\Gamma})$ behaves asymptotically as

$$\#\sigma_d(H_\alpha) = \frac{L}{\pi}(-\xi_a)^{1/2}(1 + \mathcal{O}(e^{\pi\alpha})).$$

The proof of the theorem is divided into several steps which we will describe subsequently in the following sections.

3.1 Dirichlet-Neumann bracketing

Our aim is to estimate $H_{\alpha,\Gamma}$ in the negative part of the spectrum from both sides by suitable operators acting in a tubular neighbourhood Ω_d of Γ with d sufficiently small to make the assumption (aΓ) satisfied. The first step in obtaining the estimating operators is to impose additional Dirichlet and Neumann condition at the boundary of Ω_d. Let thus the operators $H^j_{\alpha,\Gamma}$, $j = D, N$, in $L^2(\Omega_d)$ act as the Laplacian with the domains given respectively by $D(H^j_{\alpha,\Gamma}) = \{f \in \Upsilon_{\Omega_d} :\ f\tilde{\ }\alpha.bc(\Gamma),\ f\tilde{\ }j.bc(\partial\Omega_d)\}$; it is straightforward to check that operators $H^j_{\alpha,\Gamma}$ are self-adjoint. Now the well-known result [RS, Sec. XIII.15] says that

$$-\Delta^N_{\Sigma_d} \oplus H^N_{\alpha,\Gamma} \le H_{\alpha,\Gamma} \le -\Delta^D_{\Sigma_d} \oplus H^D_{\alpha,\Gamma}\,, \quad \Sigma_d := \mathbb{R}^3 \setminus \overline{\Omega}_d\,.$$

What is important is that the operators $-\Delta^j_{\Sigma_d}$ corresponding to the exterior of Ω_d do not contribute to the negative part of the spectrum because they are both positive by definition.

It is convenient to express the operators $H^j_{\alpha,\Gamma}$ in the curvilinear coordinates $q = (s, r, \theta)$; this can be done by means of the unitary transformation

$$Uf = f \circ \phi_d : L^2(\Omega_d) \to L^2(\mathcal{D}_d, g^{1/2}dq)\,, \quad \mathcal{D}_d = [0, L] \times B_d\,.$$

Then the operators $\tilde{H}^j_{\alpha,\Gamma} := UH^j_{\alpha,\Gamma}U^{-1}$ act as

$$f(x) \mapsto -(g^{-1/2}\partial_i g^{1/2} g^{ij} \partial_j f)(x) \quad \text{for} \quad x \in \Omega_d \setminus \Gamma$$

with the domains $\{f \in \Upsilon_{\Omega_d} : f\tilde{\ }\alpha.bc(\Gamma), f\tilde{\ }j.bc(\omega_r(d)), f\tilde{\ }p.bc(\omega_s(0), \omega_s(L))\}$, respectively, where we have introduced the notation

$$\omega_{q_i}(t) := \{q \in \overline{\mathcal{D}}_d : q_i = t\}.$$

To simplify it further we remove the weight $g^{1/2}$ appearing in the inner product of the space $L^2(\mathcal{D}_d, g^{1/2}dq)$. This is done by means of the another unitary map,

$$\hat{U} : L^2(\mathcal{D}_d, g^{1/2}dq) \to L^2(\mathcal{D}_d, dq)\,, \quad \hat{U}f := g^{1/4}f\,;$$

the images of $\tilde{H}^j_{\alpha,\Gamma}$ will be denoted as $\hat{H}^j_{\alpha,\Gamma} = \hat{U}\tilde{H}^j_{\alpha,\Gamma}\hat{U}^{-1}$. The aim of these unitary transformations is to find a representation where the eigenvalues – which we need to estimate the eigenvalues of $H_{\alpha,\Gamma}$ by means of the minimax principle – are easy to analyze. A straightforward calculation analogous to that performed in [DE] yields explicit formulae for $\hat{H}^j_{\alpha,\Gamma}$, $j = D, N$, which both act as[3]

$$-\partial_i g^{ij}\partial_j - \frac{1}{4}r^{-2} + V\,,$$

where V is the effective potential given by

$$V = g^{-1/4}(\partial_i g^{ij}(\partial_j g^{1/4})) + \frac{1}{4}r^{-2}, \tag{3.2}$$

while their domains are different,

$$\begin{aligned} D(\hat{H}^D_{\alpha,\Gamma}) &= \{f \in \Upsilon_{\mathcal{D}_d} :\ g^{-1/4}f \,\tilde{}\, \alpha.bc(\Gamma),\ f \,\tilde{}\, p.bc(\omega_s(0), \omega_s(L))\,, \\ &\quad\ f \,\tilde{}\, D.bc(\omega_r(d))\}\,, \\ D(\hat{H}^N_{\alpha,\Gamma}) &= \{f \in \Upsilon_{\mathcal{D}_d} :\ g^{-1/4}f \,\tilde{}\, \alpha.bc(\Gamma),\ f \,\tilde{}\, p.bc(\omega_s(0), \omega_s(L))\,, \\ &\quad\ (\partial_r f)_{r=d} = -[(g^{1/4}\partial_r g^{-1/4})f]_{r=d}\}\,, \end{aligned}$$

Remark 3.3 Notice that the boundary conditions satisfying by functions from $D(\hat{H}^j_{\alpha,\Gamma})$ on the curve Γ can be written in a simpler way. Since only the leading term in $g^{-1/4}$ is important as $r \to 0$, they are equivalent to $r^{-1/2}f \,\tilde{}\, \alpha.bc(\Gamma)$. Notice also that while the Dirichlet boundary condition at $\partial\Omega_d$ persists at the unitary transformation, the Neumann one is changed by $\hat{U}$ into a mixed boundary condition.

3.2 Estimates by operators with separated variables

While the operators $\hat{H}^j_{\alpha,\Gamma}$, $j = D, N$, give the two-sided bounds for the negative eigenvalues of H_α, they are not easy to handle. This is why we pass to a cruder, but still sufficient estimate by operators with separated variables.

