Semiclassical methods and tunneling effects. a minicourse (6 hours) at the Mittag-Leffler Institute

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Overall abstract

In 1982-1983 the so-called symmetric double well problem was rigorously analyzed in any dimension in the semi-classical context by B. Simon (announced in 1982) and Helffer-Sjöstrand (1983). This involves semi-classical Agmon estimates, WKB constructions and a very fine analysis of the so-called tunneling effect in order to establish the splitting between the lowest eigenvalues.
The strategy followed by Helffer-Sjöstrand appears to be quite efficient in many other contexts. After recalling how it works on the initial double well problem, we will focus on the Robin problem for the Laplacian in a domain where in some asymptotic regime for the Robin parameter and some specific symmetric domain (ellipse like domain) a double well appears.

We will also discuss the case of the magnetic Laplacian with large constant magnetic field in a similar domain. The optimal result in this case is still open.
The results correspond to contributions by various subsets of the following set of authors : Bonnaillie, Fournais, Helffer, Hérau, Kachmar, Morame, Pankrashkin, Popoff, Raymond, Sjöstrand,....

Various books are devoted to semi-classical analysis. I would like to mention in the domain of mathematics

- D. Robert. Autour de l'approximation semi-classique.
- B. Helffer
- Cycon-Froese-Kirsch-Simon
- P. Hislop and I. Sigal
- A. Grigis and J. Sjöstrand
- M. Dimassi and J. Sjöstrand
- A. Martinez
- M. Zworski
- N. Raymond

and for the extremely courageous students or researchers the monster book of V. Ivrii.
Concerning semi-classical methods in superconductivity, there is also the book of Fournais-Helffer (evolutive book on line).

Agmon estimates.

Since the proof of his estimates controlling the decay of eigenfunctions for N-body Schrödinger operators by Agmon was diffused at the end of the seventies, a lot of applications and variants have been found, particularly in the context of semi-classical analysis.

- Decay at $+\infty$. Combes-Thomas, Agmon, Carmona-Simon
- Agmon estimates in semi-classical analysis Simon and Helffer-Sjöstrand.
- Comparison eigenfunction–quasi-mode
- Application to tunneling
- Resonant wells
- Agmon estimates and magnetic Schrödinger operators.

Agmon estimates continued

- Agmon estimates in tight-binding (Daumer,..)
- Agmon estimates and pseudo-differential operators: Klein-Gordon, Dirac, Kac, Harper,... Discrete operators..
- Microlocal Agmon estimates
- Magnetic bottles.
- Decay estimates in superconductivity
- Decay estimates for the Robin problem.
- Agmon estimates and Landscape function.

Introduction of Carmona-Simon

We start from the introduction of the paper of Carmona-Simon (1981). The results of Agmon are known at this time [Ag1] but some are unpublished [Ag2]. Hence we learn Agmon's result through this paper.

This paper is a contribution to the large literature on the decay at infinity of eigenvectors of Schrödinger operators $-\Delta + V$, *associated to discrete spectrum Many references given. For the leading behavior of the ground state,* ϕ, *our results are definitive in the sense that we will show that:*

$$\lim_{|x|\to+\infty} -\frac{\log \phi(x)}{\rho(x)} = 1\,,$$

for an explicit function ρ *and for a large class of potentials,* V, *including general* N*-body systems.*

The upper bounds implicit above are not new: for multiparticle systems, they were found in successively more general cases by Mercuriev (1974), Deift et al., and Hoffman-Ostenhoff et al. (atoms with infinitely heavy nucleus)(1977) in the seventies and Agmon [Ag1] (1979) in the general case; for potentials going to infinity at infinity they were found by Lithner [32] (1964) and rediscovered by Agmon [Ag1]. The Lithner-Agmon upper bounds are only proven to hold in some average sense, but it is easy to get pointwise bounds with minor extra restrictions on V.
Our primary goal here will be to find lower bound complementary to these various upper bounds which show that the upper bounds are "best possible". A major source of motivation for the approach we use is the part of Agmon's work [Ag1] which identifies the function ρ.

Let us initially describe the situation for the case $V \to +\infty$*,* $V \geq 1$ *and continuous, a case treated by Lithner, with a related intuition. Agmon finds a sufficient condition for:*

$$|\phi(x)| \leq c_\epsilon \exp(1-\epsilon)\rho(x)\,,\ \forall \epsilon > 0\,,$$

is the condition

$$|\nabla \rho(x)|^2 \leq V(x)\,.$$

Related conditions were found using the Combes-Thomas method [CT] (1973).

Agmon estimates in the semi-classical context 1982-84

The application of Agmon estimates in semi-classical analysis appears chronologically along 1983 in three papers: one announcement by B. Simon [44], one preprint by Helffer-Sjöstrand [HS1] and a detailed version of his announcement by B. Simon [45] (the two last ones appear in 1984).

Energy inequalities

The main but basic tool is a very simple identity attached to the Dirichlet realization of the Schrödinger operator

$$P_{h,V} : -h^2\Delta + V\,,$$

where V is assumed to be non negative.

Proposition: Energy identity

Let Ω be a bounded open domain in $\mathbb{R}^m$ with C^2 boundary. Let $V \in C^0(\bar{\Omega};\mathbb{R})$, and ϕ a real valued lipschitzian function on $\bar{\Omega}$. Then, for any $u \in C^2(\bar{\Omega};\mathbb{R})$ with $u_{/\partial\Omega} = 0$, we have

$$\begin{array}{c}\int_\Omega |h\nabla(\exp\frac{\phi}{h}\,u)|^2\,dx + \int_\Omega (V - |\nabla\phi|^2)\exp\frac{2\phi}{h}\,|u|^2\,dx = \\ \int_\Omega \exp\frac{2\phi}{h}\,(P_{h,V}\,u)(x)\cdot u(x)\,dx\,.\end{array} \qquad (1)$$

Under some conditions on V, we can also take $\Omega = \mathbb{R}^n$. Note that the identity is universal and this is only later that we have to play with the semi-classical parameter.

Another direction initiated by Agmon was to analyze the asymptotic behavior as $|x| \to +\infty$.

Immediate applications

If u_h is an eigenfunction of $P_{h,V}$ with eigenvalue λ_h, we get:

$$\int_\Omega |h\nabla(\exp \frac{\phi}{h}\, u_h)|^2\, dx + \int_\Omega (V - |\nabla\phi|^2 - \lambda_h) \exp \frac{2\phi}{h}\, |u_h|^2\, dx = 0\,, \tag{2}$$

which implies the simple estimate

$$\int_\Omega (V - |\nabla\phi|^2 - \lambda_h) \exp \frac{2\phi}{h}\, |u_h|^2\, dx \leq 0\,, \tag{3}$$

or the weaker, assuming that $\lambda_h \leq E$,

$$\int_\Omega (V - |\nabla\phi|^2 - E) \exp \frac{2\phi}{h}\, |u_h|^2\, dx \leq 0\,. \tag{4}$$

This is true for any ϕ. Hence the question is to determine if there is a clever choice for ϕ.

The Agmon distance

The Agmon metric attached to an energy E and a potential V is defined as $(V - E)_+ dx^2$ where dx^2 is the standard metric on $\mathbb{R}^n$. This metric is degenerate and is identically 0 at points living in the "classical" region: $\{x \mid V(x) \leq E\}$. Associated to the Agmon metric, we define a natural distance

$$(x, y) \mapsto d_{(V-E)_+}(x, y)$$

by taking the infimum :

$$d_{(V-E)_+}(x, y) = \inf_{\gamma \in \mathcal{C}^{1,pw}([0,1];x,y)} \int_0^1 [(V(\gamma(t)) - E)_+]^{\frac{1}{2}} |\gamma'(t)| dt \,, \tag{5}$$

where $\mathcal{C}^{1,pw}([0, 1]; x, y)$ is the set of the piecewise (pw) C^1 paths in $\mathbb{R}^n$ connecting x and y. When there is no ambiguity, we shall write more simply $d_{(V-E)_+} = d$.

Similarly to the Euclidean case, we obtain the following properties

- Triangular inequality

$$|d(x',y) - d(x,y)| \leq d(x',x)\ ,\ \forall x, x', y \in \mathbb{R}^m\ . \qquad (6)$$

- $$|\nabla_x d(x,y)|^2 \leq (V-E)_+(x)\ , \qquad (7)$$

  almost everywhere.

We observe that the second inequality is satisfied for any derived distance like

$$d(x,U) = \inf_{y\in U} d(x,y)\ .$$

If $U = \{x \mid V(x) \leq E\}$, $d(x,U)$ measures the distance to the classical region.
All these notions being expressed in terms of metrics, they can be easily extended on manifolds.

Decay of eigenfunctions.

When u_h is a normalized eigenfunction of the Dirichlet realization in Ω satisfying $P_{h,V} u_h = \lambda_h u_h$ then the energy identity gives roughly that $\exp \frac{\phi}{h}\, u_h$ is well controlled (in L^2) in a region

$$\Omega_1(\epsilon_1, h) = \{x \mid V(x) - |\nabla\phi(x)|^2 - \lambda_h > \epsilon_1 > 0\}\,,$$

by $\exp\left(\sup_{\Omega\setminus\Omega_1} \frac{\phi(x)}{h}\right)$. The choice of a suitable ϕ (possibly depending on h) is related to the Agmon metric $(V - E)_+\, dx^2$, when $\lambda_h \to E$ as $h \to 0$.

The typical choice is $\phi(x) = (1-\epsilon)d(x)$ where $d(x)$ is the Agmon distance to the "classical" region $\{x \mid V(x) \leq E\}$. In this case we get that the eigenfunction is localized inside a small neighborhood of the classical region and we can measure the decay of the eigenfunction outside the classical region by

$$\exp(1-\epsilon)\frac{d(x)}{h}\, u_h = \mathcal{O}(\exp\frac{\epsilon}{h})\,, \tag{8}$$

for any $\epsilon > 0$.

More precisely we get for example the following theorem

Theorem: localization of eigenfunctions

Let us assume that V is C^∞, semibounded and satisfies

$$\lim \inf_{|x|\to\infty} V > \inf V = 0 \tag{9}$$

and

$$V(x) > 0 \text{ for} |x| \neq 0\ . \tag{10}$$

Let u_h be a (family of L^2-) normalized eigenfunctions s.t.

$$P_{h,V} u_h = \lambda_h u_h\ , \tag{11}$$

with $\lambda_h \to 0$ as $h \to 0$. Then for all ϵ and all compact $K \subset \mathbb{R}^m$, there exists a constant $C_{\epsilon,K}$ s.t. for h small enough

$$||h\nabla(\exp \frac{d}{h} \cdot u_h)||_{L^2(K)} + ||\exp \frac{d}{h} \cdot u_h||_{L^2(K)} \leq C_{\epsilon,K} \exp \frac{\epsilon}{h}\ . \tag{12}$$

Remark

When V has a unique non degenerate minimum the estimate can be improved when $\lambda_h \in [0, C_0 h]$, by taking

$$\phi = d - Ch \inf(\log(\frac{d}{h}), \log C)\,.$$

We observe indeed that V, d and $|\nabla d|^2$ are equivalent in the neighborhood of the well.

A universal approach to Agmon estimates

For some problems, it could be useful to have an estimate with a universal control independent of the structure of the wells. We start from the energy identity.

$$\int_\Omega |h\nabla(\exp\frac{\phi}{h}\, u)|^2\, dx + \int_\Omega (V - |\nabla\phi|^2 - \lambda)\exp\frac{2\phi}{h}\, |u_h|^2\, dx = 0\,,$$

where u is an eigenfunction corresponding to the eigenvalue $\lambda > \inf V$.

We introduce the free positive parameter $\delta > 0$ and consider the set

$$U_\delta(\lambda) = \{x, V(x) < \lambda + \delta\}\,.$$

We take as ϕ

$$\phi_\delta := d^\delta(x, U_\delta(\lambda))\,,$$

where d^δ denotes the Agmon distance relative to $(V - \lambda - \delta)_+ dx^2$.

Then we rewrite the energy identity in the following way:

$$\int_\Omega |h\nabla(\exp \tfrac{\phi}{h}\, u)|^2\, dx + \int_{\Omega\setminus U_\delta(\lambda)} (V - |\nabla\phi|^2 - \lambda) \exp \tfrac{2\phi}{h}\, |u_h|^2\, dx$$
$$= \int_{U_\delta(\lambda)} (-V + |\nabla\phi|^2 + \lambda) \exp \tfrac{2\phi}{h}\, |u_h|^2\, dx\,.$$

Using our choice of ϕ, this immediately leads to

$$\int_\Omega |h\nabla(\exp \tfrac{\phi}{h}\, u)|^2\, dx + \delta \int_{\Omega\setminus U_\delta(\lambda)} |u_h|^2\, dx$$
$$\leq (\lambda - \inf V) \int_{U_\delta(\lambda)} |u_h|^2\, dx\,.$$

We finally keep it in the form, for any $\delta > 0$, we have

$$\int_{\Omega\setminus U_\delta(\lambda)} |u_h|^2 \exp \frac{2\phi_\delta}{h}\, dx \leq \frac{1}{\delta}(\lambda - \inf V) \int_\Omega |u_h|^2\, dx\,. \qquad (13)$$

We emphasize that at this stage, the estimate is universal with no assumptions on the wells.

To get back the previous estimates, we have then to choose δ and to compare $\phi_\delta(x)$ with $d(x)$. Here we can meet suitable assumptions on the potential in the neighborhood of its infimum.

First application

We can compare different Dirichlet problems corresponding to different open sets Ω_1 and Ω_2 containing a unique well U attached to an energy E. If for example $\Omega_1 \subset \Omega_2$, one can prove the existence of a bijection b between the spectrum of $P_{(h,\Omega_1)}$ in an interval $I(h)$ tending (as $h \to 0$) to E and the corresponding spectrum of $P_{(h,\Omega_2)}$ s.t. $|b(\lambda) - \lambda| = \mathcal{O}(\exp -S/h)$ (under a weak assumption on the spectrum at $\partial I(h)$).
Here S is chosen s.t.

$$0 < S < d_{(V-E)_+}(\partial\Omega_1, U)\ .$$

This can actually be improved (using more sophisticated perturbation theory) as $\mathcal{O}(\exp -2S/h)$.

Second application: the symmetric double well problem

As discussed above, the double well problem in dimension ≥ 2 was first discussed in the note [44] immediately followed by the two detailed papers [HS1] and [45].

There is a huge litterature in (1D) including an exercise in Landau-Lipschitz, the book by Fröman-Fröman (1960), the french group in Marseille around J.M. Combes and the detailed mathematical proof for the tunneling by E. Harrell (1978) [10]. Agmon estimates are not needed because one can work directly with WKB solutions and the theory of ordinary differential equations.

Harmonic approximation–rough localization

We discuss one of the basic technics for analyzing the groundstate energy (also called lowest eigenvalue or principal eigenvalue) of a Schrödinger operator in the case the electric potential V has non degenerate minima.

