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Flux and symmetry effects on quantum tunneling

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Abstract

Motivated by the analysis of the tunneling effect for the magnetic Laplacian, we introduce an abstract framework for the spectral reduction of a self-adjoint operator to a hermitian matrix. We illustrate this framework by three applications, firstly the electro-magnetic Laplacian with constant magnetic field and three equidistant potential wells, secondly a pure constant magnetic field and Neumann boundary condition in a smoothed triangle, and thirdly a magnetic step where the discontinuity line is a smoothed triangle. Flux effects are visible in the three aforementioned settings through the occurrence of eigenvalue crossings. Moreover, in the electro-magnetic Laplacian setting with double well radial potential, we rule out an artificial condition on the distance of the wells and extend the range of validity for the tunneling approximation recently established in Fefferman et al. (SIAM J Math Anal 54: 1105–1130, 2022), Helffer & Kachmar (Pure Appl Anal, 2024), thereby settling the problem of electro-magnetic tunneling under constant magnetic field and a sum of translated radial electric potentials.

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1 Introduction

1.1 Tunneling and flux effects

The tunneling induced by symmetries is an interesting phenomenon in spectral theory featuring an exponentially small splitting between the ground state and the next excited state energies. The magnetic flux has an effect on the eigenvalue multiplicity which can lead to oscillatory patterns in the spectrum: as the magnetic flux varies, the eigenvalues may cross and split infinitely many times. Hence it is interesting to look at the interaction between symmetry and flux effects. We explore this question by investigating examples of operators involving the magnetic Laplacian $(-ih\nabla - \mathbf{A})^2$ perturbed in various ways by an electric potential, a boundary condition or a magnetic field discontinuity. We observe interesting flux effects, manifested in endless eigenvalue crossings, when adding symmetry assumptions on the electric potential, the boundary of the domain or the magnetic field discontinuity set.

A braid structure in the distribution of the low lying eigenvalues was predicted heuristically [11, Sec. 15.2.4] and confirmed numerically [4] for the magnetic Laplacian on an equilateral triangle with Neumann boundary condition and constant magnetic field. We confirm this prediction by giving a proof for smoothed equilateral triangles and for other examples on the full plane (electro-magnetic Laplacian and magnetic steps).

Let us introduce a mathematical definition of (semi-classical) *braid structure* of lowest eigenvalues. Consider a family of unbounded self-adjoint operators $(T_h)_{h\in(0,1]}$ on a Hilbert space H. Let us assume that, for every $h \in (0, 1]$, T_h is semi-bounded from below and denote by $\lambda_1(T_h), \lambda_2(T_h), \cdots$ the discrete eigenvalues below the essential spectrum of T_h, counted with multiplicity. In practical examples, the parameter h will be the semi-classical parameter, which tends to 0 and can result as the inverse of the magnetic field's intensity in problems involving strong magnetic fields.

Definition 1.1 The lowest eigenvalues of T_h, $\lambda_1(T_h)$ and $\lambda_2(T_h)$, are said to have a braid structure, if

$$\forall \epsilon > 0,\ \exists\, h_\epsilon, h'_\epsilon \in (0,\epsilon),\ \begin{cases} \lambda_2(T_{h_\epsilon}) - \lambda_1(T_{h_\epsilon}) > 0 \\ \lambda_2(T_{h'_\epsilon}) - \lambda_1(T_{h'_\epsilon}) = 0 \end{cases} .$$

According to Definition 1.1, the eigenvalues $\lambda_1(T_h)$ and $\lambda_2(T_h)$ exhibit infinitely many crossings and splittings as the parameter h varies in a right neighborhood of 0 (see Fig. 1). This phenomenon has also been observed in non-simply connected domains when considering a magnetic Laplacian and assuming an Aharonov–Bohm magnetic potential. Furthermore, it has been proven in [23] that these crossings and splittings occur in response to variations in the magnetic flux.

For the semi-classical magnetic Laplacian on a simply connected domain with Neumann boundary conditions, the spectrum is related with the spectral properties of an operator which is defined on the boundary. Hence we actually work on another non-simply connected domain (i.e. the boundary) and therefore flux effects are expected to exhibit crossings and splittings of eigenvalues. However, this is not the case when

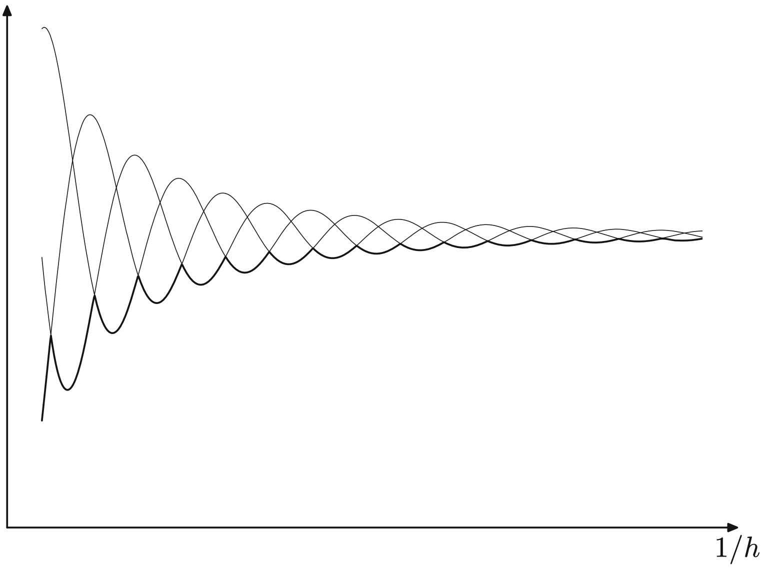

Fig. 1 A schematic figure of eigenvalues with a braid structure, occurring in the presence of trilateral symmetry. The ground state energy has multiplicity 2 infinitely many times. Observe also that the energy of the second state may have multiplicity 2 while the ground state energy is a simple eigenvalue

the boundary curvature has for example a unique non-degenerate maximum. In this case the eigenvalues split in the semi-classical limit [12]. It is when non-degenerate minima are exchanged in the presence of symmetries (like in the case of an ellipse or a smoothed equilateral triangle), that eigenvalue crossings are expected to occur along with tunneling effects [6, 11]. We will also prove such a behavior for the electro-magnetic Laplacian with 'potential' wells located on the vertices of an equilateral triangle, which to our knowledge is quite novel.

1.2 Electro-magnetic tunneling

The analysis in this paper yields new results on the electro-magnetic Laplacian on $\mathbb{R}^2$,

$$\mathcal{L}_{h,b} = (-\mathrm{i}h\nabla - b\mathbf{A})^2 + V,$$

where b, h are positive parameters, $\mathbf{A} = \frac{1}{2}(-x_2, x_1)$ is the vector field generating the unit uniform magnetic field, curl $\mathbf{A} = 1$, and V is a smooth function.

What we call the wells are the points where V attains its minimum. The pure electric case where $b = 0$ was settled for any number of wells n in [21]. We would like to address the case where $b > 0$ and $n \geq 2$. For $n = 2$, this problem was considered in [22, 25] and revisited recently in [10, 17]. The article [22] follows a perturbative approach (i.e. considers the case b relatively small) and assumes the analyticity of the electric potential V, while the results in [10, 17] hold for any $b > 0$ but under the assumption that V is non-positive and defined as a superposition of radially symmetric compactly supported functions.

1.2.1 Double wells

Suppose that the electric potential V is as follows

$$V(x) = v_0(|x - z_1|) + v_0(|x - z_2|) \tag{1.1}$$

where $v_0 \in C^\infty(\overline{\mathbb{R}_+})$ vanishes on $[a, +\infty)$, negative-valued on $[0, a)$ and has a unique and non-degenerate minimum at 0. The wells of V are then z_1 and z_2. We prove the following theorem that, in particular, rules out eigenvalue crossings for double wells.

Theorem 1.2 *Assuming $b > 0$ is fixed and V is given as in (1.1) with $z_1 = 0$, $z_2 = (L, 0)$ and $L \geq 4a$, then there exists a positive constant $\mathscr{E}_{b,L}(v_0)$ such that*

$$h \ln \big(\lambda_2(\mathcal{L}_{h,b}) - \lambda_1(\mathcal{L}_{h,b})\big) \underset{h\searrow 0}{\sim} -\mathscr{E}_{b,L}(v_0). \tag{1.2}$$

Moreover

$$\mathscr{E}_{b,L}(v_0) \underset{b\searrow 0}{\sim} 2\int_0^{L/2} \sqrt{v_0(\rho) - v_0^{\min}}\, \mathrm{d}\rho,$$

where $v_0^{\min} = \min_{r\geq 0} v_0(r)$.

Remark 1.3 i) The asymptotics in (1.2) was obtained earlier in [17] for $b = 1$ but under the assumption that

$$L > 4\Big(\sqrt{|v_0^{\min}|} + a\Big). \tag{1.3}$$

ii) The use of (1.3) in [17] was technical. In fact, assuming (1.3), it is proved in [10] that

$$\lambda_2(\mathcal{L}_{h,1}) - \lambda_1(\mathcal{L}_{h,1}) \underset{h\searrow 0}{\sim} \mathfrak{c}_h(v_0, L) \tag{1.4}$$

where $\mathfrak{c}_h(v_0, L)$ is the hopping coefficient that will be introduced in (3.15) later on. The accurate approximation of $\ln \mathfrak{c}_h(v_0, L)$ was then carried out in [17].

iii) For $b \neq 1$, by a change of semi-classical parameter, the condition in (1.3) reads as follows

$$L > 4\Big(b^{-1}\sqrt{|v_0^{\min}|} + a\Big).$$

Clearly, this is a very strong condition on L which in particular prevents us from considering the limit $b \searrow 0$. The novelty in Theorem 1.2 is in improving the previous condition which could appear as artificial. However, it is still an open question whether (1.2) holds for $2a < L < 4a$. We provide a sufficient condition on (L, a, v_0) that allows for L to be slightly below $4a$; see Assumption 3.6.

iv) The dependence on b in the expression of $\mathscr{E}_{b,L}(v_0)$ can actually be made more explicit. We have indeed

$$\mathscr{E}_{b,L}(v_0) = b\, S(b^{-2}v_0, L)\,,$$

where $S(\cdot, L)$ will be introduced in (3.18) later on.
The leading term of $\mathscr{E}_{b,L}(v_0)$ in the limit $b \searrow 0$ was calculated in [17, Rem. 1.3], and it is consistent with the existing results [20, 29] without a magnetic field, $b = 0$, thereby showing a sort of continuity of the tunneling estimate with respect to the magnetic field's strength. Studying the transition from $b = 0$ to $b > 0$ when $b = b(h)$ could be an interesting question.

1.2.2 Three wells and eigenvalue crossings

Suppose now that the electric potential V is as follows

$$V(x) = v_0(|x - z_1|) + v_0(|x - z_2|) + v_0(|x - z_3|) \tag{1.5}$$

where v_0 is the same function as in (1.5) and that the wells z_1, z_2, z_3 are located on the vertices of an equilateral triangle with side length L. We prove then the existence of a braid structure in the sense of Definition 1.1.

Theorem 1.4 *Assuming $b > 0$ is fixed and V is given as in (1.5) with*

$$|z_1 - z_2| = |z_2 - z_3| = |z_3 - z_1| = L > 4a,$$

then the lowest egigenvalues of $\mathcal{L}_{h,b}$ has a braid structure. Moreover,

$$\limsup_{h\searrow 0}\Big(h \ln\big(\lambda_2(\mathcal{L}_{h,b}) - \lambda_1(\mathcal{L}_{h,b})\big)\Big) = -\mathscr{E}_{b,L}(v_0)$$

with $\mathscr{E}_{b,L}(v_0)$ the same positive quantity as in Theorem 1.2.

Not only Theorem 1.4 establishes the existence of infinitely many eigenvalue crossings and splittings, but it also establishes an accurate estimate for the magnetic tunneling induced by three symmetric potential wells, thereby extending the recent results of [10, 17] on double wells.

1.3 Geometrically induced braid structure

We present here results on the pure magnetic Laplacian where the eigenvalue crossings are induced by a combination of the geometry and the flux in the semi-classical limit. We shall describe the results when Ω is a smoothed triangle (see Fig 2). That is, Ω is a simply connected domain, invariant under rotation by $2\pi/3$, with three points of maximum curvature that are equidistant with respect to the arc-length distance on the boundary.

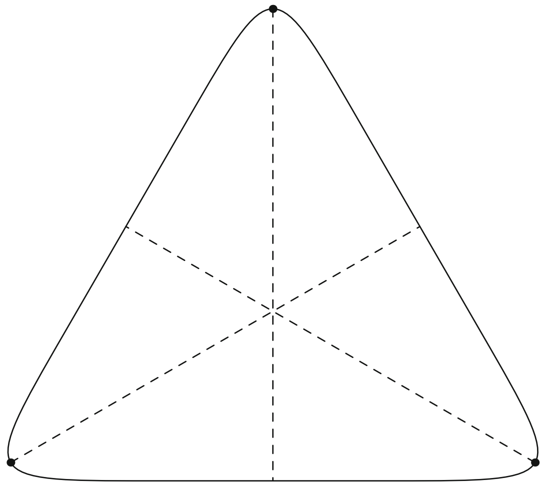

Fig. 2 Illustration of the domain Ω: a smoothed triangle invariant under the rotation by $2\pi/3$

1.3.1 The magnetic Neumann Laplacian under constant magnetic field

In the Hilbert space $L^2(\Omega)$, we consider the magnetic Neumann Laplacian $\mathscr{L}_h^N = (-ih\nabla - \mathbf{A})^2$ on Ω, with uniform magnetic field curl $\mathbf{A} = 1$ and (magnetic) Neumann condition

$$\nu \cdot (-ih\nabla - \mathbf{A})u|_{\partial\Omega} = 0.$$

Theorem 1.5 *Let the domain Ω be a smoothed triangle, invariant under the rotation by $2\pi/3$ (see Fig. 2). The lowest eigenvalues of the operator $\mathscr{L}_h^N$ have a braid structure.*

The presence of the Neumann boundary condition plays a vital role in the preceding theorem. This condition is responsible for the semi-classical localization of the bound states near the boundary of Ω and this is this localization that gives rise to the observed flux effects.

1.3.2 The Landau Hamiltonian under a magnetic step

We consider here the Landau Hamiltonian $\mathscr{L}_h^B = (-ih\nabla - \mathbf{A})^2$ on $\mathbb{R}^2$ with the discontinuous magnetic field

$$B = \operatorname{curl} \mathbf{A} = \begin{cases} 1 & \text{on } \Omega, \\ \vartheta \in (-1, 0) & \text{on } \mathbb{R}^2 \setminus \overline{\Omega}. \end{cases}$$

Such magnetic fields have been called 'magnetic steps' in the literature, and the semi-classical limit for the operator $\mathcal{L}_h^B$ has been studied recently in [3, 13] (and in [14] for $\vartheta = -1$). The bound states of the system become increasingly concentrated along the discontinuity of B in the semi-classical limit. Consequently, we expect the emergence of flux effects, and they are indeed realized when Ω is a smoothed triangle with 3-fold symmetry.

Theorem 1.6 *Assume that Ω is a smoothed triangle, invariant under the rotation by $2\pi/3$ (see Fig. 2). The lowest eigenvalues of the operator $\mathscr{L}_h^B$ have in the semi-classical limit a braid structure.*

We therefore have an example where the eigenvalues of the Landau Hamiltonian on the full plane cross and split infinitely many times. This is the consequence of having a sign changing magnetic field with a discontinuity along a simple smooth curve.

Recently, an estimate for the tunneling induced by a smooth magnetic field that vanishes non-degenerately along a smooth curve has been established in [1]. It seems natural to expect the existence of a braid structure in that setting too when adding symmetry assumptions.

1.4 Organization

The paper is organized as follows. Since we work with various symmetry configurations, Section 2 is devoted to an abstract spectral reduction to a hermitian matrix (so often called the interaction matrix in the literature on tunneling effects [16, 20]). This provides us with a robust methodology when analyzing tunneling effects in various settings. Loosely speaking, all we need is the construction of adequate quasi-modes.

In Sect. 3 we discuss the electro-magnetic Laplacian. Our investigation has two ingredients, the first is to appply the abstract methodology in Sect. 2, and the second is to control the errors produced by the interaction terms; the later task is achieved by using the analysis in the recent work [17]. Section 3 concludes with the proofs of Theorems 1.2 and 1.4.

In Sect. 4, we prove Theorem 1.5 by applying the results of Sect. 2. The control of the error terms and the computation of the interaction term were done in [6].

Finally, in Sect. 5, we prove Theorem 1.6 by applying the constructions in Sect. 2. We will be more succinct here since the analysis is similar to Sect. 4. The control of the error terms and the asymptotics of the interaction terms were done in [13] and are actually rather close to those in [6].

2 Abstract framework for a spectral reduction to a hermitian matrix

The strategy of reducing the spectral analysis of Schrödinger operators to that of a hermitian matrix goes back to [20]. It was presented in the survey works [9, 16], and was adapted to other type of operators [6, 18, 19]. Nevertheless, it should be emphasized that the scheme of proof (as described for example in [9]) can not be immediately transposed to some of the cases considered in our applications, due to the absence of optimal Agmon estimates.

In this section we consider a family of operators dependent on a positive semi-classical parameter $h \ll 1$. Assuming the existence of certain quasi-modes (see Assumption 2.1 below), we can approximate the eigenvalues of the operator with those of the matrix of its restriction on a specific basis (Proposition 2.4 below). Assuming an additional symmetry hypothesis (Assumption 2.6 below) we can relabel the eigenvalues and spot their possible crossings and splittings as the semi-classical parameter approaches 0 (Eqs. (2.20), (2.21) and Paragraphs 2.4.2, 2.4.3).

2.1 Preliminaries

Consider a Hilbert space H endowed with an inner product $\langle\cdot,\cdot\rangle$ and a family of self-adjoint unbounded operators $T_h\colon D_h \to H$, $h \in (0,1]$. Assume furthermore that, for every $h \in (0,1]$, T_h is semi-bounded from below and has a sequence of discrete eigenvalues

$$\lambda_1(h) \le \lambda_2(h) \le \lambda_3(h) \le \ldots < \Sigma_h := \inf \sigma_{\mathrm{ess}}(T_h) \in \mathbb{R} \cup \{+\infty\},$$

counted with multiplicity. By the min-max principle the eigenvalues can be represented as

$$\lambda_n(h) = \inf_{\substack{M \subset D_h \\ \dim(M)=n}} \left(\max_{\substack{\phi \in M \\ \|\phi\|=1}} \langle T_h\phi, \phi\rangle \right).$$

We will work under additional assumptions on the operators $(T_h)_{h\in(0,1]}$.

Assumption 2.1 (n wells) Let $n \ge 2$ be an integer. There exist positive constants $\mathfrak{S}_1, \mathfrak{S}_2, \mathfrak{S}_3, c, p$ and $h_0 \in (0,1]$ such that, for all $h \in (0,h_0]$, there exists a subspace $E_h = \operatorname{span}(u_{h,1},\ldots,u_{h,n}) \subset D_h$ such that:

(1) $\max_{1\le i\le n} \|T_h u_{h,i}\| = \mathcal{O}(\mathrm{e}^{-\mathfrak{S}_1/h})$.