In the first step we will make the boundary conditions in the lower bound independent of the coordinates. The boundary term involved in the definition of $D(\hat{H}^N_{\alpha,\Gamma})$ depends on s and θ. We replace the corresponding coefficient by $M := \left\|g^{1/4}\partial_r g^{-1/4}\right\|_{L^\infty(\omega_r(d))}$ passing thus to the operator

$$\dot{H}^-_{\alpha,\Gamma} := -\Delta_h \otimes I + I \otimes (-\Delta^-_\alpha) + V \le \hat{H}^N_{\alpha,\Gamma}$$

[3] We employ the usual convention that summation is performed over repeated indices keeping in mind that (g^{ij}) is diagonal.

on $L^2(0,L)\otimes L^2(B_d)$, where $-\Delta_h := -\partial_s h^{-2}\partial_s :\; D(S)\to L^2(0,L)$ and

$$\begin{aligned}
-\Delta_\alpha^- &:= -\partial_r^2 - r^{-2}\partial_\theta^2 - \frac{1}{4}r^{-2} :\; D(\Delta_\alpha^-)\to L^2(B_d)\,,\\
D(\Delta_\alpha^-) &:= \{f\in W^{2,2}_{\mathrm{loc}}(B_d\setminus\{0\}) :\; \Delta_\alpha^- f\in L^2(B_d),\; r^{-1/2}f\,\tilde{}\,\alpha.bc(0),\\
&\qquad (\partial_r f)|_{r=d} = Mf|_{r=d}\}
\end{aligned}$$

with the the boundary condition at the centre of the circle written in the simplified form mentioned in Remark 3.3. The upper bound contains no boundary term depending on s or θ so we can put

$$\dot H^+_{\alpha,\Gamma} = \hat H^D_{\alpha,\Gamma} = -\Delta_h\otimes I + I\otimes(-\Delta_\alpha^+) + V$$

which acts in the same way but the above mixed boundary condition on ∂B_d is replaced by the Dirichlet condition.

The next estimate concerns the effective potential V given by (3.2); by a straightforward calculation [DE] we can express it in terms of the curvature together with the function h and its two first derivatives with respect to the variable s as follows,

$$V = -\frac{\kappa^2}{4h^2} + \frac{h_{,ss}}{2h^3} - \frac{5(h_{,s})^2}{4h^4}\,. \tag{3.3}$$

It is important that up to an $\mathcal{O}(d)$ term this expression coincides with the potential involved in the comparison operator S. Indeed, since h is continuous on a compact set and thus bounded, by (2.1) there exists a positive C_h such that the inequalities

$$C_h^-(d)\le h^{-2}\le C_h^+(d)\quad\text{with}\quad C_h^\pm(d) := 1\pm C_h d,$$

hold for all d small enough. Since Γ is C^4 by assumption, the derivatives $h_{,s}$ and $h_{,ss}$ are also bounded; hence (3.3) yields the estimate

$$\left|V+\frac{\kappa^2}{4}\right|\le C_V d$$

with a positive C_V valid on $\mathcal{D}_d$ for all sufficiently small d. At the same time, we can apply the above bounds for h^{-2} to the longitudinal part of the kinetic term. Putting all this together we get

$$L_d^-\otimes I\le -\Delta_h\otimes I + V\le L_d^+\otimes I\,,$$

where

$$L_d^{\pm} := -C_h^{\pm}\frac{d^2}{ds^2} - \frac{\kappa^2}{4} \pm C_V d : \; D(S) \to L^2(0,L)\,.$$

Summarizing the above discussion, we can introduce a pair of operators with the longitudinal and transverse components separated, namely

$$B_\alpha^{\pm} := L_d^{\pm} \otimes I + I \otimes (-\Delta_\alpha^{\pm}) \quad \text{on} \quad L^2(0,L) \otimes L^2(B_d)\,, \tag{3.4}$$

which give the sought two-sided bounds, $\pm \dot{H}_{\alpha,\Gamma}^{\pm} \le \pm B_\alpha^{\pm}$.

3.3 Component eigenvalues estimates

In the next step we have to estimate the eigenvalues of $L_d^{\pm}$ and $-\Delta_\alpha^{\pm}$. Let us start with the longitudinal part. It is easy to check the identity

$$L_d^{\pm} = C_h^{\pm}(d)S \pm \left(C_V + C_h\frac{\kappa^2}{4}\right) d\,;$$

combining it with the minimax principle and the fact that the eigenvalues of S behave as $(\frac{2\pi}{L})^2\ell^2 + \mathcal{O}(1)$ as $\ell \to \pm\infty$, we arrive at the following conclusion:

Lemma 3.4 *There is a positive C such that the eigenvalues $l_j^{\pm}(d)$ of $L_d^{\pm}$, numbered in the ascending order, satisfy the inequalities*

$$|l_j^{\pm}(d) - \mu_j| \le Cj^2 d \tag{3.5}$$

for all $j \in \mathbb{N}$ and d small enough.

The transverse part is a bit more involved. Our aim is to show that in the strong-coupling case the influence of the boundary conditions is weak, i.e. that the negative eigenvalues of the operators $-\Delta_\alpha^{\pm}$ do not differ much from the number (2.4).

Lemma 3.5 *There exist positive numbers C_i, $1 \le i \le 4$, such that each one of the operators $-\Delta_\alpha^{\pm}$ has exactly one negative eigenvalue $t_\alpha^{\pm}$ which satisfies*

$$\xi_\alpha - S(\alpha) < t_\alpha^- < \xi_\alpha < t_\alpha^+ < \xi_\alpha + S(\alpha) \tag{3.6}$$

for α large enough negative, where

$$S(\alpha) := C_1\zeta_\alpha^2\sqrt{d\zeta_\alpha}\exp(-C_2 d\zeta_\alpha)$$

with $\zeta_\alpha := (-\xi_\alpha)^{1/2}$, provided $d\zeta_\alpha > C_3$ and $dM < C_4$.

Proof. Let us start with the eigenvalue of the operator $-\Delta_\alpha^+$ involved in the upper bound; the argument will be divided into four parts.