Upper bounds

We start with the simplest one-well problem:

$$P_{h,v} := -h^2 d^2/dx^2 + v(x) \ , \tag{14}$$

where v is a C^∞- function tending to ∞ and admitting a unique minimum at 0 with $v(0) = 0$.
Let us assume that

$$v''(0) > 0 \ . \tag{15}$$

In this very simple case, the harmonic approximation is an elementary exercise. We start with the harmonic oscillator attached to 0 :

$$-h^2d^2/dx^2+\frac{1}{2}v''(0)x^2\,. \tag{16}$$

This means that we replace the potential v by its quadratic approximation at 0 $\frac{1}{2}v''(0)x^2$ and consider the associated Schrödinger operator.
Using the dilation $x = h^{\frac{1}{2}}y$, we observe that this operator is unitarily equivalent to

$$h\left[-d^2/dy^2 + \frac{1}{2}v''(0)y^2\right] . \tag{17}$$

Consequently, the eigenvalues are given by

$$\lambda_n(h) = h \cdot \lambda_n(1) = (2n+1)h \cdot \sqrt{\frac{v''(0)}{2}} , \tag{18}$$

and the corresponding eigenfunctions are

$$u_n^h(x) = h^{-\frac{1}{4}} u_n^1(\frac{x}{h^{\frac{1}{2}}}) \tag{19}$$

with

$$u_n^1(y) = P_n(y) \exp -\sqrt{\frac{v''(0)}{2}} \frac{y^2}{2} . \tag{20}$$

We are just looking for simplicity at the first eigenvalue. We consider the function $u_1^{h,app.}$

$$x \mapsto \chi(x) u_1^h(x) = c \cdot \chi(x) h^{-\frac{1}{4}} \exp -\sqrt{\frac{v''(0)}{2}} \frac{x^2}{2h} ,$$

where χ is compactly supported in a small neighborhood of 0 and equal to 1 in a smaller neighborhood of 0. Note here that the H^1-norm of this function over the complementary of a neighborhood of 0 is exponentially small as $h \to 0$.

We now get

$$\left(P_{h,v} - h \cdot \sqrt{\frac{v''(0)}{2}}\right) u_1^{h,app.} = \mathcal{O}(h^{\frac{3}{2}}) \,.$$

The coefficients corresponding to the commutation of $P_{h,v}$ and χ give exponentially small terms and the main contribution is

$$||(v(x) - \frac{1}{2}v''(0)x^2)\chi(x)u_1^h(x)||_{L^2}$$

which is easily seen, observing that

$$|v(x) - \frac{1}{2}v''(0)x^2| \leq C|x|^3 \;, \quad \text{for } |x| \leq 1 \;,$$

as $\mathcal{O}(h^{\frac{3}{2}})$. Then the spectral theorem gives the existence for $P_{h,v}$ of an eigenvalue $\lambda(h)$ such that

$$|\lambda(h) - h \cdot \sqrt{\frac{v''(0)}{2}}| \leq C \cdot h^{\frac{3}{2}}$$

In particular, we get the inequality

$$\lambda_1(h) \leq h \cdot \sqrt{\frac{v''(0)}{2}} + C\, h^{\frac{3}{2}}\ . \tag{21}$$

Combining with other techniques, one can actually prove that

$$|\lambda_1(h) - h \cdot \sqrt{\frac{v''(0)}{2}}| \leq C \cdot h^{\frac{3}{2}} \tag{22}$$

Harmonic approximation in general: upper bounds

In the multidimensional case, we can proceed essentially in the same way. The analysis of the quadratic case

$$H(hD_x, x) := -h^2\Delta + \frac{1}{2}\langle Ax \mid x\rangle$$

can be done explicitly by diagonalizing A via an orthogonal matrix U. There is a corresponding unitary transformation on $L^2(\mathbb{R}^n)$ defined by

$$(\mathcal{U}f)(x) = f(U^{-1}x)\ ,$$

such that

$$\mathcal{U}^{-1}H\mathcal{U} = \sum_j \left(-(h\partial_{y_j})^2 + \frac{1}{2}\lambda_j y_j^2\right)\ .$$

Using the Hermite functions as quasimodes we get the upper bounds by $h\sum_j \sqrt{\frac{\lambda_j}{2}} + \mathcal{O}(h^{\frac{3}{2}})$ as in the one-dimensional case.

Case with multiple minima

When there are more than one minimum, one can apply the above construction near each of the minima. The upper bound for the ground state is obtained by taking the infimum over all the minima of the upper bound attached to each minimum.

Harmonic approximation in general: lower bounds

Here we follow the approach proposed in the book of Cycon-Froese-Kirsch-Simon [CFKS].

Given a covering of $\mathbb{R}^n$, by balls of radius R $B(x^j, R)$ ($j \in \mathcal{J}$) and a corresponding partition of unity, such that :

$$\begin{array}{l} \sum_{j\in\mathcal{J}} (\phi_j^R)^2 = 1 \,, \\ \sum_{\ell=1}^n \sum_{j\in\mathcal{J}} |D_{x_\ell}\phi_j^R|^2 \leq \frac{C}{R^2} \,, \end{array} \tag{23}$$

we can write that, for all $u \in C_0^\infty$,

$$\begin{array}{ll} \langle P_{h,V}\, u \mid u\rangle & = \sum_j \langle P_{h,V}\phi_j^R u \mid \phi_j^R u\rangle - h^2 \sum_{j,\ell} || |D_{x_\ell}\phi_j^R| u||^2 \\ & \geq \sum_j \langle P_{h,V}\phi_j^R u \mid \phi_j^R u\rangle - C\, \frac{h^2}{R^2} ||u||^2 \,. \end{array} \tag{24}$$

We can in addition assume that either the balls are centered at the minima of V, or that the balls are at a distance of $\frac{1}{C} R$ of these minima x^{j_k}.
In the first case, using the fact that the minimas of V are non degenerate, we get :

$$
|\langle P_{h,V} \phi_j^R u \mid \phi_j^R u \rangle \geq \frac{R^2}{C} ||\phi_j^R u||^2 \, .
$$

In the second case, we observe that :

$$
|\, \langle P_{h,V} \phi_j^R u \mid \phi_j^R u \rangle - \langle P^k_{h,V} \phi_j^R u \mid \phi_j^R u \rangle \,| \leq C R^3 ||\phi_j^R u||^2 \, ,
$$

where $P^k_{h,V}$ is the quadratic approximation model at the minimum x^{j_k} (replace V by its quadratic approximation $V^k(x) = \inf V + \frac{1}{2} \langle V''(x^{j_k})(x - x^{j_k} \mid (x - x^{j_k} \rangle)$ if the ball is centered at the minimum.

The optimization between the two errors leads to the choice of

$$\frac{h^2}{R^2} = R^3 \,,$$

that is $R = h^{\frac{2}{5}}$, and we then observe that $\frac{R^2}{C} = \frac{h^{\frac{4}{5}}}{C} >> h$. We then get the lower bound

$$\lambda_1(h) \geq \inf V + h(\inf_k \mu_1(h, x^{j_k})) - Ch^{\frac{6}{5}} \,, \tag{25}$$

where the infimum is over the various minima x^{j_k} (assumed to be non degenerate) and $\mu_1(h, x^{j_k})$ denotes the lowest eigenvalue of the harmonic approximation at x^{j_k} $P^k_{h,V}$.

Once the harmonic approximation is done, it is possible to construct an orthonormal basis of the spectral space attached to some interval $I(h) := [\inf V, \inf V + Ch]$ (C avoiding the eigenvalues of the approximating harmonic oscillators at each minimum), each of the elements of the basis being exponentially localized in one of the wells.
The computation of the matrix of the operator in this basis using WKB approximation leads to the so-called "interaction matrix" (See the books of Dimassi-Sjöstrand [DiSj] or Helffer [12] for a pedagogical presentation).

We consider the case with two wells, say U_1 and U_2. We assume that there is a symmetry[1] g in $\mathbb{R}^m$, s.t. $g^2 = Id$, $gU_1 = U_2$, and s.t. the corresponding action on $L^2(\mathbb{R}^m)$ defined by $gu(x) = u(g^{-1}x)$ commutes with the Laplacian.
In addition

$$gV = V\,.$$

We now define reference one well problems by introducing :

$$M_1 = \mathbb{R}^m \setminus B(U_2, \eta)\,,\; M_2 = \mathbb{R}^m \setminus B(U_1, \eta)\,.$$

With this choice, we have $gM_1 = M_2$.

[1] Typically, in 2D the symmetry with respect to $\{x_2 = 0\}$.

The parameter $\eta > 0$ is free but can always be chosen arbitrarily small.
We denote by ϕ_j the corresponding ground state of the Dirichlet realization of $-h^2\Delta + V$ in M_j and corresponding to the ground state energy $\lambda_{M_1} = \lambda_{M_2}$. According to our result on the decay, these eigenfunctions decay like $\tilde{O}(\exp - \frac{d(x,U_j)}{h})$, where $\tilde{O}(f)$ roughly[2] means $\exp \frac{\epsilon}{h} \cdot \mathcal{O}_\epsilon(f)$ for all $\epsilon > 0$ as $h \to 0$.

We can of course keep the relation

$$g\phi_1 = \phi_2 \ .$$

[2] More precisely, for any $\epsilon > 0$, one can choose above $\eta > 0$ s.t. ...

Let us now introduce θ_j, which is equal to 1 on $B(U_j, \frac{3}{2}\eta)$ and with support in $B(U_j, 2\eta)$. We introduce

$$\chi_1 = 1 - \theta_2 \;,\; \chi_2 = 1 - \theta_1 \;,$$

and we can also keep the symmetry condition :

$$g\chi_1 = \chi_2 \;.$$

Our approximate eigenspace will be generated by

$$\psi_j = \chi_j \phi_j \;,\; (j = 1, 2) \;,$$

which satisfies

$$S_h \psi_j = \lambda_M \psi_j + r_j \;,$$

with

$$r_j = h^2 (\Delta \chi_j) \phi_j + 2h^2 (\nabla \chi_j) \cdot (\nabla \phi_j) \;.$$

We note that the "smallness" of r_j can be immediately controlled using the decay estimates in $B(U_j, 2\eta) \setminus B(U_j, \frac{3}{2}\eta)$.

In order to construct an orthonormal basis of the eigenspace F corresponding to the two lowest eigenvalues near λ_M, we first project our basis ψ_j which was not far to be orthogonal and introduce:

$$v_j = \Pi_F \psi_j \; .$$

The resolvent formula shows that $v_j - \psi_j$ can be made very small (at least $\exp -\frac{S}{h}$ with $S < d(U_1, U_2)$ by chosing $\eta > 0$ small enough). More precisely, we have the following comparison.

Lemma

$$(v_j - \psi_j)(x) = \tilde{O}(\exp -\frac{\delta_j(x)}{h}) \; , \tag{26}$$

in $\mathbb{R}^m \setminus B(U_{\hat{j}}, 4\eta)$, where $\hat{1} = 2$, $\hat{2} = 1$ and

$$\delta_j(x) = d(x, U_{\hat{j}}) + d(U_1, U_2) \; .$$

Proof

Our starting point is :

$$P_{h,M_j}\psi_j = \lambda_{M_j}\psi_j + r_j \ .$$

where

$$\mathrm{supp}\, r_j \subset B(U_{\hat{j}}, 2\eta) \ ,$$

and

$$r_j = \tilde{O}(\exp -\frac{d(x,U_j)}{h}) \ .$$

We have $v_j - \Pi_F \psi_j \in F^\perp$ and the spectral theorem gives already the estimate

$$||v_j - \pi_F \psi_j|| = \tilde{O}(\exp -\frac{d(U_1, U_2)}{h}) \,. \tag{27}$$

For a suitable contour Γ_h in $\mathbb{C}$ containing the interval $I(h)$ and remaining at a suitable distance of the spectrum

$$d(\Gamma_h, \sigma(P_h)) \geq \frac{1}{C_\epsilon} \exp -\frac{\epsilon}{h}, \forall \epsilon > 0 \,, \tag{28}$$

we can write :

$$v_j - \psi_j = \frac{1}{2\pi} \int_{\Gamma_h} (\lambda_M - z)^{-1} (P_h - z)^{-1} r_j dz \,.$$

We observe by a property of the resolvent deduced from Agmon estimates that:

$$\begin{aligned}(P_h - z)^{-1} r_j &= \tilde{O}(\sup_{y \in \mathrm{supp} r_j} \exp -\frac{[d(x,y)+d(y,U_j)]}{h}) \\ &= \tilde{O}(\exp -\frac{\delta_j(x)}{h})\,.\end{aligned}$$

The separation assumption (28) permits to get the same property for $v_j - \psi_j$:

$$v_j - \psi_j = \tilde{O}(\exp -\frac{\delta_j(x)}{h})\,.$$

This is indeed an improvment of the control in L^2.
We notice that :

$$\delta_j(x) \geq d(x, U_j) \ ,$$

What we see here is that the improved estimate does not lead to improvements near $U_{\hat{j}}$, where we have modified ϕ_j into ψ_j by introducing a cut-off function but that the improvement is quite significative when keeping a large distance (in comparison with η) with $U_{\hat{j}}$.

We then orthonormalize by the Gram-Schmidt procedure.

$$e_j = \sum_k (V^{-\frac{1}{2}})_{jk} v_k \ ,$$

with

$$V_{ij} = \langle v_i \mid v_j \rangle \ .$$

We note that

$$V_{ij} - \delta_{ij} = \mathcal{O}(\exp -\frac{S}{h}) \ .$$

At each step, we control the difference $e_j - \psi_j$, which satisfies also (26).
The matrix we would like to analyze is then simply the two by two matrix

$$M_{ij} = \langle (P_h - \lambda_M) e_i \mid e_j \rangle \ .$$

The eigenvalues of this matrix measure the dispersion of the two eigenvalues around λ_M.
We observe that symmetry considerations lead to :

$$M_{12} = M_{21} \text{ and } M_{11} = M_{22} \ .$$

So the eigenvalues are easy to compute and corresponding eigenvectors are $\frac{1}{\sqrt{2}}(1,1)$ and $\frac{1}{\sqrt{2}}(-1,+1)$. As soon as we have the main behavior of M_{12}, we can deduce that the eigenvalues are simple and that the splitting between the two eigenvalues is given by $2|M_{12}|$.

It remains to explain how one can compute M_{12}. The analysis of the decay permits to show that

$$M_{12} = \frac{1}{2}\left(\langle r_2\,,\ \psi_1\rangle + \langle r_1\,,\ \psi_2\rangle\right) + \mathcal{R}_{12}\,, \tag{29}$$

with

$$\mathcal{R}_{12} = \mathcal{O}(\exp -\frac{2S}{h})\,, \tag{30}$$

for a suitable choice of $\eta > 0$ small enough.