(2) $\langle u_{h,i}, u_{h,j}\rangle = \begin{cases} 1 + \mathcal{O}(\mathrm{e}^{-\mathfrak{S}_2/h}) & i = j, \\ \mathcal{O}(\mathrm{e}^{-\mathfrak{S}_3/h}) & i \ne j. \end{cases}$

(3) $\lambda_{n+1}(h) \ge c\,h^p$.

It results from (2) above that $\dim(E_h) = n$ for h small enough. As a consequence of Assumption 2.1, we now prove that the operator T_h has precisely n eigenvalues that are *exponentially small* in h, and there is a gap to $\lambda_{n+1}(h)$, since it is at least of polynomial size in h.

Proposition 2.2 *Under Assumption 2.1, there exist positive constants C, h_1 such that, for $h \in (0,h_1]$,*

$$\lambda_n(h) \le Ce^{-\mathfrak{S}_1/h}. \tag{2.1}$$

In particular $\lambda_n(h) < \lambda_{n+1}(h)$ for h sufficiently small.

Proof Since $\dim(E_h) = n$, we can use the min-max principle. Let $\phi = \sum_j \alpha_j u_{h,j}$ be in E_h. Then, the triangle inequality and Cauchy–Schwarz inequality, together with (1) and (2) from Assumption 2.1, provide the existence of constants A_1 and A_2, such that if h is small enough,

$$\langle T_h\phi,\phi\rangle \le \sum_{j,k}|\alpha_j|\cdot|\alpha_k|\cdot\|T_hu_{h,j}\|\cdot\|u_{h,k}\| \le A_1\mathrm{e}^{-\mathfrak{S}_1/h}(1+A_2\mathrm{e}^{-\mathfrak{S}_2/h})\sum_j|\alpha_j|^2.$$

On the other hand, we can use (2) of Assumption 2.1 to bound the norm of ϕ from below. We get indeed constants A_3 and A_4 such that, if h is small enough,

$$\|\phi\|^2 \ge (1-A_3\mathrm{e}^{-\mathfrak{S}_2/h}-A_4\mathrm{e}^{-\mathfrak{S}_3/h})\sum_j|\alpha_j|^2.$$

This gives the bound in (2.1). Combining this bound with (3) in Assumption 2.1 we conclude that that $\lambda_{n+1}(h)>\lambda_n(h)$ if h is sufficiently small. □

We want to link the quasi mode constructions $\{u_{h,j}\}$ to the low-lying eigenvalues of T_h. To do this, we want to show that the symmetric matrix $\mathsf{U}_h=(\mathsf{u}_{j,k})$,

$$\mathsf{u}_{j,k}=\langle T_hu_{h,j},u_{h,k}\rangle, \tag{2.2}$$

does not differ much (component-wise) from the matrix W_h that will be constructed as the restriction of T_h to the eigenspace

$$F_h \coloneqq \bigoplus_{j=1}^{n}\mathrm{Ker}(T_h-\lambda_j(h)), \tag{2.3}$$

written in an orthonormal basis. We will do the approximation in two steps. We first consider the projected functions

$$v_{h,j}=\Pi_{F_h}u_{h,j}$$

and show that the norms $\|v_{h,j}-u_{h,j}\|$ are small. Since the span of $\{u_{h,j}\}$ is n-dimensional by Assumption 2.1 (2), it will follow that the $\{v_{h,j}\}$ are linearly independent, and thus constitute a basis for F_h.

Proposition 2.3 *If Assumption 2.1 holds for E_h, then for $h>0$ sufficiently small, we have* $\dim(F_h)=n$*, and the vectors*

$$v_{h,i}=\Pi_{F_h}u_{h,i}\quad (i\in\{1,\cdots,n\}),$$

form a basis of F_h. Moreover they satisfy

$$\max_{1\le i\le n}\|v_{h,i}-u_{h,i}\|=\mathcal{O}(h^{-p}\mathrm{e}^{-\mathfrak{S}_1/h}). \tag{2.4}$$

Proof Since we count multiplicities, we know in general that $\dim(F_h)\ge n$. However, by (3) in Assumption 2.1, we get from Proposition 2.2 that $\dim(F_h)=n$.

With $v_{h,i} = \Pi_{F_h} u_{h,i}$ we note that $u_{h,i} - v_{h,i} \in H \ominus F_h$. Since T_h, restricted to $H \ominus F_h$ is bounded below by ch^p by Assumption 2.1 (3), we find that

$$\|T(u_{h,i} - v_{h,i})\| \geq c\, h^p \|u_{h,i} - v_{h,i}\|.$$

On the other hand, According to Assumption 2.1 (1) and (2), and Proposition 2.2,

$$\|T(u_{h,i} - v_{h,i})\| \leq \|T u_{h,i}\| + \|T v_{h,i}\| \leq C\mathrm{e}^{-\mathfrak{S}_1/h}.$$

Combining these inequalities we get (2.4). From this and Assumption 2.1 (2), we find that $\{v_{h,1}, \ldots, v_{h,n}\}$ are linearly independent, and hence a basis for F_h. $\square$

2.2 Reduction to a matrix through a suitable orthonormal basis

The aim in this subsection is to find an orthonormal basis for F_h such that the matrix of the restriction of T_h in this basis can be well approximated. Later in the applications to multiple wells problems this matrix will be according to the previous literature called the interaction matrix.

The basis $\{v_{h,j}\}$ of F_h that we just constructed will, in general, not be orthogonal. We construct, by a symmetry-preserving Gram–Schmidt procedure an orthonormal basis $\{w_{h,j}\}$. The matrix W_h will be the matrix of T_h restricted to F_h, written in this new basis $\{w_{h,j}\}$.

Let us denote by $\mathsf{G}_h = (\mathsf{g}_{ij}(h))_{1\leq i,j\leq n}$ the Gram matrix of the basis $\{v_{h,1}, \ldots, v_{h,n}\}$ of F_h, where

$$\mathsf{g}_{ij} = \langle v_{h,i}, v_{h,j}\rangle. \tag{2.5}$$

Since the $\{v_{h,j}\}$ are linearly independent, the Gram matrix becomes positive definite, so $\mathsf{G}_h^{-1/2}$ is well defined and positive definite. We obtain an orthonormal basis $\mathcal{V}_h = \{w_{h,1}, \ldots, w_{h,n}\}$ of F_h as follows[1]

$$\begin{pmatrix} w_{h,1} \\ \vdots \\ w_{h,n} \end{pmatrix} = \mathsf{G}_h^{-1/2} \begin{pmatrix} v_{h,1} \\ \vdots \\ v_{h,n} \end{pmatrix}. \tag{2.6}$$

We consider the restriction of T_h to the space F_h and denote by $\mathsf{W}_h = (\mathsf{w}_{ij})_{1\leq i,j\leq n}$ its matrix in the basis $\mathcal{V}_h$, so $\mathsf{w}_{ij} = \langle T_h w_{h,i}, w_{h,j}\rangle$. The matrix W_h is hermitian, with eigenvalues $\{\lambda_1(h), \ldots, \lambda_n(h)\}$. The next proposition controls how W_h is approximated by the matrix U_h defined by (2.2).

[1] We could have worked in the basis obtained by the standard Gram–Schmidt process but the downside is that the Gram–Schmidt process does not respect the symmetry invariance that we will impose later.

Proposition 2.4 *Let*

$$\left.\begin{aligned} \Lambda_h &:= \|T_h|_{F_h}\| = \max_{1\le i\le n} |\lambda_i(h)|,\\ C_h &= h^{-p}\mathrm{e}^{-\mathfrak{S}_1/h} + \mathrm{e}^{-\min(\mathfrak{S}_2,\mathfrak{S}_3)/h},\\ \varepsilon_h &= (\Lambda_h + C_h)C_h. \end{aligned}\right\} \tag{2.7}$$

Then the matrix $\mathsf{R}_h = (\mathsf{r}_{ij})$,

$$\mathsf{R}_h := \mathsf{W}_h - \mathsf{U}_h, \tag{2.8}$$

is symmetric, and satisfies

$$\mathsf{r}_{ij} = \mathcal{O}(\varepsilon_h)\,. \tag{2.9}$$

Proof **Step 1.** Proposition 2.3 says that

$$\langle v_{h,i}, v_{h,j}\rangle = \langle u_{h,i}, u_{h,j}\rangle + \mathcal{O}(h^{-p}\mathrm{e}^{-\mathfrak{S}_1/h}).$$

With I denoting the $n\times n$ identity matrix, we get from (2) in Assumption 2.1,

$$\mathsf{G}_h = \mathsf{I} + \mathcal{O}(C_h)$$

so that

$$\mathsf{G}_h^{-1/2} = \mathsf{I} + \mathcal{O}(C_h).$$

It follows then that

$$\left.\begin{aligned} \|w_{h,i} - v_{h,i}\| &= \mathcal{O}(C_h),\\ \|T_h w_{h,i} - T_h v_{h,i}\| &= \mathcal{O}\big(\Lambda_h C_h\big) \end{aligned}\right\} \tag{2.10}$$

where in the second estimate in (2.10), we simply combine the first estimate and the definition of Λ_h.

Step 2. We may write

$$\begin{aligned} \mathsf{w}_{ij} &= \langle T_h w_{h,i}, w_{h,j}\rangle = \langle T_h v_{h,i}, v_{h,j}\rangle\\ &\quad + \langle T_h v_{h,i}, w_{h,j} - v_{h,j}\rangle + \langle T_h(w_{h,i} - v_{h,i}), w_{h,j}\rangle. \end{aligned}$$

Using this identity, (2.10) and Proposition 2.3, we get

$$\langle T_h w_{h,i}, w_{h,j}\rangle = \langle T_h v_{h,i}, v_{h,j}\rangle + \mathcal{O}(\Lambda_h C_h). \tag{2.11}$$

Then, we use

$$\langle T_h v_{h,i}, v_{h,j}\rangle = \langle T_h u_{h,i}, u_{h,j}\rangle + \langle T_h u_{h,i}, v_{h,j} - u_{h,j}\rangle + \langle v_{h,i} - u_{h,i}, T_h v_{h,j}\rangle.$$

By Proposition 2.3 and (1) in Assumption 2.1, we have

$$\begin{aligned} \langle T_h u_{h,i}, v_{h,j} - u_{h,j}\rangle &= \mathcal{O}(h^{-p}\mathrm{e}^{-2\mathfrak{S}_1/h}) = \mathcal{O}(C_h^2)\,,\\ \langle v_{h,i} - u_{h,i}, T_h v_{h,j}\rangle &= \mathcal{O}(\Lambda_h C_h). \end{aligned}$$

So we get

$$\langle T_h v_{h,i}, v_{h,j}\rangle = \langle T_h u_{h,i}, u_{h,j}\rangle + \mathcal{O}(\varepsilon_h)\,, \tag{2.12}$$

which together with (2.11) implies (2.9). $\square$

An immediate consequence of Proposition 2.4 is an improved lower bound on the lowest eigenvalue $\lambda_1(h)$.

Corollary 2.5 *If Assumption 2.1 holds, then there exist positive constants C, h_1 such that, for $h \in (0, h_1]$,*

$$\lambda_1(h) \geq -C\mathrm{e}^{-\min(\mathfrak{S}_1, 2\mathfrak{S}_2, 2\mathfrak{S}_3)/h}. \tag{2.13}$$

Proof It follows from Hölder's inequality and (1)–(2) in Assumption 2.1 that $\mathsf{u}_{ij} = \mathcal{O}(\mathrm{e}^{-\mathfrak{S}_1/h})$, where u_{ij} is introduced in (2.2). By Proposition 2.4, we have

$$\Lambda_h \leq \|\mathsf{W}_h\| \leq \|\mathsf{U}_h\| + \|\mathsf{R}_h\| = \mathcal{O}(\mathrm{e}^{-\mathfrak{S}_1/h}) + \mathcal{O}(\Lambda_h C_h + C_h^2)$$

which yields

$$\big(1 - \mathcal{O}(C_h)\big)\Lambda_h \leq \mathcal{O}(\mathrm{e}^{-\mathfrak{S}_1/h}) + \mathcal{O}(C_h^2).$$

To conclude, we just notice that $C_h = o(1)$. $\square$

As we will see in the next subsection, we can actually say much more about the spectrum of these matrices, when we impose some symmetry condition involving T_h and the choice of the $u_{h,j}$.

2.3 Implementing invariance assumptions

Our task in this subsection is to analyze the case when the matrix W_h of $T_h|_{F_h}$ enjoys certain invariance properties. We shall see that this corresponds to what occurs in the case of *symmetric* wells in the applications, starting from the double well case as mathematically considered by E. Harrell [15] and later extended to the multiple wells case in [20, 21, 28, 29]. Here we mainly follow in a more abstract way [21] and the heuristic presentation given in [11]. We denote by $\mathbb{Z}_n$ the cyclic group of order n and by $\mathfrak{g} \mapsto \rho(\mathfrak{g})$ a faithful unitary representation of $\mathbb{Z}_n$ in H. We denote by a_n its generator, so $a_n^n = e$ where e is the identity element of the group.

In addition to the properties in Assumption 2.1, we assume

Assumption 2.6 (1) The operator T_h commutes with $\rho(\mathfrak{g})$ for all $\mathfrak{g} \in \mathbb{Z}_n$.
(2) $u_{h,i+1} = \rho(a_n)u_{h,i}$ for $1 \leq i \leq n-1$.

Remark 2.7 In the applications considered in this article, the Hilbert space will be $H = L^2(\Omega)$ where Ω is a domain in $\mathbb{R}^2$. We first consider the unitary representation ρ_0 of $\mathbb{Z}_n$ as the group G_n of the n-fold rotations, i.e. the representation such that

$$\rho_0(a_n) \coloneqq g_n$$

is the rotation in $\mathbb{R}^2$ by $2\pi/n$ around the origin in $\mathbb{R}^2$.

We let the rotation g_n act on functions as

$$\big(M(g_n)u\big)(x) = u(g_n^{-1}x). \tag{2.14}$$

This gives by extension to any element of G_n a representation of G_n in $L^2(\Omega)$ if $\Omega \subset \mathbb{R}^2$ is a domain invariant by G_n and we then define ρ by

$$\rho(\mathfrak{g}) = M(\rho_0(\mathfrak{g}))\,.$$

Equivalently to Assumption 2.6, we can then write in this case

Assumption 2.8 (1) $\Omega \subset \mathbb{R}^2$ is a domain invariant by G_n and $H = L^2(\Omega)$.
(2) The operator T_h commutes with $M(g_n)$.
(3) $u_{h,i+1} = M(g_n)u_{h,i} = u_{h,1}(g_n^{-i}x)$ for $1 \le i \le n-1$.

Assumption 2.6 permits to treat more general situations which for example occur in the case of manifolds or in the case of higher dimension.

Remark 2.9 If $n = 2$ we can define another group of symmetry $\tilde{G}$ defined by the reflection $\tilde{g}_2\binom{x_1}{x_2} = \binom{-x_1}{x_2}$. We can then consider a variant of Assumption 2.6 by instead assuming that the domain Ω is invariant by the reflection $\tilde{g}_2$ and that $u_{h,2} = \overline{M(\tilde{g}_2)u_{h,1}}$. This symmetry invariance was assumed by the papers considering the magnetic tunneling induced by the geometry of the domain [1, 6, 13, 24]. Notice that $M(\tilde{g}_2)$ does not commute with T_h and that we have consequently to compose $M(\tilde{g}_2)$ with the complex conjugation Γ in order to get

$$T_h \Gamma M(\tilde{g}_2) = \Gamma M(\tilde{g}_2) T_h\,.$$

Proposition 2.10 *If Assumption 2.6 holds, then the orthonormal basis $\mathcal{V}_h = \{w_{h,1}, \dots, w_{h,n}\}$ of F_h satisfies,*

$$w_{h,i+1} = \rho(a_n)w_{h,i} \quad (1 \le i \le n-1).$$

Proof Recall that $\{w_{h,1}, \dots, w_{h,n}\}$ is defined in (2.6) by the Gram matrix starting from the basis consisting of the vectors $v_{h,i} = \Pi_{F_h}u_{h,i}$, $1 \le i \le n$. It suffices to observe that the projector Π_{F_h} on the eigenspace F_h commutes with $\rho(a_n)$. Actually, since T_h commutes with $\rho(a_n) = M(g_n)$, we get, for every z in the resolvent set of T_h, that $(z - T_h)^{-1}\rho(a_n) = \rho(a_n)(z - T_h)^{-1}$, and consequently, the identity $\Pi_{F_h}\rho(a_n) = \rho(a_n)\Pi_{F_h}$ follows from Cauchy's formula.

Let us give a more hands-on argument for this commutativity. If $\{w_{h,1}, \dots, w_{h,n}\}$ is an orthonormal basis of F_h consisting of eigenvectors of T_h, then, since T_h commutes with $\rho(a_n)$, we get that $\rho(a_n)w_{h,1}, \dots, \rho(a_n)w_{h,n}$ are eigenvectors of T_h and form an orthonormal basis of F_h. Consequently

$$\begin{aligned}\Pi_{F_h}\rho(a_n)u &= \sum_{k=1}^{n}\langle \rho(a_n)u, \rho(a_n)w_{h,k}\rangle \rho(a_n)w_{h,k}\\ &= \sum_{k=1}^{n}\langle u, w_{h,k}\rangle \rho(a_n)w_{h,k} = \rho(a_n)\Pi_{F_h}u.\end{aligned}$$

□

The matrix of $\rho(a_n)$ in the basis $\mathcal{V}_h$ is the same as the matrix of the shift operator τ on $\ell^2(\mathbb{Z}/n\mathbb{Z})$, whose matrix is given by

$$\tau_{j,k} = \delta_{j+1,k} \text{ for } 1 \leq j, k \leq n \tag{2.15}$$

where $\delta_{i,k}$ denotes the Kronecker symbol, with i computed in $\mathbb{Z}/n\mathbb{Z}$. When $n = 2$ and $n = 3$, the matrix τ is respectively given by

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

We observe that

$$\tau^{n-1} = \tau^{-1} = \tau^* .$$

The property that the operator T_h commutes with $\rho(a)$ implies that the matrix W_h (of $T_h|_{F_h}$ in the basis $\mathcal{V}_h$) commutes with τ, i.e., $\tau \mathsf{W}_h = \mathsf{W}_h \tau$. Note that this invariance condition yields that

$$\mathsf{W}_h = \sum_{k=0}^{n-1} I_k(h)\tau^k, \tag{2.16}$$

for some coefficients $I_0(h), \ldots, I_{n-1}(h) \in \mathbb{C}$. Here τ^0 denotes the identity matrix.