1. step: We will show that the number $-k_\alpha^2$ with $k_\alpha > 0$ is an eigenvalue of $-\Delta_\alpha^+$ *iff* k_α is a solution of the equation

$$x = \zeta_\alpha \eta(x)\,, \tag{3.7}$$

where ζ_α has been defined above and η is the function given by

$$\eta:\ \mathbb{R}_+ \to \mathbb{R}_+\,, \quad \eta(x) = \exp\left(-\frac{K_0(xd)}{I_0(xd)}\right)\,; \tag{3.8}$$

the symbols K_0, I_0 denote the Macdonald and the modified Bessel function, respectively [AS]. To verify this claim we note that the eigenfunction ψ of $-\Delta_\alpha^+$ corresponding to $-k_\alpha^2$ is a linear combination

$$\psi(r) = D_1 I_0(k_\alpha r) r^{1/2} + D_2 K_0(k_\alpha r) r^{1/2}$$

with the coefficients D_1, D_2 chosen in such a way that the conditions following from $\psi\,\tilde{}\,D.bc(\partial B_d)$ and $r^{-1/2}\psi\,\tilde{}\,\alpha.bc(0)$ are satisfied. Using the behaviour of K_0, I_0 at the origin

$$K_0(\rho) = -\ln\frac{\rho}{2} + \psi(1) + \mathcal{O}(\rho) \quad \text{and} \quad I_0(\rho) = 1 + \mathcal{O}(\rho)\,, \tag{3.9}$$

as $\rho \to 0$, we can readily check that ψ fulfils the needed boundary conditions *iff* $(D_1, D_2) \in \ker M(\alpha)$, where $M(\alpha)$ is the matrix given by

$$M_{ij}(\alpha) = \begin{pmatrix} I_0(k_\alpha d) & K_0(k_\alpha d) \\ 1 & \omega(\alpha, k_\alpha) \end{pmatrix}$$

with $\omega(\alpha, k_\alpha) := \psi(1) - 2\pi\alpha - \ln(k_\alpha/2)$. Of course, the condition $\ker M(\alpha) \neq \emptyset$ is equivalent to $\det M(\alpha) = 0$; the latter holds *iff* k_α is a solution of (3.7).

2. step: Our next aim is show that the equation (3.7) has at least one solution for $-\alpha$ sufficiently large, and moreover, that such a solution k_α satisfies the inequalities

$$\tilde{C}\zeta_\alpha < k_\alpha < \zeta_\alpha \tag{3.10}$$

with $\tilde{C} \in (0,1)$ independent of α. Using again (3.9) together with the asymptotic behaviour of the functions K_0, I_0 at infinity, we get for a fixed α

$$\zeta_\alpha \eta(x) \to \zeta_\alpha \quad \text{as} \quad x \to \infty$$

and

$$\zeta_\alpha \eta(x) = g_{\alpha,d}x + \mathcal{O}(x^2) \quad \text{as} \quad x \to 0\,, \tag{3.11}$$

where $g_{\alpha,d} := \frac{1}{2}\,\mathrm{e}^{-\psi(1)} d\zeta_\alpha$. It is clear that the error term is uniform with respect to α over finite intervals only, however, if

$$g_{\alpha,d} > 1 \tag{3.12}$$

then the equation (3.7) has obviously at least one solution. The second inequality in (3.10) holds trivially because $\eta(x) < 1$ for any $x > 0$. Let us assume that the first one is violated. This means that there is a sequence $\{\alpha_n\}$ with $\alpha_n \to -\infty$ as $n \to \infty$ such that $\eta(k_{\alpha_n}) \to 0$ as $n \to \infty$. This may happen only if the k_{α_n} tends to the singularity of K_0, in other words if $k_{\alpha_n} \to 0$ holds as $n \to \infty$. However, the inequality (3.12) is valid for α_n with n large enough, thus small k_{α_n} can not in view of the asymptotics (3.11) be a solution of (3.7) in contradiction with the assumption.

3. step: To show that there exists only one solution of (3.7) it suffices to check that the function $h_\alpha : \mathbb{R}_+ \mapsto \mathbb{R}$,

$$h_\alpha(x) = x - \zeta_\alpha \eta(x)\,,$$

is strictly monotonous for $x \in (\tilde{C}\zeta_\alpha, \zeta_\alpha)$ and $-\alpha$ sufficiently large. Using again the behaviour of K_0, I_0 at large values of the argument we find that the derivative $\eta'(x) \to 0$ as $x \to \infty$ which implies the result.

4. step: It remains to show that the eigenvalue $t_\alpha^+ = -k_\alpha^2$ satisfies the second one of the inequalities

$$\xi_\alpha < -k_\alpha^2 < \xi_\alpha + S(\alpha)\,. \tag{3.13}$$

Since the functions $-K_0$, I_0 are increasing and $I_0(0) = 1$ we get from (3.10) the estimate

$$\eta(k_\alpha) \geq \exp\left(-K_0(\tilde{C}\zeta_\alpha d)\right).$$

Putting now $\tilde{S}(\alpha) = \left(1 - \exp\left(-2K_0(\tilde{C}\zeta_\alpha d)\right)\right)\zeta_\alpha^2$ and using the asymptotic behaviour of K_0 at large distances one finds that

$$\tilde{S}(\alpha) \leq \tilde{C}_1 \zeta_\alpha^2 \sqrt{d\zeta_\alpha}\, \exp(-\tilde{C}_2 d\zeta_\alpha) \quad \text{as} \quad \alpha \to -\infty$$

holds with suitable constants $\tilde{C}_1$, $\tilde{C}_2$ and the inequality (3.13) is satisfied which concludes the proof for the operator $-\Delta_\alpha^+$.

Let us turn to the operator $-\Delta_\alpha^-$. The argument is similar, so we just sketch it with the emphasis on the differences. The number $t_\alpha^- = -k_\alpha^2$ is an eigenvalue of $-\Delta_\alpha^-$ *iff* k_α is a solution of the equation

$$x = \zeta_\alpha \tilde{\eta}(x)\,, \tag{3.14}$$

where $\tilde{\eta} : \mathbb{R}_+ \to \mathbb{R}_+$ is the function given by

$$\tilde{\eta}(x) = \exp\left(-\frac{S_K(xd)}{S_I(xd)}\right)\,, \quad S_F(xd) = \tilde{F}_1(xd)xd + w_d F_0(xd)$$

for $F = K, I$, where $\tilde{I}_1 = I_1$, $\tilde{K}_1 = -K_1$ and $w_d := \frac{1}{2} - Md$; we assume that

$$w_d > 0\,. \tag{3.15}$$

To proceed further, we employ again the asymptotics of functions I_n, K_n, $n = 0, 1$, for $x \to 0$ and at large values of the argument. It is easy to see that the behaviour of $x \mapsto \frac{S_K(xd)}{S_I(xd)}$ for small x is dominated by that of $K_0(\cdot)$. Thus mimicking the second step of the above argument we can show that the equation (3.8) has at least one solution for $-\alpha$ sufficiently large provided that assumption (3.12) is satisfied. Repeating the third step we can check that the solution k_α is unique for $-\alpha$ sufficiently large. By *reduction ad absurdum*, as in the second step, we can also prove that there exists $\hat{C}$ such that $\hat{C}\zeta_\alpha < k_\alpha$, which means that $k_\alpha \to \infty$ as $\alpha \to -\infty$. The constant can be made more specific: using the fact that the term $-dx\, K_1(dx)$ dominates the behaviour of $S_K(dx)$ for large x and $S_I > 0$ we get $\eta_\alpha > 1$ for $-\alpha$ sufficiently large, i.e.

