On the magnetic Quantum tunneling

Bernard Helffer (Nantes Université)

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Notes for a Minicourse at the Nantes-Rennes meeting.

– mainly (for the recent contributions) after Fefferman-Shapiro-Weinstein, Helffer-Kachmar, Helffer-Kachmar-Sundqvist and Morin–

Introduction

If the analysis of the double well problem is one of the standard examples treated in Quantum Mechnaics (this is an exercise in Landau-Lifshitz book in the $(1D)$ situation), its solution in general dimension for the Schrödinger operator $-h^2\Delta + V$ is obtained in the beginning of the eighties (B. Simon, B.Helffer and J. Sjöstrand). In the case with magnetic field, the magnetic Schrödinger operator reads $(hD - A)^2 + V$ and many various problems appear which are still unsolved or only solved recently.

Our mini-course will be two-fold:

- on one hand explain the general techniques for treating this kind of questions. Here we can mention Helffer-Sjöstrand [HelSjPise1987], Matsumoto, Martinez-Sordoni,... when V is creating a well or multiple wells.
- on the other hand focus on a recent paper by Charles Fefferman, Jakob Shapiro and Michael Weinstein [FSW2022], recently improved in three papers Helffer-Kachmar [HelKa2022-23], Helffer-Kachmar-Sundqvist [HKS2023] and Leo Morin [Mor2023], which under restrictive but physical conditions give a complete answer to the problem.

We will not discuss the case when $V = 0$ and the wells are created by the magnetic fields (see Helffer, Mohamed, Kordyukov, Raymond, Vu Ngoc,....., Colbois, Savo, Provenziano, Léna,...) and particularly the recent paper by Fournais-Morin-Raymond [FoMoRa2023]. The case with boundary will also not be discussed (see Lu, Pan, Helffer, Mohamed, Fournais, Bonnaillie, Hérau, Raymond,....). The "magnetic" book by N. Raymond [Raybook] presents many other results.

The harmonic oscillator

Let us first consider the "semi-classical" harmonic oscillator.

$$-h^2 \frac{d^2}{dx^2} + x^2 \,,$$

on the line, with $h > 0$. Its spectrum is explicitly known. It consists of a sequence of eigenvalues

$$\lambda_n(h) = (2n - 1)h \,,\; n \in \mathbb{N} \setminus \{0\}$$

and a corresponding system of eigenfunctions are given (note some homogeneity by dilation) by

$$\phi_n(x; h) = P_n(x/\sqrt{h}) e^{-x^2/h} \,.$$

Considering later more general operators, we will lose explicit expressions but we should keep in mind the following properties

- For fixed n, $\lambda_n(h)$ tends to 0 (which should be interpreted as the minimum of the function $x \mapsto V(x) = x^2$) as h tends to 0
- For fixed n, $\phi_n(x; h)$ is localized at $x = 0$.

The single well problem

We consider on $\mathbb{R}$

$$P_h := -h^2 \frac{d^2}{dx^2} + V(x)\,,$$

where

- $h > 0$ is the "semi-classical parameter.
- V is a simple well real potential with a unique non degenerate minimum x_{min},
- $\lim_{|x|\to+\infty} V(x) = +\infty$. (to simplify)

The typical examples are $V(x) = x^2$, or $V(x) = (x^2 + 1)^2$.

Under these assumptions, there is a unique selfadjoint extension of P_h (whose initial domain was $C_0^\infty(\mathbb{R})$) as an unbounded operator on $L^2(\mathbb{R})$, which has a compact resolvent. Hence there is an infinite sequence $\lambda_j(h)$ of eigenvalues tending to $+\infty$ and simple (by Sturm-Liouville theory).
As $h \to 0$,

$$\lambda_j(h) \to V(x_{min})$$

and

$$\lambda_j(h) = V(x_{min}) + (2j-1)\sqrt{V''(x_{min})/2}\, h + o_j(h)\,.$$

The philosophy is simply that we get the asymptotics as $h \to 0$ of a fixed number of eigenvalues by replacing $V(x)$ by its quadratic approximation at the minimum. Note in particular that

$$\lambda_2(h) - \lambda_1(h) = \sqrt{2V''(x_{min})}\, h + o(h)\,.$$

The double well problem

We consider on $\mathbb{R}$

$$P_h := -h^2 \frac{d^2}{dx^2} + V(x)\,,$$

where

- $h > 0$ is the "semi-classical parameter.
- V is a double well real potential with two non degenerate minima $\pm x_{min}$,
- V is symmetric $V(-x) = V(x)$
- $\lim_{|x|\to+\infty} V(x) = +\infty$.

The typical example is $V(x) = (x^2 - 1)^2$.
Notice that when considering a fixed number of eigenvalues the last condition can be replaced by

$$V(x_{min}) < \liminf_{|x|\to+\infty} V(x)\,.$$

Under these assumptions, there is a unique selfadjoint extension of P_h (whose initial domain was $C_0^\infty(\mathbb{R})$) as an unbounded operator on $L^2(\mathbb{R})$, which has a compact resolvent. Hence there is an infinite sequence $\lambda_j(h)$ of eigenvalues tending to $+\infty$ and simple (by Sturm-Liouville theory).
As $h \to 0$, $\lambda_j(h) \to \inf V$ for fixed j. Now the "exercise" in Landau-Lifschitz leads to the following result

$$\lambda_1(h) = \inf V + \sqrt{V''(x_{min})/2}h + o(h)\,.$$

$$\lambda_2(h) - \lambda_1(h) \sim ch^{-\nu} \exp -S/h\,,$$

where

$$S = \int_{-x_{min}}^{+x_{min}} \sqrt{V(x) - \inf V} dx\,.$$

Mathematically the complete proof appears only in the paper of E. Harrell in 1980 [Ha1980]. Note that

$$\lambda_3(h) - \lambda_2(h) = \sqrt{2V''(x_{min})}\, h + o(h)\,.$$

The magnetic Laplacian

We limit ourselves to the case $d = 2$ and consider the self-adjoint realization in $L^2(\mathbb{R}^2)$ of

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

where $b, h > 0$,

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

and $V \in C^\infty(\mathbb{R}^2, \mathbb{R})$.
Notice that $\mathbf{A}$ generates the constant magnetic field $\mathrm{curl}\,\mathbf{A} = 1$.
We assume that

$$V \leq 0\,, \quad \text{and} \quad \inf V < 0 \tag{2a}$$

and that

$$V \text{ is invariant by rotation by } \frac{2\pi}{n}\,. \tag{2b}$$

The symmetry $\tilde{\sigma}$ by $(x_1, x_2) \mapsto (-x_1, x_2)$ can also be considered. Note that in this case the two-form $b dx_1 \wedge dx_2$ is not preserved.

At the quantum level

$$\Sigma_n \mathcal{L}_{h,b} = \mathcal{L}_{h,b} \Sigma_n$$

where $\Sigma_n u(x) = u(g_n^{-1} x)$.
But

$$\tilde{\Sigma} \mathcal{L}_{h,b} = \mathcal{L}_{h,-b} \tilde{\Sigma}\,.$$

where $\tilde{\Sigma} u(x) = u(-x_1, x_2)$.

Coming back to the assumptions on V

Moreover, we assume that the minimum of V is attained at n non-degenerate minima and it results from the invariance property of V that these are n equidistant points of $\mathbb{R}^2 \setminus \{0\}$.

What we call the wells are the points where V attains its minimum.

Earlier results

The pure electric case where $b = 0$ was settled for any n and any d in [HelSj2-1985]. So we would like to address the case where $d = 2$, $b > 0$ and $n \geq 2$. For $n = 2$, this problem was considered in [HelSjPise1987] and revisited recently in [FSW2022, HelKa2022-23, HKS2023, Mor2023].

The paper [HelSjPise1987] follows a perturbative approach (i.e. for b relatively small) under an analytic hypothesis on the electric potential V, while the results in [FSW2022, HelKa2022-23, HKS2023, Mor2023] hold for any $b > 0$ but under the assumption that V is a superposition of radially symmetric compactly supported functions.