An integration by parts leads (observing that $\nabla\chi_1 \cdot \nabla\chi_2 \equiv 0$ for our choice of η) to the formula

$$M_{12} = h^2 \int \chi_1(\phi_2 \nabla\phi_1 - \phi_1 \nabla\phi_2)\nabla\chi_2 + \mathcal{R}_{12}\,. \tag{31}$$

A priori informations on the decay permit to restrict the integration in the right hand side of (31) to the set $\{d(x, U_1) + d(x, U_2) \leq d(U_1, U_2) + a\}$ for some $a > 0$.
A computation based on the Stokes Lemma gives then the existence of $\epsilon_0 > 0$ s.t. :

$$M_{12} = h^2 \int_\Gamma [\phi_2 \partial_n \phi_1 - \phi_1 \partial_n \phi_2] d\nu_\Gamma + \mathcal{O}(\exp -\frac{S_{12} + \epsilon_0}{h})\,. \tag{32}$$

Here $S_{12} = d(U_1, U_2)$ and Γ is an open piece of hypersurface defined in the neighborhood of the minimal geodesic $\mathrm{geod}(U_1, U_2)$ between the two points U_1 and U_2, that we assume for simplification to be unique and ∂_n denotes the normal derivative to Γ, positively oriented from U_1 to U_2 .
The last step is to observe that in a neighborhhood of the intersection γ_{12} of Γ with $\mathrm{geod}(U_1, U_2)$, one can replace the function ϕ_j (or ψ_j) modulo $\mathcal{O}(h^\infty)\exp -\frac{d(x,U_j)}{h}$ by its WKB approximation $h^{-\frac{m}{4}} a_j(x,h)\exp -\frac{d(x,U_j)}{h}$.

This leads finally to

$$M_{12} = h^{1-\frac{m}{2}} \exp -\frac{d(U_1,U_2)}{h} \times \\ \times \int_\Gamma \exp -\frac{(d(x,U_1)+d(x,U_2)-d(U_1,U_2))}{h} \times \\ \times (a_1(x,0)a_2(x,0)(\partial_n d(x,U_1) - (\partial_n d(x,U_2)) + \mathcal{O}(h))\, d\nu_\Gamma \,, \tag{33}$$

where $d\nu_\Gamma$ is the induced measure on Γ.
With natural generic additional assumptions saying that the map

$$\Gamma \ni x \mapsto (d(x,U_1) + d(x,U_2) - d(U_1,U_2))$$

vanishes exactly at order 2 at γ_{12}, this finally leads to the formula giving the splitting after use of the Laplace integral method.

WKB expansions

Inspired by the expression of the eigenfunctions of the harmonic oscillator, one looks in the case of a non degenerate well for a solution in the form

$$h^{-\frac{n}{4}} a(x,h) \exp -\frac{\varphi(x)}{h} \,.$$

where $a(x,h)$ is a formal symbol defined in a neighborhood of 0

$$a(x,h) \sim \sum_{j=0}^{+\infty} a_j(x) h^j \,.$$

The main theorem is the following (Helffer-Sjöstrand)

Theorem

There exists a C^∞-non negative function φ, a formal series

$$E(h) \sim \sum_{j\geq 1} E_j h^j \,, \text{ with } E_0 = \min V = V(0) = 0\,,$$

and a formal symbol defined in a neighborhood of 0 s.t. E_1 is the first eigenvalue of the associate harmonic oscillator and

$$(P(h) - E(h))(a(x,h) \exp -\frac{\varphi(x)}{h}) = \mathcal{O}(h^\infty) \exp -\frac{\varphi(x)}{h})\,,$$

in a neighborhood of 0 with $a_0(0) \neq 0$.

Remarks

- $\varphi(x)$ is the Agmon distance to 0 in a neighborhood of 0.
- One can extend the construction of the WKB solution in larger domains.
- In the analytic case one can work modulo $\mathcal{O}(\exp -\frac{\epsilon_0}{h})$.

Eikonal equation

The phase φ is determined by the proposition

Proposition Eikonal equation

Under the previous assumptions, there exists a unique C^∞ non negative function φ defined in a neighborhood of 0 such that

$$|\nabla\varphi|^2 = (V - E_0)\,.$$

This goes through the construction of

$$\Lambda := \{x, \nabla\varphi(x)\}\,,$$

which is living in

$$\{(x,\xi)\,:\,p(x,\xi) = E_0\}$$

where $p(x,\xi) = \xi^2 + V(x)\,.$

First transport equation

When writing term to term the necessary conditon, we have to find E_1 and a_0 such that

$$2\nabla\varphi \cdot \nabla a_0 + (\Delta\varphi - E_1)a_0 = 0\,,$$

with initial condition

$$a_0(0) \neq 0\,.$$

As a necessary condition for solving we get

$$E_1 = (\Delta\varphi(0)\,,$$

to compare with what we get from the harmonic approximation.

Comparison WKB solution–one well eigenfunction

Comparison theorem

If φ_1 is the eigenfunction of P_{M_1} with eigenvalue μ in $I(h)$ and θ_1 is the WKB solution, then, we have

$$\varphi_1 - \theta_1 = \mathcal{O}(h^\infty) \exp -\frac{d_1(x)}{h}$$

in a small neighborhhod of the minimal geodesics between U_1 and U_2 intersected with $\{d_1(x, U_1) < d(U_1, U_2)\}$.

Here we use that the Agmon distance to U_1 is indeed C^∞ in this domain of comparison and that the WKB eigenfunction is well defined there modulo $\mathcal{O}(h^\infty) \exp -\frac{d_1(x)}{h}$.

Coming back to the global strategy

What we should remember when extending this global strategy to other problems:

1. Decay estimates for the eigenfunctions of the initial problem and of suitable one well problems (Agmon estimates).
2. Rough localization of the eigenvalues permitting to identify spectral gaps (harmonic approximation)
3. Comparison of the initial problem to localized one-well problems: construction of an orthonormal basis consisting of one well localized functions generating the eigenspace relative to the spectral interval in study.
4. Compute the interaction matrix.
5. Construct WKB solutions for the one well problem.
6. Control the error term in weighted space of the difference between the WKB solution and the one well eigenfunction.

Non resonant wells

As soon as we leave the symmetric case many effects can be considered. This is analyzed by B. Simon [46] under the name of "Flea of the elephant".
This is analyzed more systematically in (the second and) third paper(s) of the series Helffer-Sjöstrand where the decay of an eigenfunction is analyzed when crossing a non resonant well.

Miniwells

Interesting questions appear when the wells are submanifolds. Then we have to define a transversal Agmon distance and a tangential Agmon distance. We will recover this situation for the two models that we want to present for the Robin problem and the problem in surface conductivity. The well will actually appear to be the boundary of the domain.
Here is an interesting toy model where the "mini-well effect" appears:

$$-h^2\frac{d^2}{dx^2} - h^2\frac{d^2}{dy^2} + (1+x^2)y^2\,.$$

The well is $\{y=0\}$, but there is a miniwell given by $(x,y)=(0,0)$.
One can also produce a double mini-well problem:

$$-h^2\frac{d^2}{dx^2} - h^2\frac{d^2}{dy^2} + (1+(1-x^2)^2)y^2\,.$$

In this situation the decay of the first eigenfunction takes a different form.

- It appears first the standard Agmon estimate corresponding to the Agmon distance to the well U like $\mathcal{O}(\exp -d((x,y),U)/h)$.
- But inside the well, it appears a tangential decay to the set of miniwells $\mathcal{O}(\exp -d_T(x)/\sqrt{h})$.

This can be understood for the first model by the following reduction.

We look first at the "normal" operator

$$-h^2 \frac{d^2}{dy^2} + (1+x^2)y^2$$

whose first eigenvalue is $h\sqrt{1+x^2}$. We then get a tangential effective Schrödinger model

$$-h^2 \frac{d^2}{dx^2} + h\sqrt{1+x^2} = h\left(-\hbar^2 \frac{d^2}{dx^2} + \sqrt{1+x^2}\right)$$

with $\hbar$ (new semi-classical parameter) given by

$$\hbar = h^{\frac{1}{2}}\,.$$

The general theory has been developed in the fifth paper of the series of Helffer-Sjöstrand devoted to the multiple wells problem. We have the assumption that the wells (corresponding to $\inf V$) are submanifolds for which the transversal Hessian at the wells are non degenerate.

Born-Oppenheimer problem

Here is the simplest models are

$$h^2 D_x^2 + D_y^2 + (1+x^2)y^2$$

resp.

$$h^2 D_x^2 + D_y^2 + (1+(1-x^2)^2)^2 y^2$$

which reduces approximately to

$$h^2 D_x^2 + \sqrt{1+x^2}\,.$$

resp.

$$h^2 D_x^2 + (1+(1-x^2)^2)\,.$$

This was analyzed in detail by A. Martinez and see the book of Nicolas Raymond for many other examples.

Application to the tight-binding

The flexibility of Agmon's approach for estimating decay estimates can also be seen in the context of the tight-binding model. Here there is no semiclassical parameter but a large parameter $R > 0$ measuring the distance between the wells. The potential has for example the form

$$V_R(x) = v(x - Re_1) + v(x + Re_1)\,,$$

where v is a potential having some decay at ∞ (the most simple case is when v has compact support but one can also consider Coulomb potential), e_1 is a non zero vector in $\mathbb{R}^n$.
Here for estimating the tunneling effect, this is the decay of the eigenfunctions at ∞ for the one-well model $-\Delta + v(x)$ which plays the important role. Hence we are coming back to the original Agmon estimates.
We refer to the work of F. Daumer [Da93, Da96] and to quite recent contributions (2018) by C. Fefferman, M. Weinstein in connection with graphene models.

The Robin problem

Let $\Omega \subset \mathbb{R}^2$ be an open domain with a smooth C^∞ compact boundary $\Gamma = \partial\Omega$. We are interested in the low-lying eigenvalues of the Robin Laplacian in $L^2(\Omega)$ with a large parameter. This is the operator

$$\mathcal{P}^\alpha = -\Delta \quad \text{in } L^2(\Omega), \tag{34}$$

with domain,

$$D(\mathcal{P}^\alpha) = \{u \in H^2(\Omega) \ : \ \nu \cdot \nabla u - \alpha\, u = 0 \quad \text{on } \partial\Omega\}\,, \tag{35}$$

where $\alpha > 0$ is a given parameter.
The unit outward normal vector of $\partial\Omega$ is denoted by ν. The operator $\mathcal{P}^\alpha$ is defined by the Friedrichs Theorem via the closed semi-bounded quadratic form, defined on $H^1(\Omega)$ by

$$u \mapsto \mathcal{Q}^\alpha(u) := ||\nabla u||^2_{L^2(\Omega)} - \alpha \int_{\partial\Omega} |u(x)|^2 ds(x)\,. \tag{36}$$

Let $(\lambda_n(\alpha))$ the sequence of min-max values of the operator $\mathcal{P}^\alpha$.
In (Pankrashkin, Pankrashkin-Popoff, Exner-Minakov-Parnovski), it is proved that, for every fixed $n \in \mathbb{N}$,

$$\lambda_n(\alpha) = -\alpha^2 - \kappa_{\mathsf{max}}\alpha + o(\alpha) \quad \text{as } \alpha \to +\infty\,, \tag{37}$$

where κ_{max} is the maximal curvature along the boundary Γ. Note that the first term in (37) has been obtained previously (see Levitin-Parnovski [31] and references therein).
Note that this does not permit to get for example the splitting between the first and the second eigenvalue as $\alpha \to +\infty$.

If the domain Ω is an exterior domain, then the operator $\mathcal{P}^\alpha$ has an essential spectrum; the essential spectrum is $[0, \infty)$. In this case, the asymptotics in (37) show that, for every fixed n, if α is selected sufficiently large, then $\lambda_n(\alpha)$ is in the discrete spectrum of the operator $\mathcal{P}^\alpha$. When the domain Ω is an interior domain, then by Sobolev embedding, the operator $\mathcal{P}^\alpha$ is with compact resolvent and its spectrum is purely discrete.

Analysis of the splitting

Our aim is to improve the two terms asymptotic expansion in (37) and to give the leading term of the spectral gap $\lambda_{n+1}(\alpha) - \lambda_n(\alpha)$ under rather generic assumptions on the boundary $\partial\Omega$. Let κ be the curvature and $\kappa_{\max}$ its maximal value of κ.

We suppose (first) that:

$$
Ass.\,(A) \left\{ \begin{array}{l} \kappa \text{ attains its maximum } \kappa_{\max} \text{ at a unique point} \\ \qquad\qquad \text{(denoted by } 0 \text{ in arc length) and} \\ \text{the maximum is non-degenerate, i.e. } k_2 := -\kappa''(0) > 0\,. \end{array} \right.
$$

This corresponds in some sense to a "one mini-well" situation inside the well which will appear to be the unique well (if the boundary is connected).

Complete asymptotics

The main result (Helffer-Kachmar) is actually more precise and reads:

Main Theorem

For any positive n, there exists a sequence $(\zeta_{j,n})_{j\in\mathbb{N}^*}$, such that the eigenvalue $\lambda_n(\alpha)$ has, as $\alpha \to +\infty$, the asymptotic expansion

$$\lambda_n(\alpha) \sim -\alpha^2 - \alpha\kappa_{\max} + (2n-1)\sqrt{\frac{k_2}{2}}\,\alpha^{1/2} + \sum_{j=0}^{+\infty} \zeta_{j,n}\alpha^{\frac{1-j}{4}}\,.$$

Actually, for all n, $\zeta_{j,n} = 0$ when j is even.

If we compare with the existing semi-classics of Schrödinger operators (see Helffer-Sjöstrand [HS1] and Simon [45] in the eighties), the curvature acts as a potential mini-well. Assumption (A) corresponds to the case of a unique mini-well inside the well which is the boundary.

Towards the tunneling

As in [HS1], a natural and interesting question is to discuss the case of multiple wells. If we replace (A) by

$$(A')\ \left\{\begin{array}{l}\kappa \text{ attains its maximum } \kappa_{\mathsf{max}} \text{ at } \{s_0, s_1, \cdots, s_j\}\,;\\ \text{and the max. are non-degenerate.}\end{array}\right.$$

then many effects can appear depending on the values of the $\kappa''(s_i)$ (as in the case of the Schrödinger operator). In case of symmetries, the determination of the tunneling effect between the points of maximal curvature is expected to play an important role.

A limiting situation is discussed in Helffer-Pankrashkin [21] when the domain Ω has two congruent corners (analysis of the tunneling).
The case of the exterior of a polygon (two term asymptotics) is discussed in a recent paper by K. Pankrashkin. The corners are no more important but instead the sides of the polygon.
In the regular case (typically an ellipse), an interesting step is the construction of WKB solutions in the spirit of a recent work by V. Bonnaillie, F. Hérau and N. Raymond [1].

Transformation into a semi-classical problem

We will first transform the initial problem into a semi-classical problem as follows. Let

$$h = \alpha^{-2}\,.$$

The limit $\alpha \to +\infty$ is now equivalent to the semi-classical limit $h \to 0_+$.

