Semiclassical methods and tunneling effects.

a videominicourse

B. Helffer (Université de Nantes)

Nantes-Beyrouth 19, 21, 26 and 28 January 2021

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.

This will be in continuation of the lectures by Ayman Kachmar in Decembre.

A first presentation of this minicourse was given at the Mittag-Leffler institute in January 2019.



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 has been obtained in 2020 by Bonnaillie-Hérau-Raymond. 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. Progress in Math. 68. Birkhäuser (1987).
- B. Helffer. Semi-classical analysis for the Schrödinger operator and applications. Lecture Notes in Mathematics, 1336 (1988).
- Cycon-Froese-Kirsch-Simon. Schrödinger operators. Lecture Notes in Physics (1987).
- P. Hislop and I. Sigal. Introduction to spectral Theory. Appl. Math. Sc 113 (1996).
- M. Dimassi and J. Sjöstrand. Spectral asymptotics in the semi-classical limit (LMS Lecture. Note Series no. 268, Cambridge, 1999)
- ► A. Martinez. An Introduction to Semiclassical and Microlocal Analysis (Universitext) 2002.
- ▶ M. Zworski. Semiclassical Analysis (2012).
- N. Raymond. Bound states of the magnetic Schrödinger Operator. EMS tracts in Mathematics. Vol. 27 (2019).

For the extremely courageous students or researchers the evoluting monster book of V. Ivrii (2019) for its last version):

Microlocal Analysis, Sharp Spectral Asymptotics and Applications. SpringerMonographs in Mathematics. Springer-Verlag, Berlin, 2019.

Concerning semi-classical methods in superconductivity, there is also the book of Fournais-Helffer.

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 (Helffer-Sjöstrand)
- Application to tunneling
- Resonant wells
- Agmon estimates and magnetic Schrödinger operators.



Agmon estimates continued

- Agmon estimates in tight-binding (Daumer,.., Feffermann-Weinstein-Thorpe)
- ► Agmon estimates and pseudo-differential operators: Klein-Gordon, Dirac, Kac, Harper,... Discrete operators...
- ▶ Microlocal Agmon estimates (Martinez,...)
- Magnetic bottles. (Mohamed-Helffer,..., Raymond)
- Decay estimates in superconductivity
- Decay estimates for the Robin problem (Pankrashkin, Helffer, Kachmar, Raymond,...).
- Decay estimates for the Stecklov problem (Hislop-Lutzer, Galkovski-Toth,...)
- Agmon estimates and Landscape function (David, Filloche, Svoboroda).



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-Ostenhof 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 [33] (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 $V \to +\infty$, $V \ge 1$ and continuous, a case treated by Lithner, with a related intuition. Agmon finds a sufficient condition for:

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

is the condition

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

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

This ends the extract of the introduction of Carmona-Simon (1981).

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 [45], one preprint by Helffer-Sjöstrand [HS1] and a detailed version of his announcement by B. Simon [46] (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 in a bounded regular domain $\underline{\Omega}$

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

where V is assumed to be non negative and h > 0 is a positive parameter.

The domain of this operator is

$$D(P_{h,V})=H^2(\Omega)\cap H^1_0(\Omega).$$

This operator is selfadjoint, has compact resolvent and its spectrum is discrete.



Proposition: Energy identity

Let Ω be a bounded open domain in \mathbb{R}^n 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

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

The proof is by an integration by parts.

(1D)-proof

We have

$$-\int_{a}^{b} u''(t)e^{2\phi(t)}u(t) dt$$

$$=\int_{a}^{b} u'(t)(e^{2\phi}u)'(t)dt - u'(b)u(b)e^{2\phi(b)} + u'(a)u(a)e^{2\phi(a)}.$$

Note that the two last term on the right hand side vanish when u(a) = u(b) = 0. Then

$$\int_{a}^{b} u'(t)(e^{2\phi}u)'(t)dt = \int_{a}^{b} u'(2\phi'u + u')e^{2\phi}dt
= \int_{a}^{b} \left((u' + \phi'u)^{2} - (\phi')^{2}u^{2} \right) e^{2\phi}dt
= \int_{a}^{b} ((e^{\phi}u)')^{2}dt - \int_{a}^{b} (\phi')^{2}(e^{\phi}u)^{2}dt.$$

This immediately gives the announced energy identity.

Under some conditions on V, for example if $V \to +\infty$ at ∞ , 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:

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

which implies the simple estimate

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

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

$$\int_{\Omega} (V - |\nabla \phi|^2 - E) \exp \frac{2\phi}{h} |u_h|^2 dx \le 0.$$
 (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:

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

where $C^{1,pw}([0,1];x,y)$ 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

$$|d(x',y)-d(x,y)| \le d(x',x) , \ \forall x,x',y \in \mathbb{R}^n . \tag{6}$$

$$|\nabla_x d(x,y)|^2 \le (V-E)_+(x)$$
, (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.



(1D) computations.

In (1D) the distance between two points a and b takes the form

$$d(a,b) = |\int_a^b \sqrt{(v(t)-E)_+}(t)dt|.$$

A particular case is when E = 0, v(a) = 0, v'(a) = 0, v''(a) > 0. So v has a local minimum. Then, for b close to a, the distance to $b \mapsto d(b, a)$ is a C^{∞} function vanishing exactly at order 2. Its quadratic approximation is easily computed by replacing v by its quadratic approximation v_q :

$$v^{q}(t) = \frac{1}{2}v''(a)(t-a)^{2}$$
.

We then find

$$d(a,b) = \frac{\sqrt{v''(a)}}{2\sqrt{2}} (b-a)^2 + \mathcal{O}(b-a)^3.$$



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 $\frac{1}{\epsilon_1} \exp\left(\sup_{\Omega \setminus \Omega_1} \frac{\phi(x)}{h}\right)$. 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

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

for $h \in (0, h(\epsilon))$ with $h(\epsilon) > 0$, $\eta(\epsilon) \to 0$ as $\epsilon \to 0$.

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

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

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

$$P_{h,V}u_h = \lambda_h u_h , \qquad (11)$$

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

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

Remarks

- An explicit proof will be given below.
- ▶ Under the assumption of the theorem, the essential spectrum is contained (Persson's Lemma) in [lim inf V, $+\infty$). The eigenvalue $\lambda(h)$ which is considered is below lim inf V hence necessarily isolated, with finite multiplicity.
- ▶ The condition inf $V < \liminf V$ implies that for any N > 0, there exists $h_N > 0$ such that for $h \in (0, h_N)$ the operator has at least N eigenvalues (counted with multiplicity).
- ▶ 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 (as already mentioned in the (1D) case) 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:

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

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

Using our choice of ϕ , this immediately leads to

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

Here note that $\phi_{\delta} = \nabla \phi_{\delta} = 0$ in $U_{\delta}(\lambda)$. We finally keep it in the form, for any $\delta > 0$, we have

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

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 connected 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 5 is chosen s.t.

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

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



Detailed proof of a weaker result

If $u^{(2)}$ is an L^2 -normalized eigenfunction of $P_{(h,\Omega_2)}$ attached to an eigenvalue $\lambda^{(2)}(h) \leq E$, then we can introduce a cut-off function χ_2 such that $\operatorname{Supp}\chi_2 \subset \Omega_1$. Then $\chi_2 u^{(2)}$ is in the domain of $P_{(h,\Omega_1)}$ and we have

$$P_{(h,\Omega_1)}(\chi_2 u^{(2)}) = \lambda^{(2)}(h)\chi_2 u^{(2)} + r_2(h),$$

with

$$r_2(h) = -h^2(\Delta \chi_2)u^{(2)} - 2h\nabla \chi_2 \cdot \nabla u^{(2)}$$
.

Now we can choose χ_2 such that the Agmon distance of U to $\operatorname{Supp}(1-\chi_2)$ is larger than S.



Using the Agmon estimates for $u^{(2)}$ and $\nabla u^{(2)}$ we obtain

$$||\chi_2 u^{(2)}|| = 1 + \mathcal{O}(e^{-S/h}),$$

and

$$||r_2|| = \mathcal{O}(e^{-S/h}).$$

By the spectral theorem applied to $P_{(h,\Omega_1)}$, we obtain the existence of $\lambda^{(1)}(h) \in \sigma(P_{(h,\Omega_1)})$ such that

$$|\lambda^{(2)}(h) - \lambda^{(1)}(h)| \le Ce^{-S/h}$$
.

Conversely we can do the same starting from an eigenfunction $u^{(1)}$. Note that the statement I gave before is more precise!

Second application: the symmetric double well problem

As discussed above, the double well problem in dimension ≥ 2 was first discussed in the note of B. Simon [45] immediately followed by the two detailed papers [HS1] and B. Simon [46].

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) [11]. Agmon estimates are not needed because one can work directly with WKB solutions and the theory of ordinary differential equations.

To treat this application, we need first to get a complete analysis of the one well problem.

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:

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

where v is a C^{∞} - function tending to ∞ and admitting a unique minimum at 0 with v(0) = 0.

Let us assume that

$$v''(0) > 0$$
 . (15)

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

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

This means that we replace the potential v by its quadratic approximation at 0 i.e. $\frac{1}{2}v''(0)x^2$ and consider the associated Schrödinger operator.