$$\zeta_\alpha < k_\alpha\,.$$

Using properties of the special functions involved here we also find that

$$\eta_\alpha(k_\alpha) \le \exp(\dot{C} K_1(d\zeta_\alpha) d\zeta_\alpha)$$

holds for any $\dot{C}$ satisfying $(w_d)^{-1} + (d\zeta_\alpha)^{-1} < \dot{C}$. Thus proceeding similarly as in the fourth step we infer that there are constants $\breve{C}_1$, $\breve{C}_2$ such that

$$\xi_\alpha - \tilde{S}(\alpha) < -k_\alpha^2 < \xi_\alpha\,, \tag{3.16}$$

where

$$\tilde{S}(\alpha) \le \breve{C}_1 \zeta_\alpha^2 \sqrt{d\zeta_\alpha}\, \exp(-\breve{C}_2 d\zeta_\alpha) \quad \text{as} \quad \alpha \to -\infty\,.$$

Finally putting together (3.12), (3.13), (3.15) and (3.16) we get the claim with $C_1 := \max\{\tilde{C}_1, \breve{C}_1\}$ and $C_2 := \min\{\tilde{C}_2, \breve{C}_2\}$. ■

3.4 Proof of Theorem 3.2 for a loop

Suppose now that Γ is a closed curve. The result will follow from combination of the above estimates. We have to couple the width of the neighbourhood Ω_d and the coupling constant α in such a way that d shrinks properly to zero as $\alpha \to -\infty$. This is achieved, e.g., by choosing

$$d(\alpha) = \mathrm{e}^{\pi\alpha} \, . \tag{3.17}$$

Proof of (a): To find the asymptotic behaviour of eigenvalues $\lambda_j(\alpha)$ of $H_{\alpha,\Gamma}$ we will rely on the decomposition (3.4), according to which we know that the negative eigenvalues of $H_{\alpha,\Gamma}$ are squeezed between $l_j^{\pm}(d) + t_\alpha^{\pm}$. Since the operators $-\Delta_\alpha^{\pm}$ have a single negative eigenvalue, the sought values $\lambda_j(\alpha)$ are ordered in the same way as $l_j^{\pm}(d)$ are. Combining (3.17) with the results of Lemmas 3.4 and 3.5 we get for the upper and lower bound

$$l_j^{\pm}(d(\alpha)) + t_\alpha^{\pm} = \xi_\alpha + \mu_j + \mathcal{O}(e^{\pi\alpha}) \quad \text{as} \quad \alpha \to -\infty \, ,$$

and of course, the same asymptotics holds for $\lambda_j(\alpha)$. Clearly, to a given integer n there exists $\alpha(n) \in \mathbb{R}$ such that $l_n^{+}(d(\alpha)) + t_\alpha^{+} < 0$ is true for all $\alpha \leq \alpha(n)$; this completes the proof of (a).

Proof of (b): Using the above asymptotic estimates and Lemma 3.4 we get

$$\nu_j^{-}(\alpha) \leq \lambda_j(\alpha) \leq \nu_j^{+}(\alpha) \, , \tag{3.18}$$

where

$$\nu_j^{\pm}(\alpha) := \xi_\alpha + j^2 \left(\left(\frac{2\pi}{L} \right)^2 + \mathcal{O}(\mathrm{e}^{\pi\alpha}) \right) \pm v$$

and $v = 4^{-1} \|\kappa^2\|_\infty$. Combining this with the minimax principle we arrive at the two-sided estimate

$$\sharp\{j : \, \nu_j^{+}(\alpha) < 0\} \leq \sharp\sigma_d(H_\alpha) \leq \sharp\{j : \, \nu_j^{-}(\alpha) < 0\} \, ,$$

which implies

$$\sharp\sigma_d(H_\alpha) = \frac{L}{\pi}(-\xi_a)^{1/2}(1 + \mathcal{O}(\mathrm{e}^{\pi\alpha})) \, .$$

3.5 A curve with free ends

The part (b) of Theorem 3.2 does not require Γ to be a closed curve. One can repeat the argument with a small modification taking for Ω_d a closed tube around Γ bordered by the additional "lid" surfaces normal to Γ at its ends. Thus instead of S we have a pair of comparison operators $S^i = -\frac{d^2}{ds^2} - \frac{\kappa^2}{4}$ on $L^2(0,L)$ with $D(S^i) := \{f \in W^{2,2}(0,L), f\tilde{\ } i.bc\}$, $i = D, N$, which give in the same way as above estimates for the eigenvalues $\lambda_j(\alpha)$ of $H_{\alpha,\Gamma}$ as $\alpha \to -\infty$, namely

$$\xi_\alpha + \mu_j^N + \mathcal{O}(\mathrm{e}^{\pi\alpha}) \le \lambda_j(\alpha) \le \xi_\alpha + \mu_j^D + \mathcal{O}(\mathrm{e}^{\pi\alpha}),$$

where μ_j^i, $j = 1, 2, \dots$, denote the eigenvalues of S^i. The fact that the latter are different for the Dirichlet and Neumann condition does not allow us to squeeze $\lambda_j(\alpha)$ sufficiently well to get its asymptotics in analogy with the claim (a) of the theorem. On the other hand, the behaviour of $\mu_j^D - \mu_j^N$ as $j \to \infty$ allows us find an asymptotic estimate for the counting function. Recall that the eigenvalues of $-\Delta^i = -\frac{d^2}{ds^2} : D(S^i) \to L^2(0,L)$ are of the form $s_j^i = j^2(\frac{\pi}{L})^2$, where $j \in \mathbb{N}$ for $i = D$ and $j \in \mathbb{N} \cup \{0\}$ for $i = N$; thus in analogy with (3.18) we can define the functions

$$\nu_j^\pm(\alpha) := \xi_\alpha + j_\pm^2 \left(\left(\frac{\pi}{L}\right)^2 + \mathcal{O}(\mathrm{e}^{\pi\alpha}) \right) \pm v\,,$$

where $j^+ = j$ and $j^- = j-1$ with $j \in \mathbb{N}$, which give a two-sided bound for $\lambda_j(\alpha)$. Combining it with the minimax principle we arrive again at the formula

$$\sharp\sigma_d(H_{\alpha,\Gamma}) = \frac{L}{\pi}(-\xi_a)^{1/2}(1 + \mathcal{O}(\mathrm{e}^{\pi\alpha})) \quad \text{as} \quad \alpha \to -\infty\,.$$