Notice the simple identity,

$$\forall\ u \in H^1(\Omega)\,, \quad \mathcal{Q}^\alpha(u) = h^{-2}\left(\int_\Omega |h\nabla u|^2 - h^{3/2}\int_{\partial\Omega} |u|^2\, ds(x)\right)\,.$$

We get the operator

$$\mathcal{L}_h = -h^2 \Delta \,, \tag{38}$$

with domain,

$$D(\mathcal{L}_h) = \{ u \in H^2(\Omega) \ : \ \nu \cdot h\nabla u - h^{1/2} u = 0 \text{ on } \partial\Omega \} \,. \tag{39}$$

Clearly,

$$\sigma(\mathcal{P}^\alpha) = h^{-2} \sigma(\mathcal{L}_h) \,.$$

If $(\mu_n(h))$ is the sequence of min-max values of the operator $\mathcal{L}_h$, the asymptotics of $\lambda_n(\alpha)$ as $\alpha \to +\infty$, directly follows from the semi-classical asymptotics of $\mu_n(h)$ as $h \to 0_+$.

Hence the previous theorem is a rephrasing of:

Theorem SC

For any positive n, there exists a sequence $(\zeta_{j,n})_{j\in\mathbb{N}^*}$, s.t. , as $h \to 0_+$, the eigenvalue $\mu_n(h)$ has the asymptotic expansion

$$\mu_n(h) \sim -h - \kappa_{\max} h^{3/2} + (2n-1)\sqrt{\frac{k_2}{2}}\, h^{7/4} + h^{15/8} \sum_{j=0}^{\infty} \zeta_{j,n} h^{j/8} .$$

Note that the dependence with respect to n appears in the third term of the expansion.

The proof of Theorem SC consists of two major steps. In the first step, we establish a three-term asymptotics

$$\mu_n(h) = -h - \kappa_{\max} h^{3/2} + (2n-1)\sqrt{\frac{k_2}{2}}\, h^{7/4} + o(h^{7/4})\,, \qquad (40)$$

which is valid under the weaker assumption that the boundary of the domain Ω is C^4 smooth.

This goes mainly through the proof of the lower bound in (40), the upper bound can be postponed to the proof of a better quasimode (at least if the boundary is sufficiently regular) whose construction does not cost more.

The next step is to construct good trial states and use the spectral theorem to establish existence of eigenvalues of the operator $\mathcal{L}_h$ satisfying the refined asymptotics,

$$\widetilde{\mu}_n(h) \sim -h - \kappa_{\max} h^{3/2} + (2n-1)\sqrt{\frac{k_2}{2}}\, h^{7/4} + h^{15/8} \sum_{j=0}^{+\infty} \zeta_{j,n} h^{j/8}\,,$$

which in light of the three-term asymptotics (lower bound) for $\mu_n(h)$, yields the equality

$$\mu_n(h) = \widetilde{\mu}_n(h)\,,$$

for $h > 0$ sufficiently small.

Reduction to a tubular neighborhood of the boundary, Agmon estimates

The eigenfunctions of the initial operator $\mathcal{L}_h$ are localized near the boundary and this localization is quantified by the following theorem:

Theorem

Let $\epsilon_0 \in (0,1)$ and $\alpha \in (0, \sqrt{\epsilon_0})$. There exist constants $C > 0$ and $h_0 \in (0,1)$ such that, for $h \in (0, h_0)$, if u_h is a normalized eigenfunction of $\mathcal{L}_h$ with eigenvalue $\mu \leq -\epsilon_0 h$, then,

$$\int_\Omega \left(|u_h(x)|^2 + h|\nabla u_h(x)|^2\right) \exp\left(\frac{2\alpha\,\mathrm{dist}(x,\Gamma)}{h^{\frac{1}{2}}}\right) dx \leq C\,.$$

Hence, this theorem is a quantitative version of the statement that the boundary is a well (in analogy with the Schrödinger model) as $h \to 0$.

Spectral reduction

We assume for simplification that the boundary is connected. Given $\delta \in (0, \delta_0)$ (with $\delta_0 > 0$ small enough), we introduce the δ-neighborhood of the boundary

$$\mathcal{V}_\delta = \{x \in \Omega \ : \ \mathrm{dist}(x, \Gamma) < \delta\}\,, \tag{41}$$

and the quadratic form, defined on the variational space

$$V_\delta = \{u \in H^1(\mathcal{V}_\delta) \ : \ u(x) = 0\,, \quad \text{for all } x \in \Omega \text{ such that } \mathrm{dist}(x, \Gamma) = \delta\}$$

by the formula

$$\forall u \in V_\delta\,, \qquad \mathcal{Q}_h^{\{\delta\}}(u) = \int_{\mathcal{V}_\delta} |h\nabla u|^2 dx - h^{\frac{3}{2}} \int_\Gamma |u|^2\, ds(x)\,.$$

In the following we will be led to take $\delta = Dh^\rho$ with $\rho \in \left(0, \frac{1}{4}\right]$. We will choose

- either $\rho < \frac{1}{4}$ with $D = 1$,
- or $\rho = \frac{1}{4}$ and $D > \mathsf{S}$ where S is the tangential Agmon distance between the wellls in order that the error term in (42) is smaller than the tunneling effect, we want to measure and which is expected to have a behavior like $\exp -S/h^{\frac{1}{4}}$.

Let us denote by $\mu_n^{\{\delta\}}(h)$ the n-th eigenvalue of the corresponding operator $\mathcal{L}_h^{\{\delta\}}$. As in our analysis of the standard double well problem (first appplication of the Agmon estimates) we get the following comparison statement:

Proposition

Let $\epsilon_0 \in (0,1)$ and $\alpha \in (0, \sqrt{\epsilon_0})$.There exist constants $C > 0$, $h_0 \in (0,1)$ such that, for all $h \in (0, h_0)$, $\delta \in (0, \delta_0)$, $n \geq 1$ such that $\mu_n(h) \leq -\epsilon_0 h$,

$$\mu_n(h) \leq \mu_n^{\{\delta\}}(h) \leq \mu_n(h) + C \exp\left(-\alpha\delta h^{-\frac{1}{2}}\right) . \tag{42}$$

This leads us to replace the initial problem by a new problem Robin-Dirichlet leaving in a δ-neighborhood of the boundary Γ.

Boundary coordinates

Near the boundary, we use specific coordinates displaying the arc-length along the boundary and the normal distance to the boundary. Let

$$\mathbb{R}/(|\partial\Omega|\mathbb{Z}) \ni s \mapsto M(s) \in \partial\Omega$$

be a parametrization of $\partial\Omega$. The unit tangent vector of $\partial\Omega$ at the point $M(s)$ of the boundary is given by

$$T(s) := M'(s).$$

We define the curvature $\kappa(s)$ by the following identity

$$T'(s) = \kappa(s)\,\nu(s),$$

where $\nu(s)$ is the unit outward normal vector. We choose the orientation s.t.

$$\det(T(s), \nu(s)) = 1, \qquad \forall s \in \mathbb{R}/(|\partial\Omega|\mathbb{Z}).$$

For all $\delta > 0$, define

$$\mathcal{V}_\delta = \{x \in \Omega \ : \ \mathrm{dist}(x, \partial\Omega) < \delta\},$$

The map Φ is defined as follows :

$$\Phi : \mathbb{R}/(|\partial\Omega|\mathbb{Z}) \times (0, t_0) \ni (s, t) \mapsto x = M(s) - t\,\nu(s) \in \mathcal{V}_{t_0}. \quad (43)$$

The determinant of the Jacobian of Φ^{-1} is given by:

$$a(s, t) = 1 - t\kappa(s).$$

For all $u \in L^2(\mathcal{V}_{t_0})$, define the function

$$\widetilde{u}(s,t) := u(\Phi(s,t)). \tag{44}$$

For all $u \in H^1(\mathcal{V}_{t_0})$, we have, with $\widetilde{u} = u \circ \Phi$,

$$\int_{\mathcal{V}_\delta} |\nabla u(x)|^2 dx = \int \Big[(1-t\kappa(s))^{-2}|\partial_s \widetilde{u}|^2 + |\partial_t \widetilde{u}|^2\Big](1-t\kappa(s))\, dsdt\,, \tag{45}$$

and

$$\int_{\mathcal{V}_{t_0}} |u(x)|^2 dx = \int_{|t|<t_0} |\widetilde{u}(s,t)|^2 (1 - t\kappa(s)) dsdt. \tag{46}$$

The associated differential operator takes in the (s,t) coordinates the form

$$\mathcal{L}_h = -h^2 a^{-1}\partial_s(a^{-1}\partial_s) - h^2 a^{-1}\partial_t(a\partial_t) \quad \left(\text{in } L^2(a\,dsdt)\right),$$

where

$$a(s,t) = 1 - t\kappa(s)\,.$$

If we neglect the curvature (but we can not !), we get the simple model

$$\mathcal{L}_h = -h^2\partial_s^2 - h^2\partial_t^2 \qquad \text{in } L^2(\mathbb{S}^1 \times \mathbb{R}^+, dsdt)\,.$$

with the Robin condition at $t = 0$ and the problem is completely decoupled.

Robin Laplacians in one dimension

It is now convenient to introduce three reference $1D$-operators and to determine their spectra. These models naturally arise in our strategy of dimensional reduction and already appeared in Helffer-Kachmar.

On a half line

As simplest model, we start with the operator, acting on $L^2(\mathbb{R}_+)$, defined by

$$\mathcal{H}_0 = -\partial_\tau^2 \tag{47}$$

with domain

$$\mathrm{Dom}\,(\mathcal{H}_0) = \{u \in H^2(\mathbb{R}_+)\ :\ u'(0) = -u(0)\}\,. \tag{48}$$

Note that this operator is associated with the quadratic form

$$V_0 \ni u \mapsto \int_0^{+\infty} |u'(\tau)|^2 \, d\tau \, - |u(0)|^2 \, ,$$

with $V_0 = H^1(0, +\infty)$.
The spectrum of this operator is $\{-1\} \cup [0, \infty)$.
The eigenspace of the eigenvalue -1 is generated by

$$u_0(\tau) = \sqrt{2} \exp\left(-\tau\right) \, . \tag{49}$$

We also consider this operator in a bounded interval $(0, T)$ with T large and Dirichlet condition at $\tau = T$.

On an interval

Let us consider $T \geq 1$ and the self-adjoint operator acting on $Ł^2(0,T)$

$$\mathcal{H}_0^{\{T\}} = -\partial_\tau^2\,, \tag{50}$$

with domain,

$$\mathrm{Dom}\,(\mathcal{H}_0^{\{T\}}) = \{u \in H^2(0,T)\,:\, u'(0) = -u(0) \quad \text{and} \quad u(T) = 0\}\,. \tag{51}$$

The spectrum of $\mathcal{H}_0^{\{T\}}$ is purely discrete and consists of a strictly increasing sequence of eigenvalues denoted by $\left(\lambda_n\left(\mathcal{H}_0^{\{T\}}\right)\right)_{n\geq 1}$.

This operator is associated with

$$V_0^{\{T\}} \ni u \mapsto \int_0^T |u'(\tau)|^2\, d\tau \, - |u(0)|^2\,,$$

with $V_0^{\{T\}} = \{v \in H^1(0,T) \,|\, v(T) = 0\}$.

The next lemma gives the localization of the two first eigenvalues $\lambda_1\left(\mathcal{H}_0^{\{T\}}\right)$ and $\lambda_2\left(\mathcal{H}_0^{\{T\}}\right)$ for T large.

Lemma

As $T \to +\infty$,

$$\lambda_1(\mathcal{H}_0^{\{T\}}) = -1 + 4\big(1 + o(1)\big)\exp\big(-2T\big) \quad \text{and} \quad \lambda_2(\mathcal{H}_0^{\{T\}}) \geq 0\,. \tag{52}$$

This can be done by explicit computation. The second term looks like a tunneling effect due to the boundary.

In a weighted space

The previous model is to rough. We should indeed use a localized $1D$-operator taking account from the curvature.
Let $B \in \mathbb{R}$, $T > 0$ s.t. $BT < \frac{1}{3}$. Consider the self-adjoint operator, acting on $L^2\big((0,T);(1-B\tau)d\tau\big)$ and defined by

$$\mathcal{H}_B^{\{T\}} = -(1-B\tau)^{-1}\partial_\tau(1-B\tau)\partial_\tau = -\partial_\tau^2 + B(1-B\tau)^{-1}\partial_\tau\,, \quad (53)$$

with domain

$$\mathrm{Dom}\,(\mathcal{H}_B^{\{T\}}) = \{u \in H^2(0,T)\ :\ u'(0) = -u(0) \quad \text{and} \quad u(T) = 0\}\,. \quad (54)$$

The operator $\mathcal{H}_B^{\{T\}}$ is the Friedrichs extension in $L^2\big((0,T);(1-B\tau)d\tau\big)$ associated with the quadratic form defined for $u \in V_h^{\{T\}} = \{H^1((0,T)) \cap \{u(T)=0\}$, by

$$q_B^{\{T\}}(u) = \int_0^T |u'(\tau)|^2(1-B\tau)\,d\tau - |u(0)|^2\,.$$

The operator $\mathcal{H}_B^{\{T\}}$ is with compact resolvent. The strictly increasing sequence of the eigenvalues of $\mathcal{H}_B^{\{T\}}$ is denoted by $(\lambda_n(\mathcal{H}_B^{\{T\}})_{n\in\mathbb{N}^*}$.

It is easy to compare the spectra of $\mathcal{H}_B^{\{T\}}$ and $\mathcal{H}_0^{\{T\}}$ as $B \to 0$.

Lemma

There exists $T_0 > 0$ and C s.t. for all $T \geq T_0$, for all $B \in (-1/(3T), 1/(3T))$ and $n \in \mathbb{N}^*$, there holds,

$$\left|\lambda_n(\mathcal{H}_B^{\{T\}}) - \lambda_n(\mathcal{H}_0^{\{T\}})\right| \leq C\,|B|\,T\Big(\,|\lambda_n(\mathcal{H}_0^{\{T\}})| + 1\Big)\,.$$

Then notice that, $\forall T > 0$, the family $\left(\mathcal{H}_B^{\{T\}}\right)_B$ is analytic for B small enough.

The next proposition states a two-term asymptotic expansion of the eigenvalue $\lambda_1(\mathcal{H}_B^{\{T\}})$.

Proposition

There exist $T_0 > 0$ and $C > 0$ s.t. $\forall T \geq T_0$, for all $B \in (-1/(3T), 1/(3T))$ there holds,

$$\left|\lambda_1(\mathcal{H}_B^{\{T\}}) - (-1 - B)\right| \leq CB^2 \,.$$

One also needs a decay estimate of $u_B^{\{T\}}$ that is a classical consequence of the positivity of the Dirichlet problem on $(0, T)$ and of an Agmon estimate.