Using the dilation $x = h^{\frac{1}{2}}y$, we observe that this operator is unitarily equivalent to

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

Consequently, the eigenvalues are given by

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

and the corresponding eigenfunctions are

$$u_n^h(x) = h^{-\frac{1}{4}} u_n^1(\frac{x}{h_2^{\frac{1}{2}}}) \tag{19}$$

with

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

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

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

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

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

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

At this stage, we do not know the labelling of this eigenvalue.



In particular, we get the inequality

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

Combining with other techniques, one can actually prove that

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

$$\mathcal{U}^{-1}\mathcal{H}\mathcal{U} = \sum_{i} \left(-(h\partial_{y_{j}})^{2} + rac{1}{2}\lambda_{j}y_{j}^{2}
ight) \; .$$

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.

For example, in (1D) suppose that there are N minima at a_1, \ldots, a_N , then we have for the ground state we have

$$\lambda_1(h) = h \inf_j \sqrt{\frac{v''(a_j)}{2}} + \mathcal{O}(h^{\frac{3}{2}}).$$

Agmon estimate will say that this ground state is exponentially localized in $\bigcup_{j} \{a_{j}\}$.

With a little more effort, one can show that it is localized in $\bigcup_{i \in \mathcal{J}} \{a_i\}$, where

$$\mathcal{J} = \{j \in \{1, \cdots, N\}, v''(a_j) = \inf_{\ell} v''(a_{\ell})\}.$$



Harmonic approximation in general: lower bounds

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

Assumptions

- ▶ If $\Omega = \mathbb{R}^n$, we assume that $\liminf V > \inf V$.
- ▶ If Ω is bounded, we assume that $\inf_{x \in \Omega} V(x) < \inf_{y \in \partial \Omega} V(y)$.
- V has N non degenerate minima.

In a more physical language, we say that these N minima create N wells.

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 :

$$\sum_{j \in \mathcal{J}} (\phi_j^R)^2 = 1 ,$$

$$\sum_{\ell=1}^n \sum_{j \in \mathcal{J}} |D_{x_\ell} \phi_j^R|^2 \le \frac{C}{R^2} ,$$
 (23)

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

$$\langle P_{h,V}u \mid u \rangle = \sum_{j} \langle P_{h,V}\phi_{j}^{R}u \mid \phi_{j}^{R}u \rangle - h^{2} \sum_{j,\ell} |||D_{x_{\ell}}\phi_{j}^{R}|u||^{2}$$

$$\geq \sum_{j} \langle P_{h,V}\phi_{j}^{R}u \mid \phi_{j}^{R}u \rangle - C \frac{h^{2}}{R^{2}}||u||^{2}.$$
(24)

We will choose the parameter R > 0 later (depending on h) but we already assumed that $R \le 1$.

We can in addition assume that

- either the balls are centered at the N minima of V,
- or the balls are at a distance of $\frac{1}{C}R$ of these minima x^{j_k} $(k = 1, \dots, N)$.

In the first case we observe that :

$$|\left\langle P_{h,V}\phi_j^Ru\mid\phi_j^Ru\right\rangle - \left\langle P_{h,V}^k\phi_j^Ru\mid\phi_j^Ru\right\rangle| \leq CR^3||\phi_j^Ru||^2\;,$$

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

In the second case, using again the fact that the minima of ${\it V}$ are non degenerate, we get :

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



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

$$\lambda_1(h) \ge \inf V + h(\inf_k \mu_1(1, x^{j_k})) - C h^{\frac{6}{5}},$$
 (25)

where the infimum is over the various minima x^{jk} and $\mu_1(h, x^{jk}) = h \, \mu_1(1, x^{jk})$ denotes the lowest eigenvalue of the harmonic approximation at x^{jk} i.e. $P_{h,V}^k$.

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 [13] for a pedagogical presentation).

We will treat in more detail the case of the symmetric double well problem and choose I(h) such that it contains only one eigenvalue of the one-well problem.

The double well symmetric problem

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

$$gV = V$$
.

We also assume that the minima are non degenerate.

We now define reference one well problems by introducing:

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

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

¹Typically, in 2D the symmetry with respect to $\{x_2 = 0\}$ $\Rightarrow x_2 \Rightarrow x_3 \Rightarrow x_4 \Rightarrow x_5 \Rightarrow x$

The parameter $\eta > 0$ is free but can always be chosen arbitrarily small and will not depend on h.

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 the Agmon estimate, these eigenfunctions decay on any compact of M_j and as $h \to 0$, like $\tilde{O}(\exp{-\frac{d(x,U_j)}{h}})$,. We can of course keep the relation

$$g\phi_1=\phi_2$$
.



Definition of \tilde{O}

Here \tilde{O} has the following meaning for given f(x, h) and g(x):

$$f(x,h) = \tilde{O}(\exp \frac{g(x)}{h})$$

if, for any $\epsilon > 0$, one can choose h_{ϵ} and C_{ϵ} s.t. for $h \in (0, h_{\epsilon}]$ we have

$$|f(x,h)| \leq C_{\epsilon} \exp \frac{\epsilon}{h} \exp \frac{g(x)}{h}$$
.

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

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

and

$$S_h = -h^2 \Delta + V$$
.

We note that the "smallness" of r_j can be immediately controlled using the decay estimates on ϕ_j in $B(U_{\hat{j}}, 2\eta) \setminus B(U_{\hat{j}}, \frac{3}{2}\eta)$, where

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:

$$v_j = \Pi_F \psi_j$$
.

Here

$$\Pi_F = \frac{1}{2i\pi} \int_{\gamma} (z - S_h)^{-1} dz$$

where γ is a simple curve in the resolvent set of S_h which surrounds λ_M and such that all the other eigenvalues are in the non bounded component of $\mathbb{C} \setminus \operatorname{Im} \gamma$. We can actually, using our knowledge of the spectrum at the bottom modulo $\mathcal{O}(h^{\frac{3}{2}})$ take a small circle centered at λ_M with radius $r(h) = hr_0$.

For the proof of this formula, we can use the spectral theorem for selfadjoint operators. We arrive at a very simple computation in complex analysis. The resolvent formula shows that $v_j - \psi_j$ can be made very small, more precisely $\exp{-\frac{S}{h}}$ with $S < d(U_1, U_2)$, the Agmon distance between U_1 and U_2 , by choosing $\eta > 0$ small enough). More precisely, we have the following comparison.

Lemma: Control of the error in weighted spaces

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

in $\mathbb{R}^n \setminus B(U_{\widehat{i}}, 4\eta)$, where $\widehat{1} = 2$, $\widehat{2} = 1$ and

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

Here we use an extended notion of \tilde{O} in comparison with the previous definition. We should add in the previous definition after $\forall \epsilon > 0$, " there exists $\eta_{\epsilon} > 0$ ".

Proof

Our starting point is :

$$S_h \psi_j = \lambda_{M_j} \psi_j + r_j \,,$$

where

- ▶ S_h is the selfadjoint realization of $(-h^2\Delta + V)$,
- •

$$\operatorname{supp} r_j \subset B(U_{\widehat{j}}, 2\eta) ,$$

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



We have $\psi_j - \prod_F \psi_j \in F^{\perp}$ by definition and the spectral theorem gives already the estimate

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

The goal is now to have a better estimate near U_j . For a suitable contour γ_h in \mathbb{C} containing λ_M (as above)

$$d(\gamma_h, \sigma(S_h)) \ge \frac{h}{C} \tag{28}$$

we can write:

$$(*) v_j - \psi_j = \frac{1}{2i\pi} \int_{\gamma_h} (z - \lambda_M)^{-1} (z - S_h)^{-1} r_j dz$$
.

Details for the previous identity (*)

We start of

$$(z-S_h)\psi_j=(z-\lambda_M)\psi_j-r_j.$$

For $z \in \gamma_h$, $(z - S_h)^{-1}$ is well defined so, composing the previous equality with $(z - \lambda_M)^{-1}(z - S_h)^{-1}$, we get

$$(z - S_h)^{-1}\psi_j = (z - \lambda_M)^{-1}\psi_j + (z - \lambda_M)^{-1}(z - S_h)^{-1}r_j.$$

Integrating along γ_h leads indeed to (*)

$$(*) v_j - \psi_j = \frac{1}{2i\pi} \int_{\gamma_h} (z - \lambda_M)^{-1} (z - S_h)^{-1} r_j dz.$$

We observe by a property of the kernel of the resolvent (see Dimassi-Sjöstrand) deduced from Agmon estimates that:

$$(z - S_h)^{-1} r_j = \tilde{O}(\sup_{y \in \operatorname{supp} r_j} \exp - \frac{[d(x, y) + d(y, U_j)]}{h})$$

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

Roughly speaking, the distribution kernel $R_h(x, y, z)$ of the resolvent satisfies in a weak sense (see Dimassi-Sjöstrand)

$$R_h(x, y, z) = \tilde{O}(\exp -d(x, y)/h),$$

and this gives a good control in weighted spaces. The separation assumption (28) permits to get the same property for $v_i - \psi_i$:

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

This is indeed an improvement 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 the cut-off function χ_j but that the improvement is quite significative when keeping a large distance (in comparison with η) with $U_{\hat{i}}$ and in particular near U_j .