Remark 3.6 While Theorem 3.2 was formulated for a single finite curve, which may not be closed for part (b), the argument easily extends to any Γ which decomposes into a finite disjoint union of such curves, up to the eigenvalue numbering. The latter may be ambiguous in case that the corresponding operator S, which is now an orthogonal sum of components of the type (3.1), exhibits an accidental degeneracy in its spectrum.

4 Infinite asymptotically straight curves

We know from [EK] that the operator $H_{\alpha,\Gamma}$ has a nonempty discrete spectrum if Γ is an infinite C^4 curve which is non straight but it is asymptotically straight in the following sense

(a$\Gamma_{\rm inf}$1) for all $s \in \mathbb{R}$ we have $|\kappa(s)| \leq M|s|^{-\beta}$, where $\beta > 5/4$ and $M > 0$.

Moreover one has to assume that

(a$\Gamma_{\rm inf}$2) there exists a constant $c \in (0,1)$ such that $|\gamma(s) - \gamma(s')| \geq c|s - s'|$.

If these conditions are satisfied then the operator $H_{\alpha,\Gamma}$ is self-adjoint and

$$\sigma_{\rm ess}(H_{\alpha,\Gamma}) = [\xi_\alpha, \infty)\,, \quad \sigma_{\rm d}(H_{\alpha,\Gamma}) \neq \emptyset\,.$$

Since the infinite curve has no free ends, the asymptotics of eigenvalues of $H_{\alpha,\Gamma}$ for $\alpha \to -\infty$ can be found in the same way as for the loop. We employ the comparison operator which now takes the form

$$S = -\frac{d^2}{ds^2} - \frac{1}{4}\kappa(s)^2 :\ D(S) \to L^2(\mathbb{R})$$

with the domain $D(S)$ equal to $W^{2,2}(\mathbb{R})$. It is a Schrödinger operator on line with a potential which is purely attractive provided $\kappa \neq 0$, and therefore

$$\sigma_{\rm d}(S) \neq \emptyset\,.$$

On the other hand, in view of the assumed decay of curvature as $|s| \to \infty$ the number $N := \sharp\sigma_{\rm d}(S)$ is finite [RS, Thm. XIII.9]. Using the symbol μ_j for the j-th eigenvalue of the operator S we get the following result.

Theorem 4.1 *Under the above stated assumptions there is $\alpha_0 \in \mathbb{R}$ such that $\sharp\sigma_{\rm d}(H_{\alpha,\Gamma}) = N$ holds for all $\alpha < \alpha_0$. Moreover, the j-th eigenvalue $\lambda_j(\alpha)$ of $H_{\alpha,\Gamma}$, $j = 1, \ldots, N$, admits the asymptotic expansion*

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

Since the proof fully analogous to that of Theorem 3.2 we omit details.

5 Spectrum for an infinite periodic curve

5.1 The Floquet–Bloch decomposition

Now we turn our attention to Hamiltonians with singular perturbations supported by a periodic C^4 curve without self-intersections. In other words we assume that there is a vector $\mathbf{K}_1 \equiv \mathbf{K} \in \mathbb{R}^3$ and a number $L > 0$ such that

$$\gamma(s+L) = \mathbf{K} + \gamma(s) \quad \text{for all} \quad s \in \mathbb{R}\,.$$

Of course, we can always choose the Cartesian system of coordinates such that $\mathbf{K} = (K, 0, 0)$ with $K > 0$, and $\gamma(0) = 0$. As usual in periodic situations we decompose the space $\mathbb{R}^3$ according to the periodicity of Γ. To this aim we define the basic period cell as

$$\mathcal{C}_0 \equiv \mathcal{C} := \{x : x = \sum_{i=1}^{3} t_i \mathbf{K}_i,\ t_1 \in [0,1),\, t_i \in \mathbb{R},\, i = 2,3\,\}\,, \qquad (5.1)$$

where $\{\mathbf{K}_i\}_{i=1}^3$ are linearly independent vectors in $\mathbb{R}^3$; without loss of generality we may suppose that $\mathbf{K}_2 \perp \mathbf{K}_3$. Then the translated cells $\mathcal{C}_n := \mathcal{C} + n\mathbf{K}$, where $n \in \mathbb{Z}$, are mutually disjoint for different values of the index and $\mathbb{R}^3 = \bigcup_{n\in\mathbb{Z}} \mathcal{C}_n$. As in the previous section we assume that Γ has no self-intersections. However, to proceed further we need an additional assumption, namely

($\mathrm{a}\Gamma_{\mathrm{per}}$) the restriction of $\Gamma_{\mathcal{C}} := \mathcal{C} \cap \Gamma$ to the interior of $\mathcal{C}$ is connected.

Let us note the choice of the point $s = 0$ is important in checking the assumption ($\mathrm{a}\Gamma_{\mathrm{per}}$), and for the same reason we do not require generally that $\mathbf{K}_1 \perp \{\mathbf{K}_2, \mathbf{K}_3\}$ (see also Remark 5.4 below).