The Hermitian property of W_h gives, in addition,

$$I_0(h) \in \mathbb{R}\,,\ I_k(h) = \overline{I_{n-k}(h)} \ \text{ for } k = 1, \ldots, n-1\,. \tag{2.17}$$

Notice that the matrix U_h introduced in (2.2) satisfies the same properties as W_h. Hence we can also write

$$\mathsf{U}_h = \sum_{k=0}^{n-1} J_k(h)\tau^k\,, \tag{2.18}$$

for some coefficients $J_0(h), \ldots, J_{n-1}(h) \in \mathbb{C}$ and the Hermitian property of U_h also implies

$$J_0(h) \in \mathbb{R}\,,\ J_k(h) = \overline{J_{n-k}(h)} \ \text{ for } k = 1, \ldots, n-1\,. \tag{2.19}$$

All these invariant matrices (W_h or U_h) share the property to be diagonalizable in the same orthonormal basis of eigenfunctions e_k ($k = 1, \dots, n$) whose coordinates in our selected basis are given by

$$(\mathrm{e}_k)_\ell = \omega_n^{(k-1)\ell}\,, \quad \text{with} \quad \omega_n := \exp(2i\pi/n)\,.$$

It is then easy to compute the corresponding eigenvalues.

In particular, we get an explicit representation of the eigenvalues of W_h which illustrates when $n = 3, 4$, the possibility of eigenvalue crossings (i.e. change of multiplicity).

- When $n = 2$, W_h assumes the form $\begin{pmatrix} I_0 & I_1 \\ I_1 & I_0 \end{pmatrix}$ with I_1 real. This matrix has two eigenvalues
$$\lambda_1 = I_0 - |I_1|\,,\ \lambda_2 = I_0 + |I_1|\,. \tag{2.20}$$
- When $n = 3$, W_h assumes the form
$$\mathsf{W}_h = \begin{pmatrix} I_0 & \overline{I_1} & I_1 \\ I_1 & I_0 & \overline{I_1} \\ \overline{I_1} & I_1 & I_0 \end{pmatrix}$$
with $I_1 = \rho e^{i\theta}$, $\rho \geq 0$, $\theta \in [0, 2\pi)$. This matrix has three eigenvalues
$$\mu_k = I_0 + 2\rho\cos\left(\theta + (k-1)\frac{2\pi}{3}\right), \quad k \in \{1, 2, 3\}. \tag{2.21}$$
- When $n = 4$, we meet the matrix
$$\mathsf{W}_h = \begin{pmatrix} I_0 & \overline{I_1} & I_2 & I_1 \\ I_1 & I_0 & \overline{I_1} & I_2 \\ I_2 & I_1 & I_0 & \overline{I_1} \\ \overline{I_1} & I_2 & I_1 & I_0 \end{pmatrix}$$
with I_2 real and $I_1 = \rho e^{i\theta}$, $\rho \geq 0$, $\theta \in [0, 2\pi)$. We refer to [11] for a further discussion of this case. Figure 3 illustrates the braid startucture of the eigenvalues of the matrix W_h.

2.4 Applications

2.4.1 Additional hypothesis

We can strengthen the estimate of Λ_h in (2.7) if we assume additionally that[2]

[2] We shall see in the applications that the rough estimate of $J_k(h)$ by Hölder's inequality and (1)–(2) in Assumption 2.1 is not sufficient to the accurate estimate of tunneling.

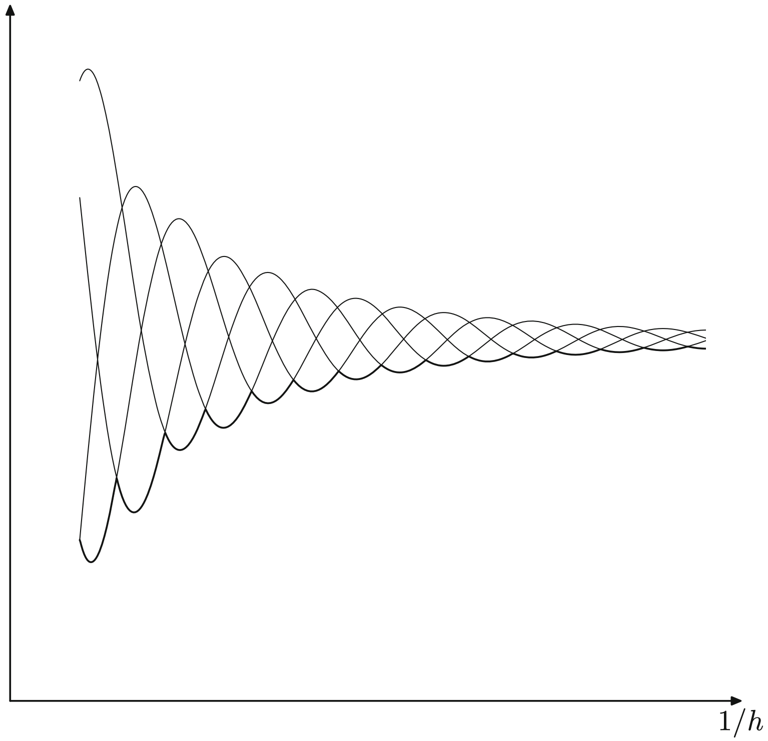

Fig. 3 A schematic figure of four eigenvalues with a braid structure in the case of a rotational symmetry of order 4

Assumption 2.11 There exists a positive constant $\mathfrak{S}$ such that

$$\mathfrak{S} < 2 \min_{1 \le j \le 3} \mathfrak{S}_j\,, \tag{2.22}$$

$$J_k(h) \underset{h \searrow 0}{=} \mathcal{O}(\mathrm{e}^{-\mathfrak{S}/h}) \quad (k = 0, \cdots, n-1), \tag{2.23a}$$

and

$$|J_1(h)| \underset{h \searrow 0}{=} \mathrm{e}^{-(\mathfrak{S}+o(1))/h}. \tag{2.23b}$$

Proposition 2.12 *There exist positive constants $C, h_0 > 0$ such that, if Assumptions 2.1 and 2.11 hold, then for all $h \in (0, h_0]$, the symmetric matrix $\mathsf{R}_h = (\mathsf{r}_{ij})$ introduced in (2.8) satisfies*

$$\|\mathsf{R}_h\| \underset{h \searrow 0}{=} \mathcal{O}\big(\mathrm{e}^{-3\mathfrak{S}/2h}\big) = o\big(|J_1(h)|\big).$$

Proof This follows by applying Proposition 2.4 (the same argument as in Corollary 2.5). Indeed, we have by the first identity in (2.23),

$$\Lambda_h = \mathcal{O}(\mathrm{e}^{-\mathfrak{S}/h}) + \mathcal{O}(C_h^2)\,. \tag{2.24}$$

Inserting (2.24) into the definition of ε_h in (2.7), we obtain that

$$\varepsilon_h = \mathcal{O}(\delta_h) \text{ where } \delta_h = C_h\mathrm{e}^{-\mathfrak{S}/h} + C_h^2 = \mathcal{O}(\mathrm{e}^{-3\mathfrak{S}/2h}). \tag{2.25}$$

We can improve the bounds (2.9) of the symmetric matrix R_h into $\mathsf{r}_{ij} = \mathcal{O}(\delta_h)$. To finish the proof, we observe that, by the second identity in (2.23), $\delta_h = o(|J_1(h)|)$. □

2.4.2 The case $n = 2$

A first consequence of the previous analysis is a full understanding of the case corresponding to $n = 2$ where the symmetry g_2 reads $(x_1, x_2) \mapsto (-x_1, -x_2)$. Assuming that Assumptions 2.8 and 2.11 hold, we get from (2.20) and Proposition 2.12

$$\lambda_2(h) - \lambda_1(h) = 2|J_1(h)| + o\big(|J_1(h)|\big). \tag{2.26}$$

2.4.3 The case $n = 3$, braid structure of eigenvalues

Suppose that Assumptions 2.8 and 2.11 hold with $n = 3$. Let $I_0(h), I_1(h)$ be as in (2.16) and let us write

$$I_1(h) = \rho(h)\mathrm{e}^{\mathrm{i}\theta(h)} \text{ where } \rho(h) \geq 0 \text{ and } \theta(h) \in [0, 2\pi).$$

Then, by (2.21), we have a relabeling $\mu_1(h)$, $\mu_2(h)$, and $\mu_3(h)$ of the eigenvalues $\lambda_1(h)$, $\lambda_2(h)$, and $\lambda_3(h)$ of T_h with $\rho = \rho(h)$ and $\theta = \theta(h)$. Moreover,

$$I_0(h) = J_0(h) + \mathcal{O}(\delta_h), \quad I_1(h) = J_1(h) + \mathcal{O}(\delta_h) \sim J_1(h) \tag{2.27a}$$

with $\delta_h = o\big(J_1(h)\big)$ defined in (2.25) and

$$J_0(h) = \langle T_h u_{h,1}, u_{h,1}\rangle, \quad J_1(h) = \langle T_h u_{h,1}, u_{h,2}\rangle. \tag{2.27b}$$

Notice that there is possibility for eigenvalue crossings between

- $\mu_1(h)$ and $\mu_2(h)$ if $\theta(h) \in \{2\pi/3, 5\pi/3\}$;
- $\mu_2(h)$ and $\mu_3(h)$ if $\theta(h) \in \{0, \pi\}$;
- $\mu_1(h)$ and $\mu_3(h)$ if $\theta(h) \in \{\pi/3, 4\pi/3\}$.

The point is then to seek an accurate approximation of $\theta(h)$. Notice that (2.27) yields $I_1(h) \underset{h\searrow 0}{\sim} J_1(h)$. Defining $\theta_1(h)$ by $J_1(h) = \rho_1(h)\mathrm{e}^{i\theta_1(h)}$, we can approximate $\theta(h)$ by $\theta_1(h)$ modulo $2\pi\mathbb{Z}$. This could confirm the predicted braid structure mentioned in [4, 11]. We will consider in detail three models where such a phenomenon holds (see Theorem 3.9, Section 4, and Section 5).

3 Electro-magnetic tunneling

3.1 Introduction

In this section, the Hilbert space is $H = L^2(\mathbb{R}^2)$, and for given $n \in \mathbb{N}$ we consider $g = g_n$ to be rotation around the origin by $2\pi/n$, and $M(g)$ to be as in (2.14). We are interested in the spectrum of the electro-magnetic Schrödinger operator

$$\mathcal{L}_{h,b} = (-\mathrm{i}h\nabla - b\mathbf{A})^2 + V,$$

where $b, h > 0$, and

$$\mathbf{A}(x) = \frac{1}{2}(-x_2, x_1)\,. \tag{3.1}$$

Notice that $\mathbf{A}$ generates the constant magnetic field curl $\mathbf{A} = 1$. For the potential V we assume that

$$V \in C^\infty(\mathbb{R}^2, \mathbb{R})\,, \tag{3.2a}$$

$$V \leq 0\,, \tag{3.2b}$$

$$V \text{ is invariant by the rotation } g_n\,. \tag{3.2c}$$

Moreover, we assume that

$$\text{The minimum of } V \text{ is attained at } n \text{ non-degenerate minima.} \tag{3.2d}$$

Then it results from the invariance property of V that these minima are n equidistant points of $\mathbb{R}^2 \setminus \{0\}$. We will refer to these points as the *wells*.

Notice that, when dealing with a fixed $b > 0$ we can reduce the analysis to the case where $b = 1$ by introducing an effective semi-classical parameter $\hbar = b^{-1}h$ so that

$$\mathcal{L}_{h,b} = b^2\big((-\mathrm{i}\hbar\nabla - \mathbf{A})^2 + b^{-2}V\big). \tag{3.3}$$

So we will assume henceforth that $b = 1$. To relate with the discussion in Sect. 2, our operator T_h is the electro-magnetic Laplacian shifted by a certain scalar $\lambda(h)$.

$$T_h := \mathcal{L}_h - \lambda(h), \quad \mathcal{L}_h = (-\mathrm{i}h\nabla - \mathbf{A})^2 + V. \tag{3.4}$$

Note that the assumption in (3.2c) implies that T_h commutes with $M(g)$. Hence the condition of invariance of the preceding section holds. The shift constant $\lambda(h)$ in (3.4) will be chosen as the ground state energy of a reference single well operator.

3.2 Single well ground states

Let us first discuss the one well operator.

3.2.1 Preliminary discussion and assumptions

There are various possible approaches to create one well problems in the presence of multiple wells. The approach considered in [20, 21] starts from a general electric potential V and introduce suitable Dirichlet conditions to create an infinite barrier leading to a one well problem. The so-called LCAO[3] approach, frequently used in Physics and Atomic Chemistry, and considered in [10, 17], particularly applies when V is a superposition of single well potentials.

As in [10, 17], we consider a radial single well potential. More precisely, we assume in this section that $V = \mathfrak{v}_0$, where $\mathfrak{v}_0 \in C_c^\infty(\mathbb{R}^2)$ is a non-positive radial function satisfying

$$\begin{cases} \mathfrak{v}_0(x) = v_0(|x|) \ \& \ v_0^{\min} := \min\limits_{r\geq 0} v_0(r) < 0\,, \\ \operatorname{supp} \mathfrak{v}_0 \subset \overline{D(0,a)} := \{x \in \mathbb{R}^2 \ : \ |x| \leq a\}\,, \\ \mathfrak{v}_0^{-1}(v_0^{\min}) = \{0\} \quad \& \quad v_0''(0) > 0\,. \end{cases} \tag{3.5}$$

We choose $\overline{D(0,a)}$ as the smallest closed disc containing $\operatorname{supp} \mathfrak{v}_0$, i.e.

$$a = a(v_0) := \inf\{r > 0 \ : \ v_0|_{[r,+\infty)} = 0\}. \tag{3.6}$$

3.2.2 Preliminary inequalities

As in [17], we will encounter various errors of exponential order which are defined in terms of the function v_0 and the constant

$$L > 2a(v_0)\,. \tag{3.7}$$

With (v_0, L) as above, $a = a(v_0)$ and with

$$d(r) = d_{v_0}(r) := \int_0^r \sqrt{\frac{\rho^2}{4} + v_0(\rho) - v_0^{\min}}\, \mathrm{d}\rho, \tag{3.8}$$

we introduce the four constants (we will often skip the depends on v_0 and L)

$$\left.\begin{aligned} S_0 &= S_0(v_0, L) := d(L), \\ S_a &= S_a(v_0, L) := d(a) + d(L-a), \\ \hat{S}_a &= \hat{S}_a(v_0, L) := d(L-a), \\ \hat{S} &= \hat{S}(v_0, L) := \inf_{0<r<a}\left[\frac{Lr}{2} + d(r) + d(L-r)\right]. \end{aligned}\right\} \tag{3.9}$$

[3] for Linear Combination of Atomic Orbitals.

Notice also that, since v_0 vanishes on $[a, +\infty)$, we can express the constant S_a as follows

$$S_a = 2\int_0^a \sqrt{\frac{r^2}{4} + v_0(r) - v_0^{\min}}\,\mathrm{d}r + \int_0^{L-a} \sqrt{\frac{r^2}{4} - v_0^{\min}}\,\mathrm{d}r.$$

It is important when comparing the errors to compare the three constants introduced in (3.9).

Proposition 3.1 *Assume that v_0 and L satisfy (3.6) and (3.7). Then we have, with $a = a(v_0)$,*

$$\hat{S}_a(v_0, L) < S_a(v_0, L) < \hat{S}(v_0, L) < \min\Big(S_0(v_0, L), \frac{La}{2} + S_a(v_0, L)\Big). \tag{3.10}$$

Moreover, if v_0 and L satisfy $L \geq 4a(v_0)$, then $2\hat{S}_a(v_0, L) > \hat{S}(v_0, L)$.

Proof The inequality $\hat{S}_a < S_a$ is obvious. The other inequalities in (3.10) are proved in [17, Prop. 3.3]. So assume that $L > 4a$ and let us prove that $2\hat{S}_a > \hat{S}$. Notice that $S_a = \hat{S}_a + d(a)$ and $\hat{S} < \frac{La}{2} + S_a$, hence

$$\begin{aligned} 2\hat{S}_a - \hat{S} > 2\hat{S}_a - S_a - \frac{La}{2} &= \int_a^{L-a} \underbrace{\sqrt{\frac{\rho^2}{4} + v_0(\rho) - v_0^{\min}}}_{\geq \rho/2}\,\mathrm{d}\rho - \frac{La}{2} \\ &\geq \frac{L^2 - 4aL}{4} > 0. \end{aligned}$$

□

3.2.3 The one well approximate eigenfunction

Consider the single well operator

$$\mathcal{L}_h^{\mathrm{sw}} = (-\mathrm{i}h\nabla - \mathbf{A})^2 + \mathfrak{v}_0 \tag{3.11}$$

whose ground state energy is

$$\lambda(h) = \inf \sigma(\mathcal{L}_h). \tag{3.12}$$

Since $\mathfrak{v}_0 \leq 0$, $\mathcal{L}_h^{\mathrm{sw}}$ is smaller (in the sense of comparison of self-adjoint operators) than the Landau Hamiltonian $(-\mathrm{i}h\nabla - \mathbf{A})^2$. Hence we have by the min-max principle

$$\lambda(h) \leq h\,. \tag{3.13}$$

In light of the conditions on v_0 in (3.5), we know from [17, Thm. 2.1] that $\lambda(h)$ is a simple eigenvalue and that $\mathcal{L}_h^{\mathrm{sw}}$ has a positive radial ground state satisfying, for any relatively compact domain K of $\mathbb{R}^2$,

$$\mathfrak{u}_h(x) = u_h(|x|), \quad \int_{\mathbb{R}^2} |\mathfrak{u}_h(x)|^2\,\mathrm{d}x = 1, \quad \|e^{d(|x|)/h}\mathfrak{u}_h(x)\|_{H^2(K)} = \mathcal{O}(h^{-1/2}), \tag{3.14}$$

An important term in the context of tunneling is the hopping coefficient defined in [10, 17] (in the case $n = 2$) by

$$\mathfrak{c}_h(v_0, L) = \int_{D(0,a)} \mathfrak{v}_0(x)\mathfrak{u}_h(x)\mathfrak{u}_h(x_1 + L, x_2)\mathrm{e}^{\frac{\mathrm{i}Lx_2}{2h}}\,\mathrm{d}x \tag{3.15}$$

where $a = a(v_0)$ (see (3.6)).

As observed in [10], the hopping coefficient is a negative real number and an accurate estimate of it was established recently in [17, Sec. 4 & Eq. (4.32)], which we recall below.[4]

Proposition 3.2 *Assume that $\mathfrak{v}_0$ and L satisfy (3.5) and (3.7). Then there exists a positive constant $S(v_0, L)$ such that*

$$\lim_{h\searrow 0}\big(h \ln |\mathfrak{c}_h(v_0, L)|\big) = -S(v_0, L). \tag{3.16}$$

Moreover,

$$S_a(v_0, L) < S(v_0, L) < \hat{S}(v_0, L) \tag{3.17}$$

where $S_a(v_0, L)$ and $\hat{S}(v_0, L)$ are introduced in (3.9).