We then orthonormalize the basis (v_1, v_2) by the Gram-Schmidt procedure.

$$e_j = \sum_k (W^{-\frac{1}{2}})_{jk} v_k \; , \; ext{for } j = 1, 2 \, ,$$

with

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

We note that

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

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 and selfadjointness lead to :

$$M_{12} = M_{21}$$
 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

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

with

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

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

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

A priori informations on the decay permit to restrict the integration in the right hand side of (31) to the set $\{d(x, U_1) + d(x, U_2) \le d(U_1, U_2) + a\}$ for some a > 0.

A computation based on the Stokes Lemma gives then the existence of $\epsilon_0 > 0$ s.t. :

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

Here $S_{12}=d(U_1,U_2)$ and Γ is an open piece of hypersurface defined in the neighborhood of the minimal geodesic $\operatorname{geod}(U_1,U_2)$ 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 neighborhood of the intersection γ_{12} of Γ with $\operatorname{geod}(U_1,U_2)$, 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 $h^{-\frac{n}{4}}a_j(x,h) \exp{-\frac{d(x,U_j)}{h}}$.

This leads finally to

$$M_{12} = h^{1-\frac{n}{2}} \exp{-\frac{d(U_{1},U_{2})}{h}} \times \\ \times \int_{\Gamma} \exp{-\frac{(d(x,U_{1})+d(x,U_{2})-d(U_{1},U_{2}))}{h}} \times \\ \times (a_{1}(x,0)a_{2}(x,0)(\partial_{n}d(x,U_{1})-(\partial_{n}d(x,U_{2}))+\mathcal{O}(h)) d\nu_{\Gamma},$$
(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 in the case of one well

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

$$E(h) \sim \sum_{j \geq 1} E_j h^j$$
, 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 $a_0(0) \neq 0$.

This reads

$$(E) (\nabla \varphi)^2 a(\cdot, h) - 2h \nabla \varphi(\cdot, h) \nabla a(\cdot, h) - h^2 \Delta a(\cdot, h) = E(h) a(\cdot, h) + \mathcal{O}(h^{\infty})$$

We will solve this equation by expanding in powers of h

Remarks

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

Eikonal equation

The phase φ is determined by looking to the coefficient of h^0 in (E) and the existence of a solution is given by the proposition

Proposition for the 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 a Lagrangian submanifold in the cotangent space $T^*\mathbb{R}^n$

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

which is living in $\{(x,\xi): p(x,\xi) = E_0\}$ where

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



The particular case when V is quadratic.

Let us assume that V(x) is quadratic (associated to a positive symmetric matrix A. Then the corresponding φ is quadratic and non degenerate. After diagonalization of A, we are reduced by separation of variable to look for

$$\varphi(x) = \sum_{j=1}^{n} \varphi_j(x_j)$$

with φ_i satisfying:

$$(\varphi_i')^2(x_j) = \lambda_j x_i^2, \ \varphi_j(0) = 0.$$

One get immediately

$$\varphi_j(x_j) = \frac{1}{2} \sqrt{\lambda_j} x_j^2.$$

For the matrix B associated with φ we get

$$B = \frac{1}{2}A^{1/2}$$
.



First transport equation

When writing term to term the necessary cone

When writing term to term the necessary conditions, 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 by considering x = 0,

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

to compare with what we get from the harmonic approximation. One can show that this condition is sufficient. One can solve along the integral curves of the vector field $\nabla \varphi$. (See my lecture Notes)



1D case

The transport equation reads (assuming that the minimum is at x = 0)

$$2\varphi'(x)a_0'(x) + (\varphi''(x) - \varphi''(0))a_0(x) = 0$$
, $a_0(0) = 1$.

We can rewrite it as

$$(\log a_0)'(x) = a_0'(x)/a_0(x) = -(\varphi''(x) - \varphi''(0))/2\varphi'(x).$$

This leads to

$$a_0(x) = e^{-\int_0^x (\varphi''(t) - \varphi''(0))/2\varphi'(t)) dt}$$
.

Useful proposition for solving transport equations

Proposition

Let X be a C^{∞} real vector field in a neighbd of 0 s. t. X(0) = 0. Suppose that the linear part of X is given by:

$$X_0 = \sum_{i=1}^n \nu_i x_i \partial_{x_i}$$
 with $\nu_i > 0$.

Let $b \in C^{\infty}$ s.t. b(0) = 0. Then $\forall g \in C^{\infty}$ s.t. g(0) = 0 and $\forall f_0 \in \mathbb{R}, \exists g \in C^{\infty}$ (unique) in a neighbd of 0 s.t.

$$(X + b)f = g \text{ and } f(0) = f_0.$$

- ▶ Note that the proof of the proposition given in my Lecture notes is only true under a non resonance unmentioned assumption permitting to use the linearization Sternberg theorem. For a general proof, one should look either to the original paper [HeSj1] or to the book of Dimassi-Sjöstrand.
- ► The proposition was applied above with $X = \nabla \varphi$ and b = 0 and will be applied below with $X = \nabla \varphi$ and $b = (\Delta \varphi E_1)$.
- Of course if X does not vanish at a point, one can always solve locally.

Higher order transport equation

The next transport equation corresponds to the coefficient of h^2 in (E) and reads

$$2\nabla\varphi\cdot\nabla a_1+(\Delta\varphi-E_1)a_1=\Delta a_0+E_2a_0\,,\,a_1(0)=0$$

Again E_2 is determined by considering the transport equation at the minimum:

$$E_2 = -(\Delta a_0/a_0)(0).$$

One can then solve this equation by integrating along the the integral curves of $\nabla \varphi$.

Comparison WKB solution-one well eigenfunction

Comparison theorem

If ϕ_1 is the normalized eigenfunction of S_{h,M_1} with an eigenvalue λ_M and θ_1 is the WKB solution renormalized by imposing that its realization has L^2 norm equal to 1, then, we have

$$\phi_1 - \theta_1 = \mathcal{O}(h^{\infty}) \exp{-\frac{d_1(x)}{h}}$$

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

Here we use that the Agmon distance $d_1(x) = d(x, U_1)$ of x 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:

- Decay estimates for the eigenfunctions of the initial problem and the eigenfunctions of suitable one well problems (Agmon estimates).
- 2. Rough localization of the eigenvalues permitting to identify spectral gaps (harmonic approximation)
- 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.



The flea on the elephant effect

As soon as we leave the symmetric case many effects can be considered. This was first analyzed by B. Simon [47] under the name of "Flea on the elephant".

Let us explain the effect following the second paper of the series Helffer-Sjöstrand.



Figure: Does the flea bite have strong consequences?

We start from the double well symmetric situation with a potential V_0 , satisfying inf $V_0 = 0$ and having two symmetric non degenerate minima denoted by U_1 and U_2 .

We consider now as new potential

$$V_{\delta}(x) = V_0(x) + \delta w(x)$$

where $0 \le w \in C_0^{\infty}(\omega)$.

We assume that

$$0 < \mathit{d}_{V_0}(\mathit{U}_1, \operatorname{supp} w) < \frac{1}{2} \mathit{d}_{V_0}(\mathit{U}_1, \mathit{U}_2) < \mathit{d}_{V_0}(\mathit{U}_2, \operatorname{supp} w) \,.$$

and that

$$\operatorname{supp} w \cap \operatorname{Geod}(U_1, U_2) = \emptyset.$$



In this situation, one can again reduce the analysis to a 2×2 matrix M^{δ} where the principal term in the off-diagonal coefficient M_{12}^{δ} is essentially unchanged

$$M_{12}^{\delta} = M_{12}^{0} + \mathcal{O}(e^{-S_{12} - \eta/h})$$
 for some $\eta > 0$.

Similarly

$$M_{22}^\delta=M_{22}^0+\mathcal{O}(e^{-S_{12}-\eta/h})$$
 for some $\eta>0$.

But M_{11}^{δ} can be estimated from below by (for $0 < \delta < \delta_0$)

$$M_{11}^{\delta} \geq M_{11}^{0} + \delta \exp{-\frac{2d_{V_0}(U_1, \operatorname{supp} w) - \epsilon}{h}}, \, \forall \epsilon > 0.$$

Formally, the main term of the perturbation is indeed

$$\delta \int wu_1^2 dx \,,$$

where u_1 is the ground state of the Dirichlet realization of $-h^2\Delta + V_0$ in M_1 .

Using a lower bound for the decay of u_1 , we get the above.

This implies, having in mind that $M_{22}^0=M_{11}^0$, the existence of $\delta_1>0$ such that, as $h\to 0$,

$$(M_{11}^{\delta}-M_{22}^{\delta})^2\gg (M_{12})^2$$
.

Actually this is still true with $\delta = \exp{-\alpha/h}$ for $\alpha > 0$ small enough.

In this situation the eigenvalues of M^{δ} satisfy

$$\lambda_{-}^{\delta} = M_{11}^{0} + \tilde{O}(e^{-S_{12}/h}),$$

and

$$\lambda_+^{\delta} \geq M_{11}^0 + \delta \exp{-\frac{2d_{V_0}(U_1, \operatorname{supp} w)}{h}}$$

and the corresponding eigenvectors are in the orthonormal basis of M, up to exponentially small terms are (0,1) and (1,0). The localization of the ground state near U_2 . The ground state is actually exponentially small near U_1 . The second eigenfunction will be localized near U_1 .