While a smooth periodic curve without self-intersections satisfies ($\mathrm{a}\Gamma$), the property ($\mathrm{a}\Gamma_{\mathrm{per}}$) ensures that we can choose a neighbourhood of $\Gamma_{\mathcal{C}}$ which is connected set contained in $\mathcal{C}$; this is important for the construction described below. In view of Theorem 2.2 the Hamiltonian with the singular perturbation supported by Γ is well defined as a self-adjoint operator in $L^2(\mathbb{R}^3)$. To perform the Floquet–Bloch reduction for $H_{\alpha,\Gamma}$ we decompose first the state Hilbert space into a direct integral

$$\mathcal{H} = \int^{\oplus}_{[-\pi/K,\pi/K)} \mathcal{H}'\, d\theta\,, \quad \mathcal{H}' := L^2(\mathcal{C})\,.$$

It is a standard matter to check that the operator $U:\, L^2(\mathbb{R}^3)\to\mathcal{H}$ given by

$$(Uf)_\theta(x)=\frac{1}{(2\pi)^{1/2}}\sum_{n\in\mathbb{Z}}\mathrm{e}^{-i\theta Kn}f(x+n\mathbf{K}) \tag{5.2}$$

on $f\in C_0^\infty(\mathbb{R}^3)$ acts isometrically, so it can be uniquely extended to a unitary operator on the whole $L^2(\mathbb{R}^3)$. We will say that the function $f\in C^2(\mathcal{C}\backslash\Gamma_{\mathcal{C}})$ *belongs to* $\Upsilon_\alpha(\theta)$ if it satisfies the condition

$$f\,\tilde{}\,\alpha.bc(\Gamma_{\mathcal{C}})\,,$$

and furthermore, for all x such that both x and $x+\mathbf{K}$ belong to $\partial\overline{\mathcal{C}}$ and $x\neq(0,0,0)$ we have

$$f^{(\nu)}(x+\mathbf{K})=\mathrm{e}^{i\theta K}f^{(\nu)}(x)\,,\quad \nu=0,1\,, \tag{5.3}$$

where $f^{(0)}:=f$, $f^{(1)}:=\partial_{x_1}f$. Now we define $H_{\alpha,\Gamma}(\theta)$ as the self-adjoint Laplace operator in $L^2(\mathcal{C})$ with the boundary conditions introduced above; more precisely, $H_\alpha(\theta)$ is the closure of

$$\begin{aligned}\dot H_{\alpha,\Gamma}(\theta):D(\dot H_{\alpha,\Gamma}(\theta)) &= \{f\in\Upsilon_\alpha(\theta):\dot H_{\alpha,\Gamma}(\theta)f\in L^2(\mathcal{C})\}\to L^2(\mathcal{C})\,,\\ \dot H_{\alpha,\Gamma}(\theta)f(x) &= -\Delta f(x)\,,\quad x\in\mathcal{C}\setminus\Gamma_{\mathcal{C}}\,.\end{aligned}$$

The following lemma states the usual unitary equivalence between $H_{\alpha,\Gamma}$ and the direct integral of its fiber components $H_{\alpha,\Gamma}(\theta)$.

Lemma 5.1 *$UH_{\alpha,\Gamma}U^{-1}=\int^{\oplus}_{[-\pi/K,\pi/K)}H_{\alpha,\Gamma}(\theta)\,d\theta$.*

Proof. Take a function f belonging to the set

$$\mathcal{L}:=\{g\in C^2(\mathbb{R}^3\backslash\Gamma)\ :\ f\,\tilde{}\,\alpha.bc(\Gamma)\,,\ \mathrm{supp}\,f\ \text{is compact}\,\} \tag{5.4}$$

then for all $i=1,2,3$ we have

$$(U\partial_i f(x))_\theta=\partial_i(Uf)_\theta(x)\,,\quad x\notin\Gamma\,,$$

and the same relations hold for the second derivatives. Thus to prove the lemma it suffices to show that any function admitting the representation $(Uf)_\theta$ with $f\in\mathcal{L}$ belongs to $\Upsilon_\alpha(\theta)$. It is easy to check that for all $x\neq(0,0,0)$ such that x and $x+\mathbf{K}$ are in $\partial\overline{\mathcal{C}}$ we have

$$((Uf)_\theta^{(\nu)}(x+\mathbf{K})=\mathrm{e}^{i\theta K}((Uf)_\theta^{(\nu)}(x))\quad\text{for}\quad\nu=0,1\,.$$

The behaviour of the function $(Uf)_\theta$ in the vicinity of $\Gamma_{\mathcal{C}}$ is characterized by the limits $\Xi((Uf)_\theta)(\cdot)$ and $\Omega((Uf)_\theta)(\cdot)$. Using the periodicity of Γ we get

$$\begin{aligned}\Xi((Uf)_\theta)(s) &= (2\pi)^{-1/2}\sum_{n\in\mathbb{Z}} \mathrm{e}^{-in\theta K}\Xi(f)(s+nL)\,, \quad s\in(0,L)\,,\\ \Omega((Uf)_\theta)(s) &= (2\pi)^{-1/2}\sum_{n\in\mathbb{Z}} \mathrm{e}^{-in\theta K}\Omega(f)(s+nL)\,, \quad s\in(0,L)\,;\end{aligned}$$

to derive these relations we used also the uniform convergence of the sums. In this way we conclude that $(Uf)_\theta\tilde{}\,\alpha.bc(\Gamma_{\mathcal{C}})$. The Laplace operator in $L^2(\mathcal{C})$ with the domain consisting of functions which admit the representation $(Uf)_\theta$ with $f\in\mathcal{L}$ is essentially self-adjoint and its closure coincides with $H_{\alpha,\Gamma}(\theta)$; this completes the proof. ■

5.2 Spectral analysis of $H_{\alpha,\Gamma}(\theta)$

As in the case of a finite curve we can now analyze the discrete spectrum of the operator $H_{\alpha,\Gamma}(\theta)$. Before doing that let us localize the essential spectrum. An argument analogous to that of Proposition 3.1 shows that the singular perturbation supported by $\Gamma_{\mathcal{C}}$ does not change the essential spectrum of the Laplacian in a slab with Floquet boundary conditions, i.e.

$$\sigma_{\mathrm{ess}}(H_{\alpha,\Gamma}(\theta)) = \big[\theta^2,\infty\big)\,. \tag{5.5}$$

To describe the asymptotic behaviour of the eigenvalues of $H_{\alpha,\Gamma}(\theta)$ we introduce a comparison operator by $S_\theta = -\frac{d^2}{ds^2}-\frac{\kappa(s)^2}{4}\,:\,D(S_\theta)\to L^2(0,L)$, where

$$D(S_\theta) := \{\, f\in W^{2,2}(0,L) :\, f(L)=\mathrm{e}^{i\theta K}f(0),\, f'(L)=\mathrm{e}^{i\theta K}f'(0)\,\}\,.$$

In analogy with Theorem 3.2 we state:

Theorem 5.2 *Under the assumption given above for a fix number n there exists $\alpha(n)\in\mathbb{R}$ such that $\sharp\sigma_d(H_\alpha(\theta))\geq n$ holds for $\alpha\leq\alpha(n)$. Moreover, the j-th eigenvalue of $H_{\alpha,\Gamma}(\theta)$ has the asymptotic expansion of the form*

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

where $\mu_j(\theta)$ is the j-th eigenvalue of S_θ and the error term is uniform with respect to θ.