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

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

so we will assume henceforth that $b = 1$. Note that the symmetry assumption for V implies that $L_{h,b}$ commutes with $M(g_n)$, where

$$M(g_n)u(x) = u(g_n^{-1}x)\,.$$

The [FSW2022] Hamiltonian

We start from $\mathfrak{v}_0 \in C_c^\infty(\mathbb{R}^2)$ such that

$$\begin{cases} \mathfrak{v}_0(x) = v_0(|x|) \text{ is radial } \& \ v_0^{\min} := \min\limits_{r \geq 0} v_0(r) < 0\,, \\ \operatorname{supp} \mathfrak{v}_0 \subset \overline{D(0,a)} := \{x \in \mathbb{R}^2 \ : \ |x| \leq a\}\,, \\ U_0 := \{\mathfrak{v}_0(x) = v_0^{\min}\} = \{0\} \quad \& \quad v_0''(0) > 0\,. \end{cases} \tag{3}$$

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

$$a = a(\mathfrak{v}_0) := \inf\{r > 0 \ : \ \operatorname{supp} \mathfrak{v}_0 \subset D(0,r)\}\,. \tag{4}$$

We introduce the *double well* potential

$$V(x) = \mathfrak{v}_0(x - z^{\ell}) + \mathfrak{v}_0(x - z^{r}) \,, \tag{5}$$

where

$$z^{\ell} = \Big(-\frac{L}{2}, 0 \Big), \quad z_r = \Big(\frac{L}{2}, 0 \Big) \,. \tag{6}$$

and

$$L > 2a(\mathfrak{v}_0) \,.$$

The potential wells of V associated with the energy v_0^{min} are z_ℓ and z_r.

Consider a constant magnetic field $b > 0$, so

$$b = \mathrm{curl}\,(\mathrm{b}\mathbf{A})$$

where $\mathbf{A}$ is defined in polar coordinates (r, θ) as follows,

$$\mathbf{A}(r, \theta) = \frac{r}{2}\begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix}. \tag{7}$$

More generally, when the magnetic field is then no more constant but still radial, one should consider above the case when $r/2$ is replaced by $\phi'(r)$, where ϕ is a solution of $\Delta\phi = B = b(r) > 0$. This reads

$$\phi''(r) + \frac{1}{r}\phi'(r) = b(r)\,.$$

One has

$$\phi'(r) = \frac{1}{r}\int_0^r b(\rho)\rho\, d\rho\,. \tag{8}$$

$$\mathbf{A}(r,\theta) = \phi'(r)\begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix}\,. \tag{9}$$

The potential function considered in [FSW2022] is not analytic, thereby making our setting significantly different from the one of [HelSjPise1987]. This will induce difficulties in deriving accurate bounds on the magnitude of the tunnel effect and highlights another interesting new phenomenon related to *tunneling* under a magnetic field compared to recent results:

- by Bonnaillie-Hérau-Raymond [BonHerRay2022] (tunneling inside the boundary Γ for the Neumann realization of the Schrödinger operator with constant magnetic field in an open set Ω)
- by Fournais-Helffer-Kachmar [FoHelKa2022] (tunneling along the discontinuity Γ of a magnetic step).
- see also a recent work (ArXiv Dec. 2022) by Khaled Abou Alfa [AbAl2022] who is considering a case where the magnetic field vanishes along a curve Γ.

Of course, in these questions an assumption of symmetry (or more generally the action of a finite group) should be done leading to the existence of symmetric (mini)-wells in Γ.

Similar problems were also appearing in papers of V. Bonnaillie-Noël and collaborators (M. Dauge, S. Fournais) (tunneling in regular polygons) (see the book of Fournais-Helffer [FoHel2010] and additional references therein). But the problem is OPEN for this example but can be solved in the [FSW2022] context (see [HKS2023]).

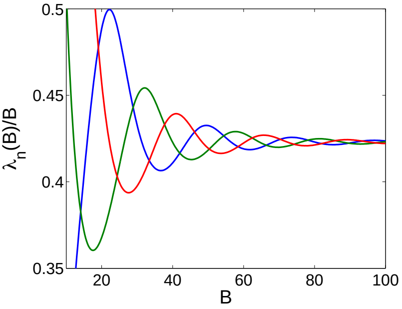


Figure: Braid structure in the case $n = 3$ associated with a magnetic flux (Bonnaillie-Dauge-Martin-Vial and Bonnaillie)

In order to exploit the connection with semi-classical analysis we consider instead

$$\mathcal{L}_h := (hD - \mathbf{A})^2 + V\,, \tag{10}$$

where $h = \lambda^{-1} \ll 1$.
With $(e_j^{\mathfrak{v}_0}(h))_{j\geq 1}$ the sequence of eigenvalues of $\mathcal{L}_h$, we will investigate the semi-classical asymptotics of

$$e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h)\,, \tag{11}$$

and prove that, if $\mathfrak{v}_0$ does not vanish in $D\big(0,a\big)$, an asymptotics of the form

$$e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h) \underset{h\to 0}{=} \exp\left(-\frac{S(\mathfrak{v}_0)+o(1)}{h}\right)$$

Our proof will be based on a mixing between what we get from the semi-classical analysis initiated in Helffer-Sjöstrand and Simon in the eighties with the approach of Fefferman-Shapiro-Weinstein.

We will also implement a recent improvement by Leo Morin [Mor2023] in order to get, for $c \neq 0$,

$$e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h) \underset{h\to 0}{=} c\, h^{\nu} \exp\left(-\frac{S(\mathfrak{v}_0)}{h}\right)$$

like in the case without magnetic field [HelSj1984, Sim1984].

Analysis of the Single well operator

Our investigation relies first on expanding the ground state $e^{\mathrm{sw}}(h)$ of the single well Hamiltonian

$$\mathcal{L}_h^{\mathrm{sw}} := (hD - \mathbf{A})^2 + \mathfrak{v}_0 \,, \tag{12}$$

under the additional assumption that $\mathfrak{v}_0$ is radial.

We show that:

Theorem OW: Existence of radial ground states and precise expansions

1. The ground state energy $e^{\mathrm{sw}}(h)$ of $\mathcal{L}_h^{\mathrm{sw}}$, is a simple eigenvalue and

$$e^{\mathrm{sw}}(h) = v_0^{\min} + h\sqrt{1 + 2v_0''(0)} + \mathcal{O}(h^{3/2})\,. \tag{13}$$

2. There exists a unique positive ground state $\mathfrak{u}_h$, with the properties
   - $\mathfrak{u}_h(x) = u_h(|x|)$ is a radial function ;
   - $\int_{\mathbb{R}^2} |\mathfrak{u}_h(x)|^2 dx = 1\,.$

Theorem continued

3. There exists a positive radial function $\mathfrak{a}_0$ on $\mathbb{R}^2$ satisfying

$$\mathfrak{a}_0(0) = \frac{1}{2}\frac{\sqrt{1+2v_0''(0)}}{\pi}\,, \tag{14}$$

and s. t. $\forall R > 0$, the ground state $\mathfrak{u}_h$ satisfies, unif. in $B(0,R)$,

$$\left| e^{\mathfrak{d}(x)/h}\mathfrak{u}_h(x) - h^{-1/2}\mathfrak{a}_0(x) \right| = \mathcal{O}(h^{1/2})\,, \tag{15}$$

where

$$\mathfrak{d}(x) = d(|x|) = \int_0^{|x|} \sqrt{\frac{\rho^2}{4} + v_0(\rho) - v_0^{\min}}\, d\rho\,. \tag{16}$$

More generally, for radial positive magnetic fields (see (8)), one will have

$$d(r) = \int_0^r \sqrt{\phi'(\rho)^2 + v_0(\rho) - v_0^{\min}}\, d\rho\,. \tag{17}$$

choosing ϕ such that $\phi'(0) = 0$.

Proof of Theorem OW

Except the "radial" statement, this is rather standard in semi-classical analysis since the works of [HelSj1984] and [Sim1983]. Let us recall the main tools.

The magnetic harmonic approximation

Consider the case where $\mathfrak{v}_0(x) = \mu|x|^2$, where μ is a positive constant. This means that we have replaced $\mathfrak{v}_0$ by its quadratic approximation at 0. The single well operator $\mathcal{L}_h^{sw}$ becomes approximated by

$$\mathcal{L}_h^{\mathrm{swap}} = (hD - \mathbf{A})^2 + \mu|x|^2 \,.$$

After rescaling[1] we get

$$\sigma(\mathcal{L}_h^{\mathrm{swap}}) = h\sigma(L_\mu^{\mathrm{mag}})$$

where

$$L_\mu^{\mathrm{mag}} = (D - \mathbf{A})^2 + \mu|x|^2 \,.$$

[1] We do the change of variable $y = h^{-1/2}x$.