Conclusion about the role of the flea



The elephant does not feel a flea-bite. ...

Figure: Is it true?

No the proverb is not true! We have shown that it is not true for the localization of the groundstate. An exponentially small perturbation, relatively far from the minima can have a strong effect: hence the name "the flea on the elephant".

Miniwells

Interesting questions appear when the minima (= wells) are submanifolds. Then we could have to define a transversal Agmon distance and an Agmon distance inside the wells. We will recover this situation for many models that we want to present for the Robin problem and the problem in surface superconductivity. The well will actually appear to be the boundary of the domain.

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 $O(\exp{-d(x, U)/h})$.
- ▶ But inside the well, it appears a tangential decay to the set of miniwells $\mathcal{O}(\exp{-d_{Tang}(x)}/\sqrt{h})$.

Analysis of a toy model

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 a more accurate exhibit a miniwell phenomenon given by (x, y) = (0, 0). The ground state will actually live as $h \to 0$ at (0, 0).

Rough decay estimates

Very roughly, the inequalities

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

and

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

suggest that the decay of the ground state will be in any compact $K \subset \mathbb{R}^2$ like $\mathcal{O}(\exp{-\alpha_K \frac{y^2}{h}} \exp{-\beta_K \frac{x^2}{\sqrt{h}}})$ for positive constants α_K, β_K .

A more accurate point of view: "harmonic approximation"

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

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

One can also produce a double mini-well problem:

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

We will then see a tunnelling effect (inside the well) between (-1,0) and (1,0) leading to a splitting between the two first eigenvalues of order $\exp{-\frac{S_{-+}}{\sqrt{h}}}$.

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 the simplest models are

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

resp.

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

which reduces approximately to

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

resp.

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

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



The Robin problem

We come back to the problem described in the course of Ayman Kachmar. This time we assume that no magnetic field is present but we would like to have more accurate results leading to the analysis of the splitting.

Ayman Kachmar was analyzing the case of a disk (hence with constant curvature), we will here exhibit the role of the variation of the curvature.

In this Robin problem, the well will be the boundary of the domain and the variation of the curvature will create miniwells (at the boundary). 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,

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

where $\alpha > 0$ is a given parameter.

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

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

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

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

where κ_{max} is the maximal curvature along the boundary Γ . Note that the first term in (40) has been obtained previously (see Levitin-Parnovski [32] and references therein).

For the disk (= the constant curvature case), you recognize the result presented by Ayman Kachmar in his course (but with no magnetic field!).

Note that this does not permit to get for example the splitting between the first and the second eigenvalue as $\alpha \to +\infty$. Actually all the eigenvalues have the same asymptotics modulo $o(\alpha)$.

The Steklov problem

A close problem, which is very popular in the recent years is the following.

This time we are looking for the $\alpha \in \mathbb{R}$'s for which there exists a non trivial solution for

$$\mathcal{P}^{\alpha}u=0. \tag{38}$$

It can be shown when $\partial\Omega$ is compact that there is an infinite sequence of α_i tending to $+\infty$ such that this property holds.

Another way to present the problem is to introduce the Dirichlet-to-Neumann operator which associates to $u_0 \in H^{\frac{1}{2}}(\partial\Omega)$ minus the normal derivative of u at the boundary where u is the unique solution in $H^1(\Omega)$ of the non homogeneous Dirichlet problem

$$-\Delta u = 0$$
, $u_{/\partial\Omega} = u_0$.



The Steklov problem is then interpreted as the problem to determine the spectrum (α_j) of the Dirichlet-to-Neumann operator which can be seen as a positive selfadjoint operator with compact resolvent on $L^2(\Gamma)$ with domain $H^1(\Gamma)$.

The Robin-Steklov problem

More generally, we can look for the pairs $\alpha, \lambda \in \mathbb{R}$ for which there exists a non trivial solution for

$$\mathcal{P}^{\alpha}u = \lambda u. \tag{39}$$

For fixed α , we recover the Robin problem.

For $\alpha=0$, we are dealing with the Neumann problem and in the limit $\alpha\to-\infty$ we recover the Dirichlet problem.

For fixed λ , we get a generalization of the Steklov problem which corresponds to $\lambda = 0$.



If the domain Ω is an exterior domain, then the operator \mathcal{P}^{α} has an essential spectrum; the essential spectrum is $[0,\infty)$. In this case, the asymptotics in (40) 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}^{α} . When the domain Ω is an interior domain, then by Sobolev embedding, the operator \mathcal{P}^{α} is with compact resolvent and its spectrum is purely discrete.

Analysis of the splitting (after Helffer-Kachmar-Raymond)

Our aim is to improve the two terms asymptotic expansion in

$$\lambda_n(\alpha) = -\alpha^2 - \kappa_{\text{max}}\alpha + o(\alpha) \quad \text{as } \alpha \to +\infty,$$
 (40)

and to give the leading term of the spectral gap $\lambda_2(\alpha) - \lambda_1(\alpha)$ under rather generic assumptions on the boundary $\partial\Omega$.

Let κ be the curvature and κ_{max} its maximal value of κ . We suppose (first) that:

$$\text{Ass. (A)} \left\{ \begin{array}{l} \kappa \text{ attains its maximum } \kappa_{\text{max}} \text{ at a unique point} \\ \text{ (denoted by 0 in arc length) and} \\ \text{ the maximum is non-degenerate, i.e. } \kappa_2 := -\kappa''(0) > 0 \,. \end{array} \right.$$

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

$$\lambda_{\it n}(lpha) \sim -lpha^2 - lpha \kappa_{\sf max} + (2\it n-1) \sqrt{rac{k_2}{2}} \, lpha^{1/2} + \sum_{j=0}^{+\infty} \zeta_{j,\it n} lpha^{rac{1-j}{4}} \, .$$

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



If we compare with the existing semi-classical litterature for Schrödinger operators (see Helffer-Sjöstrand [HS1] and Simon [46] 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

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

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 [22] 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

$$\mathcal{L}_h = -h^2 \Delta \,, \tag{41}$$

with domain,

$$D(\mathcal{L}_h) = \{ u \in H^2(\Omega) : \nu \cdot h \nabla u - h^{1/2} u = 0 \text{ on } \partial \Omega \}.$$
 (42)

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 HK

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 HK consists of two major steps. In the first step, we establish a three-term asymptotics

$$\mu_n(h) = -h - \kappa_{\text{max}} h^{3/2} + (2n - 1)\sqrt{\frac{k_2}{2}} h^{7/4} + o(h^{7/4}), \quad (43)$$

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 (43), 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,

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

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

$$V_{\delta} = \{x \in \Omega : \operatorname{dist}(x, \Gamma) < \delta\},$$
 (44)

and the quadratic form, defined on the variational space

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

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 $\rho \in (0, \frac{1}{4}]$. We will choose

- either $\rho < \frac{1}{4}$ with D = 1,
- or $\rho=\frac{1}{4}$ and D>S where S is the tangential Agmon distance between the wells in order that the error term in (45) 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 $\mu_n(h) \leq -\epsilon_0 h$,

$$\mu_n(h) \le \mu_n^{\{\delta\}}(h) \le \mu_n(h) + C \exp\left(-\alpha \delta h^{-\frac{1}{2}}\right)$$
 (45)

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.

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



For all $\delta > 0$, define

$$V_{\delta} = \{x \in \Omega : \operatorname{dist}(x, \partial \Omega) < \delta\},\$$

The map Φ is defined as follows:

$$\Phi: \mathbb{R}/(|\partial\Omega|\mathbb{Z})\times(0,t_0)\ni (s,t)\mapsto x=M(s)-t\,\nu(s)\in\mathcal{V}_{t_0}.$$
 (46)

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

$$\widetilde{u}(s,t) := u(\Phi(s,t)).$$
 (47)

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

$$\int_{\mathcal{V}_{\delta}} |\nabla u(x)|^2 dx = \int \left[(1 - t\kappa(s))^{-2} |\partial_s \widetilde{u}|^2 + |\partial_t \widetilde{u}|^2 \right] (1 - t\kappa(s)) \, ds dt \,, \tag{48}$$

and

$$\int_{\mathcal{V}_{t_0}} |u(x)|^2 dx = \int_{|t| < t_0} |\widetilde{u}(s, t)|^2 (1 - t\kappa(s)) ds dt. \tag{49}$$

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

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

where

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

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

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

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 1*D*-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

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

with domain

$$Dom(\mathcal{H}_0) = \{ u \in H^2(\mathbb{R}_+) : u'(0) = -u(0) \}.$$
 (51)



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

$$u_0(\tau) = \sqrt{2} \exp(-\tau) . \tag{52}$$

We also consider this operator in a bounded interval (0, T) with T large and Dirichlet condition at $\tau = T$. We refer for this analysis to the course by Ayman Kachmar.

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

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

where

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

in the re-scaled boundary coordinates

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

and get

$$(L_h/h)(s, t, \partial_s, \partial_t) = \widetilde{\mathcal{L}}_h(\sigma, \tau, \partial_\sigma, \partial_\tau).$$

The Robin condition in this new coordinates reads

$$\partial_{\tau} u(\sigma,0) = -u(\sigma,0)$$
.