Proposition

There exist $T_0 > 0$, $\alpha > 0$ and $C > 0$ s.t. $\forall T \geq T_0$, $\forall B \in (-1/(3T), 1/(3T))$,

$$\|e^{\alpha\tau} u_B^{\{T\}}\|_{L^2\left((0,T);(1-B\tau)d\tau\right)} \leq C\,.$$

We will apply these results with $T = Dh^{-r}$, $r \in (0, \frac{1}{2})$, $B = h^{\frac{1}{2}}\kappa$ and $h \in (0, h_0)$.

Lower bound

This goes (implicitly) through the construction of a Grushin's problem. This is possible under the condition that we have obtained an a priori information on the eigenfunctions (Agmon estimates) corresponding to eigenvalues $\lambda(h)$'s satisfying

$$\lambda(h) \leq -h - \kappa_{\max} h^{3/2} + Ch^{\frac{7}{4}} .$$

The idea is that we can "project" an eigenfunction of $\mathcal{L}_h$ (roughly speaking, we take the product with $\sqrt{2}\, h^{-\frac{1}{4}} \exp -\frac{t}{\sqrt{h}}$) to get an approximate eigenfunction of an harmonic oscillator living (after scaling, see below) in $L^2(\mathbb{R}_\sigma)$:

$$-\partial_\sigma^2 - \frac{\kappa''(0)}{2}\sigma^2$$

In a very close context this approach was used in Fournais-Helffer in the context of surface superconductivity.

Accurate quasimodes (double scaling)

We can now sketch the proof of the complete asymptotics which goes from a rescaling. We compute the expression of the operator $\mathcal{L}_h/h$ in the re-scaled boundary coordinates

$$(\sigma,\tau) = (h^{-1/8}s, h^{-1/2}t)\,.$$

Here we recall that

$$\mathcal{L}_h = -h^2 a^{-1}\partial_s(a^{-1}\partial_s) - h^2 a^{-1}\partial_t(a\partial_t) \quad (\text{in } L^2(a\,dsdt))\,,$$

where

$$a(s,t) = 1 - t\kappa(s)\,.$$

We then consider the formal expansion of the operator $\mathcal{L}_h$. This is obtained by the Taylor expansion of the coefficients of the rescaled operator at $\tau = 0, \sigma = 0$. This leads to an expansion in powers of $h^{\frac{1}{8}}$.

$$h^{-1}\mathcal{L}_h = P_0 + h^{1/2}P_2 + h^{3/4}P_3 + h^{7/8}P_{\frac{7}{2}} + \cdots \,, \qquad (55)$$

where

$$P_0 = -\partial_\tau^2 \,,$$
$$P_2 = \kappa(0)\partial_\tau = \kappa_{\mathrm{max}}\partial_\tau \,,$$
$$P_3 = -\partial_\sigma^2 + \frac{\kappa''(0)}{2}\sigma^2\partial_\tau \,.$$

We will use below the notation

$$k_2 = -\kappa''(0) \,.$$

Let $n \in \mathbb{N}^*$. We will construct a sequence of real numbers $(\zeta_{j,n})_{j=0}^{\infty}$ and two sequences of real-valued Schwartz functions $(v_{n,j})_{j=1}^{\infty} \subset \mathcal{S}(\mathbb{R})$, $(g_{n,j})_{j=0}^{\infty} \subset \mathcal{S}(\mathbb{R} \times \overline{\mathbb{R}_+})$ s.t. ,

$$\forall\ j, \quad \partial_\tau g_{n,j}\Big|_{\tau=0} = -g_{n,j}\Big|_{\tau=0},$$

and the function

$$\Psi_n(\sigma,\tau) \sim u_0(\tau) f_n(\sigma) + \sum_{j=1}^{\infty} h^{j/8} u_0(\tau) v_{n,j}(\sigma) + h^{7/8} \sum_{j=0}^{+\infty} h^{j/8} g_{n,j}(\sigma,\tau) \tag{56}$$

satisfies

$$\left(\widetilde{\mathcal{L}}_h - \mu_h\right)\Psi_n = \mathcal{O}(h^\infty)\,, \tag{57}$$

where

$$\mu_n \sim -1 - h^{1/2}\kappa_{\max} + h^{3/4}\sqrt{\frac{k_2}{2}}\,(2n-1) + h^{7/8}\sum_{j=0}^{\infty} \zeta_{j,n} h^{j/8}\,. \tag{58}$$

Let us mention that, for every j, our definition of the function $g_{n,j}(\sigma,\tau)$ ensures that it is a finite sum of functions having the simple form $F(\sigma)\times U(\tau)$.
Remember that $u_0(\tau)=\sqrt{2}\,\exp(-\tau)$ and $f_n(\sigma)$ is the n-th normalized eigenfunction of the harmonic oscillator $H_{\rm harm}=-\partial_\sigma^2+\frac{k_2}{2}\sigma^2$.

Before we proceed in the construction of the aforementioned sequences, we show how they give us refined expansions of the eigenvalues of the operator $\mathcal{L}_h$. Let χ_1 be a cut-off function. Define a function ϕ_n in $L^2(\Omega)$ by means of the boundary coordinates as follows,

$$\Phi_n(s,t) = \chi_1\left(\frac{s}{|\partial\Omega|}\right)\chi_1\left(\frac{t}{h^{1/8}}\right)\Psi_n(h^{-1/8}s, h^{-1/2}t)\,. \tag{59}$$

The function ϕ_n is in the domain of the operator $\mathcal{L}_h$ because the functions $g_{n,j}$ and u_0 satisfy the Robin condition at $\tau = 0$. Since all involved functions in the expression of Ψ_n are in the Schwartz space, then multiplying by cut-off functions will produce small errors in the various calculations–all the error terms are $\mathcal{O}(h^\infty)$. Also, since the function $u_0(\tau)f_n(\sigma)$ is normalized in $L^2(\mathbb{R}\times\mathbb{R}_+)$, then the norm of Φ_n in $L^2(\Omega)$ is equal to $1+o(1)$, as $h\to 0_+$.

The spectral theorem now gives us:

Thm-quasimodes

Let $n \in \mathbb{N}$. There exists an eigenvalue $\widetilde{\mu}_n(h)$ of the operator $\mathcal{L}_h$ such that, as $h \to 0_+$,

$$\widetilde{\mu}_n(h) \sim -h - h^{3/2}\kappa_{\max} + h^{3/4}\sqrt{\frac{k_2}{2}}\,(2n-1) + h^{7/8}\sum_{j=0}^{\infty}\zeta_{j,n}h^{j/8}\,.$$

Proof of the expansion

We now proceed to the construction of the numbers $\zeta_{j,n}$ and the functions Ψ_n. This is done by an iteration process.
The first equations (corresponding to the vanishing of the first powers of $h^{\frac{1}{8}}$) are easy to solve and lead to determination of the first term

$$\psi_{n,0}(\sigma,\tau) = u_0(\tau) f_n(\sigma)\,,$$

and the determination of the three-term asymptotics.
In this way, we cancel all the coefficients of the expansion (the coefficient of $h^{\frac{3}{4}}$ included. This is enough for this asymptotics.

Continuing the asymptotics

We now want to cancel the coefficient of $h^{\frac{7}{8}}$.
A simple calculation leads to the following condition,

$$(P_0 + 1)\psi_{n,7} + (F_1 - \mu_7)\psi_{n,0} + (P_3 - \mu_6)\psi_{n,1} = 0\,. \tag{60}$$

with

$$\psi_{n,1}(\sigma,\tau) = \varphi_{n,1}(\sigma)u_0(\tau)\,.$$

Note that $\zeta_0 = \mu_7$.
The operator F_1 takes the form

$$F_1 = q_{1,0}(\sigma,\tau)\partial_\tau + q_{2,0}(\sigma,\tau)\partial_\sigma^2 + q_{3,0}(\sigma,\tau)\partial_\sigma$$

with the functions $q_{k,0}(\sigma,\tau)$ being polynomials depending on both variables σ and τ.
We determine μ_7 by multiplying by $u_0(\tau)\varphi_0(\sigma)$:

$$\mu_7 = \langle F_1\psi_{n,0} \,|\, \psi_{n,0}\rangle\,. \tag{61}$$

We now come back to (60), multiply by $u_0(\tau)$ and integrate over τ. This gives:

$$\left(\int ((F_1 - \mu_7)\psi_0)(\sigma,\tau)\, u_0(\tau))\, d\tau\right) + (P_3 - \mu_6)\varphi_1 = 0\,. \tag{62}$$

This can be written in the form

$$(P_3 - \mu_6)\varphi_1 = \vartheta(\sigma)\,, \tag{63}$$

where $\vartheta(\sigma)$ is orthogonal to $\varphi_0(\sigma)$ as a consequence of the choice of μ_7. We choose φ_1 as the solution of (63) which is orthogonal to φ_0.

We write:

$$\psi_7(\sigma,\tau)) = \varphi_7(\sigma)u_0(\tau) + \psi_7^0(\sigma,\tau)$$

where

$$\int \psi_7^0(\sigma,\tau)u_0(\tau)\, d\tau = 0\,.$$

It remains to solve

$$((P_0+1)\psi_7^0)(\sigma,\tau)=\Theta_7(\sigma,\tau)$$

with

$$\int \Theta_7(\sigma,\tau)d\tau = 0\,.$$

This is clearly solvable (we are on the orthogonal to the space $\{(\mathbb{R}u_0)\times L^2(\mathbb{R}_\sigma)\}$). More explicitly

$$\Theta_7(\sigma,\tau)=\sum_\ell \kappa_\ell(\sigma)\nu_\ell(\tau)$$

with $\nu_\ell(\tau)$ orthogonal to u_0 and in $\mathcal{S}(\overline{\mathbb{R}^+})$.

The solution is then given by

$$\psi_7^0(\sigma,\tau) = \sum_\ell \kappa_\ell(\sigma)\hat{\nu}_\ell(\tau)$$

with $\hat{\nu}_\ell$ solution of the Robin problem in the orthogonal space to u_0:

$$(P_0+1)\hat{\nu}_\ell = \nu_\ell\,,$$

and $\int \hat{\nu}_\ell(\tau)u_0(\tau)d\tau = 0$.

The same method can be used for the cancellation of the coefficients of $h^{\frac{j}{8}}$ for $j>7$. At the step j, this cancellation permits to determine μ_j, φ_{j-6} and ψ_j^0.

Definition of the simple mini-well operator

Let ω be an (open) interval in the circle of length $2L$ identified with the interval $(-L, L]$. We can view ω as a (curved) segment in the boundary of Ω by means of the length parametrization.

The operator $\widehat{\mathcal{L}}^{T}_{r,\hbar} = \widehat{\mathcal{L}}_r$ is defined as follows.

We assume that ω contains a unique point s_ω of maximum curvature (i.e. $\kappa(s_\omega) = \kappa_{\mathrm{max}}$) that is non degenerate.

The form domain $\widehat{V}_r$ and the domain $\widehat{\mathcal{D}}_r$ of this operator are defined as follows,

$$
\begin{aligned}
&\widehat{\mathcal{V}}_r = \omega \times (0, T)\,,\\
&\widehat{V}_r = \{u \in H^1(\widehat{\mathcal{V}}_r)\ :\ u = 0 \text{ on } \tau = T \text{ and } \partial\omega \times (0, T)\}\,,\\
&\widehat{\mathcal{D}}_r = \{u \in H^2(\widehat{\mathcal{V}}_r) \cap \widehat{V}_r\ :\ \partial_\tau u = -u \text{ on } \tau = 0\}\,.
\end{aligned}
\tag{64}
$$

The operator $\widehat{\mathcal{L}}_r$ is the self-adjoint operator on $L^2(\widehat{\mathcal{V}}_r; \widehat{a}\, d\sigma\, d\tau)$ with domain $\widehat{\mathcal{D}}_r$ and

$$\widehat{\mathcal{L}}_r = -\hbar^4\, \widehat{a}^{-1}(\partial_\sigma \widehat{a}^{-1})\partial_\sigma - \widehat{a}^{-1}(\partial_\tau \widehat{a})\partial_\tau\,. \tag{65}$$

We denote by $\mu_r(\hbar)$ its lowest eigenvalue.
The corresponding positive and L^2-normalized eigenfunction is denoted by $\phi_{\hbar,r}$.
Let $\mu_{2,r}(\hbar)$ be the second eigenvalue of the operator $\widehat{\mathcal{L}}_r$.
The previous analysis yields that, for $\hbar$ small, $\mu_r(\hbar)$ is a simple eigenvalue and

$$\mu_{2,r}(\hbar) - \mu_r(\hbar) = 3\gamma\, \hbar^{7/4} + \hbar^{7/4} o(1) \quad \text{as } \hbar \to 0_+\,, \tag{66}$$

where $\gamma = \sqrt{\frac{-\kappa''(s_\omega)}{2}}$.

WKB approach for the ground state

If the previous method was satisfactory to get the complete expansions of the first eigenvalues in powers of h, they are not sufficient for controlling later the tunneling effect. If we compare with our treatment of the standard double well problem, we have at this stage proposed a refined version of the harmonic approximation.
Hence we need a substitute for the WKB solution for the one mini-well problem.

Here we follow what was done by S. Lefebvre (1986) for a model in Born-Oppenheimer

$$h^2\, D_x^2 + D_y^2 + (1 + x^2) y^2$$

which reduces to the model

$$h^2 D_x^2 + \sqrt{1 + x^2}\,,$$

and more recently Bonnaillie-Hérau-Raymond (2014) in [1] for the problem arising in superconductivity (see the last part of the lectures).

We only scale in the t variable

$$t = h^{\frac{1}{2}}\tau\,,$$

and expand $\mathcal{L}_h/h$ in powers of $h^{\frac{1}{2}}$

$$\widehat{L}_h := -\partial_\tau^2 - h\partial_s^2 + h^{\frac{1}{2}}\kappa(s)\partial_\tau + 2h^{\frac{3}{2}}\tau\kappa(s)\partial_s^2 + h^{\frac{3}{2}}\tau\kappa'(s)\partial_s + \dots.$$

The idea is to look (like in Born-Oppenheimer) for a WKB vector-valued expansion in the form

$$\Psi^{WKB}(s,\tau,h) \sim \exp -\frac{\vartheta(s)}{h^{\frac{1}{4}}}\left(\sum_\ell a_\ell(s,\tau)h^{\frac{\ell}{4}}\right)$$

and a corresponding eigenvalue

$$\mu^{WKB}(h) \sim \sum_\ell \mu_\ell h^{\frac{\ell}{4}}\,.$$

We first determine the "formal" operator

$$\widehat{L}_h^\vartheta := \exp \frac{\vartheta(s)}{h^{\frac{1}{4}}} \, \widehat{L}_h \, \exp - \frac{\vartheta(s)}{h^{\frac{1}{4}}} \, .$$

Expanding in powers of $h^{\frac{1}{4}}$ we get

$$\widehat{L}_h^\vartheta = \sum_\ell Q_\ell^\vartheta \, h^{\frac{\ell}{4}}$$

with

$$\begin{array}{ll} Q_0^\vartheta & = -\partial_\tau^2 \, , \\ Q_1^\vartheta & = 0 \, , \\ Q_2^\vartheta & = +\kappa(s)\partial_\tau - \vartheta'(s)^2 \, , \\ Q_3^\vartheta & = 2\vartheta'(s)\partial_s + \vartheta''(s) \\ Q_4^\vartheta & = -\partial_s^2 \ldots \end{array}$$

Taking $\mu_0 = -1$, the first equation reads (with Robin condition)

$$(Q_0 + 1) a_0(s, \tau) = 0 \, .$$

This leads to take $a_0(s, \tau) = \xi_0(s) u_0(\tau)$.