We decompose the operator L_μ^{mag} via the orthogonal projections on the Fourier modes as follows

$$L_\mu^{\mathrm{mag}} \simeq \bigoplus_{m\in\mathbb{Z}} H_{m,\mu}$$

where

$$H_{m,\mu} := \pi_m L_\mu^{\mathrm{mag}} \pi_m^* = -\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} + \left(\frac{1}{4} + \mu\right) r^2 + \frac{m^2}{r^2} - m\,.$$

The min-max principle yields for $m < 0$

$$\lambda_1(H_{m,\mu}) > \inf_{u \neq 0} \frac{\left\langle \left(-\Delta + \left(\frac{1}{4} + \mu\right) |x|^2\right) u, u \right\rangle_{L^2(\mathbb{R}^2)}}{\|u\|_{L^2(\mathbb{R}^2)}} = 2\sqrt{\frac{1}{4} + \mu}\,.$$

Moreover, the rescaling $r \mapsto (1+4\mu)^{1/4} r$ yields the reduction to the unitary equivalent Landau Hamiltonian,

$$\widehat{H}_{m,\mu} = \sqrt{1+4\mu}\, H_{m,0} + \left(\sqrt{1+4\mu} - 1\right) m\,.$$

Consequently, we get

$$\inf_{m \in \mathbb{Z}} \lambda_1(H_m) = \lambda_1(H_0) = \sqrt{1+4\mu}\,, \quad \inf_{\substack{m \in \mathbb{Z} \\ m \neq 0}} \lambda_1(H_m) > \sqrt{1+4\mu}\,.$$

This implies that

$$\lambda_1(L_\mu^{\mathrm{mag}}) = \sqrt{1+4\mu}$$

is a simple eigenvalue and that its (normalized) associated eigenfunction is radial:

$$\phi_\mu^{\mathrm{mag}}(x) = \pi^{-1/2}(1+4\mu)^{1/4}\exp\left(-\frac{\sqrt{1+4\mu}}{2}|x|^2\right).$$

The case with magnetic field

Let us consider two situations.

V has a non degenerate minimum.

The first case is the case when V has a non degenerate minimum at 0. In this case the model which gives the approximation is

$$\sum_{j=1}^{n}(hD_{x_j} - A_j^0)^2 + \frac{1}{2}\langle V''(0)x \mid x\rangle \,,$$

where A_j^0 is a linear magnetic potential attached to the constant magnetic field $B_{jk} = B_{jk}(0)$,

$$A_j^0(x) = \frac{1}{2}\left(\sum_k B_{jk}x_k\right) \,,$$

so that in a suitable gauge (note that by a linear gauge, one can first reduce to the case when $A(0) = 0$) is such that $A(x) - A^0(x) = \mathcal{O}(|x|^2)$.

After the dilation $x = h^{\frac{1}{2}} y$, we get

$$h \left(\sum_{j=1}^{n} (D_{y_j} - A_j^0)^2 + \frac{1}{2} \langle V''(0) y \mid y \rangle \right) ,$$

whose spectrum can be determined explicitly (see [Mel], Hörmander (Vol III) and more specifically for this case [Mat]). One then get easily the upper bound.

2-dimensional harmonic oscillator.

Let us treat the 2-dimensional case as an exercice. [Mat] gives an alternative explicit computation (after another gauge transformation). We start from

$$D_{x_1}^2 + (D_{x_2} + Bx_1)^2 + \frac{\lambda_1}{2} x_1^2 + \frac{\lambda_2}{2} x_2^2 \ .$$

A partial Fourier transform, leads to

$$D_{x_1}^2 + (\xi_2 + Bx_1)^2 + \frac{\lambda_1}{2} x_1^2 + \frac{\lambda_2}{2} D_{\xi_2}^2 \ .$$

A dilation leads to the standard Schrödinger operator

$$D_t^2 + D_s^2 + (\sqrt{\frac{\lambda_2}{2}} s + Bt)^2 + \frac{\lambda_1}{2} t^2 \ .$$

So we have proved the isospectrality of the initial operator to a standard Schrödinger operator, with potential

$$V^{new}(s,t) = (\sqrt{\frac{\lambda_2}{2}}s + Bt)^2 + \frac{\lambda_1}{2}t^2$$

Its groundstate is immediately computed as

$$\lambda(B) = \sqrt{\lambda(0)^2 + B^2} \text{ with } \lambda(0) = \left(\sqrt{\lambda_1} + \sqrt{\lambda_2}\right)/\sqrt{2}\,.$$

On this explicit formula, one immediately observes what is called the diamagnetic effect. One also recovers the property that the ground state energy is simple.

Lower bounds.

The lower bound is obtained similarly once we have observed that

$$\Re\langle P_{h,A,V}u \mid u\rangle \\ = \sum_j \langle P_{h,A,V}\phi_j^R u \mid \phi_j^R u\rangle - h^2 \sum_{j,\ell} |||D_{x_\ell}\phi_j^R|u||^2 \,. \qquad (18)$$

Magnetic wells

We would also like to describe the rather generic case when $B(z) \in C^\infty(\overline{\Omega})$ satisfies, for some $z_0 \in \Omega$:

$$B(z) > b := B(z_0) > 0,\ \forall\, z \in \overline{\Omega} \setminus \{z_0\}, \tag{19}$$

and we assume that the minimum is non degenerate :

$$\mathrm{Hess}\, B(z_0) > 0\ . \tag{20}$$

We introduce in this case the notation :

$$a = \mathrm{Tr}\left(\frac{1}{2}\mathrm{Hess}\, B(z_0)\right)^{1/2}\ . \tag{21}$$

Theorem Helffer-Mohamed

If $A \in C^\infty(\overline{\Omega};\mathbb{R}^2)$, and if the hypotheses (19) and (20) are satisfied, then

$$\mu(h) = [b + \frac{a^2}{2b} h]h + o(h^2)\ . \qquad (22)$$

The detailed proof can be found in [HelMo1996]. It is based on the analysis of the simpler model where near 0

$$B(z) = b + \alpha x^2 + \beta y^2. \tag{23}$$

In this case, we can also choose a gauge $A(z)$ such that

$$A_1(z) = 0 \text{ and } A_2(z) = bx + \frac{\alpha}{3}x^3 + \beta xy^2 . \tag{24}$$

This has been later improved in papers by Helffer, Kordyukov, Vu Ngoc, Raymond,...
The associated tunneling effect for the corresponding magnetic double wells in analyzed in [FoMoRa2023] with techniques similar to what we will present in this course.
The radial case can get ($\alpha = \beta$) special care ! But after a gauge transform, one can again show that the ground state energy (= lowest eigenvalue) is simple !

Eigenvalue asymptotics and radial ground states

We come back to the [FSW] case.
We now have an accurate description of the spectrum of the operator $\mathcal{L}_h^{\rm sw}$ but only keeps here:

Proposition [OW1]

For every fixed $j \in \mathbb{N}$, the j'th eigenvalue of $\mathcal{L}_h^{\rm sw}$ satisfies,

$$\lambda_j(\mathcal{L}_h^{\rm sw}) = v_0^{\sf min} + h\,\lambda_j(L_\mu^{\rm mag}) + \mathcal{O}(h^{3/2}) \quad (h \to 0_+)\,,$$

with $\mu = \frac{v_0''(0)}{2}$.
Moreover, the lowest eigenvalue of $\mathcal{L}_h^{\rm sw}$ is simple with a radial ground state.

Agmon estimates

If f is a radial function, then

$$\mathcal{L}_h^{\mathrm{sw}} f = -h^2 \Delta f + \mathfrak{w} f \tag{25}$$

with

$$\mathfrak{w}(\rho) = \mathfrak{v}_0(\rho) + \frac{1}{4}\rho^2 .$$

Recall that the free Laplacian in polar coordinates reads

$$\Delta = \frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho} + \frac{1}{\rho^2}\frac{d^2}{d\theta^2} .$$

Therefore, when restricting the action of $\mathcal{L}_h^{\mathrm{sw}}$ to radial functions, we consider $\mathfrak{w}$ as the effective potential.
Hence, we can apply the semi-classical analysis relative to the Schrödinger operator without magnetic potential as considered in [HelSj1984] or [Sim1983] (see [Hel1988] or [DS1999] for a more pedagogical presentation). Another way would be to use the $(1D)$-technique but we have less developed techniques in semi-classical context (outside a huge literature in physics).