We then consider the formal expansion of the operator $\widetilde{\mathcal{L}_h}$.

This is obtained by the Taylor expansion of the coefficients of the rescaled operator at $\tau=0, \sigma=0$. This depends only on the Taylor expansion of the curvature at 0, the point of maximal curvature. This leads to an expansion in powers of $h^{\frac{1}{8}}$.

$$h^{-1}\mathcal{L}_h \sim P_0 + h^{1/2}P_2 + h^{3/4}P_3 + h^{7/8}P_{\frac{7}{2}} + \cdots,$$
 (53)

where

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

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 $(v_{n,j})_{i=1}^{\infty} \subset \mathcal{S}(\mathbb{R}), (g_{n,j})_{i=0}^{\infty} \subset \mathcal{S}(\mathbb{R} \times \overline{\mathbb{R}_+})$ s.t. ,

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

and the function

$$\Psi_{n}(\sigma,\tau) \sim u_{0}(\tau)f_{n}(\sigma) + \sum_{j=1}^{\infty} h^{j/8}u_{0}(\tau)v_{n,j}(\sigma) + h^{7/8} \sum_{j=0}^{+\infty} h^{j/8}g_{n,j}(\sigma,\tau)$$
(54)

satisfies

$$\left(\widetilde{\mathcal{L}}_h - \mu_h\right) \Psi_n = \mathcal{O}(h^{\infty}), \qquad (55)$$

where

$$\mu_n \sim -1 - h^{1/2} \kappa_{\mathsf{max}} + h^{3/4} \sqrt{\frac{k_2}{2}} (2n - 1) + h^{7/8} \sum_{j=0}^{\infty} \zeta_{j,n} h^{j/8} \,.$$
 (56)

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

$$H_{\text{harm}} = -\partial_{\sigma}^2 + \frac{k_2}{2}\sigma^2$$
.

From the formal construction to the quasi-mode

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,

$$\Phi_n(s,t) = \chi_1\left(\frac{s}{|\partial\Omega|}\right) \chi_1\left(\frac{t}{h^{1/8}}\right) \Psi_n(h^{-1/8}s, h^{-1/2}t).$$
 (57)

Detail.

For Ψ_n which is only a formal construction, we actually take a finite sum (of arbitrary length)

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

and will get an arbitrarily small remainder, i.e. $\mathcal{O}(h^{N/8})$ with N arbitrarily large.

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 $h \to 0_+$,

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

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 with

$$\mu_{n} \sim -1 - h^{1/2} \kappa_{\mathsf{max}} + h^{3/4} \sqrt{rac{k_{2}}{2}} \left(2n - 1\right) + o(h^{rac{3}{4}}) \,.$$

Details for the three first terms

We write, observing that

$$u_0'=-u_0\,,$$

$$(P_{0} + h^{1/2}P_{2} + h^{3/4}P_{3})(\psi_{n,0})(\sigma,\tau)$$

$$= \left(-\partial_{\tau}^{2} + h^{\frac{1}{2}}\kappa(0)\partial_{\tau} - h^{\frac{3}{4}}(\partial_{\sigma}^{2} + \frac{\kappa''(0)}{2}\sigma^{2}\partial_{\tau})\right)u_{0}(\tau)f_{n}(\sigma)$$

$$= \left(-1 - h^{\frac{1}{2}}\kappa(0)\right)\psi_{n,0} + h^{\frac{3}{4}}u_{0}(\tau)\left((-\partial_{\sigma}^{2} - \frac{\kappa''(0)}{2}\sigma^{2})f_{n}(\sigma)\right)$$

$$= \left(-1 - h^{\frac{1}{2}} + h^{\frac{3}{4}}\sqrt{\frac{k_{2}}{2}}(2n-1)\right)\psi_{n,0}$$

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,

$$(P_0+1)\psi_{n,7}+(F_1-\mu_7)\psi_{n,0}+(P_3-\mu_6)\psi_{n,1}=0.$$
 (58)

with

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

Note that $\zeta_0 = \mu_7$ and that μ_6 has been already determined

$$\mu_6 = \sqrt{\frac{k_2}{2}} (2n-1)$$
.

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 .

Note that we already know $\psi_{n,0}$.



We determine μ_7 by multiplying by $u_0(\tau)\varphi_0(\sigma)$:

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

and integrating in all the variables. We get as a necessary condition for the existence of a solution:

$$\mu_7 = \langle F_1 \psi_{n,0} \, | \, \psi_{n,0} \rangle \,. \tag{59}$$

We now come back to (58) (recalled above), multiply by $u_0(\tau)$ and integrate this time only in the variable τ . This gives:

$$\left(\int ((F_1 - \mu_7)\psi_0)(\sigma, \tau) u_0(\tau) d\tau\right) + (H_{\text{harm}} - \mu_6)\varphi_1(\sigma) = 0.$$
(60)

This can be written in the form, having in mind that μ_6 is an eigenvalue of $H_{\rm Harm}$,

$$(H_{\text{Harm}} - \mu_6)\varphi_1(\sigma) = \theta(\sigma), \qquad (61)$$

where

$$\theta(\sigma) = -\left(\int ((F_1 - \mu_7)\psi_0)(\sigma, \tau) u_0(\tau)\right) d\tau$$

 θ is orthogonal to φ_0 as a consequence of the choice of μ_7 .

We choose φ_1 as the solution of (61) which is orthogonal to φ_0 . We write:

$$\psi_{n,7}(\sigma,\tau) = \varphi_1(\sigma)u_0(\tau) + \psi_{n,7}^0(\sigma,\tau)$$

where

$$\int \psi_{n,7}^0(\sigma,\tau)u_0(\tau)\,d\tau=0\,.$$

It remains to solve

$$((P_0+1)\psi_{n,7}^0)(\sigma,\tau)=\Theta_7(\sigma,\tau)$$

with

$$\int_0^{+\infty} \Theta_7(\sigma,\tau) u_0(\tau) d\tau = 0.$$

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

More explicitly, if we write

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

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

The solution is then given by

$$\psi_{n,7}^0(\sigma,\tau) = \sum_\ell \kappa_\ell(\sigma) \hat{\nu}_\ell(\tau)$$

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
$$\int_0^{+\infty} \hat{\nu}_{\ell}(\tau) u_0(\tau) d\tau = 0$$
.

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 .

We have achieved the construction of quasi-modes permitting the localize the spectrum modulo $\mathcal{O}(h^{\infty})$.

This is only a first step in the general strategy that we have described in the case of the Schrödinger operator. At this stage the constructed quasi-modes do not have the right decay.

There is a need for a WKB construction.

Moreover in the case of multiple minima for the curvature, we have to explain how we construct "one mini well" problems.

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 $\widehat{\mathcal{L}}_{s_{\omega},h}^{T}$ is defined as follows.

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

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

$$\widehat{\mathcal{V}} = \omega \times (0, T),
\widehat{V}_{s_{\omega}, T} = \{ u \in H^{1}(\widehat{\mathcal{V}}_{r}) : u = 0 \text{ on } t = T \text{ and } \partial \omega \times (0, T) \},
\widehat{\mathcal{D}}_{s_{\omega}, T} = \{ u \in H^{2}(\widehat{\mathcal{V}}_{r}) \cap \widehat{V}_{s_{\omega}, T} : \partial_{t} u = -h^{-\frac{1}{2}} u \text{ on } t = 0 \}.$$
(62)

The operator $\widehat{\mathcal{L}}_{s_{\omega},T}$ is the self-adjoint operator on $L^2(\widehat{\mathcal{V}}; a\,dsdt)$ with domain $\widehat{\mathcal{D}}_r$.

Let $\mu_{j,s_{\omega},T}(h)$ be the *j*-th eigenvalue of the operator $\widehat{\mathcal{L}}$.

The previous analysis yields that, for h small, $\mu_{1,s_{\omega},T}(h)$ is a simple eigenvalue and

$$\mu_{2,\mathbf{s}_{\omega},T}(h) - \mu_{1,\mathbf{s}_{\omega},T}(h) = 3\gamma h^{7/4} + h^{7/4}o(1) \quad \text{as } h \to 0_+, \quad (63)$$
 where $\gamma = \sqrt{\frac{-\kappa''(\mathbf{s}_{\omega})}{2}}$.

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 there is a need for the construction of a 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

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

More recently Bonnaillie-Hérau-Raymond (2014) in [1] use this technique for a problem arising in superconductivity (see the last part of the lectures).

We recall that

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

where

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

This time 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

$$\Psi^{WKB}(s, au,h)\sim \exp{-rac{artheta(s)}{h^{rac{1}{4}}}}\left(\sum_{\ell}\mathsf{a}_{\ell}(s, au)h^{rac{\ell}{4}}
ight)$$

and a corresponding eigenvalue

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

We first determine the "formal" operator

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

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

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

with

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

Taking $\mu_0 = -1$, the first equation reads (with Robin condition and $Q_0 = Q_0^{\vartheta}$)

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

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

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

At this stage ξ_0 , ξ_1 and ϑ are undetermined.

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 $\vartheta(s) \ge 0$.

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

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

and to determine ξ_0 .

This looks at this stage identical to what we were doing for the Schrödinger operator in (1D) and suggests that there is an effective hamiltonian in the s variable.