The second equation (with $\mu_1 = 0$) reads

$$(Q_0 + 1)a_1(s, \tau) = 0$$

This leads to take

$$a_1(s, \tau) = \xi_1(s)u_0(\tau)\,.$$

The third equation reads

$$(Q_0 + 1)a_2 + (Q_2 - \mu_2)a_0 = 0\,.$$

This gives

$$(Q_0+1)a_2+u_0(\tau)(-\kappa(s)-\vartheta'(s)^2-\mu_2)\xi_0(s)=0\,.$$

Multiplying by u_0 and integrating over τ leads to the eikonal equation

$$-\kappa(s)-\vartheta'(s)^2-\mu_2=0\,.$$

We consequently take $\mu_2=-\kappa(0)$ and ϑ is determined once we assume $\vartheta(0)=0$ and $\vartheta(s)\geq 0$.
We have to take a_2 in the form

$$a_2(s,\tau)=\xi_2(s)u_0(\tau)\,.$$

The next equation reads

$$(Q_0+1)a_3+(Q_2-\mu_2)a_1+(Q_3-\mu_3)a_0=0\,.$$

Multiplying by u_0 and integrating over τ leads to the first transport equation

$$2\vartheta'(s)\xi_0'(s)+(\vartheta''(s)-\mu_3)\xi_0(s)=0\,.$$

This leads to

$$\mu_3=\vartheta''(0)=\sqrt{-\frac{1}{2}\kappa''(0)}\,,$$

and to determine ξ_0.
This also leads to choose

$$a_3(s,\tau)=\xi_3(s)u_0(\tau)\,.$$

and so on....

Towards the analysis of the tunneling

The idea is that the "one well" eigenfunction is well approximated by the WKB approximation in large domains of the boundary. In the case of an ellipse, we expect a tunneling in the form

$$\mu_2 - \mu_1 \sim h^{-\nu} a_0(h^{\frac{1}{4}}) \exp -\frac{S_0}{h^{\frac{1}{4}}} \,,$$

where S_0 is the tangential Agmon distance between the two points of maximal curvature on the boundary associated with the metric $\sqrt{\kappa_{max} - \kappa(s)}\, ds^2$.

Tunneling effect

We now consider the "multiwell" case.

Assumption T1

The curvature κ on the boundary Γ attains its maximum κ_{max} at a finite number N of points on Γ and these maxima are non degenerate.

In the case when $N = 2$ in Ass.T1 we will carry out a refined analysis valid under the following stronger (geometric) assumption:

Assumption T2

i) Ω is symmetric with respect to the y-axis.

ii) The curvature κ on the boundary Γ attains its maximum at a_1 and a_2 which are not on the symmetry axis and belong to the same connected component of the boundary.

iii) The second derivative of the curvature (w.r.t. arc-length) at a_1 and a_2 is negative.

In this case we write

$$a_1 = (a_{1,1}, a_{1,2}) \in \Gamma \quad \text{and} \quad a_2 = (a_{2,1}, a_{2,2}) \in \Gamma\,,$$

s.t. $a_{1,1} > 0$ and $a_{2,1} < 0$.
A simple example of a domain satisfying all the assumptions is the full ellipse

$$\left\{(x,y)\ :\ \frac{x^2}{a^2} + \frac{y^2}{b^2} < 1\right\}\,,\ \text{with } 0 < b < a\,.$$

The two points in the boundary of maximal curvature are $(\pm a, 0)$.
The second example is the complementary:

$$\left\{(x,y)\ :\ \frac{x^2}{a^2} + \frac{y^2}{b^2} > 1\right\}\,,\ \text{with } 0 < a < b\,.$$

The two points of maximal curvature in the boundary are $(\pm a, 0)$.

We recall that our problem is equivalent to the semiclassical analysis of the operator

$$\mathcal{L}_h = -h^2 \Delta\,, \tag{67}$$

with domain

$$\mathcal{D}(\mathcal{L}_h) = \{u \in H^2(\Omega) \ : \ \nu \cdot h^{\frac{1}{2}} \nabla u - u = 0 \text{ on } \Gamma\}\,, \tag{68}$$

where ν is the *outward* pointing normal and $h > 0$ is the semiclassical parameter.

About semiclassical tunneling on the circle

The aim is to analyze the splitting $\mu_2(h) - \mu_1(h)$ under the symmetry Assumption T2 ($M = 2$). We will see that the proof is reduced to the case when Γ has only one component (the one, by assumption unique, where κ attains its maximum). The candidate for the splitting is obtained by considering the splitting for the operator

$$\mathcal{M}_h^{\mathrm{eff}} = -h - \kappa_{\max} h^{\frac{3}{2}} + h^2 D_s^2 + h^{\frac{3}{2}} \mathfrak{v}(s) \,, \qquad \mathfrak{v} = \kappa_{\max} - \kappa \,, \quad (69)$$

acting on the periodic functions in $L^2(\mathbb{R}/(2L)\mathbb{Z})$, where

$$L = \frac{|\Gamma|}{2} \,,$$

and s the arc-length.

Equivalently $\mathcal{M}_h^{\text{eff}}$ can be considered as the Schrödinger operator on the compact one dimensional manifold Γ.

This is a double well problem which can be treated as a particular case of Helffer-Sjöstrand [HS1] with the effective semiclassical parameter being $\hbar := h^{\frac{1}{4}}$.

We denote by $\mu_j^{\text{eff}}(h)$ the j-th eigenvalue of $\mathcal{M}_h^{\text{eff}}$ (counting multiplicities).

Let us recall the splitting formula for the Schrödinger operator

$$\mathcal{M}_{\hbar}^{\mathrm{circ}} := \hbar^2 D_s^2 + \mathfrak{v}(s)$$

on the circle of length $2L$ when $\mathfrak{v}$ has two symmetric non degenerate wells at say s_{r} and s_ℓ with $\mathfrak{v}(s_{\mathrm{r}}) = \mathfrak{v}(s_\ell) = 0$ and $\mathfrak{v}''(s_{\mathrm{r}}) = \mathfrak{v}''(s_\ell) > 0$.

We can follow the exposition of the first part except that we are on the disk (see the Lecture Notes in Semi-Classical Analysis in 1988, the PHD of A. Outassourt 1987 and the more recent presentation in Bonnaillie-Hérau-Raymond [2]). Because there are two geodesics between the two wells, the discussion depends on the comparison between the lengths of these two geodesics.

For that purpose, we introduce

$$\begin{aligned} \mathsf{S} &= \min\left(\mathsf{S}_{\mathsf{u}}, \mathsf{S}_{\mathsf{d}}\right)\,, \\ \mathsf{S}_{\mathsf{u}} &= \int_{[s_{\mathsf{r}}, s_\ell]} \sqrt{\mathfrak{v}(s)}\,ds\,, \\ \mathsf{S}_{\mathsf{d}} &= \int_{[s_\ell, s_{\mathsf{r}}]} \sqrt{\mathfrak{v}(s)}\,ds\,, \end{aligned}$$

where $[p, q]$ denotes the arc joining p and q in Γ counter-clockwise.

Note that in the case of the ellipse, we have an additional symmetry, hence $S_u = S_d$.

The splitting formula for the operator $\mathcal{M}_\hbar^{\mathrm{circ}}$ is obtained by adding the contributions of each geodesic and reads

$$\begin{aligned} \lambda_2(\hbar) - \lambda_1(\hbar) & \\ &= 4\hbar^{\frac12}\pi^{-\frac12}\gamma^{\frac12}\left(\mathsf{A}_{\mathsf{u}}\sqrt{\mathfrak{v}(0)}e^{-\frac{\mathsf{S}_{\mathsf{u}}}{\hbar}} + \mathsf{A}_{\mathsf{d}}\sqrt{\mathfrak{v}(L)}e^{-\frac{\mathsf{S}_{\mathsf{d}}}{\hbar}}\right) \\ &\qquad + \mathcal{O}(\hbar^{\frac32}e^{-\frac{\mathsf{S}}{\hbar}}), \end{aligned} \tag{70}$$

where

$$\begin{aligned} \mathsf{A}_{\mathsf{u}} &= \exp\left(-\int_{[s_{\mathsf{r}},0]}\frac{(\mathfrak{v}^{\frac12})'(s)+\gamma}{\sqrt{\mathfrak{v}(s)}}ds\right), \\ \mathsf{A}_{\mathsf{d}} &= \exp\left(-\int_{[s_\ell,L]}\frac{(\mathfrak{v}^{\frac12})'(s)-\gamma}{\sqrt{\mathfrak{v}(s)}}ds\right), \\ \gamma &= \left(\mathfrak{v}''(s_{\mathsf{r}})/2\right)^{\frac12} = \left(\mathfrak{v}''(s_\ell)/2\right)^{\frac12}. \end{aligned}$$

Then, for the particular model $\mathcal{M}_h^{\text{eff}}$, we notice that

$$\mu_2^{\text{eff}}(h) - \mu_1^{\text{eff}}(h) = h^{\frac{3}{2}}(\lambda_2(\hbar) - \lambda_1(\hbar))\,, \tag{71}$$

so that, under Assumption T2, we have ($h^{\frac{1}{4}} = \hbar$)

$$\begin{aligned} &\mu_2^{\text{eff}}(h) - \mu_1^{\text{eff}}(h) \\ &\quad = 4h^{\frac{13}{8}}\pi^{-\frac{1}{2}}\gamma^{\frac{1}{2}}\left(\mathsf{A_u}\sqrt{\mathfrak{v}(0)}\exp -\frac{\mathsf{S_u}}{h^{\frac{1}{4}}} + \mathsf{A_d}\sqrt{\mathfrak{v}(L)}\exp -\frac{\mathsf{S_d}}{h^{\frac{1}{4}}}\right) \\ &\qquad + \mathcal{O}\left(h^{\frac{13}{8}+\frac{1}{4}}\exp -\frac{\mathsf{S}}{h^{\frac{1}{4}}}\right)\,. \end{aligned} \tag{72}$$

Note that, if we assume that $\mathfrak{v}$ is invariant under the symmetry exchanging the upper and lower parts, we have $\mathfrak{v}(0) = \mathfrak{v}(L)$, $\mathsf{S_u} = \mathsf{S_d}$ and $\mathsf{A_u} = \mathsf{A_d}$.

Statement of the main Tunneling result

Tunneling Theorem (Helffer-Kachmar-Raymond (2015))

Under Assumptions T1 and T2, we have

$$\mu_2(h) - \mu_1(h) \underset{h\to 0}{\sim} \mu_2^{\mathrm{eff}}(h) - \mu_1^{\mathrm{eff}}(h)\,, \tag{73}$$

where $\mu_j^{\mathrm{eff}}(h)$ is defined before and where $\mu_2^{\mathrm{eff}}(h) - \mu_1^{\mathrm{eff}}(h)$ is computes on the $(1D)$-effective model on the circle.

Tunneling Theorem shows a tunneling effect induced by the geometry of the domain (comparing with the semi-classical analysis of degenerate wells, the boundary acts as the well and the points of maximal curvature as the mini-wells).

About other points of the proof

The general strategy described in the case of the initial double well problem can be achieved in this case.

We have explained

1. How to find asymptotics of eigenvalues;
2. The decoupling between the mini-wells;
3. How to use Agmon estimates in the normal direction.
4. the WKB construction in the one mini-well situation.

An important tool, to justify the decoupling, is also to establish like in the mini-well situation a tangential decay estimate near the boundary.
The starting formula for the splitting is the same as in the standard double well problem.

When the domain Ω has corners and symmetries (e.g. the interior of an isosceles triangle), the tunneling effect is analyzed by Helffer-Pankrashkin in [21]. One difference between the setting here and that appears in the spectral reduction to the reference problems. In [21], the reference problem is a two-dimensional problem in an infinite sector which has an explicit groundstate. In this paper, the limiting reference problem is a direct sum of two one-dimensional operators. To prove our Tunneling Theorem, we need to compare the eigenfunctions of the operator $\mathcal{L}_h$ with WKB approximate eigenfunctions.

Other questions around ...

- Look at

$$u \mapsto \mathcal{Q}^\alpha(u) := ||\nabla u||^2_{L^2(\Omega)} + \alpha \int_{\partial\Omega} b(x)|u(x)|^2 ds(x)\,. \qquad (74)$$

  This is considered in Daners-Kennedy (who refers to Yuan Lou and Meijun Zhu). The ground state is localized at the boundary near the maxima of b:

$$\lambda \sim -\alpha^2 b_{max}^2\,.$$

- Look at the higher dimension. See Pankrashkin-Popoff [39, 40] for the 2-term expansion.
- Introduce a more systematic reduction to the boundary and analyze the resulting semi-classical problem at the boundary.

Magnetic bottles in semi-classical analysis.

Here we refer to papers with A. Morame, Y. Kordyukov, N. Raymond and S. Vu-Ngoc from 1996 to 2017. A good reference is the recent book by N. Raymond (2017) [42].
When no electric potential $V(x)$ is present we can still have localization through the magnetic field.

To simplify, we describe the case of dimension 2. We assume that the magnetic field $B(x) = \mathrm{curl} A$ is positive and that

$$0 \leq \inf B < \lim \inf_{|x| \to +\infty} B(x)\,.$$

Considering $P_{hA,0}$ one can show that the spectrum below $h \liminf_{|x|\to+\infty} B$ is discrete and we would like to localize the groundstate (as $h \to 0$).

The question is then:

Does it exists a substitute for the Agmon strategy ?

So we should look for an effective electric potential. Here we simply observe that

$$\langle P_{h,A,0} u, u \rangle \geq h \int B(x) |u(x)|^2 \, dx \,.$$

This suggest to take $hB(x)$ as an effective electric potential. More precisely, we use the previous inequality in the form

$$\langle P_{hA,0} u, u \rangle \geq (1-\epsilon) h \int B(x) |u(x)|^2 \, dx + \epsilon \langle P_{h,A,0} u, u \rangle \,,$$

and look for an optimal $\epsilon \in (0,1)$.

A magnetic Agmon distance d_B is associated with $B - \inf B$ and one expects, assuming a unique minimum at 0, a decay in $\exp -\alpha \frac{d_B(x,0)}{\sqrt{h}}$, for some $\alpha > 0$.

Note that the double well problem in the case considered by the above mentioned authors is completely open. We are here thinking of a (2D)-situation where the magnetic field is positive and admit two symmetric non degenerate minima.