Radial case, b non constant (see (8))

More generally, we get with b non constant

$$\mathfrak{w}(\rho) = v_0(\rho) + a(\rho)^2 \,.$$

with

$$a(r) = \frac{1}{r} \int_0^r b(\rho)\rho \, d\rho \,.$$

When $v_0 = 0$, we have simply $\mathfrak{w}(\rho) = a(\rho)^2$.

Energy identity and Agmon estimates

The identity above and an integration by parts yield the following result

Proposition

For all $R > 0$, if $\phi \in C^0(\overline{D_R};\mathbb{R})$ and $u \in C^2(\overline{D_R};\mathbb{R})$ are radial functions such that ϕ is Lipschitz and $u = 0$ on ∂D_R, then

$$\int_{D_R} \left(h^2|\nabla(e^{\phi/h}u)|^2 + (\mathfrak{w} - |\nabla\phi|^2|e^{\phi/h}u|^2 \right) dx = \int_{D_R} e^{2\phi/h} u\, \mathcal{L}_h^{\mathrm{sw}} u\, dx\,.$$

Application to the decay

We have the following standard application of this proposition on the decay.

Proposition D

For all $\delta \in (0,1)$, there exist $a(\delta), C_\delta, h_0 > 0$ such that $\lim_{\delta \to 0_+} a(\delta) = 0$ and, if $\mathfrak{u}_h$ is a ground state of $\mathcal{L}_h^{\mathrm{sw}}$ and $h \in (0, h_0]$, then we have,

$$\left\| \nabla \left(e^{(1-\delta)\mathfrak{d}(x)/h} \mathfrak{u}_h \right) \right\|^2 + \left\| e^{(1-\delta)\mathfrak{d}(x)/h} \mathfrak{u}_h \right\|^2 \leq C_\delta \, e^{a(\delta)/h} \, \|\mathfrak{u}_h\|^2 \,,$$

where $\mathfrak{d}$ is the Agmon distance associated with $\mathfrak{w} - v_0^{min}$.

WKB approximation

For all $S > 0$, we introduce the set $B_{\mathfrak{d}}(S) = \{x \in \mathbb{R}^2 \ : \ \mathfrak{d}(x) < S\}$, where $\mathfrak{d}$ is the Agmon distance to 0. We can then perform the WKB construction:

Proposition WKB1

There exist $N_0 \geq 1$ and two sequences $(E_k)_{k\geq 0} \subset \mathbb{R}$ and $(\mathfrak{a}_k)_{k\geq 0} \subset C^\infty(\mathbb{R}^2)$ s. t. , for all $N \geq 1$ and $S > 0$,

$$e^{\mathfrak{d}(x)/h}\Big(\mathcal{L}_h^{\mathrm{sw}} - E^N(h)\Big)\vartheta^N = \mathcal{O}(h^{N-N_0}) \quad \text{on } B_{\mathfrak{d}}(S)\,,$$

where

$$E^N(h) = \sum_{k=0}^{N} E_k h^k\,, \quad E_0 = v_0^{\min}, \quad E_1 = \sqrt{1 + 2v_0''(0)}$$

$$\vartheta^N(x) = h^{-1/2}\left(\sum_{k=0}^{N} \mathfrak{a}_k(x) h^k\right) e^{-\mathfrak{d}(x)/h}, \quad \mathfrak{a}_0(0) = \frac{1}{2}\sqrt{\frac{1 + 2v_0''(0)}{\pi}}\,.$$

The function $\mathfrak{a}_0$ satisfies the transport equation

$$2\nabla\mathfrak{d}\cdot\nabla\mathfrak{a}_0+(\Delta\mathfrak{d}-E_1)\mathfrak{a}_0=0\,.$$

Since $\mathfrak{d}$ and $\mathfrak{a}_0$ are radial, we get

$$\mathfrak{a}_0(x)=a_0(|x|):=\frac{1}{2}\sqrt{\frac{1+2v_0''(0)}{\pi}}\exp\left(-\int_0^{|x|}f(\rho)d\rho\right)\,,$$

where

$$f(\rho)=\frac{1}{4}\frac{u'(\rho)}{u(\rho)}+\frac{1}{2\rho}-\frac{E_1}{2\sqrt{u(\rho)}}\,,$$

and

$$u(\rho)=\frac{\rho^2}{4}+v_0(\rho)-v_0^{\min}\,.$$

Proposition WKB2

There exists $N_0 \geq 1$, and for all $h \in (0, h_0]$, there exists a normalized ground state $\mathfrak{u}_h$ of $\mathcal{L}_h^{\mathrm{sw}}$ s. t. for any N and any $R > 0$ the following holds

$$\left\| e^{\mathfrak{d}(x)/h}(\mathfrak{u}_h - \vartheta^N) \right\|_{H^2(D(0,R))} = \mathcal{O}(h^{N-N_0}).$$

This ends the sketch of the proof of Theorem OW.

Coming back to the main theorem

Our "one well" theorem OW in particular clarifies the hypotheses imposed in Fefferman-Shapiro-Weinstein which states then that when

$$\mathfrak{v}_0 \leq 0 \text{ and } L > 4\left(\sqrt{|v_0^{\min}|} + a(\mathfrak{v}_0)\right)\,, \tag{26}$$

then

$$\exp\left(-\frac{L^2 + 4\sqrt{|v_0^{\min}|}L + \gamma(\mathfrak{v}_0)}{4h}\right) \leq e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h) \tag{27}$$

where $\gamma(\mathfrak{v}_0)$ is a positive constant, and

$$e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h) \leq Ch^{-5/2}\exp\left(-\frac{(L - a(\mathfrak{v}_0))^2 - a(\mathfrak{v}_0)^2}{4h}\right)\,. \tag{28}$$

The most important was here to give a lower bound (non optimal upper bounds are easy using Agmon estimates) but we will see that these estimates are far from optimal.
We will also improve the assumption on L.

Interaction matrix or hopping coefficient

The bounds above follow from the asymptotics [FSW2022]

$$e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h) \underset{h\to 0}{\sim} \left| 2 \int_{D(0,a)} \mathfrak{v}_0(x)\mathfrak{u}_h(x)\mathfrak{u}_h(x_1 + L, x_2) e^{\frac{iLx_2}{2h}}\, dx \right| \tag{29}$$

where $\mathfrak{u}_h$ is the radial ground state of $\mathcal{L}_h^{\mathrm{sw}}$.
The integral in the right hand side is called in Solid State Physics the *hopping coefficient* which can be written in a more symmetric way as

$$\mathrm{Hop}(\mathfrak{v}_0, h, L) := \int \mathfrak{v}_0(x - z_\ell)\mathfrak{u}_h(x - z_\ell)\mathfrak{u}_h(x - z_r) e^{\frac{iLx_2}{2h}}\, dx$$

Heuristics leading to the hopping coefficient

We explain first the case without magnetic field. We have two approximate states u_ℓ and u_r constructed by using u_0 eigenfunction of the one well operator with eigenvalue λ_0

$$u_\ell(x) = u_0(x - z_\ell)\,,\; u_r(x) = u_0(x - z_r)\,,$$

and we admit that "essentially" the true eigenspace is very close to the span of u_ℓ and u_r and that u_ℓ and u_r are "essentially" orthogonal. Then to compute the matrix of

$$\mathcal{L}_h - \lambda_0 = -h^2\Delta + V - \lambda_0$$

relative to this eigenspace in this "essentially orthogonal" basis, we just consider the off diagonal term

$$\langle (\mathcal{L}_h - \lambda_0)u_\ell, u_r\rangle\,.$$

But by construction

$$(\mathcal{L}_h - \lambda_0)u_\ell = v_r u_\ell\,, \text{with } v_r(x) = v_0(x - z_r)\,.$$

Note here that $u_r(x) = u_\ell(-x) = u_0(x - z_r)$.