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 the ellipse, where we have two maxima for the curvature and a symmetry, we expect a tunneling in the form

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

where S_0 is the tangential Agmon distance between the two points of maximal curvature on the boundary associated with the metric $\sqrt{\kappa_{max} - \kappa(s)} \, ds^2$ and a_0 has a complete. expansion in powers of $h^{\frac{1}{4}}$ starting with $a(0) \neq 0$.

This is this kind of example that we want to treat. Here we follow a paper by Helffer-Kachmar-Raymond [HKR].



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

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

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

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

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

$$\mathcal{L}_h = -h^2 \Delta \,, \tag{64}$$

with domain

$$\mathcal{D}(\mathcal{L}_h) = \{ u \in H^2(\Omega) : \nu \cdot h^{\frac{1}{2}} \nabla u - u = 0 \text{ on } \Gamma \}, \qquad (65)$$

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

$$\mathcal{M}_{h}^{\text{eff}} = -h - \kappa_{\text{max}} h^{\frac{3}{2}} + h^{2} D_{s}^{2} + h^{\frac{3}{2}} v(s), \qquad v = \kappa_{\text{max}} - \kappa,$$
 (66)

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

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

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

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

$$\begin{split} S &= min\left(S_u, S_d\right)\,, \\ S_u &= \int_{\left[s_r, s_\ell\right]} \sqrt{\mathfrak{v}(s)} ds\,, \\ S_d &= \int_{\left[s_\ell, s_r\right]} \sqrt{\mathfrak{v}(s)} ds\,, \end{split}$$

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 $\mathcal{M}_{\hbar}^{\text{circ}}$ is obtained by adding the contributions of each geodesic and reads

$$\lambda_{2}(\hbar) - \lambda_{1}(\hbar) = 4\hbar^{\frac{1}{2}}\pi^{-\frac{1}{2}}\gamma^{\frac{1}{2}} \left(\mathsf{A}_{\mathsf{u}}\sqrt{\mathfrak{v}(\mathsf{0})}e^{-\frac{\mathsf{S}_{\mathsf{u}}}{\hbar}} + \mathsf{A}_{\mathsf{d}}\sqrt{\mathfrak{v}(\mathsf{L})}e^{-\frac{\mathsf{S}_{\mathsf{d}}}{\hbar}} \right) + \mathcal{O}(\hbar^{\frac{3}{2}}e^{-\frac{\mathsf{S}}{\hbar}}), \tag{67}$$

where

$$\begin{split} \mathsf{A}_{\mathsf{u}} &= \mathsf{exp}\left(-\int_{[s_{\mathsf{r}},0]} \frac{(\mathfrak{v}^{\frac{1}{2}})'(s) + \gamma}{\sqrt{\mathfrak{v}(s)}} ds\right) \;, \\ \mathsf{A}_{\mathsf{d}} &= \mathsf{exp}\left(-\int_{[s_{\ell},L]} \frac{(\mathfrak{v}^{\frac{1}{2}})'(s) - \gamma}{\sqrt{\mathfrak{v}(s)}} ds\right) \;, \\ \gamma &= (\mathfrak{v}''(s_{\mathsf{r}})/2)^{\frac{1}{2}} = (\mathfrak{v}''(s_{\ell})/2)^{\frac{1}{2}} \;. \end{split}$$

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

$$\mu_2^{\text{eff}}(h) - \mu_1^{\text{eff}}(h) = h^{\frac{3}{2}}(\lambda_2(\hbar) - \lambda_1(\hbar)),$$
 (68)

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

$$\mu_{2}^{\text{eff}}(h) - \mu_{1}^{\text{eff}}(h) = 4h^{\frac{13}{8}}\pi^{-\frac{1}{2}}\gamma^{\frac{1}{2}} \left(A_{u}\sqrt{\mathfrak{v}(0)} \exp{-\frac{S_{u}}{h^{\frac{1}{4}}}} + A_{d}\sqrt{\mathfrak{v}(L)} \exp{-\frac{S_{d}}{h^{\frac{1}{4}}}} \right) + \mathcal{O}\left(h^{\frac{13}{8} + \frac{1}{4}} \exp{-\frac{S}{h^{\frac{1}{4}}}}\right).$$
(69)

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

Statement of the main Tunneling result

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

Under Assumptions T1 and T2, we have

$$\mu_2(h) - \mu_1(h) \underset{h \to 0}{\sim} \mu_2^{\text{eff}}(h) - \mu_1^{\text{eff}}(h),$$
 (70)

where $\mu_j^{\text{eff}}(h)$ is defined before and where $\mu_2^{\text{eff}}(h) - \mu_1^{\text{eff}}(h)$ 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 [22]. One difference between the setting here and that appears in the spectral reduction to the reference problems. In [22], 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.

More recent results (relative to the Steklov problem) have been obtained recently (Daudé-Helffer-Nicoleau) on the flea on the elephant effect.

We have no time for presenting the last part.

Many thanks to the audience and particularly to Ayman Kachmar and Wafaa Saad who organize the course.

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) [43]. 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) = curl A is positive and that

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

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

$$\mathcal{L}_{\hbar} = (-i\hbar\nabla + \mathbf{A})^2, \tag{71}$$

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 $\psi \in H^1(\Omega)$ by

$$Q_{\hbar}(\psi) = \int_{\Omega} |(-i\hbar\nabla + \mathbf{A})\psi|^2 dx_1 dx_2.$$



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

$$\lambda_n(\hbar) = \Theta_0 \hbar - C_1 \kappa_{\text{max}} \hbar^{3/2} + (2n - 1)C_1 \Theta_0^{1/4} \sqrt{\frac{3k_2}{2}} \hbar^{7/4} + o(\hbar^{7/4}),$$
(72)

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 $L^2(\mathbb{R}/\ell\mathbb{Z}, ds)$, determines the semiclassical spectral asymptotics:

$$\mathcal{L}_{\hbar}^{\text{eff}} = \Theta_0 \hbar + \frac{\mu''(\zeta_0)}{2} (\hbar D_s + \gamma_0 - \zeta_0 \hbar^{\frac{1}{2}} + \alpha_0 \hbar)^2 - C_1 \kappa(s) \hbar^{\frac{3}{2}}, \qquad \gamma_0 = \frac{|\Omega|}{\ell},$$
(73)

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 $\mathcal{L}_{\hbar}^{\text{eff}}$ 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

$$\Theta_0 \hbar + \frac{\mu''(\zeta_0)}{2} \hbar^2 D_s^2 - C_1 \kappa(s) \hbar^{\frac{3}{2}},$$
 (74)

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.

$$\lambda_n(\hbar) \underset{\hbar \to 0}{\sim} \hbar \sum_{j \geq 0} \lambda_{n,j} \hbar^{\frac{1}{4}},$$

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

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



Continued

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

$$(\mathcal{L}_{\hbar} - \lambda_{n}(\hbar)) \left(a_{n} e^{-i\frac{s}{\hbar} \left(\gamma_{0} - \zeta_{0} \hbar^{1/2} \right)} e^{-\Phi/\hbar^{\frac{1}{4}}} \right) = \mathcal{O} \left(\hbar^{\infty} \right) e^{-\Phi/\hbar^{\frac{1}{4}}},$$

and

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

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

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

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:

$$\Omega = \left\{ (x_1, x_2) \in \mathbb{R}^2 : \frac{x_1^2}{a^2} + \frac{x_2^2}{b^2} < 1 \right\}, \quad a > b > 0.$$
 (75)

Theorem BHR

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

Continued

where

$$S = \sqrt{\frac{2C_1}{\mu''(\zeta_0)}} \int_0^{\frac{\ell}{2}} \sqrt{\kappa(0) - \kappa(s)} \, \mathrm{d}s,$$

$$A = \exp\left(-\int_{[0,\frac{\ell}{4}]} \frac{\partial_s \sqrt{\kappa(0) - \kappa(s)} - \sqrt{\frac{k_2}{2}}}{\sqrt{\kappa(0) - \kappa(s)}} \, \mathrm{d}s\right).$$

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

We denote by $\mu(\zeta)$ the first eigenvalue of this operator and by u_{ζ} a corresponding positive L²-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 $\zeta \in \mathbb{R}$, $\sigma \in \mathbb{R}/\ell\mathbb{Z}$, $\tau \in I_h$,

$$\mathcal{H}_{\sigma,\zeta,h} = -m(\sigma,h\tau)^{-1}\partial_{\tau}m(\sigma,h\tau)\partial_{\tau} +m(\sigma,h\tau)^{-1}\left(\zeta-\tau+h\frac{\tau^{2}}{2}\kappa(\sigma)\right)m(\sigma,h\tau)^{-1}\left(\zeta-\tau+h\frac{\tau^{2}}{2}\kappa(\sigma)\right) +\mathcal{O}(h^{2}).$$
(76)

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 $\tau \in \mathbb{R}^+$,

$$\mathcal{H}_{\sigma,\zeta,h} = \mathcal{H}_{\zeta} + h\kappa(\sigma) \left(\partial_{\tau} + 2\tau(\zeta - \tau)^2 + \tau^2(\zeta - \tau) \right) + \mathcal{O}(h^2). \tag{77}$$