We shall use Proposition 3.2 later on in the proof of Proposition 3.5 when dealing with n potential wells ($n \geq 2$). Let us recall the definition of $S(v_0, L)$ given in [17, Eq. (4.25) and (4.26)]. We have

$$S(v_0, L) := -F(\mathfrak{v}_0) + \inf_{\substack{r\in[0,a]\\ t\in(0,+\infty)}} \Psi(r, t), \tag{3.18}$$

where $a = a(v_0)$ is introduced in (3.6) and, with d introduced in (3.8),

$$\left.\begin{aligned} F(v_0) &:= \frac{a}{4}\sqrt{a^2 + 4|v_0^{\min}|} + \frac{|v_0^{\min}|}{2}\ln\frac{\big(\sqrt{a^2+4|v_0^{\min}|}+a\big)^2}{4|v_0^{\min}|} - d(a),\\ \Psi(r,t) &:= d(r) + \frac{r^2+L^2}{4}(2t+1) + \frac{|v_0^{\min}|}{2}\ln\left(1+\frac{1}{t}\right) - Lr\sqrt{t(t+1)}. \end{aligned}\right\} \tag{3.19}$$

The following proposition deals with a term similar to the hopping coefficient and plays a key role in the approximation of various error terms that we will encounter later, e.g. when we verify Assumption 2.1 for an electro-magnetic Schrödinger operator with multiple wells, as in Proposition 3.4.

[4] Notice that the estimate of $\mathfrak{c}_h(v_0, L)$ does not require the assumption $L > 4\big(a(v_0) + \sqrt{v_0^{\min}}\big)$ imposed in [10] (see also [17, Theorem 1.4]).

Proposition 3.3 *We have, as $h \to 0$,*

$$w := \int_{D(0,L)} \mathfrak{u}_h(x)\mathfrak{u}_h(x_1 + L, x_2)\mathrm{e}^{\frac{\mathrm{i}Lx_2}{2h}}\,\mathrm{d}x = \mathcal{O}\left(\mathrm{e}^{\frac{-S_a+o(1)}{h}}\right),$$

where $a = a(v_0)$, $L > 2a$ and S_a is defined in (3.9b).

Proof We can estimate w in the same way as the hopping coefficient $\mathfrak{c}_h(\mathfrak{v}_0, L)$ was estimated in [17, Prop. 3.5].

The only difference is that in the expression of $\mathfrak{c}_h(v_0, L)$ (see (3.15)) we encounter the potential energy term v_0 in the integrand and the integral is consequently over the smaller disc $D(0, a)$. Hence the new term to estimate corresponds to w_2 below, w_3 being of the same type as w_1 after a symmetry.

We decompose the integral defining w into three terms

$$\begin{aligned}
w &= w_1 + w_2 + w_3\,,\\
w_1 &= \int_{D(0,a)} \mathfrak{u}_h(x)\mathfrak{u}_h(x_1 + L, x_2)\mathrm{e}^{\frac{\mathrm{i}Lx_2}{2h}}\,\mathrm{d}x\,,\\
w_2 &= \int_{D(0,L-a)\setminus D(0,a)} \mathfrak{u}_h(x)\mathfrak{u}_h(x_1 + L, x_2)\mathrm{e}^{\frac{\mathrm{i}Lx_2}{2h}}\,\mathrm{d}x\,,\\
w_3 &= \int_{D(0,L)\setminus D(0,L-a)} \mathfrak{u}_h(x)\mathfrak{u}_h(x_1 + L, x_2)\mathrm{e}^{\frac{\mathrm{i}Lx_2}{2h}}\,\mathrm{d}x\,.
\end{aligned}$$

Step 1: Contribution of the integral in $D(0, a)$. We express the integral defining w_1 in polar coordinates

$$w_1 = \int_0^{2\pi}\int_0^a u_h(r)u_h\big(\sqrt{r^2 + L^2 + 2Lr\cos\theta}\big)\mathrm{e}^{\frac{\mathrm{i}Lr\sin\theta}{2h}}\,r\,\mathrm{d}r. \tag{3.20}$$

In light of the decay property in (3.14), we get

$$w_1 = \mathcal{O}(h^{-1}\mathrm{e}^{-\tilde{S}/h}),$$

where

$$\tilde{S} = \inf_{0<\theta<2\pi}\left\{\inf_{0<r<a}\Big[d(r) + d(\sqrt{r^2 + L^2 + 2Lr\cos\theta})\Big]\right\}.$$

Since $\sqrt{r^2 + L^2 + 2Lr\cos\theta} > L - r$ and since $r \mapsto d(r)$ is non-decreasing,

$$\tilde{S} \geq \inf_{0<r<a}\big(d(r) + d(L - r)\big) = d(a) + d(L - a) = S_a$$

where S_a is introduced in (3.9b). Notice that the penultimate identity follows from the fact that

$$\frac{\mathrm{d}}{\mathrm{d}r}[d(r)+d(L-r)] = \sqrt{\frac{r^2}{4}+v_0(r)-v_0^{\min}} - \sqrt{\frac{(L-r)^2}{4}-v_0^{\min}} < 0 \quad (0<r<a).$$

Therefore, we have that

$$w_1 = \mathcal{O}(h^{-1}\mathrm{e}^{-S_a/h}). \tag{3.21}$$

Step 2: Contribution of the integral in $D(0,L)\setminus D(0,L-a)$**.** We argue as in Step 1. Expressing the integral defining w_3 in polar coordinates

$$w_3 = \int_0^{2\pi}\int_{L-a}^{L} u_h(r)u_h\big(\sqrt{r^2+L^2+2Lr\cos\theta}\big)\mathrm{e}^{\frac{\mathrm{i}Lr\sin\theta}{2h}}\, r\,\mathrm{d}r, \tag{3.22}$$

we get

$$w_3 = \mathcal{O}(h^{-1}\mathrm{e}^{-\tilde{S}'/h}),$$

where

$$\begin{aligned}\tilde{S}' &= \inf_{0<\theta<2\pi}\left(\inf_{L-a<r<L}\Big(d(r)+d\big(\sqrt{r^2+L^2+2Lr\cos\theta}\big)\Big)\right)\\ &\geq \inf_{L-a<r<L}\big(d(r)+d(L-r)\big) = \inf_{0<t<a}\big(d(t)+d(L-t)\big) = S_a.\end{aligned}$$

Therefore, we have that

$$w_3 = \mathcal{O}(h^{-1}\mathrm{e}^{-S_a/h}). \tag{3.23}$$

Step 3: Contribution of the integral in $D(0,L-a)\setminus D(0,a)$**.** We express the integral defining w_2 as follows

$$w_2 = \int_a^{L-a} u_h(r)\left(\int_0^{2\pi} K_h(r,\theta)d\theta\right) r\,\mathrm{d}r\,, \tag{3.24}$$

where

$$K_h(r,\theta) = u_h\left(\sqrt{r^2+L^2+2Lr\cos\theta}\right) e^{\frac{\mathrm{i}Lr\sin\theta}{2h}}\,.$$

Observing that for $a<r<L-a$, we have $a<L-r<L-a$ and

$$\rho := \sqrt{r^2+L^2+2Lr\cos\theta} \geq L-r > a,$$

so $u_h(\rho)$ has a nice integral representation [10, Eq. (2.9)]. Consequently, the integral of K_h with respect to θ is computed as in [10, Prop. 5.1]. In fact, we have (see [17, Eq. (3.23)-(3.24)])

$$\int_0^{2\pi} K_h(r,\theta)d\theta = C_h \exp\left(-\frac{r^2+L^2}{4h}\right)\int_0^{+\infty} G_h(r,t)\,\mathrm{d}t\,, \tag{3.25}$$

where

$$G_h(r,t) = \exp\left(-\frac{(r^2+L^2)t}{2h}\right) t^{\alpha-1}(1+t)^{-\alpha} I_0\left(\frac{Lr\sqrt{t(t+1)}}{h}\right), \tag{3.26}$$

C_h, α are constants and $z \mapsto I_0(z)$ is the modified Bessel's function of order 0 (see [17, Lem. 5.2]).

Let $\eta \in (0,1)$ and observe that [17, Lem. 4.1],

$$\begin{aligned}
&\int_a^{L-a} u_h(r)\Big(C_h \exp\Big(-\frac{r^2+L^2}{4h}\Big)\int_0^{\eta} G_h(r,t)dt\Big) r\,\mathrm{d}r\\
&= \mathcal{O}(\mathrm{e}^{c\sqrt{\eta}/h})\int_a^{L-a} u_h(r)u_h(\sqrt{L^2+r^2}) r\,\mathrm{d}r.
\end{aligned}$$

By the decay properties of u_h in (3.14), we get (using also (3.10) for the last estimate)

$$\begin{aligned}
\int_a^{L-a} u_h(r)\Big(C_h \exp\Big(-\frac{r^2+L^2}{4h}\Big)\int_0^{\eta} G_h(r,t)dt\Big) r\,\mathrm{d}r &= \mathcal{O}(\mathrm{e}^{(c\sqrt{\eta}-S_0)/h})\\
&= \mathcal{O}(\mathrm{e}^{-S_a/h}),
\end{aligned}$$

for sufficiently small η.

Now we deal with the following integral

$$\int_a^{L-a} u_h(r)\Big(C_h \exp\Big(-\frac{r^2+L^2}{4h}\Big)\int_{\eta}^{+\infty} G_h(r,t)dt\Big) r\,\mathrm{d}r,$$

which is asymptotically equivalent to [17, Lem. 4.4]

$$\frac{\mathfrak{m}(v_0)}{\sqrt{2\pi h}}\int_a^{L-a}\sqrt{r}\,a_0(r)\int_{\eta}^{+\infty} g_0(t)\exp\Big(-\frac{\Psi(r,t)-F(v_0)}{h}\Big)\,\mathrm{d}t\,\mathrm{d}r,$$

where $F(v_0)$, $\Psi(r,t)$ are introduced in (3.19) and $\mathfrak{m}(v_0)$, $g_0(t)$ are introduced in [17, Eq. (3.17) and (4.5)] as follows

$$\begin{aligned}
\mathfrak{m}(v_0) &= \frac{\sqrt{1+2v_0''(0)}}{2\pi}\sqrt{\frac{2a|v_0^{\min}|}{\pi}}\,\frac{\big(a^2+4|v_0^{\min}|\big)^{1/4}}{\sqrt{a^2+4|v_0^{\min}|}+a},\\
g_0(t) &= \frac{1}{t^{5/4}(t+1)^{1/4}}\left(1+\frac{1}{t}\right)^{\frac{1}{2}(\sqrt{1+2v_0''(0)}-1)},
\end{aligned}$$

and the function a_0 is defined as follows

$$a_0(r) = \frac{1}{2}\sqrt{\frac{1+2v_0''(0)}{\pi}}\exp\left(-\int_0^r \frac{1}{2}\frac{d''(\rho)}{d'(\rho)} + \frac{1}{2\rho} - \frac{\sqrt{1+2v_0''(0)}}{2d'(\rho)}d\rho\right).$$

Of importance to us is that

$$-F(\mathfrak{v}_0) + \inf_{(r,t)\in[a,L-a]\times\mathbb{R}_+} \Psi(r,t) \geq S_a,$$

which follows by the same argument as used in the proof of [17, Prop. 4.5]; for convenience, we provide details in Appendix A.

We get eventually

$$w_2 = \mathcal{O}(\mathrm{e}^{(-S_a+o(1))/h}). \tag{3.27}$$

With (3.21) and (3.23), this achieves the proof of the proposition. □

3.3 Verifying Assumption 2.1—superposition of single well potentials

We study the specific case where the potential V is given by

$$V(x) = \sum_{k=1}^{n} \mathfrak{v}_0(x - z_k)\,, \tag{3.28}$$

where $\mathfrak{v}_0$ is the non-positive radial function satisfying (3.5) and (we identify $\mathbb{C}$ and $\mathbb{R}^2$)

$$z_k := \frac{L}{\sqrt{2-2\cos(2\pi/n)}}\mathrm{e}^{2\mathrm{i}k\pi/n}, \quad L > 0. \tag{3.29}$$

The wells in this setting are the points $\{z_k\}_{1\leq k\leq n}$ which are selected so that

$$\mathrm{dist}(z_k, z_{k+1}) = L. \tag{3.30}$$

Let us verify that V satisfies (3.2c). Our construction of the points z_k is such that $z_{k+1} = gz_k$, for $k \in \mathbb{Z}/n\mathbb{Z}$. Since $\mathfrak{v}_0$ is radial, we have

$$\mathfrak{v}_0(g^{-1}x - z_k) = v_0(|g^{-1}(x - gz_k)|) = \mathfrak{v}_0(x - z_{k+1}).$$

Consequently, (3.2c) holds and T_h commutes with $M(g)$. We still have to check that Assumption 2.1 holds with the choice in Assumption 2.8 (3).

We introduce the functions

$$u_{h,k}(x) = \chi(x - z_k)\mathfrak{u}_h(x - z_k)\mathrm{e}^{-\mathrm{i}z_k\cdot\mathbf{A}(x)/h} \quad (1 \leq k \leq n), \tag{3.31}$$

where

- $(z_k)_{1\le k\le n}$ are the points introduced in (3.29);
- $\mathbf{A}$ is the vector field introduced in (3.1);
- $\chi \in C_c^\infty(\mathbb{R}^2;[0,1])$ is a radial cut-off function satisfying $\chi = 1$ on $D(0,L)$ and $\operatorname{supp}\chi \subset D(0,L+\eta)$ with $\eta \in (0,1)$ fixed arbitrarily.

The phase term in (3.31) is due to the effect of *magnetic* translation, which ensures that $\psi_{h,k}(x) = \mathfrak{u}_h(x-z_k)\mathrm{e}^{-\mathrm{i}z_k\cdot\mathbf{A}(x)/h}$ satisfies

$$\mathcal{L}^{\mathrm{sw}}_{h,k}\psi_{h,k} = \lambda(h)\psi_{h,k} \quad \text{where} \quad \mathcal{L}^{\mathrm{sw}}_{h,k} := (-\mathrm{i}h\nabla - \mathbf{A})^2 + \mathfrak{v}_0(\cdot - z_k). \tag{3.32}$$

The above constructions ensures that Assumption 2.8 (3) holds (since $z\cdot\mathbf{A}(g_n^{-1}x) = (g_n z)\cdot\mathbf{A}(x)$). Moreover, the next proposition shows that Assumption 2.1 holds too.

Proposition 3.4 *Let T_h and $\lambda(h)$ be as in (3.4) and (3.12) respectively. The conditions in Assumption 2.1 hold with the following choices:*

(a) $\{u_{h,1},\ldots,u_{h,n}\}$ *are as in (3.31);*
(b) *any constants* $\mathfrak{S}_1, \mathfrak{S}_2, \mathfrak{S}_3, p$ *satisfying*

$$\mathfrak{S}_1 \in (0,\hat{S}_a), \quad \mathfrak{S}_2 \in (0,2\hat{S}_a), \quad \mathfrak{S}_3 \in (0,\hat{S}_a), \quad p \in (0,1], \tag{3.33}$$

where $\hat{S}_a$ is introduced in (3.9).

Proof **Step 1.** We have by (3.31) and (3.32),

$$r_{h,k} := T_h u_{h,k} = \Big(-h^2(\Delta\chi_k) + 2\mathrm{i}h(\nabla\chi_k)\cdot(-\mathrm{i}h\nabla - \mathbf{A}) + \chi_k\sum_{i\ne k}\mathfrak{v}_0(x-z_i)\Big)\psi_{h,k}, \tag{3.34}$$

where $\chi_k(x) = \chi(x-z_k)$.

Since $r_{h,k}$ is supported in $D(z_k, L+\eta)\setminus D(z_k, L-a)$, we get by using (3.14) and the decay of the ground state $\mathfrak{u}_h$ that

$$\|r_{h,k}\| = \mathcal{O}(h^{-1/2}\mathrm{e}^{-\hat{S}_a/h}). \tag{3.35}$$

Step 2. We have

$$\|u_{h,k}\|^2 = \|\mathfrak{u}_h\|^2 - \int_{\mathbb{R}^2}(1-\chi^2)|\mathfrak{u}_h|^2\,\mathrm{d}x.$$

Since $1-\chi^2$ is supported in $\mathbb{R}^2\setminus D(0,L)$, we get by the decay of $\mathfrak{u}_h$ that

$$\|u_{h,k}\|^2 = 1 + \mathcal{O}(h^{-1}\mathrm{e}^{-2S_0/h})$$

where S_0 is introduced in (3.9a).

Let us now consider $i \ne j$. We first inspect the case where $|z_i - z_j| = L$, which occurs only if $j = i \pm 1$. By a change of variable, we check that (thanks to the invariance by rotation)

$$\langle u_{h,i}, u_{h,j}\rangle = \begin{cases} \langle u_{h,1}, u_{h,2}\rangle & \text{if } j = i+1 \\ \overline{\langle u_{h,1}, u_{h,2}\rangle} & \text{if } j = i-1. \end{cases}$$

By (3.31), the function $u_{h,1}\overline{u_{h,2}}$ is supported in $D(z_1, L+\eta) \cap D(z_2, L+\eta)$. Then, we perform the following decomposition

$$\langle u_{h,1}, u_{h,2}\rangle = \mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3$$

where,

$$\begin{aligned}
\mathcal{E}_1 &:= \int_{D(z_1,L)} \mathrm{u}_h(x-z_1)\mathrm{u}_h(x-z_2)\mathrm{e}^{-\mathrm{i}(z_1-z_2)\cdot\mathbf{A}(x)}\,\mathrm{d}x,\\
\mathcal{E}_2 &:= -\int_{|x-z_1|<L} (1-\chi(x-z_2))\mathrm{u}_h(x-z_1)\mathrm{u}_h(x-z_2)\mathrm{e}^{-\mathrm{i}(z_1-z_2)\cdot\mathbf{A}(x)}\,\mathrm{d}x\\
&= \mathcal{O}(h^{-1/2}\mathrm{e}^{-S_0/h})\\
\mathcal{E}_3 &:= \int_{\substack{L<|x-z_1|<L+\eta\\ 0<|x-z_2|<L+\eta}} u_{h,1}(x)\overline{u_{h,2}(x)}\,\mathrm{d}x = \mathcal{O}(h^{-1/2}\mathrm{e}^{-S_0/h}).
\end{aligned}$$

In fact, in $D(z_1, L) \cap D(z_2, L+\eta)$, we have

$$u_{h,1}(x)\overline{u_{h,2}(x)} = \chi(x-z_2)\mathrm{u}_h(x-z_1)\mathrm{u}_h(x-z_2)\mathrm{e}^{-\mathrm{i}(z_1-z_2)\cdot\mathbf{A}(x)},$$

with u_h a radial function. By a change of variable (the translation $x \mapsto x - z_1$ followed by the rotation by the angle α defined by $z_1 - z_2 = |z_1 - z_2|\mathrm{e}^{\mathrm{i}\alpha}$), we get

$$|\mathcal{E}_1| = \left|\int_{D(0,L)} \mathrm{u}_h(x)\mathrm{u}_h(x_1+L, x_2)\mathrm{e}^{\frac{\mathrm{i}Lx_2}{2h}}\,\mathrm{d}x\right|,$$

and by Proposition 3.3, we get

$$\mathcal{E}_1 = \mathcal{O}(h^{-1/2}\mathrm{e}^{-(S_a+o(1))/h}) + \mathcal{O}(h^{-1/2}\mathrm{e}^{-S_0/h}) = \mathcal{O}(\mathrm{e}^{-\hat{S}_a/h}),$$

where in the last step we used the inequalities $\hat{S}_a < S_a < S_0$ from Proposition 3.1.