Proof. The argument follows closely that of Theorem 3.2; the only difference is the replacement of periodic boundary condition by the Floquet one. The fact that the error is uniform w.r.t. θ is a consequence of Lemma 3.4 and continuity of the functions $\mu_j(\cdot)$. ■

5.3 Spectral analysis of $H_{\alpha,\Gamma}$ in terms of $H_{\alpha,\Gamma}(\theta)$

Now our aim is to express the spectrum of $H_{\alpha,\Gamma}$ in the terms of $H_{\alpha,\Gamma}(\theta)$. First, let us note that combining (5.5) with standard results [RS, Sec. XIII.16] we get the following equivalence for the positive part of spectrum

$$\sigma(H_{\alpha,\Gamma}) \cap [0,\infty) = \bigcup_{\theta\in[-\pi/K,\pi/K)} \sigma(H_{\alpha,\Gamma}(\theta)) \cap [0,\infty) = [0,\infty).$$

The negative part of spectrum is more interesting being given by the union of ranges of the functions $\lambda_j(\alpha,\cdot)$. They give rise to well-defined spectral bands because the latter are continuous in the Brillouin zone $[-\pi/K,\pi/K)$. This can be seen by checking in the usual way, putting θ into the operator and showing that the θ dependent part is an analytic perturbation. Alternatively, one can take $g = (Uf)_\theta$ with $f \in \mathcal{L}$ as defined by (5.4) and investigate the functions

$$\theta \mapsto q_g(\theta) := (g, H_{\alpha,\Gamma}(\theta)g)_{L^2(\mathcal{C})} = \frac{1}{2\pi}\sum_{n,m\in\mathbb{Z}} \mathrm{e}^{-i(n-m)\theta}(f_n, H_{\alpha,\Gamma}f_m)_{L^2(\mathcal{C})}\,,$$

where $f_n(x) := f(x+n\mathbf{K})$. In view of (5.2) and the uniform convergence of the respective sums such a $q_g(\cdot)$ is continuous for g runing over a common core of all $H_{\alpha,\Gamma}(\theta)$. Thus by the minimax priciple we get the continuity of $\lambda_j(\alpha,\cdot)$ and combining this fact with the results of [RS] we get $\sigma(H_{\alpha,\Gamma}) \cap (-\infty,0] = (-\infty,0]$. Finally we arrive at

$$\sigma(H_\alpha) = \bigcup_{\theta\in[-\pi/K,\pi/K)} \sigma(H_\alpha(\theta))\,.$$

These results together with Theorem 5.2 allow to describe the band structure of $H_{\alpha,\Gamma}$, in particular, the existence of gaps. Notice that this operator as well as $S = -\frac{d^2}{ds^2} - \frac{\kappa(s)^2}{4}$ in $L^2(\mathbb{R})$ commute with the complex conjugation, so their Floquet eigenvalues are generically twice degenerate depending on $|\theta|$ only.

For the comparison operator thus width of the $j-$th gap is

$$G_j(S) = \mu_{j+1}(\pi/K) - \mu_j(\pi/K) \qquad \text{for odd } j$$
$$\mu_{j+1}(0) - \mu_j(0) \qquad \text{for even } j$$

and similarly for $H_{\alpha,\Gamma}$. The expansion of Theorem 5.2 then gives

$$G_j(H_{\alpha,\Gamma}) = G_j(S) + \mathcal{O}(\, e^{\pi\alpha})\,.$$

In combination with the known result about existence of gaps for one-dimensional Schrödinger operators we arrive at the following conclusion.

Corollary 5.3 *Suppose that in addition to the above assumption the function* $\kappa(\cdot)$ *is nonconstant. In the generical case when* S *has infinitely many open gaps, one can find to any* $n \in \mathbb{N}$ *an* $\alpha(n) \in \mathbb{R}$ *such that the operator* $H_{\alpha,\Gamma}$ *has at least* n *open gaps in its spectrum if* $\alpha < \alpha(n)$*. If the number of gaps in* $\sigma(S)$ *is* $N < \infty$*, then* $\sigma(H_{\alpha,\Gamma})$ *has the same property for* $-\alpha$ *large enough.*

Notice that this property is determined by the curvature alone. Thus the result does not apply not only to the trivial case of a straight line, but also to screw-shaped spirals Γ for which κ is nonzero but constant.

Remark 5.4 It is not always possible to choose $\mathcal{C}$ in the form of a rectangular slab (5.1) as we did above, which would satisfy the assumption (aΓ_{per}); counterexamples can be easily found. However, if we choose instead another period cell $\mathcal{C}$ with a smooth boundary for which the property (aΓ_{per}) is valid, the argument modifies easily and the claim of Theorem 5.2 remains valid. On the other hand, such a decomposition may not exist if the topology of Γ is non-trivial; a simple counterexample is given by a "crotchet-shaped" curve. While we conjecture that the claim of Theorem 5.2 is still true in this situation, a different method is required to demonstrate it.