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 $h \to 0$,

$$\int_{0}^{\infty} \mathcal{H}_{\sigma,\zeta,h} u_{\zeta}(\tau) u_{\zeta}(\tau) d\tau =$$

$$\int_{0}^{\infty} \mathcal{H}_{\zeta} u_{\zeta}(\tau) u_{\zeta}(\tau) d\tau + h\kappa(\sigma) \int_{0}^{\infty} \left(\partial_{\tau} + 2\tau(\zeta - \tau)^{2} + \tau^{2}(\zeta - \tau)\right) u_{\zeta}(\tau)$$
(78)

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

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

Putting these two expressions in (78), we get, as $h \to 0$, $\sigma \to 0$ and $\zeta \to \zeta_0$,

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

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

Let us now define $\mathcal{M} = \{\sigma_1, \sigma_2, \cdots, \sigma_N\}$ the set of all curvilinear abcissa where κ_{max} is attained . The preceding asymptotics remain true with $\sigma \to 0$ replaced by $\operatorname{dist}(\sigma, \mathcal{M}) \to 0$, where $\operatorname{dist}(\sigma, \mathcal{M})$ 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

$$\mathfrak{L}_{h}^{\text{eff}} = \Theta_0 + \frac{\mu''(\zeta_0)}{2} \left(h D_\sigma + \frac{\gamma_0}{h} - \zeta_0 + \alpha_0 h \right)^2 - C_1 \kappa(\sigma) h, \quad (79)$$

acting on $L^2(\mathbb{R}/\ell\mathbb{Z}, d\sigma)$, and up to controlled errors.

The operator defined in (79) appears to be a magnetic Schrödinger operator with a smooth potential on $\mathbb{R}/\ell\mathbb{Z}$. After rescaling, we get the effective operator (73).

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.

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

There exists on \mathcal{V} ,

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

s.t.

$$\left(\mathfrak{L}_{h}-\lambda_{n}(h)\right)\left(a_{n}\mathrm{e}^{-i\frac{\sigma}{h}\left(\frac{\gamma_{0}}{h}-\zeta_{0}\right)}\mathrm{e}^{-\Phi/h^{\frac{1}{2}}}\right)=\mathcal{O}\left(h^{\infty}\right)\mathrm{e}^{-\Phi/h^{\frac{1}{2}}}.$$

We also have

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

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

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

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

$$\mathfrak{L}_{h}^{\mathsf{wg}} = e^{\Phi(\sigma)/h^{\frac{1}{2}}} e^{i\frac{\sigma}{h} \left(\frac{\gamma_{0}}{h} - \zeta_{0}\right)} \mathfrak{L}_{h} e^{-i\frac{\sigma}{h} \left(\frac{\gamma_{0}}{h} - \zeta_{0}\right)} e^{-\Phi(\sigma)/h^{\frac{1}{2}}}.$$

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

$$\mathfrak{L}_{h}^{\text{wg}}a - \lambda a \sim 0.$$



We may write

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

where

$$\mathfrak{L}_{0} = D_{\tau}^{2} + (\zeta_{0} - \tau)^{2},
\mathfrak{L}_{1} = 2(\zeta_{0} - \tau)i\Phi'(\sigma),
\mathfrak{L}_{2} = \kappa(\sigma)\partial_{\tau} + 2\left(D_{\sigma} + \kappa(\sigma)\frac{\tau^{2}}{2}\right)(\zeta_{0} - \tau) - \Phi'(\sigma)^{2} + 2\kappa(\sigma)(\zeta_{0} - \tau)^{2}\tau,
\mathfrak{L}_{3} = \left(D_{\sigma} + \kappa(\sigma)\frac{\tau^{2}}{2}\right)(i\Phi'(\sigma)) + (i\Phi'(\sigma))\left(D_{\sigma} + \kappa(\sigma)\frac{\tau^{2}}{2}\right) +
+ 4i\Phi'(\sigma)\tau\kappa(\sigma)(\zeta_{0} - \tau).$$

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

$$(\mathfrak{L}_0 - \lambda_0)a_2 = (\lambda_2 - \mathfrak{L}_2)a_0 - \mathfrak{L}_1a_1.$$

After computation, the equation becomes

$$\begin{aligned} &(\mathfrak{L}_{0} - \lambda_{0})\tilde{a}_{2} \\ &= f_{0} \left(\lambda_{2} u_{\zeta_{0}} + \frac{\mu''(\zeta_{0})}{2} \Phi'^{2} u_{\zeta_{0}} \right. \\ &\left. + \kappa \left(-\partial_{\tau} u_{\zeta_{0}} - 2(\zeta_{0} - \tau)^{2} \tau u_{\zeta_{0}} - \tau^{2} (\zeta_{0} - \tau) u_{\zeta_{0}} \right) \right), \end{aligned}$$

where

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

We now get the equation

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

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

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

This leads to take

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

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

$$\begin{aligned} (\mathfrak{L}_{0} - \lambda_{0}) \hat{a}_{2} &= \lambda_{2} u_{\zeta_{0}} + \frac{\mu''(\zeta_{0})}{2} \Phi'^{2} u_{\zeta_{0}} \\ &+ \kappa \left(-\partial_{\tau} u_{\zeta_{0}} - 2(\zeta_{0} - \tau)^{2} \tau u_{\zeta_{0}} - \tau^{2} (\zeta_{0} - \tau) u_{\zeta_{0}} \right) , \end{aligned}$$

and f_2 has to be determined.

This procedure can be continued at any order.

About Theorem BHR

As suggested by our formal effective operator (79), 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 $L^2_{2\pi-per}(\mathbb{R}, \mathrm{d}x)$ 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

$$V_2 = \sqrt{\frac{V''(0)}{2}}. (80)$$

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

for
$$j = 1, 2$$
, $\rho_j(\varepsilon) = V_2 \varepsilon + o(\varepsilon)$ as $\varepsilon \to 0$.

Continued

With

$$S = \int_{[0,\pi]} \sqrt{V(x)} \, \mathrm{d}x, \quad \text{and} \quad A = \exp\left(-\int_{[0,\frac{\pi}{2}]} \frac{\partial_x \sqrt{V} - V_2}{\sqrt{V}} \, \mathrm{d}x\right),$$
(81)

we have the spectral gap estimate

$$\rho_{2}(\varepsilon) - \rho_{1}(\varepsilon) = 8\varepsilon^{1/2} \mathsf{A} \sqrt{V\left(\frac{\pi}{2}\right)} \sqrt{\frac{V_{2}}{\pi}} \left| \cos\left(\frac{\xi_{0}\pi}{\varepsilon}\right) \right| e^{-\mathsf{S}/\varepsilon} + \varepsilon^{3/2} \mathcal{O}\left(e^{-\mathsf{S}/\varepsilon}\right). \tag{82}$$

The main point is that one can see on the previous formula the global topological 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 $\mathcal{L}_{\hbar}^{\mathsf{eff}}$.

Proposition

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

$$\lambda_{2}^{\text{eff}}(\hbar) - \lambda_{1}^{\text{eff}}(\hbar) \underset{\hbar \to 0}{\sim} \hbar^{\frac{13}{8}} A \frac{2^{\frac{5}{2}} C_{1}^{\frac{3}{4}}}{\sqrt{\pi}} \left| \kappa''(0) \mu''(\zeta_{0}) \right|^{\frac{1}{4}} \left(\kappa(0) - \kappa\left(\frac{\ell}{4}\right) \right)^{\frac{1}{2}} \times \left| \cos\left(\frac{\ell}{2} \left(\frac{\gamma_{0}}{\hbar} - \frac{\zeta_{0}}{\hbar^{\frac{1}{2}}} + \alpha_{0}\right) \right) \right| e^{-S/\hbar^{\frac{1}{4}}},$$

where

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

The theorem 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 $\mathcal{L}_{\hbar}^{\text{eff}}$.

Bibliography



S. Agmon.

On exponential decay of solutions of second order elliptic equation in unbounded domains.

Proc. A. Pleijel Conf., Uppsala, September 1979.



S. Agmon.

Lectures on exponential decay of solutions of second order elliptic equations: bounds on eigenfunctions of N-body Schrödinger operators, Princeton Univ. Press, NJ, 1982.



D. Arnold, G. David, D. Jerison, S. Mayboroda, and M. Filoche.

The effective confining potential of quantum states in disordered media.

arXiv:1505.02684 and Physical Review letters (2016).



D. Arnold, G. David, M. Filoche, D. Jerison, S. Mayboroda. Localization of eigenfunctions via an effective potential. arXiv:1712.02419v4 [math.AP] 3 Oct 2018.

V. Bonnaillie, F. Hérau, and N. Raymond. Magnetic WKB expansions.

HAL: hal-00966003, version 2, arXiv: 1405.7157 (2014).

V. Bonnaillie, F. Hérau, and N. Raymond.
Semiclassical tunneling and magnetic flux effects on the circle.
J. Spectr. Theory (2015)

V. Bonnaillie, F. Hérau, and N. Raymond. Purely magnetic tunneling effect in two dimensions arXiv:1912.04035 [pdf, other] math.SP math.AP

M. Born, R. Oppenheimer. Zur Quantentheorie der Molekeln.
 Ann. Phys.
 84, 457-484 (1927).

R. Brummelhuis.

Exponential decay in the semi-classical limit for eigenfunctions of Schrödinger operators with magnetic fields and potentials which degenerate at infinity, *Comm.in PDE*, (1991).