This is no more the case in the magnetic case, where we have to use the magnetic translation for defining u_r and u_ℓ

$$u_r(x) = e^{iLx_2/2h} u_0(x - z_r)$$

$$\frac{L}{2} x_2 = \frac{L}{2} e_1 \wedge (x - z_r)\,.$$

$$u_\ell(x) = e^{-iLx_2/2h} u_0(x - z_r)$$

Interaction matrix

Under different conditions, it can be derived through a reduction to the restriction of $\mathcal{L}_h$ on a two dimensional space, yielding an *interaction matrix* like in [Hel1988] or [DS1999].
The hopping coefficient corresponds with the off diagonal term in the 2×2 interaction matrix.
The question is effectively (see at the end of the notes the details if time permit) is to measure the errors which are done in the heuristic discusssion (each time that I have written "esssentially").

Coming back to the hopping coefficient

Using the improved expansion of the ground state $\mathfrak{u}_h$, we improve the bounds on the hopping coefficient and thereby on $e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h)$ provided $\mathfrak{v}_0$ satisfies the conditions in (3).

Besides its role in capturing the tunneling asymptotics, precise estimates of the hopping coefficient (or the so-called interaction matrix) are key ingredients in the understanding of tight binding reductions in Solid State Physics (see [ShWe2022] and earlier [Out1987, Dau1994, DS1999] for mathematical contributions).

Our main result, on the eigenvalue splitting, is

[HK]-Theorem: Sharp asymptotics of the eigenvalue splitting

Under the previous assumptions, if $\mathfrak{v}_0 < 0$ in $D\big(0,a)\big)$, then we have

$$h \ln\left(e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h)\right) \underset{h\to 0}{\sim} -S(\mathfrak{v}_0)\,,$$

where $S(\mathfrak{v}_0)$ is a positive explicit constant.

Leo Morin [Mor2023] improves the result a few weeks ago by proving that

$$e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h) \underset{h\to 0}{\sim} c\, h^{\nu}\, e^{-S(\mathfrak{v}_0)/h}\,,$$

with explicit c and ν.

The formula for $S(\mathfrak{v}_0)$

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

where

$$\Psi(r,t) := d(r) + \frac{r^2+L^2}{4}(2t+1) + \frac{|v_0^{\min}|}{2}\ln\left(1+\frac{1}{t}\right) - Lr\sqrt{t(t+1)} \tag{30}$$

and

$$F(\mathfrak{v}_0) = \frac{a}{4}\sqrt{a^2+4|v_0^{\min}|} + \frac{1}{2}|v_0^{\min}|\ln\frac{\left(\sqrt{a^2+4|v_0^{\min}|}+a\right)^2}{4|v_0^{\min}|} - d(a) \tag{31}$$

Analyzing the infimum of Ψ

If $L > 2a$, then

$$\min_{(r,t)\in[0,a]\times\mathbb{R}_+} \Psi(r,t) = \Psi(a, t_a)\,,$$

where

$$t_a = \sqrt{\frac{1}{4} + s_+(a, L, v_0^{\min})} - \frac{1}{2}$$

and

$$s_+(a, L, v_0^{\min}) := \frac{2|v_0^{\min}|(L^2 + a^2) + L^2 a^2}{2(L^2 - a^2)^2} + \frac{1}{L^2 - a^2}\sqrt{\frac{(2|v_0^{\min}|(L^2 + a^2) + L^2 a^2)^2}{4(L^2 - a^2)^2} - |v_0^{\min}|^2}\,.$$

Moreover, (a, t_a) is the unique minimum of Ψ.

New formulas for $S(\mathfrak{v}_0)$

This was motivated by the discussions between the authors of [HeIKa2022-23] and [FoMoRa2023] in order to compare the formulations of [HeIKa2022-23], [HKS2023] and [Mor2023].

Lemma [HKS2023]

Assume that $L > 2a$. Let $(r_0, t_0) \in (0, L) \times \mathbb{R}_+$. Then t_0 is a critical point of Ψ with respect to t if, and only if, the following condition holds:

$$t_0 = t(r_0, L, v_0^{\text{min}}) := \sqrt{\frac{1}{4} + s(r_0, L, v_0^{\text{min}})} - \frac{1}{2} \tag{32}$$

with

$$s(r_0, L, v_0^{\text{min}}) := \frac{2|v_0^{\text{min}}|(L^2 + r_0^2) + L^2 r_0^2}{2(L^2 - r_0^2)^2} + \frac{1}{L^2 - r_0^2}\sqrt{\frac{(2|v_0^{\text{min}}|(L^2 + r_0^2) + L^2 r_0^2)^2}{4(L^2 - r_0^2)^2} - |v_0^{\text{min}}|^2}\,. \tag{33}$$

Moreover, this critical point is non degenerate.

In particular, for each $r_0 \in [a, L]$ we have

$$\Psi_{min} = \Psi(r_0, t(r_0, L, v_0^{\mathrm{min}}))$$

Hence we can play with r_0 for getting various expressions for $S(\mathfrak{v}_0)$.

Proof of the lemma

Starting with

$$\partial_t \Psi(r_0, t) := \frac{r_0^2 + L^2}{2} - \frac{|v_0^{\min}|}{2t(t+1)} - \frac{Lr_0(2t+1)}{2\sqrt{t(t+1)}}$$

we get

$$\partial_t \Psi(r_0, t) = \frac{1}{2s} g(s),$$

where $s = t^2 + t > 0$ and

$$g(s) = (L^2 + r_0^2)s - |v_0^{\min}| - Lr_0\sqrt{s}\sqrt{4s+1}.$$

The equation $g(s) = 0$ reads

$$(*) \quad (L^2 + r_0^2)s - |v_0^{\min}| = Lr_0\sqrt{s(4s+1)}.$$

This implies that a zero $\hat{s}$ of g necessarily satisfies

$$(L^2 + r_0^2)\hat{s} - |v_0^{\min}| > 0.$$

This also implies by taking the square on both sides of (*),

$$(L^2 - r_0^2)^2 \hat{s}^2 - \left(2(L^2 + r_0^2)|v_0^{\min}| + L^2 r_0^2\right)\hat{s} + |v_0^{\min}|^2 = 0\,,$$

which has two solutions $s_\pm$ of opposite sign given by explicit formulas.
Notice that, if $g(\hat{s}) = 0$, then

$$g'(\hat{s}) = \frac{(L^2 - r_0^2)^2}{(L^2 + r_0^2)\hat{s} - |v_0^{\min}|}\left(\hat{s} - \frac{2(L^2 + r_0^2)|v_0^{\min}| + L^2 r_0^2}{2(L^2 - r_0^2)^2}\right)\,.$$

So we get assuming that s_+ or s_- are zeroes of g

$$g'(s_\pm) = \pm \frac{L^2 - r_0^2}{(L^2 + r_0^2)s_\pm - |v_0^{\min}|}\sqrt{\frac{(2|v_0^{\min}|(L^2 + r_0^2) + L^2 r_0^2)^2}{4(L^2 - r_0^2)^2} - |v_0^{\min}|^2}\,.$$

At this stage we know, since $g(0) < 0$ and $\lim_{s \to +\infty} g(s) = +\infty$, that g has at least one zero and we can show that the unique zero of g is s_+.

We also get that

$$g'(s_+) > 0\,.$$

Coming back to Ψ, this yields that $\partial_t \Psi(r_0, t) = 0$ if, and only if, t satisfies

$$t^2 + t = s_+(r_0, L, v_0^{\min})$$

Solving the previous equation, we end up with a unique positive solution

$$t_0 := t_+(r_0, L, v_0^{\min}) = -\frac{1}{2} + \sqrt{\frac{1}{4} + s_+(L, r_0, v_0^{\min})}\,.$$

We get also that for all $r_0 \in [a, L)$, $t \mapsto \Psi(r_0, t)$ has a unique non degenerate minimum at $t = t_+(r_0, L, v_0^{min})$.

This will be useful later when applying Laplace integral method.

Reminder on Laplace integrals

Laplace Integral Theorem (LIT)

Let Φ be a real C^∞ phase defined in a neighborhood $\mathcal{V}$ of the closure of the ball $B(0,1)$ in $\mathbb{R}^n$ such that

- $\Phi \geq 0$ on $B(0,1)$, $\Phi > 0$ on $\partial B(0,1)$
- $\Phi(0) = \nabla\Phi(0) = 0$
- Φ has a unique non degenerate minimum at 0.