5.4 Compactly disconnected periodic curves

So far we have considered a single periodic connected curve. A slightly stronger result about the existence of gaps in spectrum of $H_{\alpha,\Gamma}$ as $\alpha \to -\infty$ can be obtained for compactly disconnected periodic curves in $\mathbb{R}^3$, i.e. such that they decompose into a disjoint union in which each of the connected components is compact. To be more specific, we consider a family of curves obtained by translations of a loop Γ_0 (being a graph of a function γ_0) generated by an r-tuple $\{\mathbf{K}_i\}$ linearly independent vectors, where $r = 1, 2, 3$. The curve Γ in question is then a union $\Gamma = \bigcup_{n\in\mathbb{Z}^r} \Gamma_n$, where Γ_n are graphs of

$$\gamma_n := \gamma_0 + \sum_{n\in\mathbb{Z}^r} n_i \mathbf{K}_i : \; [0, L] \to \mathbb{R}^3 , \quad n = \{n_i\} ;$$

for the sake of brevity we put here $\Gamma_{n_0} = \Gamma_0$, $\gamma_{n_0} = \gamma_0$, where $n_0 := (0, 0, 0)$. We assume that Γ_0 *is contained in the interior* of the period cell

$$\mathcal{C} = \left\{ \sum_{i=0}^{r-1} t_i \mathbf{K}_i : 0 \le t_i < 1 \right\} \times \{\mathbf{K}_i\}^{\perp} ,$$

which is noncompact if $r = 1, 2$ and compact otherwise. Similarly as before we can make Floquet-Bloch decomposition of $H_{\alpha,\Gamma}$ into a direct integral of the fiber operators $H_{\alpha,\Gamma}(\theta)$. However now, since $\mathrm{dist}(\partial\mathcal{C}, \Gamma_{\mathcal{C}}) > 0$ holds by assumption, the comparison operator $S = S(\theta)$ is now independent of the quasimomentum $\theta \in \prod^{\times}_{1\le i\le r} [-\pi|\mathbf{K}_i|^{-1}, \pi|\mathbf{K}_i|^{-1})$. While in the previous case some gaps of $S(\theta)$ might be closed, now they are all open. As a result each gap in the spectrum of $\sigma(H_{\alpha,\Gamma})$, which depends of course on θ, will eventually open for $-\alpha$ large enough.

Theorem 5.5 *Under the assumptions stated above the spectrum of $H_{\alpha,\Gamma}(\theta)$ is purely discrete if $r = 3$, and $\sigma_{\mathrm{ess}}(H_{\alpha,\Gamma}(\theta)) = [\sum_{i=1}^{r} \theta_i^2, \infty)$ if $r = 1, 2$. The j-th eigenvalue of $H_{\alpha,\Gamma}(\theta)$ admits the asymptotic expansion of the following form,*

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

where μ_j is the j-th eigenvalue of S and the error is uniform w.r.t. θ. Consequently, for any $n \in \mathbb{N}$ there is $\alpha(n) \in \mathbb{R}$ such that the operator $H_{\alpha,\Gamma}$ has at least n open gaps in its spectrum if $\alpha < \alpha(n)$.

6 Concluding remarks

(a) The results obtained in the previous discussion can be rephrased as a *semiclassical approximation.* To see this let us consider the Hamiltonian $H_{\alpha,\Gamma}(h)$ with the Planck's constant h reintroduced; the latter is understood in the mathematical sense, i.e. as a parameter which allows us to investigate the asymptotic behaviour as $h \to 0$. The operator in question then acts as

$$H_{\alpha,\Gamma}(h)f(x) = -h^2\Delta f(x)\,, \quad x \in \mathbb{R}^3 \setminus \Gamma\,,$$

and has the domain

$$D(H_{\alpha,\Gamma}(h)) = \{f \in \Upsilon_{\mathbb{R}^3} : f\tilde{\ }\alpha(h).bc(\Gamma)\}\,,$$

where

$$\alpha(h) := \alpha + \frac{1}{2\pi}\ln h\,. \tag{6.6}$$

This definition of $H_{\alpha,\Gamma}(h)$ requires a comment. In the case $\operatorname{codim}\Gamma = 1$ discussed in [Ex] the Hamiltonian is defined by the natural quadratic form, hence introducing h means a multiplicative change of the coupling parameter, $\alpha \to \alpha h^{-2}$; one can see that also from the approximation of such an operator by means of scaled regular potentials [EI].

In contrast to that a two-dimensional point interaction involves a complicated nonlinear coupling constant renormalization [AGHH, Sec. I.5], so introducing Planck's constant is in this case arbitrary to a certain extent. We choose the simplest way noticing that the relation between the free operators $-\Delta$ and $-h^2\Delta$ can expressed by means of the scaling transformation $x \mapsto hx$, and require the similar behavior for the singular interaction term; it is well known that a scaling for a two-dimensional point interaction is equivalent to a logarithmic shift of the coupling parameter – cf. [EGŠT]. In view of (6.6) the semiclassical limit $h \to 0$ is within this convention for a fixed coupling constant α equivalent to $\alpha(h) \to -\infty$ which means a strong coupling again. Since $H_{\alpha,\Gamma}(h) = h^2 H_{\alpha(h),\Gamma}(1)$ we see that the eigenvalues $\lambda_j(\alpha, h)$ of $H_{\alpha,\Gamma}(h)$ take then the following form,

$$\lambda_j(\alpha, h) = \xi_\alpha + \mu_j h^2 + \mathcal{O}(h^{5/2}) \quad \text{as} \quad h \to 0\,.$$

In the same way we find the counting function which is given by

$$\#\sigma_d(H_\alpha(h)) = \frac{L}{\pi h}(-\xi_\alpha)^{1/2}(1 + \mathcal{O}(h^{1/4}))\,.$$

(b) Let us finally list some *open problems* related to the present subject:

- One is naturally interested in the asymptotic expansion in the situation when Γ is a curve with free ends and the present method allows us to treat the counting function only; the analogous question stands for planar curves [EY1] and surfaces with a boundary [Ex]. We *conjecture* that the expansion of Theorem 3.2 holds again with μ_j corresponding to the comparison operator which acts according to (3.1) with *Dirichlet* boundary conditions at the boundary of Γ.

- The results can be extended to higher dimensions provided $\operatorname{codim}\Gamma \leq 3$ so that the singular interaction Hamiltonian is well defined.

- The smoothness assumption is crucial in our argument. A self-similar curve such as a broken line consisting of two halflines joined at a point provides an example of a situation where the asymptotic behaviour differs from that of Theorem 3.2. One can ask, e.g., how the asymptotics looks like for a piecewise smooth curve with non-zero angles at a discrete set of points.

- Another important question concerns the *absolute continuity* of the spectrum in case when Γ is a periodic curve or a family of curves. The answer in known if $\operatorname{codim}\Gamma = 1$ and the elementary cell is compact [BSŠ, SŠ]. The cases of a single connected periodic curve or a periodic surface diffeomorphic to the plane are open, and the same is true for periodic curve(s) in $\mathbb{R}^3$, i.e. the situation with $\operatorname{codim}\Gamma = 2$.

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