An infinite number of wells in the semi-classical limit, Asympt. Anal. 3 (1990), 189–214.



Pointwise Bounds on Eigenfunctions and Wave Packets in *N*-Body Quantum Systems V. Lower Bounds and Path Integrals.

Commun. Math. Phys. 80, 59-98 (1981).

R. Carmona, W. Masters, and B. Simon. Relativistic Schrödinger operators: Asymptotic behavior of the eigenfunctions.

J. Funct. Anal. 91 (1990), 117-142

J.M. Combes, L. Thomas. Commun. Math. Phys. 34, 251-276 (1973).

D. Daners, J.B. Kennedy.

On the asymptotic behavior of the eigenvalues of a Robin problem.

Arxiv: 0812.0318v1 (1999).



F. Daumer.

Equation de Schrödinger avec champ electrique périodique et champ magnétique constant dans l'approximation du tight-binding.

Comm. in PDE 18, n⁰ 5-6, p. 1021-1041 (1993)



F. Daumer.

Equations de Schrödinger avec potentiels singuliers et à longue portée dans l'approximation de liaison forte.

Ann. Inst. Henri Poincaré, Phys. Théor. 64, n° 1, p. 1-31 (1996).



M. Dimassi, J. Sjöstrand.

Spectral asymptotics in the semi-classical limit, London Mathematical

- Society Lecture Note Series, vol. 268, Cambridge University Press, 1999.
- P. Exner, A. Minakov, L. Parnovski. Asymptotic eigenvalue estimates for a Robin problem with a large parameter. Portugal. Math. **71** (2) 141-156 (2014).
- S. Fournais, B. Helffer. Spectral Methods in Surface Superconductivity. Progress in Nonlinear Differential Equations and Their Applications, Vol. 77, Birkhäuser (2010).
- S. Fournais, B. Helffer. Accurate eigenvalue asymptotics for the magnetic Neumann Laplacian. *Ann. Inst. Fourier.* **56** (1) 1-67 (2006).
- P. Freitas, D. Krejcirik.
 The first Robin eigenvalue with negative boundary parameter. arXiv:1403.6666v2 [math.SP] 15 May 2014.
- T. Giorgi, R. Smits.

Eigenvalue estimates and critical temperature in zero fields for enhanced surface superconductivity.

Z. angew. Math. Phys. 57 (2006), 1–22.



E. Harrell.

On the rate of asymptotic eigenvalue degeneracy. Comm. Math. Phys. 60, (1978), 73-95.



E. Harrell.

The band-structure of a one-dimensional, periodic system in a scaling limit

Annals of Physics, Volume 119, Issue 2, June 1979, p. 351 - 369.



B. Helffer.

Semi-classical analysis for the Schrödinger operator and applications

Lecture notes in mathematics, vol. 1336, 1988.



B. Helffer.

Décroissance exponentielle pour les fonctions propres d'un modèle de Kac en dimension > 1.

Operator Theory: Advances and Applications, Vol.57 (1992), p. 99-115.



B. Helffer, A. Kachmar, and N. Raymond. Tunneling for the Robin Laplacian in smooth planar domains. Communications in Contemporary Mathematics 19(1), September 2015.



B. Helffer and Y. Kordyukov. Semiclassical analysis of Schrödinger operators with magnetic wells.

Six papers 2008-2016



B. Helffer and A. Mohamed.

Caractérisation du spectre essentiel de l'opérateur de Schrödinger avec un champ magnéetique (French) Ann. Inst. Fourier (Grenoble) 38 No. 2 (1988), 95-112.



B. Helffer, A. Morame.

Magnetic bottles in connection with superconductivity.

J. Func. Anal. 181 (2) 604-680 (2001).



B. Helffer and A. Morame.

Magnetic bottles for the Neumann problem: curvature effects in the case of dimension 3 - (general case), Ann. Sci. Ecole Norm. Sup. **37** (1) (2004), 105-170.



B. Helffer, J. Nourrigat.

Décroissance à l'infini des fonctions propres de l'opérateur de Schrödinger avec champ électromagnétique polynômial. Journal d'Analyse Mathématique de Jérusalem 58, p.263-275, (1992).



B. Helffer, X-B. Pan.

Upper critical field and location of surface nucleation of superconductivity.

Ann. Inst. H. Poincaré Anal. Non Linéaire 20 (2003), no. 1, 145–181.





B. Helffer, B. Parisse.

Effet tunnel pour Klein-Gordon,

Annales de l'IHP, Section Physique théorique, Vol.60, n°2, p. 147-187 (1994).

B. Helffer and J. Sjöstrand.

Multiple wells in the semiclassical limit I.

Comm. Partial Differ. Equations 9 (4) 337-408 (1984).

B. Helffer, J. Sjöstrand.

Multiple wells in the semiclassical limit III. Non resonant wells

Math. Nachrichten.

B. Helffer, J. Sjöstrand. Multiple wells in the semiclassical limit V. The case of miniwells.

B. Helffer and J. Sjöstrand.

Effet tunnel pour l'équation de Schrödinger avec champ magnétique,

Ann. Scuola Norm. Sup. Pisa, Vol XIV, 4 (1987) p. 625-657.



B. Helffer, J. Sjöstrand.

Analyse semi-classique pour l'équation de Harper (avec application à l'équation de Schrödinger avec champ magnétique).

Mémoire de la Société Mathématique de France 34 (1988).



A. Kachmar.

On the ground state energy for a magnetic Schrödinger operator and the effect of the de Gennes boundary conditions. C.R. Math. Acad. Sci. Paris **332**, 701-706 (2006).



A. Kachmar.

On the ground state energy for a magnetic Schrödinger operator and the effect of the de Gennes boundary conditions.

J. Math. Phys. **47**(7), 072106, 32 pp (2006).



A. Kachmar, M. Persson.

On the essential spectrum of magnetic Schrödinger operators in exterior domains.

Arab J. Math. Sci. 19 (2) 217-222 (2013).



Semiclassical analysis of the operator $h^2D_x^2 + D_y^2 + (1+x^2)y^2$. Manuscript June 1986. Unpublished.

M. Levitin, L. Parnovski.

On the principal eigenvalue of a Robin problem with a large parameter.

Math. Nachr. 281, 272-281 (2008).

L. Lithner.

Ark. for Mat. Astron. Pys. 5, 281-285 (1964).

A. Martinez.

Microlocal exponential estimates and applications to tunneling, in Microlocal Analysis and Spectral theory, NATO ASI Series C, Vol. 490 (L. Rodino ed.), Kluwer Acad. Publ., p. 349-376 (1997).



An introduction to semi-classical and microlocal analysis. Springer (2002).



A. Martinez.

Développements asymptotiques et effet tunnel dans l'approximation de Born-Oppenheimer.

Ann. Inst. Henri Poincaré, Sect. Phys. Théor. **50** (3), 239-257 (1989).



V.P. Maslov.

Global exponential asymptotics of the solutions of the tunnel equations and the large deviation problems (Russ.).

Tr. Mosk. Inst. Akad. Nauk 163 (1984), p.150-180. (Engl. transl. in *Proc. Stecklov Inst. Math* 4 (1985).)



A. Outassourt.

Comportement semi-classique pour l'opérateur de Schrödinger à potentiel périodique.

Journal of Functional Analysis 72, 65-93 (1987).



K. Pankrashkin.

On the asymptotics of the principal eigenvalue problem for a Robin problem with a large parameter in a planar domain.

Nanosystems: Physics, Chemistry, Mathematics, 2013 4 (4), 474-483.



K. Pankrashkin.

On the Robin eigenvalues of the Laplacian in the exterior of a convex polygon

arXiv:1411.1956. Nanosystems: Physics, Chemistry, Mathematics 6:1 (2015) 46-56.



K. Pankrashkin, N. Popoff.

Mean curvature bounds and eigenvalues of Robin Laplacians. arXiv:1407.3087. Calc. Var. PDE. 54 (2015) 1947-1961.



K. Pankrashkin, N. Popoff.

An effective Hamiltonian for the eigenvalue for the asymptotics of the Robin Laplacian with a large parameter. arXiv:1502.00877v2 [math.SP] 28 Apr 2015.

T.F. Pankratova.

Quasimodes and splitting of eigenvalues (Russ.). Dokl. Akad. Nauk SSSR 276:4 (1984), p. 795-798. (Engl. translation in Sov. Math. Dok 29 (1984).)

N. Raymond. Bound States of the Magnetic Schrödinger Operator. EMS Tracts in Mathematics (2017).

B. Simon.

Semiclassical analysis of low lying eigenvalues, I. Nondegenerate minima: Asymptotic expansions, Ann. Inst. H. Poincaré 38 (1983), 295-307.

B. Simon. Instantons, double wells and large deviations, Bull. A.M.S., Vol 8, no 9, March 1983, 323-326

B. Simon.

Semi-classical analysis of low lying eigenvalues II. Tunneling. Ann. of Math. 120 (1984), 89–118.



B. Simon.

Two other papers in the eighties. Periodic potentials and the flea of the elephant.



X.P. Wang.

Puits multiples pour l'opérateur de Dirac.

Ann. IHP (Sect. Phys. Th.) 43, p. 260-319 (1985).