Semiclassical analysis for Schrödinger operators, Laplace integrals and transfer operators in large dimension: an introduction

Bernard Helffer
Ecole Normale Supérieure,
UA 762 du CNRS, DMI,
45 rue d'Ulm
F-75230 Paris Cédex, FRANCE
and
Université Paris-Sud,
Département de Mathématiques,
UA 760 du CNRS, Bat. 425,
F-91405 Orsay Cedex, FRANCE
DEA 1995

January 30, 1998

Abstract

The aim of this course, presented in February-May 1995 in Orsay, is to explain how the semiclassical analysis can be useful in statistical mechanics. After some presentation of the origin of the problem in statistical mechanics, which is partly inspired by a course by M.Kac, we shall analyze in parallel three situations where an asymptotic behavior with respect to the dimension or to a small parameter has to be considered

- Laplace integrals,
- Schrödinger operators,

- transfer operators.

In these three cases the starting point is a family $V^{(m)}$ of C^∞ potentials on $\mathbb{R}^m$ parametrized by m which appears as the sum of a quadratic term $\sum_j x_j^2$ and of an interaction which is in the simplest case of the form $\sum_j I(x_j, x_{j+1})$.
The main techniques which are presented here have been initiated, in the large dimension context, by J. Sjöstrand.

Résumé

On se propose dans ce cours (présenté en Février-Mai 1995 à l'université Paris-Sud) comment les techniques semi-classiques développées pour l'essentiel pour l'étude de l'opérateur de Schrödinger peuvent être utiles pour comprendre certains problèmes de mécanique statistique. Cette démarche est celle de M. Kac qui développa cette thèse dans un cours à Brandeis en 1966. L'analyse semi-classique ayant fait beaucoup de progrès ces 15 dernières années, il était naturel de voir si l'on était plus armé pour mettre sur des bases rigoureuses son programme. Force est de constater que 30 ans plus tard, l'approche proposée par M. Kac a plus posé de questions que proposé de réponses définitives.
Il nous a semblé toutefois intéressant de proposer un cours charnière entre les deux disciplines : analyse semi-classique et mécanique statistique, destiné simultanément aux étudiants des deux disciplines.
Nous nous sommes finalement concentrés, faute de temps, sur un aspect du problème qui consiste à analyser l'existence de solutions WKB. Nous nous sommes cependant efforcés de donner au lecteur, en fonction des besoins, quelques connaissances en mécanique statistique, en théorie spectrale, en géométrie symplectique ou en systèmes dynamiques, en essayant toutefois d'arriver de manière autocontenue et relativement rapide à l'objet même du cours consistant à analyser des problèmes de grande dimension.
Comme il ressort de travaux récents de J. Sjöstrand dont nous tâcherons de présenter les techniques, il y a une grande unité d'approche entre trois problèmes au départ disjoints faisant tous cependant intervenir un petit paramètre, qui, bien que n'étant pas nécessairement relié à la constante de Planck, sera souvent noté h.
On considèrera donc simultanément des intégrales de Laplace de la

forme

$$\frac{1}{m}\left[\ln((1/h\pi)^{\frac{m}{2}}\int \exp{(-\frac{V^{(m)}(x)}{h})}\,dx)\right]\ ,$$

ou des opérateurs de transfert définis sur l'espace $L^2(I\!R^m)$ par

$$K^{(m)}(h) = \exp{(-\frac{V^{(m)}(x)}{2})}\cdot \exp{(h^2\Delta^{(m)})}\cdot \exp{(-\frac{V^{(m)}(x)}{2})},$$

ou enfin des opérateurs de Schrödinger

$$S^{(m)}(h) = -h^2\Delta^{(m)} + V^{(m)}(x).$$

Dans les deux derniers cas, $\Delta^{(m)}$ est le Laplacien sur l'espace de Hilbert $L^2(I\!R^m)$ qu'il est sans doute mieux d'interpréter comme le produit tensoriel $\otimes^m L^2(I\!R)$.
Dans les trois cas, le point de départ est une famille $V^{(m)}$ de potentiels définis sur $I\!R^m$ paramétré par m qui a une structure particulière provenant de la mécanique statistique. L'entier m est à interpréter comme le nombre de points d'un sous réseau Λ de $Z\!\!Z$ et $I\!R^m$ comme l'espace $\times_{k\in\Lambda} I\!R$.
Le cas le plus typique est celui où