If $|z_i - z_j| \neq L$, then $\langle u_{h,i}\,,\,u_{h,j}\rangle = \mathcal{O}(h^{-1/2}\mathrm{e}^{-(S_a+o(1))/h}) + \mathcal{O}(h^{-1/2}\mathrm{e}^{-S_0/h})$ by a similar argument.

Step 3. Let us now estimate $\lambda_{n+1}(h)$ from below. Consider a partition of unity on $\mathbb{R}^2$, $\sum_{k=0}^{n}\zeta_k^2 = 1$, where

$$\text{for } 1 \le k \le n, \quad \zeta_k = 1 \text{ on } D\left(z_k, \frac{L}{2}\right), \quad \operatorname{supp}\zeta_k \subset D(z_k, L-a),$$

and

$$\operatorname{supp}\zeta_0 \subset \Omega_0 := \mathbb{R}^2 \setminus \bigcup_{k=1}^{n} D\left(z_k, \frac{L}{2}\right).$$

Then, we have,

$$\mathfrak{v}_0(x - z_i)\zeta_k(x) = 0 \text{ for } i \neq k\,,\ 1 \leq k \leq n\,,$$

and

$$\mathfrak{v}_0(x - z_i)\zeta_0(x) = 0 \text{ for } 1 \leq i \leq n\,.$$

Pick a function f in the domain of $\mathcal{L}_h$. We have the decomposition formula

$$\begin{aligned}\langle T_h f, f\rangle \ &= \sum_{k=1}^{n} \langle \mathcal{L}_h^{\mathrm{sw}}(\zeta_k f_h), \zeta_k f_h\rangle + \langle(-\mathrm{i}h\nabla - \mathbf{A})^2(\zeta_0 f_h), \zeta_0 f_h\rangle \\ &\quad -h^2 \sum_{k=0}^{n} \||\nabla\zeta_k| f_h\|^2 - \lambda(h).\end{aligned}$$

By the min-max principle, we have

$$\forall j \geq 1, \quad \lambda_j(h) \geq \lambda_j\Big((-\mathrm{i}h\nabla - \mathbf{A})^2 \bigoplus \oplus_{k=1}^{n} \mathcal{L}_h^{\mathrm{sw}}\Big) - \lambda(h) - M_0 n h^2,$$

where

$$M_0 = \max_{0 \leq k \leq n} \|\nabla\zeta_k\|_\infty^2.$$

Finally, we use the well known asymptotics (see [17, Prop. A.1])

$$\lambda(h) = \lambda_1(\mathcal{L}_h^{\mathrm{sw}}) = v_0^{\min} + E_1 h + \mathcal{O}(h^{3/2}), \quad \lambda_2(\mathcal{L}_h^{\mathrm{sw}}) = v_0^{\min} + E_2 h + \mathcal{O}(h^{3/2}),$$

where $E_1 = \sqrt{1 + 2v_0''(0)}$ and $E_2 > E_1$, and we conclude that

$$\lambda_{n+1}(h) \geq (E_2 - E_1)h + \mathcal{O}(h^{3/2}).$$

$\square$

The next proposition allows us to verify Assumption 2.11.

Proposition 3.5 *With $J_0(h) = \langle T_h u_{h,1}, u_{h,1}\rangle$ and $J_1(h) = \langle T_h u_{h,1}, u_{h,2}\rangle$ we have*

$$J_0(h) = \mathcal{O}(h^{-1} \mathrm{e}^{-2\hat{S}_a(v_0, L)/h})$$

and

$$J_1(h) = \mathrm{e}^{-\mathrm{i}\phi_n/2h}\mathfrak{c}_h(v_0, L) + \mathcal{O}(h^{-1}\mathrm{e}^{-S_0(v_0,L)/h}),$$

where $\mathfrak{c}_h(v_0, L)$ *is the hopping coefficient introduced in (3.15),* $\hat{S}_a(v_0, L)$ *and* $S_0(v_0, L)$ *are introduced in (3.9) and*

$$\phi_n = -\frac{L^2\sin(2\pi/n)}{2-2\cos(2\pi/n)}.$$

Moreover,

$$h\ln|J_1(h)| \underset{h\searrow 0}{\sim} -S(v_0, L),$$

where $S(v_0, L)$ *is introduced in (3.18).*

Proof From (3.34), we have

$$\begin{aligned} J_0(h) = \langle(\mathcal{L}_h - \lambda(h))u_{h,1}, u_{h,1}\rangle &= \int_{L-a\le|x-z_1|\le L+\eta} r_{h,1}(x)\overline{u_{h,1}(x)}\,\mathrm{d}x \\ &= \mathcal{O}(h^{-1}\mathrm{e}^{-2\hat{S}_a/h}). \end{aligned}$$

We now move to estimate $J_1(h)$. First let us recall that the symmetry relations in Assumption 2.8 (3) imply that $u_{h,1} = M(g)u_{h,n}$ and[5]

$$J_1(h) = \langle T_h u_{h,1}, u_{h,2}\rangle = \langle T_h u_{h,n}, u_{h,1}\rangle = \overline{\langle T_h u_{h,1}, u_{h,n}\rangle}.$$

Similarly to the previous estimate of $J_0(h)$, by (3.32) and (3.34) we have

$$J_1(h) = J_1^{\mathrm{app}}(h) + \mathcal{O}(h^{-1}\mathrm{e}^{-S_0/h}),$$

where

$$J_1^{\mathrm{app}}(h) = \int_{D(z_n,a)} \mathfrak{v}_0(x-z_n)\mathfrak{u}_h(x-z_1)\mathfrak{u}_h(x-z_n)\mathrm{e}^{-\mathrm{i}(z_n-z_1)\cdot\mathbf{A}(x)/h}\,\mathrm{d}x.$$

Notice that $(z_n - z_1)\cdot\mathbf{A}(x) = (z_n - z_1)\cdot\mathbf{A}(x - z_n + z_1)$. By a translation, we get

$$J_1^{\mathrm{app}}(h) = \mathrm{e}^{-\mathrm{i}(z_n-z_1)\cdot\mathbf{A}(z_1)/h}\int_{D(0,a)} \mathfrak{v}_0(y)\mathfrak{u}_h(y+z_n-z_1)\mathfrak{u}_h(y)\mathrm{e}^{-\mathrm{i}(z_n-z_1)\cdot\mathbf{A}(y)/h}\,\mathrm{d}y.$$

With $\ell_n = \frac{L}{\sqrt{2-2\cos(2\pi/n)}}$, we have $z_n = (\ell_n, 0)$ and $z_1 = \big(\ell_n\cos(2\pi/n), \ell_n \sin(2\pi/n)\big)$. Hence

$$(z_n - z_1)\cdot\mathbf{A}(z_1) = z_n\cdot\mathbf{A}(z_1) = \frac{\phi_n}{2}.$$

[5] This formulation will be helpful since z_n lies on the x-axis.

Observing that $|z_n - z_1| = L$, we write $z_n - z_1 = L\mathrm{e}^{\mathrm{i}\beta_n}$ where $\beta_n \in (0, \pi]$. We denote by R_{β_n} the rotation by β_n around the origin. Noticing that

$$u \cdot \mathbf{A}(R_{\beta_n} v) = (R_{\beta_n}^{-1} u) \cdot \mathbf{A}(u) \quad (u, v \in \mathbb{R}^2),$$

we get that

$$(z_n - z_1) \cdot \mathbf{A}(R_{\beta_n} x) = \begin{pmatrix} L \\ 0 \end{pmatrix} \cdot \begin{pmatrix} -x_2/2 \\ x_1/2 \end{pmatrix} = -\frac{L x_2}{2}.$$

The change of variable $y \mapsto x = R_{\beta_n}^{-1} y$ yields

$$J_1^{\mathrm{app}}(h) = \mathrm{e}^{-\mathrm{i}\phi_n/2h} \int_{D(0,a)} \mathfrak{v}_0(x) \mathfrak{u}_h(x_1 + L, x_2) \mathfrak{u}_h(x) \mathrm{e}^{\mathrm{i}L x_2/h} \, \mathrm{d}y$$

where we used that the functions $\mathfrak{v}_0, \mathfrak{u}_h$ are radial and that

$$|R_{\beta_n} x + z_n - z_1| = |x + R_{\beta_n}^{-1}(z_n - z_1)| = |(x_1 + L, x_2)|.$$

Now we have that $\mathrm{e}^{-\mathrm{i}\phi_n/2h} J_1^{\mathrm{app}}(h) = \mathfrak{c}_h(v_0, L)$ and by Proposition 3.2

$$h \ln |J_1^{\mathrm{app}}(h)| \underset{h \searrow 0}{\sim} -S(v_0, L).$$

The same asymptotics holds for $|J_1(h)|$ because $S_0(v_0, L) > S(v_0, L)$. $\square$

From now on, we work under the following assumption on (v_0, L).

Assumption 3.6 With $a = a(v_0)$ introduced introduced in (3.6) and $L > 2a$, the function v_0 satisfies $2\hat{S}_a(v_0, L) > S(v_0, L)$, where $\hat{S}_a(v_0, L)$ and $S(v_0, L)$ are introduced in (3.9) and (3.18) respectively.

Remark 3.7 By Proposition 3.1, Assumption 3.6 holds if $L \geq 4a(v_0)$.

We fix the choice of $\mathfrak{S}_1, \mathfrak{S}_2, \mathfrak{S}_3$ as in (3.33) but with the additional condition that

$$S(v_0, L) < 2 \min_{1 \leq j \leq 3} \mathfrak{S}_j.$$

This is possible under Assumption 3.6 since $S(v_0, L) < 2\hat{S}_a(v_0, L)$. Therefore, (2.22) holds with $S = S(v_0, L)$ and Proposition 3.5 ensures that the other conditions in Assumption 2.11 hold too[6].

[6] This is explicitly done for $n = 2, 3$ and can be easily justified for $n \geq 4$.

3.4 The case $n = 2$: Double wells

We choose here V to be the *double well* potential defined by (3.28) for $n = 2$. We therefore have two wells

$$z_1 = \Big(-\frac{L}{2}, 0\Big), \quad z_2 = \Big(\frac{L}{2}, 0\Big), \quad L > 2a > 0. \tag{3.36}$$

A straightforward application of (2.26), Propositions 3.4 and 3.5 (and Section 2.4.2) yields the following.

Theorem 3.8 *Assuming the conditions in (3.5) and in Assumption 3.6 are fulfilled, then the following asymptotics holds,*

$$h \ln\big(\lambda_2(h) - \lambda_1(h)\big) \underset{h \searrow 0}{\sim} -S(v_0, L), \tag{3.37}$$

where $S(v_0, L)$ is the constant introduced in (3.18).

3.4.1 Discussion

Let us introduce the following classes[7] of admissible (v_0, L), where v_0 satisfies the conditions in (3.5), and

$$\begin{aligned}
\mathscr{A} &= \{(v_0, L) \;:\; L > 2a(v_0) \text{ and } (3.37) \text{ holds}\},\\
\mathscr{A}^{\mathrm{FSW}} &= \{(v_0, L) \;:\; L > 4(a(v_0) + \sqrt{|v_0^{\min}|})\},\\
\overline{\mathscr{A}}^{\mathrm{HKS}} &= \{(v_0, L) \;:\; v_0 \text{ satisfies Assumption } 3.6\}\\
\underline{\mathscr{A}}^{\mathrm{HKS}} &= \{(v_0, L) \;:\; L \geq 4a(v_0)\}.
\end{aligned}$$

By Proposition 3.1, we have

$$\underline{\mathscr{A}}^{\mathrm{HKS}} \subset \overline{\mathscr{A}}^{\mathrm{HKS}}$$

and by Theorem 3.8

$$\overline{\mathscr{A}}^{\mathrm{HKS}} \subset \mathscr{A}.$$

The earlier results in [10, 17] yield that

$$\mathscr{A}^{\mathrm{FSW}} \subset \mathscr{A}.$$

However, our results are much stronger since $\mathscr{A}^{\mathrm{FSW}}$ is a proper subset of $\underline{\mathscr{A}}^{\mathrm{HKS}}$.

[7] $\mathscr{A}^{\mathrm{FSW}}$ is the admissible class introduced by Fefferman-Shapiro-Weinstein and HKS refers to the admissible classes introduced in this paper.

3.4.2 Proof of Theorem 1.2

In light of (3.3), it suffices to apply Theorem 3.8 with the effective semi-classical parameter $\hbar = b^{-1}h$ and the effective potential defined by $b^{-2}v_0$. We then obtain $\mathscr{E}_{b,L}(v_0) = bS(b^{-2}v_0, L)$.

3.5 The case $n = 3$: Three wells and flux effects

Let us assume that $n = 3$ so that V defined by (3.28) is a potential with three wells

$$z_1 = \frac{L}{2\sqrt{3}}(-1, \sqrt{3}), \quad z_2 = \frac{L}{2\sqrt{3}}(-1, -\sqrt{3}), \quad z_3 = \frac{L}{\sqrt{3}}(1, 0),$$

which are located on the vertices of an equilateral triangle with side length L and let $D \subset \mathbb{R}^2$ be its interior. The area of D is then $\frac{\sqrt{3}}{4}L^2$. The flux of the magnetic field in D is

$$\Phi := \frac{1}{2\pi}\int_D \operatorname{curl} \mathbf{A}\, \mathrm{d}x = \frac{\sqrt{3}L^2}{8\pi}. \tag{3.38}$$

By Proposition 3.5, we have and

$$J_0(h) = \mathcal{O}(\mathrm{e}^{-2\hat{S}_a/h}) \text{ with } S(\mathfrak{v}_0, L) < 2\hat{S}_a\,.$$

and

$$|J_1(h)| \underset{h\searrow 0}{\sim} |\mathfrak{c}_h(v_0, L)| = \exp\left(-\frac{S(\mathfrak{v}_0, L) + o(1)}{h}\right).$$

Recall that it was proved in [10] that $\mathfrak{c}_h(v_0, L)$ is a negative real number. So we infer from Proposition 3.5,

$$\mathrm{e}^{-2\pi\mathrm{i}\Phi/h} J_1(h) \underset{h\searrow 0}{\sim} \mathfrak{c}_h(v_0, L) \quad \text{and} \quad \mathfrak{c}_h(v_0, L) \underset{h\searrow 0}{\sim} -|J_1(h)|.$$

Therefore, we conclude that

$$J_1(h) \underset{h\searrow 0}{\sim} -|J_1(h)|\mathrm{e}^{2\pi\mathrm{i}\Phi/h} = |J_1(h)|\mathrm{e}^{2\pi\mathrm{i}\Phi/h + \mathrm{i}\pi}, \quad |J_1(h)| \underset{h\searrow 0}{=} \exp\left(-\frac{S(\mathfrak{v}_0, L) + o(1)}{h}\right).$$

Recall that by (2.27),

$$I_1(h) \underset{h\searrow 0}{\sim} J_1(h), \tag{3.39}$$

and that $I_1(h) = |I_1(h)|\mathrm{e}^{\mathrm{i}\theta(h)}$, with $\theta(h) \in [0, 2\pi)$. It results from (3.39) that $|I_1(h)| \sim |J_1(h)|$, and also

$$\mathrm{e}^{\mathrm{i}\theta(h) - 2\pi\mathrm{i}\Phi/h - \mathrm{i}\pi} \sim 1. \tag{3.40}$$

If for a given constant $c_0 \in (0,1)$ we introduce the set

$$\mathcal{N}(c_0) = \left\{ h \in (0,1],\ \operatorname{dist}\left(\frac{\Phi}{h} + \frac{1}{2}, \mathbb{Z}\right) \geq c_0 \right\}, \tag{3.41}$$

then

$$\forall h \in \mathcal{N}(c_0), \quad 0 < c_0 \leq \frac{\Phi}{h} + \frac{1}{2} - \left\lfloor \frac{\Phi}{h} + \frac{1}{2} \right\rfloor \leq 1 - c_0 < 1,$$

and it results from (3.40) that (since $\theta(h) \in [0, 2\pi)$ in the definition of $I_1(h)$)

$$\theta(h) \underset{\substack{h \searrow 0 \\ h \in \mathcal{N}(c_0)}}{=} 2\pi \left(\frac{\Phi}{h} + \frac{1}{2} - \left\lfloor \frac{\Phi}{h} + \frac{1}{2} \right\rfloor \right) + o(1). \tag{3.42}$$

Now by paragraph 2.4.3 we get crossing of eigenvalues quantified via the following functions

$$\begin{aligned} \mathsf{a}(x) &= \cos\left(x + \frac{2\pi}{3}\right) - \cos(x), \\ \mathsf{b}(x) &= \cos\left(x + \frac{4\pi}{3}\right) - \cos\left(x + \frac{2\pi}{3}\right). \end{aligned} \tag{3.43}$$

Theorem 3.9 *Assume that the conditions in (3.5) are fulfilled and that V is defined by (3.28) with $n = 3$. If Assumption 3.6 holds, then there is a relabeling $\mu_1(h), \mu_2(h), \mu_3(h)$ of the eigenvalues $\lambda_1(h), \lambda_2(h), \lambda_3(h)$ of the electro-magnetic Schrödinger operator $\mathcal{L}_h$ such that the asymptotics*

$$\begin{aligned} \mu_2(h) - \mu_1(h) &\underset{h \searrow 0}{=} \big(\mathsf{a}(\Phi/h) + o(1)\big) \exp\left(\frac{-S(v_0, L) + o(1)}{h}\right) \\ \mu_3(h) - \mu_2(h) &\underset{h \searrow 0}{=} \big(\mathsf{b}(\Phi/h) + o(1)\big) \exp\left(\frac{-S(v_0, L) + o(1)}{h}\right) \end{aligned} \tag{3.44}$$

hold for all $L > 2a(v_0)$.

Moreover, there exists a sequence $\big(h_1(k), h_2(k), h_3(k)\big)_{k \geq k_0}$ which converges to 0 such that, for all $k \geq k_0$ we have

$$0 < h_1(k+1) < h_3(k) < h_2(k) < h_1(k) < 1$$

and

$$\mu_1\big(h_1(k)\big) = \mu_3\big(h_1(k)\big),\ \mu_1\big(h_2(k)\big) = \mu_2\big(h_2(k)\big),\ \mu_2\big(h_3(k)\big) = \mu_3\big(h_3(k)\big).$$

Proof To get the asymptotics in (3.44), we use the computations in Paragraph 2.4.3 and (3.39). Then we approximate $|J_1(h)|$ by Proposition 3.5.