Decay estimates and tunneling in superconductivity

Here we refer to works with A. Morame, X. Pan, S. Fournais and the more recent works by Bonnaillie–Hérau-Raymond between 2002 till 2018. We refer to our book with S. Fournais for the state of the art in 2009.

The so-called Surface Superconductivity is strongly related with the Neumann realization of the Schrödinger operator with magnetic field (which in the initial papers is assumed to be constant and then variable). Here we observe a phenomenon of localization at the boundary (which plays the role of the well) and the role of the Agmon distance is played by the distance to the boundary.

More accurate localization is given in dimension 2 by the curvature of the boundary (an effect predicted by Bernoff-Sternberg and proven by Helffer-Morame).

The decay along the boundary is measured by a tangential Agmon distance associated with the curvature. Again the Agmon's strategy plays an important role.

The magnetic case in superconductivity

We now consider the semiclassical analysis of the magnetic Laplacian on a smooth domain of the plane carrying Neumann boundary conditions.
One would like to discuss a conjecture of magnetic tunneling when the domain is an ellipse.

The Neumann realization for the magnetic Laplacian

Let Ω be an open, bounded and simply connected domain of $\mathbb{R}^2$.
We consider the magnetic Laplacian

$$\mathcal{L}_\hbar = (-i\hbar\nabla + \mathbf{A})^2, \tag{75}$$

with Neumann condition on the boundary, wher
e $\mathbf{A}(x_1, x_2) = \frac{1}{2}(x_2, -x_1)$ is a vector potential associated with the magnetic field $\mathbf{B} = \nabla \times \mathbf{A} = 1$.
We mainly consider the smooth case (corners are also interesting).
The operator $\mathcal{L}_\hbar$ is associated with the quadratic form defined for $\psi \in \mathrm{H}^1(\Omega)$ by

$$Q_\hbar(\psi) = \int_\Omega |(-i\hbar\nabla + \mathbf{A})\psi|^2 \,\mathrm{d}x_1\,\mathrm{d}x_2.$$

The aim is to analyze the low lying eigenvalues of $\mathcal{L}_\hbar$ and their associated (quasi)modes, especially when there are symmetries and multiple points of maximal curvature on the boundary, and we will focus on the case of ellipses.

Semiclassical spectral gap

We are interested in the the eigenvalues $\lambda_n(\hbar)$ of $\mathcal{L}_\hbar$ and especially in the gap

$$\lambda_2(\hbar) - \lambda_1(\hbar)\,.$$

The question of estimating the gap between the magnetic eigenvalues was initially raised in Fournais-Helffer (2006) in the case of constant magnetic fields in two dimensions. Fournais and Helffer have shown the fundamental role of the curvature of the boundary in the semiclassical expansion of the gap (and improved the previous contribution by Helffer and Morame (2001) where only the first eigenvalue was considered).

Let us recall the result.

Theorem (Fournais-Helffer)

If the curvature κ of $\partial\Omega$ has a unique and non-degenerate maximum (attained at a point of the boundary with curvilinear abscissa 0). Then, we have

$$\lambda_n(\hbar) = \Theta_0 \hbar - C_1 \kappa_{\max} \hbar^{3/2} + (2n-1) C_1 \Theta_0^{1/4} \sqrt{\frac{3k_2}{2}} \hbar^{7/4} + o(\hbar^{7/4}), \tag{76}$$

where $\Theta_0 \in (0,1)$ and $C_1 > 0$ are constants related to the De Gennes operator and $k_2 = -\kappa''(0)$.

N. Raymond (with coauthors) has estimated the spectral gap in the case of varying magnetic fields in two dimensions (see his little magnetic book in EMS and references therein)

As for the Robin question, the following operator, acting on $\mathrm{L}^2(\mathbb{R}/\ell\mathbb{Z},\, \mathrm{d}s)$, determines the semiclassical spectral asymptotics:

$$\mathcal{L}_\hbar^{\mathsf{eff}} = \Theta_0\hbar + \frac{\mu''(\zeta_0)}{2}(\hbar D_s + \gamma_0 - \zeta_0\hbar^{\frac{1}{2}} + \alpha_0\hbar)^2 - C_1\kappa(s)\hbar^{\frac{3}{2}}, \qquad \gamma_0 = \frac{|\Omega|}{\ell}, \tag{77}$$

where $D_s = -i\partial_s$, $\ell = |\partial\Omega|$, $\zeta_0 = \sqrt{\Theta_0}$, $C_1 > 0$ and α_0 is a constant related to the De Gennes operator.

The spectral behavior of $\mathcal{L}_\hbar^{\mathrm{eff}}$ is well known. If κ has a unique and non-degenerate maximum, then the first eigenfunctions are localized near this maximum and a local (semi-global) change of gauge reduces the investigation to

$$\Theta_0 \hbar + \frac{\mu''(\zeta_0)}{2} \hbar^2 D_s^2 - C_1 \kappa(s) \hbar^{\frac{3}{2}}, \tag{78}$$

for which the standard semi-classical analysis applied, in particular the harmonic approximation applies, as well as the WKB constructions.

If κ has two symmetric maxima, such a change of gauge is not allowed since there is, in general, no global change of gauge to cancel the flux term (there is a phase shift between the two wells (Outassourt (1988), Bonnaillie-Hérau-Raymond (2016)).
For this problem, many steps of the "general strategy" are working but some are still missing !

WKB construction (Bonnaillie-Hérau-Raymond)

The next result is a local WKB construction (near the unique maximum of the curvature) reflecting the formal approximation by the effective (1D)-operator. In the statement in a tubular coordinates (s, t) near the boundary.

Theorem–WKB form, Curvature induced magnetic bound states

There exists $\Phi = \Phi(s)$ in a nhd $\mathcal{V}$ of $(0, 0)$ s.t. $\Phi''(0) > 0$, and $(\lambda_{n,j})_{j \geq 0}$ s.t.

$$\lambda_n(\hbar) \underset{\hbar \to 0}{\sim} \hbar \sum_{j \geq 0} \lambda_{n,j} \hbar^{\frac{j}{4}},$$

with $\lambda_{n,0} = \Theta_0$, $\lambda_{n,1} = 0$, $\lambda_{n,2} = -C_1 \kappa_{\max}$ and $\lambda_{n,3} = (2n-1) C_1 \Theta_0^{1/4} \sqrt{\frac{3k_2}{2}}$.

Continued

There exists a formal series of $\mathrm{a}_n \underset{\hbar\to 0}{\sim} \sum_{j\geq 0} \mathrm{a}_{n,j}\hbar^{\frac{j}{4}}$ on $\mathcal{V}$ s.t.

$$(\mathcal{L}_\hbar - \lambda_n(\hbar))\left(\mathrm{a}_n \mathrm{e}^{-i\frac{s}{\hbar}(\gamma_0-\zeta_0\hbar^{1/2})}\mathrm{e}^{-\Phi/\hbar^{\frac{1}{4}}}\right) = \mathcal{O}(\hbar^\infty)\,\mathrm{e}^{-\Phi/\hbar^{\frac{1}{4}}},$$

and

$$\mathrm{a}_{n,0}(s,t) = f_{n,0}(s)u_{\zeta_0}(\hbar^{-\frac{1}{2}}t)\,.$$

Moreover, for all $n \geq 1$, there exists > 0 s.t. for $\hbar$ small enough, we have

$$\mathcal{B}\Big(\Theta_0\hbar - C_1\kappa_{\max}\hbar^{\frac{3}{2}} + \lambda_{n,3}\hbar^{\frac{7}{4}}, c\hbar^{\frac{7}{4}}\Big) \cap \mathrm{sp}(\mathcal{L}_\hbar) = \{\lambda_n(\hbar)\},$$

and $\lambda_n(\hbar)$ is a simple eigenvalue.

Tunneling effect for the ellipse

Considering the effective operator leads to the following conjecture in the case of an ellipse:

$$\Omega = \left\{(x_1, x_2) \in \mathbb{R}^2 : \frac{x_1^2}{a^2} + \frac{x_2^2}{b^2} < 1\right\}, \quad a > b > 0. \tag{79}$$

Conjecture

$$\lambda_2(\hbar) - \lambda_1(\hbar) \underset{\hbar\to 0}{\sim} \hbar^{\frac{13}{8}} \mathsf{A} \frac{2^{\frac{5}{2}} C_1^{\frac{3}{4}}}{\sqrt{\pi}} \left(k_2 \mu''(\zeta_0)\right)^{\frac{1}{4}} \left(\kappa(0) - \kappa\left(\frac{\ell}{4}\right)\right)^{\frac{1}{2}} \times \left|\cos\left(\frac{\ell}{2}\left(\frac{\gamma_0}{\hbar} - \frac{\zeta_0}{\hbar^{\frac{1}{2}}} + \alpha_0\right)\right)\right| \mathrm{e}^{-\mathsf{S}/\hbar^{\frac{1}{4}}},$$

Continued

where

$$
\begin{aligned}
S &= \sqrt{\frac{2C_1}{\mu''(\zeta_0)}} \int_0^{\frac{\ell}{2}} \sqrt{\kappa(0)-\kappa(s)}\,\mathrm{d}s, \\
A &= \exp\left(- \int_{[0,\frac{\ell}{4}]} \frac{\partial_s \sqrt{\kappa(0)-\kappa(s)} - \sqrt{\frac{k_2}{2}}}{\sqrt{\kappa(0)-\kappa(s)}}\,\mathrm{d}s \right).
\end{aligned}
$$

$2S$ corresponds to the tangential Agmon distance between the two "mini-wells" inside the boundary.

Formal analysis of the operator symbol

In order to understand the main Theorem and the Conjecture, let us formally describe the mechanism responsible for the WKB constructions. Before analyzing the spectral properties of $\mathfrak{L}_h$, let us recall fundamental properties of the De Gennes operator. For $\zeta \in \mathbb{R}$, let us introduce

$$\mathcal{H}_\zeta = D_\tau^2 + (\tau - \zeta)^2.$$

defined on $\mathrm{L}^2(\mathbb{R}^+)$ with Neumann conditions on the boundary.

We denote by $\mu(\zeta)$ the first eigenvalue of this operator and by u_ζ a corresponding positive L^2-normalized eigenfunction. The behavior of μ is now well known.

Proposition

The functions $\zeta \mapsto \mu(\zeta)$ and $\zeta \mapsto u_\zeta$ are real analytic with respect to ζ. There exists $\zeta_0 > 0$ s.t. μ is decreasing on $(-\infty, \zeta_0)$ and increasing on $(\zeta_0, +\infty)$, and we have

$$\Theta_0 := \mu(\zeta_0) = \zeta_0^2, \qquad \mu'(\zeta_0) = 0, \qquad |u_{\zeta_0}(0)|^2 = \frac{\mu''(\zeta_0)}{2\zeta_0}.$$

The operator symbol and its lowest eigenvalue

The operator $\mathfrak{L}_h$ can be seen as an operator valued operator. Its semiclassical operator symbol is obtained by replacing $hD_\sigma + \frac{\gamma_0}{h}$ by ζ and using symbolic calculus.
Up to an $\mathcal{O}(h^2)$ error term (which is nevertheless an unbounded operator), the semiclassical operator symbol is given by the one dimensional operator in the τ-variable, with parameters $\zeta \in \mathbb{R}$, $\sigma \in \mathbb{R}/\ell\mathbb{Z}$, $\tau \in I_h$,

$$\begin{aligned}\mathcal{H}_{\sigma,\zeta,h} = & -m(\sigma, h\tau)^{-1}\partial_\tau m(\sigma, h\tau)\partial_\tau \\ & +m(\sigma, h\tau)^{-1}\left(\zeta - \tau + h\frac{\tau^2}{2}\kappa(\sigma)\right) m(\sigma, h\tau)^{-1}\left(\zeta - \tau + h\frac{\tau^2}{2}\kappa(\sigma)\right) \\ & +\mathcal{O}(h^2)\,.\end{aligned} \tag{80}$$

We will study this operator thanks to the De Gennes operator and the Feynman-Hellmann formulas. We first compute the asymptotic expansion of operator $\mathcal{H}_{\sigma,\zeta,h}$ as $h \to 0$.
Since $m(\sigma, h\tau) = 1 - h\tau\kappa(\sigma)$, we have for $\sigma \in \mathbb{R}/\ell\mathbb{Z}$, $\tau \in I_h$,

$$m(\sigma, h\tau)^{-1} = 1 + h\tau\kappa(\sigma) + \mathcal{O}(h^2).$$

Since $I_h \to \mathbb{R}_+$ as $h \to 0$, we replace $m(\sigma, h\tau)^{-1}$ by $1 - h\tau\kappa(\sigma) + \mathcal{O}(h^2)$, supposed to be defined on $\mathbb{R}/\ell\mathbb{Z} \times \mathbb{R}_+$.

We therefore get for $\mathcal{H}_{\sigma,\zeta,h}$ for $\sigma \in \mathbb{R}/\ell\mathbb{Z}$ and $\tau \in \mathbb{R}^+$,

$$\mathcal{H}_{\sigma,\zeta,h} = \mathcal{H}_\zeta + h\kappa(\sigma)\left(\partial_\tau + 2\tau(\zeta-\tau)^2 + \tau^2(\zeta-\tau)\right) + \mathcal{O}(h^2). \quad (81)$$

with

$$\mathcal{H}_\zeta = D_\tau^2 + (\tau-\zeta)^2\,.$$

The lowest eigenvalue $\nu(\sigma, \zeta, h)$ of $\mathcal{H}_{\sigma,\zeta,h}$ is simple and isolated. One follows the Born-Oppenheimer strategy and compute for $\sigma \in \mathbb{R}/\ell\mathbb{Z}$ and $\zeta \in \mathbb{R}$ the integral, as $h \to 0$,

$$\int_0^\infty \mathcal{H}_{\sigma,\zeta,h} u_\zeta(\tau) u_\zeta(\tau)\, \mathrm{d}\tau =$$
$$\int_0^\infty \mathcal{H}_\zeta u_\zeta(\tau) u_\zeta(\tau)\, \mathrm{d}\tau + h\kappa(\sigma) \int_0^\infty \left(\partial_\tau + 2\tau(\zeta-\tau)^2 + \tau^2(\zeta-\tau)\right) u_\zeta(\tau). \tag{82}$$

Using theTaylor expansion of $\mu(\zeta)$ at ζ_0, we get, as $\zeta \to \zeta_0$,

$$\int_0^{\infty} \mathcal{H}_\zeta u_\zeta(\tau) u_\zeta(\tau)\, \mathrm{d}\tau = \mu(\zeta) = \Theta_0 + \frac{\mu''(\zeta_0)}{2}(\zeta - \zeta_0)^2 + \mathcal{O}((\zeta - \zeta_0)^3).$$

Putting these two expressions in (82), we get, as $h \to 0$, $\sigma \to 0$ and $\zeta \to \zeta_0$,

$$\int_0^\infty \mathcal{H}_{\sigma,\zeta,h} u_\zeta(\tau) u_\zeta(\tau)\, \mathrm{d}\tau = \Theta_0 + \frac{\mu''(\zeta_0)}{2}(\zeta - \zeta_0 + \alpha_0 h)^2 - C_1 h\kappa(\sigma) + \mathcal{O}(h^2) + \mathcal{O}(h\sigma^2(\zeta-\zeta_0)) + \mathcal{O}(h(\zeta-\zeta_0)^2$$

where α_0 is defined by $\mu''(\zeta_0)\alpha_0 = C_2\kappa_{\max}$.