Let a be a C^∞ function defined on $\mathcal{V}$ and let us consider, for $h \in (0, h_0]$ the Laplace integral

$$I(a,\Phi,h) = \int_{B(0,1)} a(x)\, e^{-\Phi(x)/h}\, dx\,.$$

theorem continued

Then, as $h \to 0$,

$$I(a, \Phi, h) \sim h^{n/2} \sum_{j \geq 0} \alpha_j h^j \,,$$

with

$$\alpha_0 = (2\pi)^{n/2} a(0) (\mathrm{det Hess} \Phi(0))^{-1/2} \,.$$

When Φ is complex valued, holomorphic, with $\Re\Phi \geq 0$, there are similar results obtained by deformation of contour in the complex. Although we will meet Laplace integral with complex phase, we will avoid this kind of theorem or more precisely, we will use it in very special cases.

An important representation formula for the first one well eigenfunction

This is a combination of

- an observation of [FSW2022] about the solution of the Kummer equation
- the existence of a WKB expansion.

The first one is very particular and related to solutions in $[a, +\infty)$ tending to 0 at $+\infty$ of

$$-\frac{1}{r}\frac{d}{dr}r\frac{d}{dr}+\frac{r^2}{4}-\lambda\,.$$

The second one is quite general and not related to $1D$.

This leads to

Representation formula [RF1]

The radial ground state $\mathfrak{u}_h$ has the following representation for $\rho \geq a$,

$$u_h(\rho) = C_h \exp\left(-\frac{\rho^2}{4h}\right) \int_0^{+\infty} \exp\left(-\frac{\rho^2 t}{2h}\right) t^{\alpha-1}(1+t)^{-\alpha} dt\,,$$

where

$$\alpha = \frac{1}{2h}|v_0^{\min}| - \frac{1}{2}\left(\sqrt{1+2v_0''(0)} - 1\right) + \mathcal{O}(h^{1/2}) \underset{h\to 0}{\sim} \frac{1}{2h}|v_0^{\min}|\,,$$

and

$$C_h \underset{h\to 0}{\sim} C_h^{\mathrm{asy}} := \mathfrak{m}(v_0) h^{-1} \exp\left(\frac{F(\mathfrak{v}_0)}{h}\right)\,.$$

Here $a = a(\mathfrak{v}_0)$ and

$$F(\mathfrak{v}_0) = \frac{a}{4}\sqrt{a^2 + 4|v_0^{\min}|} + \frac{1}{2}|v_0^{\min}| \ln \frac{\left(\sqrt{a^2 + 4|v_0^{\min}|} + a\right)^2}{4|v_0^{\min}|} - d(a)$$

$$m(\mathfrak{v}_0) = \mathfrak{a}_0(0)\sqrt{\frac{2a|v_0^{\min}|}{\pi}}\left(a^2 + 4|v_0^{\min}|\right)^{1/4}\left(\sqrt{a^2 + 4|v_0^{\min}|} + a\right)^{-1}.$$

$$\alpha = \frac{1}{2} - \frac{1}{2h} e^{\mathrm{sw}}(h).$$

Proof

The representation is obtained in [FSW2022, Eq. (2.9)], with

$$\alpha = \frac{1}{2} - \frac{1}{2h} e^{\mathrm{sw}}(h)\,. \tag{34}$$

So the asymptotics of α is just a consequence of the harmonic approximation.

To determine the constant C_h, we have to match the WKB expansion which gives

$$u_h(a) \underset{h\to 0}{\sim} \mathfrak{a}_0(0)h^{-1/2}e^{-\frac{d(a)}{h}},$$

where $\mathfrak{a}_0(0)$ is given in (14), and what we get by applying the Laplace method to the representation formula [RF1].

So we get

$$u_h(a) \underset{h\to 0}{\sim} C_h \sqrt{\frac{2\pi h}{|v_0^{\min}|(1+2t_*(a))}}(1+t_*(a))e^{-\frac{\eta(a)}{h}} ,$$

with

$$t_*(a) = \frac{1}{2}\left(\sqrt{1+\frac{4}{a^2}|v_0^{\min}|}-1\right)$$

and

$$\eta(a) = \frac{1}{4}(1+2t_*(a))a^2 + \frac{|v_0^{\min}|}{2}\ln\left(1+\frac{1}{t_*(a)}\right) .$$

Consequently, we have

$$C_h \underset{h\to 0}{\sim} \frac{\sqrt{|v_0^{\min}|(1+2t_*(a))}}{\sqrt{2\pi}(1+t_*(a))} h^{-1} e^{-\frac{d(a)-\eta(a)}{h}}$$

which eventually yields the announced formula.

Second representation formula for the hopping coefficient

We recall that

$$\mathrm{Hop}(\mathfrak{v}_0, h, L) := \int \mathfrak{v}_0(x - z_\ell)\mathfrak{u}_h(x - z_\ell)\mathfrak{u}_h(x - z_r)e^{\frac{iLx_2}{2h}}\, dx$$

We start by expressing the hopping coefficient in polar coordinates

$$\mathrm{Hop}(\mathfrak{v}_0, h, L) = \int_0^a r\, v_0(r)u_h(r)\left(\int_0^{2\pi} K_h(r,\theta)d\theta\right) dr\,, \qquad (35)$$

where

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

After a gauge transformation u_h represents the "left" approximate eigenfunction (localized at $r = 0$) and K_h the " right" eigenfunction.

Note that with the assumption on v_0, it is the same to integrate over $(0, a)$ or over $(0, +\infty)$.

The integral of K_h with respect to θ is computed in [FSW2022, Prop. 5.1] as follows

$$\int_0^{2\pi} K_h(r,\theta)d\theta = C_h \exp\left(-\frac{r^2+L^2}{4h}\right)\int_0^{+\infty} G_h(r,t)dt\,, \tag{36}$$

where

$$G_h(r,t) = \exp\left(-\frac{(r^2+L^2)t}{2h}\right)t^{\alpha-1}(1+t)^{-\alpha}I_0\left(\frac{Lr\sqrt{t(t+1)}}{h}\right) \tag{37}$$

and

$$z \mapsto I_0(z) = \frac{1}{2\pi}\int_0^{\pi} e^{z\cos\theta}d\theta\,.$$

The advantage of the second representation formula is the absence of the oscillatory complex term and moreover, the integrand G_h is a positive function.
The function $I_0(z)$ has (by Theorem [LIT]) the following asymptotic for large $z > 0$,

$$I_0(z) \underset{z \to +\infty}{\sim} \frac{e^z}{\sqrt{2\pi z}} \,.$$

In addition we have the universal upper bound

$$I_0(z) \leq e^z \,.$$

The complex term disappears by using the following formula, for $\beta > \xi$

$$\int_0^{2\pi} \exp(i\xi \sin\theta + \beta\cos\theta)\, d\theta = \int_0^{2\pi} \exp(-\sqrt{\beta^2 - \xi^2}\cos\theta)\, d\theta\,,$$

which is obtained by translation in the complex.
Let us observe for later that we get similar formulas by partial differentiation with respect to β or ξ.

Third representation formula

As observed by [FoMoRa2023] and exploited in [Mor2023], it is better to come back to the trick appearing in [HelSj1984] and in the magnetic case in [HelSjPise1987].
Here we have the simplification that we can avoid to introduce a cut-off since our approximate eigenfunctions are defined in $\mathbb{R}^2$.

If we consider an open set Ω containing $B(z_\ell, a)$ and with empty intersection with $B(z_r, a)$ and denote its boundary by $\Sigma = \partial\Omega$, we can always write [HM2]

$$Hop(L, v_0) = ih \int_\Sigma \Big(u_\ell \cdot \overline{(-ih\nabla - A)u_r \cdot \vec{n}} + \overline{u_r} \cdot (-ih\nabla - A)u_\ell \cdot \vec{n} \Big) d\sigma \,,$$

where $\vec{n}$ is the outward normal to Σ.
Notice that the left hand side is independent of Σ, hence we have the freedom for the choice of Σ.
There are two natural choices for Σ:

- Take the line $x_1 = 0$ with in mind the symmetry $(x_1, x_2) \mapsto (-x_1, x_2)$
- Use the radial character of say the "left" u_ℓ and consider $\Omega = B(z_\ell, R)$ and polar coordinates centered on z_ℓ

L. Morin [Mor2023] takes the first choice. In continuation of [HelKa2022-23], we will consider below the second choice.

Application

As mentioned above, after an integration by parts, we get for $r = R$ an integral over the circle of radius R with $R \in [a, L - a)$ and consider radial coordinates centered at z_ℓ.
Choosing the natural gauge, $\vec{A}$ is tangent to Σ and $\vec{n} \cdot \nabla = \frac{d}{dr}$.