As indicated in (3.42), the function $h \mapsto \theta(h)$ will not be continuous on any open right neighborhood of 0, since, as h decreases towards 0, it will necessarily make infinite many jumps of size 2π. Given $\epsilon > 0$ we can, however, avoid the jumps by restricting θ to the union of an infinite number of small disjoint intervals $\mathcal{I}_k$, $k \in \mathbb{N}$, with the right endpoint of $\mathcal{I}_{k+1}$ is less than the left endpoint of $\mathcal{I}_k$, and moreover such that θ maps each such interval continuously *onto* the interval $(\epsilon, 2\pi - \epsilon)$. This follows from (3.40) and the fact that $h \mapsto I_1(h)$ is continuous. In each interval $\mathcal{I}_k$ we can find $h_1(k)$, $h_2(k)$ and $h_3(k)$ such that

$$\theta(h_1(k)) = \frac{\pi}{3}, \quad \theta(h_2(k)) = \frac{2\pi}{3}, \quad \theta(h_3(k)) = \pi.$$

In fact, since $h \mapsto \Phi/h + 1/2$ is strictly monotone and since $\pi/3$, $2\pi/3$ and π are well separated, we can, eventually by starting our counting on a larger k (which means that we consider smaller h), impose that $h_1(k) > h_2(k) > h_3(k)$ holds. We conclude that we get the eigenvalue crossings as indicated in Paragraph 2.4.3. $\square$

4 Smoothed triangles and Neumann boundary condition

4.1 Introduction

4.1.1 Geometric setting

In this section, Ω is a bounded open set of $\mathbb{R}^2$ with C^∞ boundary Γ. The Hilbert space is $H = L^2(\Omega)$ and we will assume (see below for the invariance assumption) that we are in the situation considered in Remark 2.7.

We assume that Γ is a simple curve and denote its length by $|\Gamma| = 2L$. Let $\mathbb{R}/2L\mathbb{Z} \ni s \mapsto \gamma(s)$ be the arc-length parameterization of Γ such that the unit tangent vector $\tau(s) := \dot\gamma(s)$ turns counterclockwise. Let us denote by k the curvature along Γ defined as follows

$$\ddot\gamma(s) = k(s)\nu(s)$$

where $\nu(s)$ is the unit normal to Γ at $\gamma(s)$ pointing inward Ω.

Definition 4.1 We introduce the maximal curvature along Γ as follows

$$k_{\max} = \max_{s\in\mathbb{R}/2L\mathbb{Z}} k(s) \tag{4.1}$$

and call a point $z_0 \in \Gamma$ a *curvature well* if $z_0 = \gamma(s_0)$ and $k(s_0) = k_{\max}$. The point z_0 is said to be a non-degenerate curvature well if furthermore $k''(s_0) < 0$. We denote by Γ_0 the set of curvature wells.

Consider a positive integer n and the rotation by $2\pi/n$ denoted by g_n. We assume that

$$\Omega \text{ is invariant by the rotation } g_n \tag{4.2a}$$

and that we have n non-degenerate curvature wells

$$\Gamma_0 = \{z_1 = \gamma(s_1), \cdots, z_n = \gamma(s_n)\} \tag{4.2b}$$

with[8]

$$s_j = (j-1)\frac{2L}{n}, \quad k''(s_j) < 0 \quad (1 \le j \le n). \tag{4.2c}$$

The symmetry assumption yields that

$$z_{j+1} = g_n z_j \quad (1 \le j \le n-1). \tag{4.2d}$$

and

$$\gamma\left(s + \frac{2L}{n}\right) = g_n \gamma(s), \quad k\left(s + \frac{2L}{n}\right) = k(s) \quad (s \in \mathbb{R}/2\pi\mathbb{Z}). \tag{4.2e}$$

4.1.2 The magnetic Neumann Laplacian

We are interested in the magnetic Neumann Laplacian $\mathscr{L}_h^N = (-\mathrm{i}h\nabla - \mathbf{A})^2$, in the Hilbert space $L^2(\Omega)$, where the magnetic field $B = \operatorname{curl}\mathbf{A} = 1$ is uniform[9] and generated by the magnetic potential $\mathbf{A}$ introduced in (3.1). The operator $\mathscr{L}_h^N$ acts on functions $u \in H^2(\Omega)$ satisfying the (magnetic) Neumann condition

$$\nu \cdot (-\mathrm{i}h\nabla - \mathbf{A})u|_\Gamma = 0.$$

The case of double curvature wells corresponding to $n = 2$ was treated in [6], where the symmetry was generated by the reflection $\tilde{g}_2$ (see Remark 2.9). Here we focus on the case with $n \ge 3$ curvature wells and where the symmetry is generated by a rotation. When $n = 3$, a typical example is the smoothed triangle (Fig. 2). When Ω is an equilateral triangle the heuristic discussion is given in [11] but no rigorous result can be given since the authors were unable to have a sufficiently accurate control of the tunneling. Numerically, this has been computed in [4] which in particular gives the enlightening picture predicting eigenvalue crossings (Fig. 4). We refer to [5, Sec. 5] for rigorous analysis in the case of polygons and to [27] for a comprehensive study of the magnetic Laplacian.

The investigation of $\mathscr{L}_h^N$ can be connected with Section 2 after shifting by a constant $\ell(h)$ and taking the operator T_h as follows

$$T_h = \mathscr{L}_h^N - \ell(h). \tag{4.3}$$

The shift constant $\ell(h)$ will be defined by the ground state energy of an operator with a single curvature well.

8 We identify $\mathbb{R}/2L\mathbb{Z}$ and $[0, 2L)$.

9 We can handle any magnetic field intensity $b > 0$ by a change of semi-classical parameter.

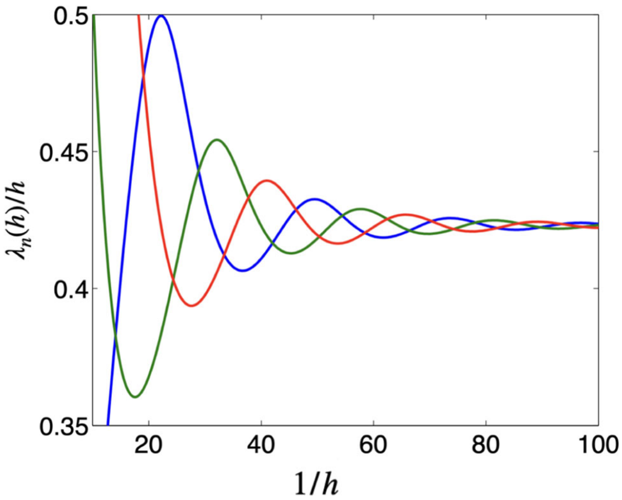

Fig. 4 Eigenvalue crossings in an equilateral triangle

Two constants are important in our analysis. First we meet a magnetic flux like term that controls the eigenvalue crossings and is defined by

$$\Phi_0 = |\Omega| - |\Gamma|\xi_0 = |\Omega| - 2L\xi_0, \tag{4.4a}$$

Secondly the following constant controls the strength of the tunneling and is defined by

$$\mathsf{S}_n = \sqrt{\frac{2C_1}{(\mu_1^N)''(\xi_0)}} \int_0^{2L/n} \sqrt{k_{\max} - k(s)}\, \mathrm{d}s. \tag{4.4b}$$

The definition of Φ_0 and S_n involves universal constants related to the de Gennes model. We recall that, for $\xi \in \mathbb{R}$, $\mu_1^N(\xi)$ denotes the lowest eigenvalue of the Neumann realization of the Harmonic oscillator on the semi-axis $\mathbb{R}_+$:

$$\mathfrak{h}^N[\xi] = -\frac{d^2}{d\tau^2} + (\xi + \tau)^2 \tag{4.5a}$$

Minimizing over $\xi \in \mathbb{R}$ we get the de Gennes constant

$$\Theta_0 = \inf_{\xi \in \mathbb{R}} \mu_1^N(\xi) = \mu_1^N(\xi_0), \text{ where } \xi_0 = -\sqrt{\Theta_0}\,. \tag{4.5b}$$

Denoting by u_0 the positive L^2- normalized ground state of $\mathfrak{h}^N[\xi_0]$, the constant C_1 appearing in (4.4b) is defined by

$$C_1 = \frac{|u_0(0)|^2}{3}\,. \tag{4.5c}$$

4.2 Reduction to tubular domain

In a tubular neighborhood of the boundary, we can work with adapted coordinates $(s, t) \in \mathbb{R}/2L\mathbb{Z} \times \mathbb{R}_+$ that are linked to Cartesian coordinates as follows

$$(x_1, x_2) = \mathscr{T}(s, t) := \gamma(s) - t\nu(s). \tag{4.6}$$

There exists a geometric constant $\varepsilon_0 > 0$ such that the above transformation is invertible when $0 < t < \varepsilon_0$; the image of Φ is the tubular neighborhood of Γ

$$\Gamma(\varepsilon_0) = \{x \in \Omega \ : \ \mathrm{dist}(x, \partial\Omega) < \varepsilon_0\} \tag{4.7}$$

and for $x \in \Gamma(\varepsilon_0)$, $(s, t) = \mathscr{T}^{-1}(x)$ means that s is the arc-length coordinate of the projection of x on Γ and t is the normal distance from x to Γ. We will refer to s as the tangential variable and to t as the normal variable.

Let us understand the action of the operator in (2.14) in these adapted coordinates. Let u be supported in $\Gamma(\varepsilon_0)$ and $v = M(g)u$. Then by (4.2e), $\tilde{v}(s, t) = v \circ \mathscr{T}$ satisfies

$$\tilde{v}(s, t) = \tilde{u}\left(s - \frac{2L}{n}, t\right), \quad \tilde{u} = u \circ \mathscr{T}. \tag{4.8}$$

The Hilbert space $L^2(\Gamma(\varepsilon_0))$ is transformed to the weighted space

$$L^2\big((\mathbb{R}/2L\mathbb{Z}) \times (0, \varepsilon_0); a\,\mathrm{d}s\,\mathrm{d}t\big), \quad a(s, t) = 1 - tk(s).$$

After a gauge transformation to eliminate the normal component of $\mathbf{A}$, see [11, App. F], the action of the operator $\mathscr{L}_h^N$ is transformed into

$$\begin{aligned} \tilde{\mathscr{L}}_h := -h^2 a^{-1}\partial_t a \partial_t + a^{-1}\left(-\mathrm{i}h\partial_s + \gamma_0 - t + \frac{k(s)}{2}t^2\right) \\ \times a^{-1}\left(-\mathrm{i}h\partial_s + \gamma_0 - t + \frac{k(s)}{2}t^2\right) \end{aligned}$$

where

$$\gamma_0 = \frac{|\Omega|}{2L} = \frac{\pi}{L}\Phi \tag{4.9}$$

and

$$\Phi = \frac{1}{2\pi}\int_\Omega B\,\mathrm{d}x \text{ is the magnetic flux in } \Omega\,.$$

The change of variables, $t = h^{1/2}\tau$ and $s = \sigma$, transforms $\mathbb{R}/2L\mathbb{Z} \times (0, \varepsilon_0)$ and the measure to $a\,\mathrm{d}s\,\mathrm{d}t$ to

$$\tilde{\Gamma}_h = (\mathbb{R}/2L\mathbb{Z}) \times (0, \varepsilon_0 h^{-1/2}) \quad \text{and} \quad \tilde{a}_h(\sigma, \tau) = 1 - h^{1/2}\tau k(\sigma).$$

Moreover, it transforms the Hilbert space $L^2\big((\mathbb{R}/2L\mathbb{Z}) \times (0, \varepsilon_0); a\, \mathrm{d}s\, \mathrm{d}t\big)$ to the Hilbert space $L^2\big(\tilde{\Gamma}_h; \tilde{a}_h\, \mathrm{d}\sigma\, \mathrm{d}\tau\big)$, and the operator $\tilde{\mathscr{L}_h}$ to $h\tilde{\mathscr{N}_h}$ where

$$\tilde{\mathscr{N}_h} = -\tilde{a}_h^{-1}\partial_\tau \tilde{a}_h \partial_\tau + \tilde{a}_h^{-1}\left(-\mathrm{i}h^{1/2}\partial_\sigma + h^{-1/2}\gamma_0 - \tau + h^{1/2}\frac{k(\sigma)}{2}\tau^2\right) \\ \times \tilde{a}_h^{-1}\left(-\mathrm{i}h^{1/2}\partial_\sigma + h^{-1/2}\gamma_0 - \tau + h^{1/2}\frac{k(\sigma)}{2}\tau^2\right). \tag{4.10}$$

Let us consider $\tilde{\mathscr{N}_h}$, in $L^2\big(\tilde{\Gamma}_h; \tilde{a}_h\, \mathrm{d}\sigma d\tau\big)$, with domain[10]

$$\mathsf{Dom}(\tilde{\mathscr{N}_h}) = \{u \in L^2\big(\tilde{\Gamma}_h; d\sigma d\tau\big) \ : \ \partial_\tau^2 u, \partial_\sigma^2 u \in L^2\big(\tilde{\Gamma}_h; d\sigma d\tau\big), \\ \partial_\tau u|_{\tau=0} = 0,\ u|_{\tau=\varepsilon_0 h^{-1/2}} = 0\}.$$

The study of the eigenvalues of $\mathscr{L}_h^N$, can then be compared with those of $\tilde{\mathscr{N}_h}$ (see [6, Prop. 2.7]).

Proposition 4.2 *Let $N \in \mathbb{N}$ and S_n be the constant introduced in (4.4b). There exist $K > \mathsf{S}_n$, $C, h_0 > 0$ such that, for all $h \in (0, h_0]$ and $1 \le k \le N$, we have,*

$$\lambda_k(\mathscr{L}_h^N) - Ce^{-K/h^{\frac14}} \le h\lambda_k(\tilde{\mathscr{N}_h}) \le \lambda_k(\mathscr{L}_h^N) + Ce^{-K/h^{\frac14}} \ ,$$

where $\lambda_k(\mathscr{L}_h^N)$ and $\lambda_k(\tilde{\mathcal{N}}_h)$ are the k-th eigenvalues, counting multiplicity, of the operators $\mathscr{L}_h^N$ and $\tilde{\mathscr{N}_h}$, respectively.

Recall that we are interested in applying the results in Sect. 2 to the operator T_h obtained by shifting the operator $\mathscr{L}_h^N$ (see (4.3)). Effectively, that is related to the operator obtained by doing the corresponding shift to the operator $\tilde{\mathscr{N}_h}$,

$$\tilde{T}_h = \tilde{\mathscr{N}_h} - h^{-1}\ell(h). \tag{4.11}$$

Our next task is to verify Assumptions 2.1 and 2.8 (they will both hold for $\tilde{T}_h$ and T_h) and this will require the construction of certain quasi-modes $(u_{h,i})_{1\le i\le n}$. Let us make the following two observations:

(i) The assumption in (4.2a) implies that $\tilde{T}_h$ commutes with $M(g_n)$, hence the condition of invariance by rotation holds.
(ii) For every fixed labeling n, the eigenfunctions of $\tilde{T}_h$ corresponding to the n'th eigenvalue decay exponentially in the (rescaled) tangential variable; more precisely, given an eigenfunction f_n of $\tilde{T}_h$ with corresponding eigenvalue $\lambda_n(\tilde{T}_h$, there exist positive constants C_n, h_n, α_n such that

$$\forall\, h \in (0, h_n], \quad \int_{\tilde{\Gamma}_h} \mathrm{e}^{\alpha_k \tau}\big(|\partial_\tau f_n|^2 + |f_n|^2\big)\, \mathrm{d}s\, \mathrm{d}\tau \le C_k \int_{\tilde{\Gamma}_h} |f_n|^2\, \mathrm{d}s\, \mathrm{d}\tau.$$

[10] Since $\tilde{a}_h = \mathcal{O}(\varepsilon_0\|k\|_\infty)$, and $\varepsilon_0 \ll 1$, the vector space with weighted measure $L^2\big(\tilde{\Gamma}_h; \tilde{a}_h\, \mathrm{d}\sigma d\tau\big)$ is the same as the space with the flat measure $L^2\big(\tilde{\Gamma}_h; d\sigma d\tau\big)$ with equivalent norm.

The relevance of (i) above is that we can construct quasi-modes of $\tilde{T}_h$ obeying the symmetry invariance properties as in Assumption 2.8, and in turn we can use these quasi-modes to produce quasi-modes for the initial operator T_h in (4.3). The observation in (ii) asserts that the eigenfunctions of $\tilde{T}_h$, once rescaled to the initial tangential variable $t = h^{1/2}\tau$, can be ignored in the interior of the domain Ω.

The expression of the operator $\mathscr{N}_h$ (and hence $\tilde{T}_h$) involves the effective semi-classical parameter $\hbar := h^{1/2}$. This leads us to adjust our setting by working with the operators

$$\mathscr{T}_\hbar = \mathscr{N}_\hbar - \lambda(\hbar) \tag{4.12}$$

and

$$\begin{aligned}\mathscr{N}_\hbar = -a_\hbar^{-1}\partial_\tau a_\hbar \partial_\tau + a_\hbar^{-1}\left(-\mathrm{i}\hbar\partial_\sigma + \hbar^{-1}\gamma_0 - \tau + \hbar\frac{k(\sigma)}{2}\tau^2\right)\\ \times a_\hbar^{-1}\left(-\mathrm{i}\hbar\partial_\sigma + \hbar^{-1}\gamma_0 - \tau + \hbar\frac{k(\sigma)}{2}\tau^2\right)\end{aligned} \tag{4.13}$$

where

$$a_\hbar(\sigma,\tau) = 1 - \hbar\tau k(\sigma) = \tilde{a}_h(\sigma,\tau), \quad \lambda(\hbar) = h^{-1}\ell(h)\,.$$

4.3 The single well problem

4.3.1 Definition of the operator

Let us recall that by (4.2a) and (4.2b), we have on the interval $(-2L/n, 2L/n)$ a single non-degenerate maximum, $s_1 = 0$, of the curvature $k(s)$. Let us fix a positive $\eta < \min(\frac{1}{4}, \frac{L}{4n})$ and consider the following set

$$\tilde{\Gamma}^{(1)}_{\hbar,\eta} = \left(-\frac{2L}{n} + \eta, \frac{2L}{n} - \eta\right) \times (0, \varepsilon_0 \hbar^{-1}).$$

Now we consider the operator

$$\begin{aligned}\mathscr{N}^{(1)}_\hbar = -a_\hbar^{-1}\partial_\tau a_\hbar \partial_\tau + a_\hbar^{-1}\left(-\mathrm{i}\hbar\partial_\sigma + \hbar^{-1}\gamma_0 - \tau + \hbar\frac{k(\sigma)}{2}\tau^2\right)\\ \times a_\hbar^{-1}\left(-\mathrm{i}\hbar\partial_\sigma + \hbar^{-1}\gamma_0 - \tau + \hbar\frac{k(\sigma)}{2}\tau^2\right)\end{aligned} \tag{4.14}$$

with domain

$$\begin{aligned}\mathsf{Dom}(\mathscr{N}^{(1)}_\hbar) = \{u \in L^2\big(\tilde{\Gamma}^{(1)}_{\hbar,\eta}; d\sigma d\tau\big) \ :\ &\partial_\tau^2 u, \partial_\sigma^2 u \in L^2\big(\tilde{\Gamma}^{(1)}_{\hbar,\eta}; d\sigma d\tau\big),\\ &\partial_\tau u|_{\tau=0} = 0,\ u|_{\tau=\varepsilon_0 h^{-1/2}}\\ &= 0,\ u|_{\sigma=\pm(2L/n-\eta)} = 0\}.\end{aligned}$$

We denote by $\lambda(\hbar)$ the ground state energy of the operator $\mathscr{N}_\hbar^{(1)}$; it is simple and can be expanded as follows [7, 12]

$$\lambda(\hbar) \underset{\hbar\to 0}{\sim} \Theta_0 - 3C_1 k_{\max}\hbar + C_1\Theta_0^{1/4}\sqrt{\frac{3|k_2|}{2}}\hbar^{3/2} + \sum_{j\geq 4}\delta_{1,j}\hbar^{j/2}. \tag{4.15a}$$

where $(\delta_{1,j})_{j\geq 1}$ are real constants and $k_2 = k_2''(0) < 0$. Moreover there exist real constants $(\delta_{2,j})_{j\geq 1}$ such that the second eigenvalue satisfies

$$\lambda_2(\hbar) \underset{\hbar\to 0}{\sim} \Theta_0 - 3C_1 k_{\max}\hbar + 3C_1\Theta_0^{1/4}\sqrt{\frac{3|k_2|}{2}}\hbar^{3/2} + \sum_{j\geq 4}\delta_{2,j}\hbar^{j/2} \tag{4.15b}$$

and there is a spectral gap

$$\lambda_2(\hbar) - \lambda(\hbar) \underset{\hbar\to 0}{\sim} 2C_1\Theta_0^{1/4}\sqrt{\frac{3|k_2|}{2}}\hbar^{3/2}.$$

Functions in the domain of $\mathscr{N}_\hbar^{(1)}$ can be extended to the full half-plane $\mathbb{R}^2_+ = \mathbb{R}\times\mathbb{R}_+$ after multiplication by a suitable cutoff function. We could have considered the single well problem in an alternative manner by truncating the curvature and extending it by 0 outside $\hat{\Gamma}^{(1)}_{\hbar,\eta}$ and also the weight function $a_\hbar$ to get an operator in $\mathbb{R}^2_+$. Due to the exponential decay of bound states, the spectra agree up to exponentially small errors that are negligible compared with the estimate of the tunneling [6, Prop. 2.7].