Let us now define $\mathcal{M} = \{\sigma_1, \sigma_2, \cdots, \sigma_N\}$ the set of all curvilinear abcissa where $\kappa_{\max}$ is attained . The preceding asymptotics remain true with $\sigma \to 0$ replaced by $\mathrm{dist}(\sigma, \mathcal{M}) \to 0$, where $\mathrm{dist}(\sigma, \mathcal{M})$ stands for the curvilinear distance between σ and the set $\mathcal{M}$. Therefore, at a formal level, and coming back to operators in variable σ, one expects that the low lying spectrum of the operator $\mathfrak{L}_h$ should be asymptotically the same as the one of

$$\mathfrak{L}_h^{\text{eff}} = \Theta_0 + \frac{\mu''(\zeta_0)}{2} \left(hD_\sigma + \frac{\gamma_0}{h} - \zeta_0 + \alpha_0 h \right)^2 - C_1 \kappa(\sigma) h, \quad (83)$$

acting on $\mathrm{L}^2(\mathbb{R}/\ell\mathbb{Z},\, \mathrm{d}\sigma)$, and up to controlled errors.
The operator defined in (83) appears to be a magnetic Schrödinger operator with a smooth potential on $\mathbb{R}/\ell\mathbb{Z}$. After rescaling, we get the effective operator (77).

WKB constructions in the simple well case

Let us now explain the main steps in the proof of the Theorem.

Theorem

There exists

$$\Phi : \sigma \mapsto \Phi(\sigma) = \left(\frac{2C_1}{\mu''(\zeta_0)}\right)^{1/2} \left| \int_0^\sigma (\kappa(0) - \kappa(\varsigma))^{1/2}\, \mathrm{d}\varsigma \right|,$$

defined in a nhd $\mathcal{V}$ of $(0,0)$ s.t. $\Phi''(0) > 0$, and $(\lambda_{n,j})_{j\geq 0}$ s.t.

$$\lambda_n(h) \underset{h\to 0}{\sim} \sum_{j\geq 0} \lambda_{n,j} h^{\frac{j}{2}}.$$

There exists on $\mathcal{V}$,

$$a_n \underset{h \to 0}{\sim} \sum_{j \geq 0} a_{n,j} h^{\frac{j}{2}}$$

s.t.

$$(\mathfrak{L}_h - \lambda_n(h)) \left(a_n \mathrm{e}^{-i \frac{\sigma}{h} \left(\frac{\gamma_0}{h} - \zeta_0 \right)} \mathrm{e}^{-\Phi / h^{\frac{1}{2}}} \right) = \mathcal{O}\left(h^\infty\right) \mathrm{e}^{-\Phi / h^{\frac{1}{2}}}.$$

We also have

$$\lambda_{n,0} = \Theta_0\,,\; \lambda_{n,1} = 0\,,\; \lambda_{n,2} = -C_1\kappa_{\max}$$

and $\lambda_{n,3} = (2n-1)C_1\Theta_0^{1/4}\sqrt{\frac{3k_2}{2}}$.
The main term in the Ansatz is

$$a_{n,0}(\sigma,\tau) = f_{n,0}(\sigma)u_{\zeta_0}(\tau).$$

Moreover, for all $n \geq 1$, there exists $c > 0$ s.t. for $\hbar$ small enough

$$\mathcal{B}\left(\lambda_{n,0} + \lambda_{n,2}h + \lambda_{n,3}h^{\frac{3}{2}}, ch^{\frac{3}{2}}\right) \cap \mathrm{sp}\,(\mathfrak{L}_h) = \{\lambda_n(h)\},$$

and $\lambda_n(h)$ is a simple eigenvalue.

Sketch of proof.

Let us introduce a phase function $\Phi = \Phi(\sigma)$ defined in a neighborhood of $\sigma = 0$ which is the unique and non degenerate maximum of the curvature $\kappa = \kappa(0)$. We consider the conjugate operator

$$\mathfrak{L}_h^{\mathsf{wg}} = \mathrm{e}^{\Phi(\sigma)/h^{\frac{1}{2}}} \mathrm{e}^{i\frac{\sigma}{h}\left(\frac{\gamma_0}{h}-\zeta_0\right)} \mathfrak{L}_h \mathrm{e}^{-i\frac{\sigma}{h}\left(\frac{\gamma_0}{h}-\zeta_0\right)} \mathrm{e}^{-\Phi(\sigma)/h^{\frac{1}{2}}} .$$

As usual, we look for

$$a \sim \sum_{j\geq 0} h^{\frac{j}{2}} a_j , \qquad \lambda \sim \sum_{j\geq 0} \lambda_j h^{\frac{j}{2}} ,$$

s.t. , in the sense of formal series we have

$$\mathfrak{L}_h^{\mathsf{wg}} a - \lambda a \sim 0.$$

We may write

$$\mathfrak{L}_h^{wg} \sim \mathfrak{L}_0 + h^{\frac{1}{2}}\mathfrak{L}_1 + h\mathfrak{L}_2 + h^{\frac{3}{2}}\mathfrak{L}_3 + \dots,$$

where

$$\begin{aligned}
\mathfrak{L}_0 &= D_\tau^2 + (\zeta_0 - \tau)^2,\\
\mathfrak{L}_1 &= 2(\zeta_0 - \tau) i\Phi'(\sigma),\\
\mathfrak{L}_2 &= \kappa(\sigma)\partial_\tau + 2\left(D_\sigma + \kappa(\sigma)\frac{\tau^2}{2}\right)(\zeta_0 - \tau) - \Phi'(\sigma)^2 + 2\kappa(\sigma)(\zeta_0 - \tau)^2\tau,\\
\mathfrak{L}_3 &= \left(D_\sigma + \kappa(\sigma)\frac{\tau^2}{2}\right)(i\Phi'(\sigma)) + (i\Phi'(\sigma))\left(D_\sigma + \kappa(\sigma)\frac{\tau^2}{2}\right) +\\
&\qquad + 4i\Phi'(\sigma)\tau\kappa(\sigma)(\zeta_0 - \tau).
\end{aligned}$$

Let us now solve the formal system.
The first equation is

$$\mathfrak{L}_0 a_0 = \lambda_0 a_0\,,$$

and leads to take

$$\lambda_0 = \Theta_0\,, \qquad a_0(\sigma,\tau) = f_0(\sigma) u_{\zeta_0}(\tau)\,,$$

where f_0 has to be determined.

The second equation is

$$(\mathfrak{L}_0 - \lambda_0)a_1 = (\lambda_1 - \mathfrak{L}_1)a_0 = (\lambda_1 - 2(\zeta_0 - \tau)i\Phi'(\sigma))u_{\zeta_0}(\tau)f_0(\sigma).$$

Due to the Fredholm alternative, we must take $\lambda_1 = 0$ and

$$a_1(\sigma,\tau) = i\Phi'(\sigma)f_0(\sigma)\left(\partial_\zeta u\right)_{\zeta_0}(\tau) + f_1(\sigma)u_{\zeta_0}(\tau),$$

where f_1 is to be determined in a next step.

Then the third equation is

$$(\mathfrak{L}_0 - \lambda_0)a_2 = (\lambda_2 - \mathfrak{L}_2)a_0 - \mathfrak{L}_1 a_1 .$$

After computation, the equation becomes

$$\begin{aligned}
&(\mathfrak{L}_0 - \lambda_0)\tilde{a}_2 \\
&\quad = f_0 \Big(\lambda_2 u_{\zeta_0} + \tfrac{\mu''(\zeta_0)}{2} \Phi'^2 u_{\zeta_0} \\
&\qquad + \kappa(-\partial_\tau u_{\zeta_0} - 2(\zeta_0 - \tau)^2 \tau u_{\zeta_0} - \tau^2(\zeta_0 - \tau) u_{\zeta_0}) \Big) ,
\end{aligned}$$

where

$$\tilde{a}_2 = a_2 - (\partial_\zeta u)_{\zeta_0}(i\Phi' f_1 - i\partial_\sigma f_0) + \tfrac{1}{2}(\partial_\zeta^2 u)_{\zeta_0} \Phi'^2 f_0 .$$

We now get the equation

$$\lambda_2 + \frac{\mu''(\zeta_0)}{2}\Phi'^2(\sigma) + C_1\kappa(\sigma) = 0, \qquad \text{with} \qquad C_1 = \frac{u_{\zeta_0}^2(0)}{3}.$$

Here we recognize an *eikonal equation* of a pure electric problem in dimension one whose potential is given by the curvature. Thus we take

$$\lambda_2 = -C_1\kappa(0),$$

and

$$\Phi(\sigma) = \left(\frac{2C_1}{\mu''(\zeta_0)}\right)^{1/2}\left|\int_0^\sigma (\kappa(0)-\kappa(\varsigma))^{1/2}\,\mathrm{d}\varsigma\right|.$$

In particular we have

$$\Phi''(0) = \left(\frac{k_2 C_1}{\mu''(\zeta_0)}\right)^{1/2}, \qquad \text{with} \quad k_2 = -\kappa''(0) > 0.$$

This leads to take

$$\begin{aligned} a_2 = f_0 \hat{a}_2 + (\partial_\zeta u)_{\zeta_0} (i\Phi' f_1 - i\partial_\sigma f_0) \\ -\tfrac{1}{2}(\partial_\eta^2 u)_{\zeta_0} \Phi'^2 f_0 + f_2 u_{\zeta_0}, \end{aligned}$$

where $\hat{a}_2$ is the unique solution, orthogonal to u_{ζ_0} for all σ, of

$$\begin{aligned} (\mathfrak{L}_0 - \lambda_0)\hat{a}_2 &= \lambda_2 u_{\zeta_0} + \tfrac{\mu''(\zeta_0)}{2} \Phi'^2 u_{\zeta_0} \\ &\quad + \kappa \left(-\partial_\tau u_{\zeta_0} - 2(\zeta_0 - \tau)^2 \tau u_{\zeta_0} - \tau^2(\zeta_0 - \tau) u_{\zeta_0}\right), \end{aligned}$$

and f_2 has to be determined.
This procedure can be continued at any order.

About the conjecture

Let us finally discuss the last Conjecture. As suggested by our formal effective operator (83), we first recall a result of tunneling type on a circle.

Let us consider the self-adjoint realization, denoted $\mathfrak{P}_\varepsilon$, of the electro-magnetic Laplacian $(\varepsilon D_x + a(x))^2 + V(x)$ on $\mathrm{L}^2_{2\pi-per}(\mathbb{R}, \mathrm{d}x)$ where the vector potential a and the electric potential V are smooth, 2π-periodic functions. By a gauge transform, this operator is unitarily equivalent to the following operator

$$\mathcal{P}_\varepsilon = (\varepsilon D_x + \xi_0)^2 + V(x),$$

with

$$\xi_0 = \int_{-\pi}^{\pi} a(x)\,\mathrm{d}x\,.$$

Here we can consider that ξ_0 is the Floquet parameter, in the analysis of $(\varepsilon D_x + \xi_0)^2 + V(x)$ on the line.

Theorem

Assume that the function V admits exactly two non-degenerate minima at 0 and π with $V(0) = V(\pi) = 0$ and satisfies $V(x) = V(\pi - x) = V(-x)$. We let

$$V_2 = \sqrt{\frac{V''(0)}{2}}. \tag{84}$$

Then, as ε is small enough, there are only two eigenvalues of $\mathcal{P}_\varepsilon$ in the interval $(-\infty, 2\kappa\varepsilon)$ and they both satisfy

$$\text{for } j = 1, 2, \qquad \rho_j(\varepsilon) = V_2\varepsilon + o(\varepsilon) \quad \text{as } \varepsilon \to 0.$$

Continued

With

$$S = \int_{[0,\pi]} \sqrt{V(x)}\, \mathrm{d}x, \qquad \text{and} \qquad A = \exp\left(-\int_{[0,\frac{\pi}{2}]} \frac{\partial_x \sqrt{V} - V_2}{\sqrt{V}}\, \mathrm{d}x\right), \tag{85}$$

we have the spectral gap estimate

$$\rho_2(\varepsilon) - \rho_1(\varepsilon) = 8\varepsilon^{1/2} A \sqrt{V\left(\frac{\pi}{2}\right)} \sqrt{\frac{V_2}{\pi}} \left|\cos\left(\frac{\xi_0 \pi}{\varepsilon}\right)\right| \mathrm{e}^{-S/\varepsilon} + \varepsilon^{3/2} \mathcal{O}\left(\mathrm{e}^{-S/\varepsilon}\right). \tag{86}$$

The main point is that one can see on the previous formula the global topologic effect of the flux ξ_0. The result is originally due to E. Harrell (1979) in 1D. In the general case this appears in the eighties in two papers of B. Simon on one side and Outassourt on the other side.

We now apply the result to our effective operator $\mathcal{L}_{\hbar}^{\text{eff}}$.

Proposition

The spectral gap of the effective operator $\mathcal{L}_{h}^{\text{eff}}$ is given by

$$\lambda_2^{\text{eff}}(\hbar)-\lambda_1^{\text{eff}}(\hbar) \underset{\hbar\to 0}{\sim} \hbar^{\frac{13}{8}} \mathsf{A} \frac{2^{\frac{5}{2}} C_1^{\frac{3}{4}}}{\sqrt{\pi}} \left|\kappa''(0)\mu''(\zeta_0)\right|^{\frac{1}{4}} \left(\kappa(0)-\kappa\left(\frac{\ell}{4}\right)\right)^{\frac{1}{2}} \times \left|\cos\left(\frac{\ell}{2}\left(\frac{\gamma_0}{\hbar}-\frac{\zeta_0}{\hbar^{\frac{1}{2}}}+\alpha_0\right)\right)\right| \mathrm{e}^{-\mathsf{S}/\hbar^{\frac{1}{4}}},$$

where

$$\begin{aligned} \mathsf{S} &= \sqrt{\frac{2C_1}{\mu''(\zeta_0)}} \int_0^{\frac{\ell}{2}} \sqrt{\kappa(0)-\kappa(s)}\,\mathrm{d}s, \\ \mathsf{A} &= \exp\left(-\int_{[0,\frac{\ell}{4}]} \frac{\partial_s\sqrt{\kappa(0)-\kappa(s)}-\sqrt{-\frac{\kappa''(0)}{2}}}{\sqrt{\kappa(0)-\kappa(s)}}\,\mathrm{d}s\right). \end{aligned}$$

The conjecture of Bonnaillie-Hérau-Raymond says that the spectral gap for the initial problem $\mathcal{L}_\hbar$ is the same as the one of the effective operator $\mathcal{L}_\hbar^{\mathrm{eff}}$.

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