Hence the hopping matrix appears as the sum of the three terms

1.
$$Rhu_h'(R)\int_0^{2\pi} u_h(\sqrt{R^2+L^2+2LR\cos\theta})e^{\frac{iR\sin\theta}{2h}}\,d\theta$$

2.
$$-Ru_h(R)\int_0^{2\pi}(R+L\cos\theta)(\frac{h\,u_h'}{r})(\sqrt{R^2+L^2+2LR\cos\theta})e^{\frac{iR\sin\theta}{2h}}\,d\theta$$

3.
$$R^2u_h(R)\int_0^{2\pi}\sin\theta\, u_h(\sqrt{R^2+L^2+2LR\cos\theta})e^{\frac{iR\sin\theta}{2h}}\,d\theta$$

One also has to verify that there are no cancellation for the main term. A natural choice for the choice of R could be $R=L/2$. Note nevertheless that the two first terms are not symmetric.

We now show that we can proceed essentially like in the [FSW2022] or [HelKa2022-23] approach with the simplification that we have no integration with respect to r.
Considering the first term, we will use the semi-classical approximation of $u_h(R)$ and use the second representation formula for

$$\int_0^{2\pi} u_h(\sqrt{R^2 + L^2 + 2LR\cos\theta})e^{\frac{iR\sin\theta}{2h}}\,d\theta = \int_0^{2\pi} K_h(R,\theta)d\theta\,.$$

Following the [HelKa2022-23] previous proof, we proceed in three steps

- Go back to a Laplace integral with real phase
- Apply the Laplace method with respect to θ
- Apply the Laplace method with the phase $t \mapsto \Psi(R,t)$.

Let us have a look at the other terms.

1. $$\int_0^{2\pi} \left(\frac{h\, u_h'}{r}\right)\left(\sqrt{R^2 + L^2 + 2LR\cos\theta}\right) e^{\frac{iR\sin\theta}{2h}}\, d\theta$$

2. $$\int_0^{2\pi} \cos\theta \left(\frac{h\, u_h'}{r}\right)\left(\sqrt{R^2 + L^2 + 2LR\cos\theta}\right) e^{\frac{iR\sin\theta}{2h}}\, d\theta$$

3. $$\int_0^{2\pi} \sin\theta\, u_h \left(\sqrt{R^2 + L^2 + 2LR\cos\theta}\right) e^{\frac{iR\sin\theta}{2h}}\, d\theta$$

For the first case, the difference is that u_h is replaced by hu_h'/r. Coming back to the. representation formula for u_h which reads

$$u_h(\rho) = C_h \int_0^{+\infty} \exp\left(-\frac{\rho^2(2t+1)}{4h}\right) t^{\alpha-1}(1+t)^{-\alpha} dt\,,$$

we get

$$hu_h'(\rho)/\rho = -\frac{1}{2} C_h \int_0^{+\infty} \exp\left(-\frac{\rho^2(2t+1)}{4h}\right) (2t+1) t^{\alpha-1}(1+t)^{-\alpha} dt\,,$$

We can then proceed as before (only the amplitude in the Laplace integral has changed).

For the second term, another change is the presence of $\cos\theta$ in the integration with respect to θ. Here we have to verify that the complex phase disappears as previously and come back to the [FSW2022] lemma. The complex term disappears by using the following formula

$$\int_0^{2\pi} \cos\theta \exp(i\xi\sin\theta + \beta\cos\theta)\, d\theta \\ = -\int_0^{2\pi} \frac{\beta}{(\beta^2-\xi^2)^{\frac{1}{2}}} \cos\theta \exp(-\sqrt{\beta^2-\xi^2}\cos\theta)\, d\theta\,,$$

which is obtained by partial differentiation with respect to β. Again we can continue with the main analysis. Only the amplitude has changed

For the third term, the change is the presence of $\sin\theta$ in the integration with respect to θ. Here we have the following formula

$$\int_0^{2\pi} \sin\theta \exp(i\xi\sin\theta + \beta\cos\theta)\,d\theta \\ = \int_0^{2\pi} \frac{\xi}{(\beta^2-\xi^2)^{\frac{1}{2}}} \cos\theta \exp(-\sqrt{\beta^2-\xi^2}\cos\theta)\,d\theta\,,$$

which is obtained by partial differentiation with respect to ξ. Again we can continue with the main analysis. Only the amplitude has changed !

Conclusion for the hopping coefficient

If $L > 2a$, we get the Morin's result for the hopping coefficient.
To solve the initial question, we have to control the errors.

A general abstract result.

Following [HelSj1984, HelSj2-1985] and [HKS2023], we try to present an abstract procedure permitting to treat the previous case and many other cases with symmetry.
Here the goal in the application is to determine under which condition on L (the distance between the wells) the error estimate appears to be small in comparison with respect to the main term in the semi-classical limit.
The conjecture is that $L > 2a$ is enough.

- [FSW2022, HelKa2022-23] gets the condition $L > 4(\sqrt{|v^{min} + a})$.
- We prove in [HKS2023] the result under condition $L > 4a$.
- Using the more accurate approach of [HKS2023] which will be presented below, we get, as announced in [Mor2023], the result under the condition $L \geq (2 + \sqrt{3})a$.

About approximation of the interaction matrix

Consider a Hilbert space H endowed with an inner product $\langle\cdot,\cdot\rangle$ and a family of self-adjoint unbounded operators

$$T_h : D_h \to H,\ h \in (0,1]\,.$$

Assume furthermore that 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.

We work under additional assumptions on the operators $(T_h)_{h\in(0,1]}$. This involves our family of approximate eigenfunctions.

Assumption H1

Let $n \geq 2$ be an integer. There exist positive constants $\mathfrak{S}_1, \mathfrak{S}_2, \mathfrak{S}_3, c, p, q$ and $h_0 \in (0,1]$ such that $p < q$ and for all $h \in (0, h_0]$, there exists a subspace $E_h = \mathrm{Span}(u_{h,1}, \dots, u_{h,n}) \subset D_h$ such that:

1. $\max_{1\leq i\leq n} \| T_h u_{h,i} \| = \mathcal{O}(e^{-\mathfrak{S}_1/h})$.
2. $\langle u_{h,i}, u_{h,j}\rangle = \begin{cases} 1 + \mathcal{O}(e^{-\mathfrak{S}_2/h}) & i = j, \\ \mathcal{O}(e^{-\mathfrak{S}_3/h}) & i \neq j. \end{cases}$
3. $\lambda_1(h) \geq -ch^q$.
4. $\lambda_{n+1}(h) \geq c\, h^p$.

It results from the assumption above that $\dim(E_h) = n$ for h small enough. We can prove that the operator T_h has precisely n eigenvalues that are *exponentially small* in h, and that there is a gap to $\lambda_{n+1}(h)$.

Proposition A1

There exist positive constants C, h_1 such that, for $h \in (0, h_1]$,

$$\lambda_n(h) \leq C e^{-\mathfrak{S}_1/h}. \tag{38}$$

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

Toward the measure of the error

We want to link the quasi mode constructions $\{u_{h,j}\}$ to the low-lying eigenvalues of T_h. To do this, we show that the symmetric matrix

$$\mathfrak{U}_{j,k} = \langle T_h u_{h,j}, u_{h,k} \rangle,$$

does not differ much (component-wise) from the matrix $\mathfrak{W}_h$ that is the restriction of T_h to the eigenspace

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

written in an orthonormal basis.

We 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 [H1], it will follow that the $\{v_{h,j}\}$ are linearly independent, and thus constitute a basis for F_h.

Proposition A2

For $h > 0$ sufficiently small, we have $\mathrm{dim}(F_h) = n$, 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

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

Reduction to a matrix through a suitable orthonormal basis

The aim 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 $\mathfrak{W}_h$ will be the matrix of T_h restricted to F_h, written in this new basis $\{w_{h,j}\}$.