4.3.2 Approximation of ground states

The ground states of $\mathscr{N}_\hbar^{(1)}$ concentrate near the curvature well $s_1 = 0$ [6, Corol.6.1] and one can expand them in a WKB form.

Let $\phi_{\hbar,1}$ be a normalized ground state of $\mathscr{N}_\hbar^{(1)}$. We introduce the function

$$\Phi_1(\sigma) = \sqrt{\frac{2C_1}{(\mu_1^N)''(\xi_0)}}\int_{[0,\sigma]}\sqrt{k_{\max} - k(\varsigma)}\,\mathrm{d}\varsigma, \tag{4.16}$$

where $[0,\sigma]$ is the segment joining 0 to σ oriented counter-clockwise; in particular $\int_{[0,\sigma]} = \int_\sigma^0$ if $\sigma < 0$ and $\int_{[0,\sigma]} = \int_0^\sigma$ if $\sigma > 0$. The ground state $\phi_{\hbar,1}$ is approximated as follows. Let $K \subset \left(-\frac{L}{2n} + \eta, \frac{L}{2n} - \eta\right)$ be a compact interval, then we have [6, Prop. 6.3 & Eq. (2.5)]

$$\left\| \langle\tau\rangle e^{\Phi_1/\sqrt{\hbar}}\big(\phi_{\hbar,1} - e^{-i\gamma_0\sigma/\hbar^2}\psi_{\hbar,1}\big)\right\|_{C^1(K;L^2(\mathbb{R}_+))} = \mathcal{O}(h^\infty), \tag{4.17a}$$

where $\langle\tau\rangle = (1+|\tau|^2)^{1/2}$ and γ_0 is introduced in (4.9).

The function $\psi_{\hbar,1}$ is defined as follows

$$\psi_{\hbar,1} = \chi \Psi_{\hbar,1} \tag{4.17b}$$

where $\chi \in C^\infty(\mathbb{R}; [0, 1])$ satisfies

$$\chi = 1 \text{ on } \left(-\frac{L}{2n} + 2\eta, \frac{L}{2n} - 2\eta\right), \ \operatorname{supp}\chi \subset \left(-\frac{L}{2n} + \eta, \frac{L}{2n} - \eta\right) \tag{4.17c}$$

and the function $\Psi_{\hbar,1}$ has the following expansion [6, Thm. 2.8]

$$e^{\Phi_1(\sigma)/\hbar^{\frac{1}{2}}} e^{-i\sigma\xi_0/\hbar} \Psi_{\hbar,1}(\sigma, \tau) \underset{\hbar\to 0}{\sim} \hbar^{-\frac{1}{8}} \sum_{j\geq 0} b_j(\sigma, \tau)\hbar^{\frac{j}{2}}, \tag{4.17d}$$

where

$$b_0(\sigma, \tau) = f_0(\sigma)u_0(\tau)$$

and the sequence of functions $(b_j(\sigma, \tau))_{j\geq 1}$ can be constructed by recursion [7, Thm. 5.6].

4.4 Construction of quasi-modes

Now we can introduce the following quasi-modes for $\mathscr{T}_\hbar$

$$\tilde{\phi}_{\hbar,1} := \chi\phi_{\hbar,1}, \quad \tilde{\phi}_{\hbar,2} := \mathscr{M}_n\tilde{\phi}_{\hbar,1}, \ldots \quad \tilde{\phi}_{\hbar,n} := \mathscr{M}_n\tilde{\phi}_{\hbar,n-1}, \tag{4.18}$$

where (see (4.8))

$$\mathscr{M}_n u(\sigma, \tau) = u\left(\sigma - \frac{L}{2n}, \tau\right). \tag{4.19}$$

Notice that $\tilde{\phi}_{\hbar,i}$ is supported in $\tilde{\Gamma}^{(i)}_{\hbar,\eta}$ defined as follows

$$\tilde{\Gamma}^{(i)}_{\hbar,\eta} = \left((i-2)\frac{2L}{n} + \eta, i\frac{2L}{n} - \eta\right) \times (0, \varepsilon_0\hbar^{-1/2}).$$

This yields quasi-modes for the operator $\tilde{T}_h$ in (4.3) obtained from $\mathscr{T}_\hbar$ by the change of parameter $\hbar = h^{1/2}$; more precisely, we introduce

$$\tilde{u}_{h,i} = \tilde{\phi}_{\hbar,i} \qquad (\hbar = h^{1/2},\ 1 \leq i \leq n). \tag{4.20}$$

Notice that by (4.17a),

$$e^{\Phi_2(\sigma,\tau)/\sqrt{\hbar}}\big(\tilde{u}_{\hbar,2}(\sigma, \tau) - e^{2i\gamma_0 L/n\hbar^2} e^{-i\gamma_0\sigma/\hbar^2}\tilde{\psi}_{\hbar,1}(\sigma - 2L/n, \tau)\big) = \mathcal{O}(h^\infty),$$

and by (4.2e),

$$\Phi_2(\sigma) = \Phi_1\left(\sigma - \frac{2L}{n}\right) \text{ on } \tilde{\Gamma}^{(2)}_{\hbar,\eta}$$

$$\Phi_2(\sigma) + \Phi_1(\sigma) = \sqrt{\frac{2C_1}{(\mu_1^N)''(\xi_0)}} \int_{\sigma-\frac{2L}{n}}^{\sigma} \sqrt{k_{\max} - k(\varsigma)}\, \mathrm{d}\varsigma$$
$$= \mathsf{S}_n \text{ on } \tilde{\Gamma}^{(2)}_{\hbar,\eta} \cap \tilde{\Gamma}^{(1)}_{\hbar,\eta}$$

where S_n is introduced in (4.4b).

To obtain quasi-modes for the operator T_h in (4.3), we truncate, re-scale and pull back the quasi-modes $\tilde{u}_{h,i}$ to the Cartesian coordinates via the transformation in (4.6) and finally renormalize. More precisely, we introduce

$$u_{h,i}(x) = h^{-1/4}\chi_0\big(t(x)/h^{1/2}\big)\tilde{u}_{h,i}\big(s(x), h^{-1/2}t(x)\big) \tag{4.21}$$

where $\chi_0 \in C_c^\infty(\mathbb{R}; [0, 1])$ satisfies $\operatorname{supp}\chi_0 \subset (-\varepsilon_0, \varepsilon_0)$ and $\chi_0 = 1$ on $[-\varepsilon_0/2, \varepsilon_0/2]$.

4.5 Estimates of interaction coefficients

We need to estimate

$$J_0(h) = \langle T_h u_{h,1}, u_{h,1}\rangle \text{ and } J_1(h) = \langle T_h u_{h,1}, u_{h,2}\rangle.$$

By the exponential decay of $u_{h,1}$ and $u_{h,2}$, we may write

$$\tilde{J}_0(h) = h\tilde{J}_0 + \mathcal{O}(\mathrm{e}^{-K'/h^{1/4}}), \quad J_1(h) = h\tilde{J}_1 + \mathcal{O}(\mathrm{e}^{-K'/h^{1/4}})$$

where $K' > \mathsf{S}_n$ and

$$\tilde{J}_0 = \langle \mathscr{T}_\hbar \tilde{\phi}_{\hbar,1}, \tilde{\phi}_{\hbar,1}\rangle, \quad \tilde{J}_1 = \langle \mathscr{T}_\hbar \tilde{\phi}_{\hbar,1}, \tilde{\phi}_{\hbar,2}\rangle$$

The term $\tilde{J}_0$ is estimated as $\mathcal{O}(\mathrm{e}^{(-2\mathsf{S}_n + c\eta)/\hbar^{1/2}})$ where c is a positive constant independent of $\hbar$ and η. We fix now the choice of $\eta \ll 1$ so that $2\mathsf{S}_n - c\eta > \mathsf{S}_n$.

The term $\tilde{J}_1$ is calculated as in [6, Sec. 7.2.1] (see also [8, 26])

$$\tilde{J}_1 = \mathrm{e}^{2\mathrm{i}(\gamma_0 - \xi_0)L/n\hbar}\mathrm{e}^{-\mathsf{S}_n/\hbar^{1/2}}\big(\hbar^{5/4}C_* + \mathcal{O}(\hbar^{7/4})\big)$$

where $C_* \in \mathbb{C} \setminus \{0\}$ is a constant independent of $\hbar$.

Writing $C_* = |C_*|\mathrm{e}^{\mathrm{i}\alpha_0}$ and recalling the definition of Φ_0 in (4.4a) and the relation $\hbar = h^{1/2}$, we get

$$J_1(h) \underset{h\searrow 0}{\sim} |C_*|h^{13/8}\mathrm{e}^{\mathrm{i}\alpha_0 + 2\mathrm{i}\Phi_0/nh^{1/2}}\mathrm{e}^{-\mathsf{S}_n/h^{1/4}} \tag{4.22a}$$

and

$$J_0(h) \underset{h\searrow 0}{=} o\big(J_1(h)\big). \tag{4.22b}$$

4.6 Application when $n = 3$.

Let us assume that $n = 3$. The functions $u_{h,i}$ introduced in (4.21) satisfy the conditions in Assumptions 2.1, 2.8 (in Remark 2.7) and 2.11. In fact,

- By (4.18) and (4.20), we check that the symmetry invariance in Assumption 2.8 is respected.
- The symmetry invariance and (4.17a) ensure that $u_{h,i}$ satisfy the conditions in Assumption 2.1 with $\mathfrak{S}_1, \mathfrak{S}_2, \mathfrak{S}_3 \in (0, \mathsf{S}_n)$ arbitrarily close to S_n; we fix the choice so that $\mathsf{S}_n < 2\min_{1\le j\le 3}\mathfrak{S}_j$.
- The estimates in (4.22) ensure that Assumption 2.11 holds with $\mathfrak{S} = \mathsf{S}_n$.

Applying (2.21), we get a similar result to Theorem 3.9 (by following exactly the same argument). In fact, there is a relabeling $\mu_1(h), \mu_2(h), \mu_3(h)$ of the eigenvalues $\lambda_1(h), \lambda_2(h), \lambda_3(h)$ of the Neumann magnetic Laplacian $\mathcal{L}_h^N$ with the asymptotics

$$\begin{aligned} \mu_2(h) - \mu_1(h) &\underset{h\searrow 0}{=} \big(\mathsf{a}(\Phi_0/3\sqrt{h} + \alpha_0) + o(1)\big)|C_*| \exp\left(\frac{-\mathsf{S}_3}{h^{1/2}}\right) \\ \mu_3(h) - \mu_2(h) &\underset{h\searrow 0}{=} \big(\mathsf{b}(\Phi_0/3\sqrt{h} + \alpha_0) + o(1)\big)|C_*| \exp\left(\frac{-\mathsf{S}_3}{h^{1/2}}\right) \end{aligned} \tag{4.23}$$

where $\mathsf{a}(\cdot)$ and $\mathsf{b}(\cdot)$ are introduced (3.43).

Moreover, there exists a sequence $\big((h_1(k), h_2(k), h_3(k)\big)_{k\ge k_0}$ which converges to 0 such that, for all $k \ge k_0$ we have

$$0 < h_1(k+1) < h_3(k) < h_2(k) < h_1(k) < 1$$

and

$$\mu_1\big(h_1(k)\big) = \mu_3\big(h_1(k)\big),\ \ \mu_1\big(h_2(k)\big) = \mu_2\big(h_2(k)\big),\ \ \mu_2\big(h_3(k)\big) = \mu_3\big(h_3(k)\big).$$

In particular, this finishes the proof of Theorem 1.5.

5 Magnetic steps

5.1 Introduction

In this section, we work in the plane and the Hilbert space is $H = L^2(\mathbb{R}^2)$. Consider a positive integer n and denote by $g = g_n$ the rotation in $\mathbb{R}^2$ by $2\pi/n$. We are then in the setting of Remark 2.7 with the domain being all of $\mathbb{R}^2$. Recall the definition of the transformation

$$M(g)u(x) = u(g^{-1}x) \quad (u \in L^2(\mathbb{R}^2)).$$

Let $\Omega \subset \mathbb{R}^2$ be an open bounded subset of $\mathbb{R}^2$ with C^∞ boundary Γ. We assume that Ω satisfies the conditions in (4.2).

Let $\mathbf{A} : \mathbb{R}^2 \to \mathbb{R}^2$ be a vector field such that

$$B := \operatorname{curl} \mathbf{A} = \begin{cases} 1 & \text{on } \Omega \\ \vartheta & \text{on } \mathbb{R}^2 \setminus \overline{\Omega} \end{cases} \tag{5.1}$$

where $-1 < \vartheta < 0$ is a fixed constant. The magnetic field $B = B_{\vartheta,\Omega}$ is a step function, hence called a *magnetic step* ([3] and references therein). The boundary Γ is the discontinuity curve of the magnetic step, and sometimes is called the *magnetic edge* ([13] and references therein).

Consider the Landau Hamiltonian on $\mathbb{R}^2$

$$\mathscr{L}_h^B = (-\mathrm{i}h\nabla - \mathbf{A})^2 \tag{5.2}$$

with semi-classical parameter h and magnetic field B as in (5.1). The symmetry conditions in (4.2) allow us to prove that the eigenvalues of $\mathscr{L}_h^B$ exhibit a braid structure in the semi-classical limit. The proof and the construction are very similar to those for the Neumann problem in Section 4 modulo the following slight modifications:

i) Use the model operator on the full real line from [2].
ii) Introduce adapted coordinates on a curved strip defined by the boundary Γ, via the signed normal distance to Γ and the tangential arc-length distance along Γ.
iii) Use a modified single well operator, with magnetic steps, analyzed in [3].
iv) Construct quasi-modes and apply the abstract results in Section 2.

Most of the computations were carried out in [3, 13] so we will be rather succinct and just present the key constructions.

5.2 Model on the real line

On $L^2(\mathbb{R})$, consider the family of Schrödinger operators, parameterized by $\xi \in \mathbb{R}$,

$$\mathfrak{h}_\vartheta[\xi] = -\frac{d^2}{d\tau^2} + V_\vartheta(\xi, \tau), \tag{5.3}$$

where $\xi \in \mathbb{R}$ is a parameter and

$$V_\vartheta(\xi, \tau) = \big(\xi + b_\vartheta(\tau)\tau\big)^2, \quad b_\vartheta(\tau) = \mathbf{1}_{\mathbb{R}_+}(\tau) + \vartheta \mathbf{1}_{\mathbb{R}_-}(\tau)\,. \tag{5.4}$$

We denote by $\mu_\vartheta(\xi)$ the ground state energy of $\mathfrak{h}_\vartheta[\xi]$, and according to [2], we can introduce the constants β_ς, ζ_ϑ as follows

$$\beta_\vartheta := \inf_{\xi\in\mathbb{R}} \mu_\vartheta(\xi) = \mu_\vartheta(\zeta_\vartheta)\,, \tag{5.5}$$

where $\zeta_\vartheta < 0$, is the unique minimum of $\mu_\vartheta(\cdot)$ and we have $\mu''_\vartheta(\zeta_\vartheta) > 0$.

Let ϕ_ϑ be the positive L^2-normalized ground state of $\mathfrak{h}_\vartheta[\zeta_\vartheta]$. We introduce the negative constant [2]

$$M_3(\vartheta) = \frac{1}{3}\Big(\frac{1}{\vartheta} - 1\Big)\zeta_\vartheta \phi_\vartheta(0)\phi'_\vartheta(0). \tag{5.6}$$

5.3 Adapted coordinates and single well problem

Recall that $\gamma : \mathbb{R}/2L\mathbb{Z} \to \mathbb{R}^2$ is a counter-clockwise oriented arc-length parameterization of the curve Γ and that, for $s \in \mathbb{R}/2L\mathbb{Z}$, $\nu(s)$ is the unit normal to Γ at $\gamma(s)$ which points to the interior of the Γ. We can adjust the coordinates (s,t) introduced in (4.6), by allowing t to have negative values. We therefore set

$$\mathscr{T}(s,t) := \gamma(s) - t\nu(s) \qquad ((s,t) \in \mathbb{R}/2L\mathbb{Z} \times \mathbb{R}).$$

We introduce the curved strip

$$\hat{\Gamma}(\varepsilon_0) = \{x \in \mathbb{R}^2 \ : \ \mathrm{dist}(x,\Gamma) < \varepsilon_0\}$$

and we choose $\varepsilon_0 > 0$ so that $\mathscr{T}$ is one-to-one on $\mathbb{R}/2L\mathbb{Z} \times (-\varepsilon_0, \varepsilon_0)$ and that $\hat{\Gamma}(\varepsilon_0)$ is the image of $\mathbb{R}/2L\mathbb{Z} \times (-\varepsilon_0, \varepsilon_0)$ by $\mathscr{T}$.

We assign to a function u defined on $\hat{\Gamma}(\varepsilon_0)$ the function $\tilde{u} = u \circ \mathscr{T}$ defined on $\mathbb{R}/2L\mathbb{Z} \times (-\varepsilon_0, \varepsilon_0)$. The Hilbert space $L^2(\hat{\Gamma}(\varepsilon_0))$ is then transformed to the weighted space

$$L^2\big((\mathbb{R}/2L\mathbb{Z}) \times (-\varepsilon_0, \varepsilon_0); a\,\mathrm{d}s\,\mathrm{d}t\big), \quad a(s,t) = 1 - tk(s)$$

and the action of the transformation $M(g)$ is still given by (4.8).

Note that the action of $\mathscr{L}_h^B$ on $\hat{\Gamma}(\varepsilon_0)$ is transformed to (after, possibly, a gauge transformation)

$$\begin{aligned}\tilde{\mathscr{L}_h^B} \ := -h^2 a^{-1}\partial_t a \partial_t + a^{-1}\left(-\mathrm{i}h\partial_s + \gamma_0 - b_\vartheta(t)t + \frac{k(s)}{2}b_\vartheta(t)t^2\right)\\ \times a^{-1}\left(-\mathrm{i}h\partial_s + \gamma_0 - b_\vartheta(t)t + \frac{k(s)}{2}b_\vartheta(t)t^2\right)\end{aligned}$$

where the constant γ_0 and the function b_ϑ are introduced in (4.9) and (5.4) respectively.

We do the scaling $(\sigma,\tau) = (s, h^{-1/2}t)$ and introduce the effective semi-classical parameter $\hbar = h^{1/2}$. We obtain the operator

$$\begin{aligned}\mathscr{N}_{\hbar,\vartheta} = -a_\hbar^{-1}\partial_\tau a_\hbar \partial_\tau + a_\hbar^{-1}\left(-\mathrm{i}\hbar\partial_\sigma + \hbar^{-1}\gamma_0 - b_\vartheta\tau + \hbar\frac{k(\sigma)}{2}b_\vartheta\tau^2\right)\\ \times a_\hbar^{-1}\left(-\mathrm{i}\hbar\partial_\sigma + \hbar^{-1}\gamma_0 - b_\vartheta\tau + \hbar\frac{k(\sigma)}{2}b_\vartheta\tau^2\right)\end{aligned} \tag{5.7}$$

where[11]

$$a_\hbar(\sigma,\tau) = 1 - \hbar\tau k(\sigma).$$

Our single well problem is defined as follows. Fix a positive $\eta < \min(\frac{1}{4}, \frac{L}{4n})$ and consider

$$\hat{\Gamma}^{(1)}_{\hbar,\eta} = \Big(-\frac{2L}{n} + \eta, \frac{2L}{n} - \eta\Big) \times (-\varepsilon_0\hbar^{-1}, \varepsilon_0\hbar^{-1}).$$

We introduce the operator on $L^2\big(\hat{\Gamma}^{(1)}_{\hbar,\eta}; a_\hbar\, \mathrm{d}\sigma\, \mathrm{d}\tau\big)$,

$$\mathscr{N}^{(1)}_{\hbar,\vartheta} = \mathscr{N}_{\hbar,\vartheta} \tag{5.8}$$

with domain

$$\begin{aligned}\mathsf{Dom}(\mathscr{N}^{(1)}_{\hbar,\vartheta}) = \{u \in L^2\big(\hat{\Gamma}^{(1)}_{\hbar,\eta}; \mathrm{d}\sigma\, \mathrm{d}\tau\big) \ : \ \partial_\tau^2 u, \partial_\sigma^2 u \in L^2\big(\hat{\Gamma}^{(1)}_{\hbar,\eta}; \mathrm{d}\sigma\, \mathrm{d}\tau\big),\\ u|_{\tau=\pm\varepsilon_0 h^{-1/2}} = 0,\ u|_{\sigma=\pm(2L/n-\eta)} = 0\}.\end{aligned}$$

We denote by $\lambda(\hbar)$ the ground state energy of the operator $\mathscr{N}^{(1)}_{\hbar,\vartheta}$; it is simple and can be expanded as follows [3, 13]

$$\lambda(\hbar) \underset{\hbar\to 0}{\sim} \beta_\varsigma + M_3(\vartheta)k_{\max}\hbar + \sqrt{\frac{k_2 M_3(\vartheta)\mu''_\vartheta(\zeta_\vartheta)}{4}}\hbar^{3/2}, \tag{5.9}$$

and the splitting between $\lambda(\hbar)$ and the second eigenvalue $\lambda_2(\hbar)$ is estimated as follows

$$\lambda_2(\hbar) - \lambda(\hbar) \underset{\hbar\to 0}{\sim} \sqrt{\frac{k_2 M_3(\vartheta)\mu''_\vartheta(\zeta_\vartheta)}{4}}\hbar^{3/2}.$$

5.4 Quasi-modes and application

In order to apply the results in Section 2 we introduce the operator

$$\mathcal{T}_h = \mathscr{L}_h^B - \ell(h)$$

and construct suitable quasi-modes. With $\hbar = h^{1/2}$, we choose $\ell(h) = h\lambda(\hbar)$, where $\lambda(\hbar)$ is the ground state energy of the single well operator $\mathscr{N}^{(1)}_{\hbar,\vartheta}$ introduced in (5.8).

Let $\phi^\vartheta_{\hbar,1}$ be a normalized ground state of $\mathscr{N}^{(1)}_{\hbar,\vartheta}$ and choose $\chi \in C^\infty(\mathbb{R}; [0,1])$ satisfying (4.17c). We introduce the quasi-modes

$$\tilde{\phi}^\vartheta_{\hbar,1} := \chi\phi^\vartheta_{\hbar,1}, \quad \tilde{\phi}^\vartheta_{\hbar,2} := \mathscr{M}_n\tilde{\phi}^\vartheta_{\hbar,1}, \ldots \quad \tilde{\phi}^\vartheta_{\hbar,n} := \mathscr{M}_n\tilde{\phi}^\vartheta_{\hbar,n-1}, \tag{5.10}$$

[11] The function b_ϑ now depends on the variable τ.

where $\mathscr{M}_n$ is introduced in (4.19). We obtain quasi-modes for the operator T_h by truncation, re-scaling and pulling back to Cartesian coordinates; more precisely we introduce

$$u_{h,i}^{\vartheta}(x) = h^{-1/4}\chi_0\big(t(x)/h^{1/2}\big)\tilde{u}_{h,i}^{\vartheta}\big(s(x), h^{-1/2}t(x)\big) \tag{5.11}$$

where $\chi_0 \in C_c^\infty(\mathbb{R}; [0, 1])$ is as in (4.21) and $\tilde{u}_{h,i}^{\vartheta} = \tilde{\phi}_{\hbar,i}^{\vartheta}$, with $\hbar = h^{1/2}$.

We move then to the calculation of the following two terms

$$J_0(h) = \langle \mathcal{T}_h u_{h,1}^{\vartheta}, u_{h,1}^{\vartheta}\rangle \text{ and } J_1(h) = \langle \mathcal{T}_h u_{h,1}^{\vartheta}, u_{h,2}^{\vartheta}\rangle.$$

That is essentially done in [13]. We introduce the following 'distance'

$$\mathsf{S}_n(\vartheta) = \sqrt{\frac{-2M_3(\vartheta)}{\mu_\vartheta''(\zeta_\vartheta)}}\int_0^{2L/n}\sqrt{k_{\max} - k(s)}\,\mathrm{d}s$$

and the flux like term

$$\Phi_\vartheta = |\Omega| - 2L\zeta_\vartheta.$$

We have

$$J_0(h) = \mathcal{O}(\mathrm{e}^{(-2\mathsf{S}_n(\vartheta)+c\eta)/h^{1/4}})$$

where c is a positive constant independent of $\hbar$ and η, and

$$\tilde{J}_1(h) = \mathrm{e}^{2\mathrm{i}\Phi_\vartheta/n\hbar}\mathrm{e}^{-\mathsf{S}_n(\vartheta)/h^{1/4}}\big(C_*(\vartheta)h^{13/8} + \mathcal{O}(h^{15/8})\big)$$

where $C_*(\vartheta) \in \mathbb{C}\setminus\{0\}$ is a constant independent of $\hbar$.

We fix now the choice of $\eta \ll 1$ so that $2\mathsf{S}_n(\vartheta) - c\eta > \mathsf{S}_n(\vartheta)$ and we write $C_*(\vartheta) = |C_*(\vartheta)|\mathrm{e}^{\mathrm{i}\alpha_0(\vartheta)}$. We get

$$J_1(h) \underset{h\searrow 0}{\sim} |C_*(\vartheta)|h^{13/8}\mathrm{e}^{\mathrm{i}\alpha_0(\vartheta)+2\mathrm{i}\Phi_\vartheta/nh^{1/2}}\mathrm{e}^{-\mathsf{S}_n(\vartheta)/h^{1/4}} \tag{5.12a}$$

and

$$J_0(h) \underset{h\searrow 0}{=} o\big(J_1(h)\big). \tag{5.12b}$$

Let us now assume that $n = 3$, which corresponds to the setting in Theorem 1.6. The functions $u_{h,i}^{\vartheta}$ introduced in (4.21) satisfy the conditions in Assumptions 2.1, 2.8 (in Remark 2.7) and 2.11. Applying (2.21), we get a relabeling $\mu_1(h), \mu_2(h), \mu_3(h)$ of the eigenvalues $\lambda_1(h), \lambda_2(h), \lambda_3(h)$ of the Landau hamiltonian $\mathscr{L}_h^B$ with the asymptotics

$$\mu_2(h) - \mu_1(h) \underset{h\searrow 0}{=} \big(\mathsf{a}(\Phi_\vartheta/3\sqrt{h} + \alpha_0(\vartheta)) + o(1)\big)|C_*(\vartheta)|\exp\left(\frac{-\mathsf{S}_3(\vartheta)}{h^{1/2}}\right)$$

$$\mu_3(h) - \mu_2(h) \underset{h\searrow 0}{=} \big(\mathsf{b}(\Phi_\vartheta/3\sqrt{h} + \alpha_0(\vartheta)) + o(1)\big)|C_*(\vartheta)|\exp\left(\frac{-\mathsf{S}_3(\vartheta)}{h^{1/2}}\right)$$

where $\mathsf{a}(\cdot)$ and $\mathsf{b}(\cdot)$ are introduced (3.43).

Moreover, there exists a sequence $\big((h_1(k), h_2(k), h_3(k)\big)_{k\geq k_0}$ which converges to 0 such that, for all $k \geq k_0$ we have

$$0 < h_1(k+1) < h_3(k) < h_2(k) < h_1(k) < 1$$

and

$$\mu_1\big(h_1(k)\big) = \mu_3\big(h_1(k)\big),\ \mu_1\big(h_2(k)\big) = \mu_2\big(h_2(k)\big),\ \mu_2\big(h_3(k)\big) = \mu_3\big(h_3(k)\big).$$

In particular, this finishes the proof of Theorem 1.6.

Appendix A Minimizing the function $\Psi(r, t)$.

Let Ψ be the function introduced in (3.19). Using the inequality $\sqrt{t(t+1)} \leq t + \frac{1}{2}$ we get

$$\Psi(r,t) \geq d(r) + \frac{|v_0^{\min}|}{2}\ln\Big(1+\frac{1}{t}\Big) + \frac{(L-r)^2}{2}\left(t+\frac{1}{2}\right). \tag{A.1}$$

Consequently, the minimum of $\Psi(r,t)$ over $[a, L-a]\times\overline{\mathbb{R}}_+$ is attained at $(r_0, t_0) \in [a, L-a]\times\mathbb{R}_+$. By [17, Remark 4.8],

$$\inf_{(r,t)\in[a,L-a]\times\mathbb{R}_+}\Psi(r,t) \geq \inf\left\{\inf_{(r,t)\in[0,a]\times\mathbb{R}_+}\Psi(r,t),\ \inf_{t\in\mathbb{R}_+}\Psi(L-a,t)\right\}. \tag{A.2}$$

Recalling $F(v_0)$ from (3.19), we have by [17, Eq. (4.18) and Prop. 4.5],

$$-F(v_0) + \inf_{(r,t)\in[0,a]\times\mathbb{R}_+}\Psi(r,t) = S(v_0, L) \geq S_a \tag{A.3}$$

where $S(v_0, L)$ and S_a are introduced in (3.9).

The function

$$G(t) := \frac{|v_0^{\min}|}{2}\ln\Big(1+\frac{1}{t}\Big) + \frac{a^2}{2}\left(t+\frac{1}{2}\right)$$

has a unique minimum on $\mathbb{R}_+$,

$$t_* = \sqrt{\frac{1}{4}+\frac{|v_0^{\min}|}{a^2}} - \frac{1}{2}.$$

By (A.1) (for $r = L - a$), we get

$$\inf_{t\in\mathbb{R}_+} \Psi(L-a,t) \ge d(L-a) + G(t_*)$$
$$= d(L-a) + \frac{a}{4}\sqrt{a^2+4|v_0^{\min}|} + \frac{|v_0^{\min}|}{2} \ln \frac{\left(\sqrt{a^2+4|v_0^{\min}|}+a\right)^2}{4|v_0^{\min}|}.$$

Consequently,

$$-F(v_0) + \inf_{t\in\mathbb{R}_+} \Psi(L-a,t) \ge d(L-a) + d(a) = S_a. \tag{A.4}$$

Collecting (A.3) and (A.4), we infer from (A.2) that

$$-F(v_0) + \inf_{(r,t)\in[a,L-a]\times\mathbb{R}_+} \Psi(r,t) \ge S_a.$$

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Declarations

Conflict of interest The authors have no conflict of interest to declare.

References

1. Abou Alfa, K.: Tunneling effect in two dimensions with vanishing magnetic fields. Preprint arXiv:2212.04289 (2022)
2. Assaad, W., Kachmar, A.: Lowest energy band function for magnetic steps. J. Spectr. Theory **12**(2), 813–833 (2022)
3. Assaad, W., Helffer, B., Kachmar, A.: Semi-classical eigenvalue estimates under magnetic steps. Anal. PDE **17**(2), 535–585 (2024)
4. Bonnaillie-Noël, V., Dauge, M., Martin, D., Vial, G.: Numerical computations of fundamental eigenstates for the Schrödinger operator under constant magnetic field. Comput. Methods Appl. Mech. Engng. **196**, 3841–3858 (2007)

5. Bonnaillie-Noël, V., Dauge, M.: Asymptotics for the low-lying eigenstates of the Schrödinger operator with magnetic field near corners. Ann. Henri Poincaré **7**, 899–931 (2006)
6. Bonnaillie-Noël, V., Hérau, F., Raymond, N.: Purely magnetic tunneling effect in two dimensions. Invent. Math. **227**(2), 745–793 (2022)
7. Bonnaillie-Noël, V., Hérau, F., Raymond, N.: Magnetic WKB constructions. Arch. Ration. Mech. Anal. **221**(2), 817–891 (2016)
8. Bonnaillie-Noël, V., Hérau, F., Raymond, N.: Semiclassical tunneling and magnetic flux effects on the circle. J. Spectr. Theory **7**(3), 771–796 (2017)
9. Dimassi, M.: J. Sjöstrand. Spectral asymptotics in the semi-classical limit. London Math. Soc. Lecture Note Ser., Vol. 268 (1999)
10. Fefferman, C., Shapiro, J., Weinstein, M.: Lower bound on quantum tunneling for strong magnetic fields. SIAM J. Math. Anal. **54**(1), 1105–1130 (2022)
11. Fournais, S., Helffer, B.: Spectral methods in surface superconductivity. Progress in Nonlinear Differential Equations and Their Applications 77. Birkhäuser, Basel (2010)
12. Fournais, S., Helffer, B.: Accurate eigenvalue asymptotics for the magnetic Neumann Laplacian. Ann. Inst. Fourier **56**(1), 1–67 (2006)
13. Fournais, S., Helffer, B., Kachmar, A.: Tunneling effect induced by a curved magnetic edge. Frank, R.L. (ed.) et al., The physics and mathematics of Elliott Lieb. The 90-th anniversary. Volume I. Berlin: European Mathematical Society (EMS). 315–350 (2022)
14. Fournais, S., Helffer, B., Kachmar, A., Raymond, N.: Effective operators on an attractive magnetic edge. J. de l'École polytechnique Mathématiques **10**, 917–944 (2023)
15. Harrell, E.: Double wells. Commun. Math. Phys. **75**, 239–261 (1980)
16. Helffer, B.: Semi-classical analysis for the Schrödinger operator and applications. Lecture Notes in Mathematics, vol. 1336. Springer-Verlag, Berlin (1988)
17. Helffer, B., Kachmar, A.: Quantum tunneling in deep potential wells and strong magnetic field revisited. Pure Appl. Anal. (in press). arXiv:2208.13030v4 (2022)
18. Helffer, B., Kachmar, A., Raymond, N.: Tunneling for the Robin Laplacian in smooth planar domains. Commun. Contemp. Math. **19**(1), 1650030 (2017)
19. Helffer, B., Pankrashkin, K.: Tunneling between corners for Robin Laplacians. J. Lond. Math. Soc. (2) **91**(1), 225–248 (2015)
20. Helffer, B., Sjöstrand, J.: Multiple wells in the semi-classical limit I. Commun. Partial Differ. Equ. **9**, 337–408 (1984)
21. Helffer, B., Sjöstrand, J.: Puits multiples en limite semi-classique. II Interaction moléculaire. Symétries. Perturbation. Ann. IHP, Section A **42**(2), 127–212 (1985)
22. Helffer, B., Sjöstrand, J.: Effet tunnel pour l'équation de Schrödinger avec champ magnétique. Ann. Sc. Norm. Super. Pisa, Cl. Sci., IV. Ser. **14**(4), 625–657 (1987)
23. Helffer, B., Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T., Owen, M.P.: Nodal sets for ground states of Schrödinger operators with zero magnetic field in non simply connected domains. Commun. Math. Phys. **202**(3), 629–649 (1999)
24. Kachmar, A., Raymond, N.: Tunnel effect in a shrinking shell enlacing a magnetic field. Rev. Mat. Iberoam. **35**(7), 2053–2070 (2019)
25. Nakamura, S.: Tunneling estimates for magnetic Schrödinger operators. Commun. Math. Phys. **200**(1), 25–34 (1999)
26. Outassourt, A.: Comportement semi-classique pour l'opérateur de Schrödinger à potentiel périodique. J. Funct. Anal. **72**(1), 65–93 (1987)
27. Raymond, N.: Bound states of the magnetic Schrödinger operator. EMS Tracts Math., 27 (2017)
28. Simon, B.: Semiclassical analysis of low lying eigenvalues, I. Non-degenerate minima: asymptotic expansions. Ann. Inst. H. Poincaré **38**, 295–307 (1983)
29. Simon, B.: Semiclassical analysis of low lying eigenvalues. II. Tunneling. Ann. Math. **120**, 89–118 (1984)