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

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

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 $\mathcal{V}_h = \{w_{h,1}, \dots, w_{h,n}\}$ of F_h

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

We consider the restriction of T_h to the space F_h and denote by $\mathfrak{W}_h = (\mathsf{w}_{ij})_{1 \le i,j \le n}$ its matrix in the basis $\mathcal{V}_h$, so

$$\mathfrak{W}_{ij} = \langle T_h w_{h,i}, w_{h,j} \rangle .$$

The matrix $\mathfrak{W}_h$ is hermitian, with eigenvalues $\{\lambda_1(h), \dots, \lambda_n(h)\}$.

The next proposition controls how $\mathfrak{W}_h$ is approximated by the matrix $\mathfrak{U}_h$.

Proposition A3

Let

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

Then the symmetric "error" matrix satisfies

$$\mathfrak{R}_h := \mathfrak{W}_h - \mathfrak{U}_h, = \mathcal{O}(\varepsilon_h)\,.$$

An immediate consequence of Proposition [A3] is an improved lower bound on the lowest eigenvalue $\lambda_1(h)$.

Corollary [C]

There exist positive constants C, h_1 such that, for $h \in (0, h_1]$,

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

Implementing invariance assumptions

Our task is to analyze the case when the matrix $\mathfrak{W}_h$ of $T_h|_{F_h}$ enjoys certain invariance properties. 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 [Ha1980] and later extended to the multiple wells case in [HelSj1984, HelSj2-1985, Sim1983, Sim1984].
Here we mainly follow in a more abstract way [HelSj2-1985] and the heuristic presentation given in [FoHel2010]. 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 previous assumptions, we assume

Symmetry Assumption [H2]

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 $1 \leq i \leq n-1$.

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

$$\rho_0(a_n) := g_n$$

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

$$\big(M(g_n)u\big)(x) = u(g_n^{-1}x). \tag{39}$$

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 we can then write in this case

Assumption [H2bis]

1. $\Omega \subset \mathbb{R}^2$ is a domain invariant by G 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 $1 \leq i \leq n-1$.

Proposition A4

Under the symmetry assumption [H2], the orthonormal basis $\mathcal{V}_h = \{w_{h,1}, \ldots, w_{h,n}\}$ of F_h satisfies,

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

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

$$\tau_{j,k} = \delta_{j+1,k} \text{ for } 1 \leq j, k \leq n \tag{40}$$

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

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

The property that the operator T_h commutes with $\rho(a)$ implies that

$$\mathfrak{W}_h = \sum_{k=0}^{n-1} I_k(h)\tau^k, \qquad (41)$$

for some coefficients $I_0(h), \ldots, I_{n-1}(h) \in \mathbb{C}$.

The Hermitian property of $\mathfrak{W}_h$ gives, in addition,

$$I_0(h) \in \mathbb{R}\,,\; I_k(h) = \overline{I_{n-k}(h)} \;\text{ for } k = 1, \ldots, n-1\,. \qquad (42)$$

Notice that the matrix $\mathfrak{U}_h$ satisfies the same properties as $\mathfrak{W}_h$. Hence we can also write

$$\mathfrak{U}_h = \sum_{k=0}^{n-1} J_k(h)\tau^k \,, \tag{43}$$

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

$$J_0(h) \in \mathbb{R}\,,\; J_k(h) = \overline{J_{n-k}(h)} \;\text{ for } k = 1, \ldots, n-1\,. \tag{44}$$

All these invariant matrices ($\mathfrak{W}_h$ or $\mathfrak{U}_h$) share the property to be diagonalizable in the same orthonormal basis of eigenfunctions ϵ_k $(k = 1, \ldots, n)$ whose coordinates in our selected basis are given by

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

It is then easy to compute the corresponding eigenvalues.

$n = 3$

$\mathfrak{W}_h$ assumes the form

$$\mathfrak{W}_h = \begin{pmatrix} l_0 & \overline{l_1} & l_1 \\ l_1 & l_0 & \overline{l_1} \\ \overline{l_1} & l_1 & l_0 \end{pmatrix}$$

with $l_1 = \rho e^{i\theta}$, $\rho \geq 0$, $\theta \in [0, 2\pi)$. This matrix has three eigenvalues

$$\mu_k = l_0 + 2\rho \cos\left(\theta + (k-1)\frac{2\pi}{3}\right), \quad k \in \{1, 2, 3\}. \tag{45}$$

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 $(x_1, x_2) \mapsto (-x_1, -x_2)$. We get

$$\lambda_2(h) - \lambda_1(h) = 2|J_1(h)| + o\big(|J_1(h)|\big). \tag{46}$$

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

Let $I_0(h), I_1(h)$ as before and let us write

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

Then, we have a relabeling $\mu_1(h), \mu_2(h)$, $\mu_3(h)$ of $\lambda_1(h), \lambda_2(h)$, $\lambda_3(h)$

Moreover,

$$I_0(h) = J_0(h) + \mathcal{O}(\delta_h), \quad I_1(h) = J_1(h) + \mathcal{O}(\delta_h) \sim J_1(h) \qquad (47a)$$

with

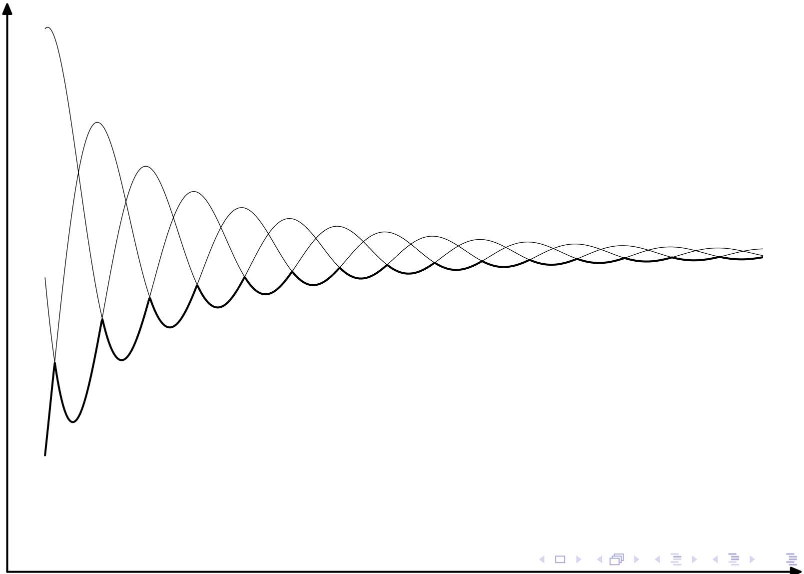
$$J_0(h) = \langle T_h u_{h,1}, u_{h,1} \rangle, \quad J_1(h) = \langle T_h u_{h,1}, u_{h,2} \rangle. \qquad (47b)$$

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 $\theta(h)$.

A schematic figure of eigenvalues with a braid structure, occurring in the presence of trilateral symmetry.



Additional hypothesis

We can strengthen the estimate of Λ_h if we assume additionally that

Assumption [H3]

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

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

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

and

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

Proposition A5

There exist positive constants $C, h_0 > 0$ such that if [H1]-[H3] holds, then for all $h \in (0, h_0]$, the symmetric matrix $\mathfrak{R}_h = (\mathfrak{r}_{ij})$ satisfies

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

Application to [FSW]

Proposition A6

Let T_h and $\lambda(h)$ corresponding to the [FSW2022] operator minus the ground state energy of the one well problem $\lambda_1(\mathcal{L}_h^{\rm sw}$. The conditions hold with the following choices:

1. $L > (2+\sqrt{3})a$
2. $u_{h,1} = u_{h,\ell}$, $u_{h,2} = u_{h,r}$;
3. any constants $\mathfrak{S}_1, \mathfrak{S}_2, \mathfrak{S}_3, p, q$ satisfying

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

where $\hat{S}_a$ can be explicitly computed.

This achieves, using the asymptotics of J_1 the proof of the announced result of [Mor2023] (improving [FSW2022] and [HelKa2022-23]) and their extension to a larger number of wells [HKS2023].

$$e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h) \underset{h\to 0}{=} c\, h^{\nu} \exp\left(-\frac{S(\mathfrak{v}_0)}{h}\right)$$

MERCI !

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