$$V^{(m)}(x_1,\cdots,x_m) = \sum_{j=1}^{m} v(x_j) + a|x_j - x_{j+1}|^2\ ,$$

où v est une fonction définie sur $I\!R$, par exemple $v(x) = (x^2-1)^2$.
Dans un premier temps nous présentons un grand nombre d'exemples tirés de la mécanique statistique et conduisant aux problèmes que nous étudierons.
Nous insisterons alors principalement sur deux aspects de ce problème: l'approximation harmonique et les constructions WKB, en essayant de faire découvrir les problèmes nouveaux liés au contrôle par rapport à la dimension.
Les principales techniques présentées ici dans le cadre de la grande dimension ont été initialisées par J. Sjöstrand dans le cadre de l'équation de Schrödinger et des intégrales de Laplace. Les résultats semi-classiques concernant l'opérateur de transfert sont nouveaux (souvent non encore publiés) et principalement dus à l'auteur.
Notre présentation est ici nécessairement très limitée (même si nous avons essayé dans quelques notes en bas de page de signaler d'autres

résultats) et nous renvoyons à notre article de synthèse [He94e] pour une revue plus complète des techniques existantes mais beaucoup moins détaillée dans la présentation des démonstrations.

1 Introduction

1.1 On the way of a program by M.Kac

In this course we shall present results concerning semiclassical techniques in statistical mechanics. We planed at the beginning to present also maximum principle techniques but it finally appears to be a too ambitious program and we refer to the Survey [He94e] for this part.
After some presentation of the origin of the problem in statistical mechanics which is mainly inspired by a course by M.Kac [Ka66] we analyze in parallel three situations concerning asymptotic behavior with respect to the dimension or to a small parameter: Laplace integrals, Schrödinger operators and Kac operators (which are more commonly called transfer operators or transfer matrices). Of course we are limited in this course by the time. The survey [He94e] gives more information. Historical references will not be given systematically inside this manuscript (see however [He94e] for recent results or [He88] for the more standard semi-classical analysis) in order to make the reading for the student easier. We have tried in general to give detailed proofs outside some cases where we indicate references when details are missing.
In these three cases, the starting point is a family $V^{(m)}$ of C^∞ functions on $\mathbb{R}^m$ parametrized by m which play the role of the potential in classical mechanics. These potentials will of course have a very special structure adapted to the statistical mechanics. The most simple examples take the form

$$V^{(m)}(x) = \sum_{j=1}^{m} v(x_j) + \sum_j I(x_j, x_{j+1}) \ , \tag{1.1.1}$$

where x_{m+1} is identified with x_1, $I(x,y)$ describes the interaction between two nearest neighbors and satisfies $I(x,y) = I(y,x)$ and v is the one-particle potential. In the case when the Schrödinger operator $-h^2\Delta + V^{(m)}(x)$ is involved, it is probably better to understand the Hilbert space $L^2(\mathbb{R}^m)$, on which it is defined, as the tensor product $\otimes_{j=1}^m L^2(\mathbb{R})$.

1.2 Presentation of the mathematical problems

We have selected the following problems.

(I)
Study of the asymptotic behavior of the Laplace integral

$$\frac{1}{m}\left[\ln((1/h\pi)^{\frac{m}{2}}\int \exp\,(-\frac{V^{(m)}(x)}{h})\;dx)\right]\;, \tag{1.2.1}$$

as m tends to ∞, and control of the limit with respect to h as h tends to $+0$. As the potential $V^{(m)}$ admits a decomposition of the type (1.1.1), it could be more intuitive to understand that the measure $\exp\,(-\frac{V^{(m)}(x)}{h})\;dx$ can ve written in the form $\exp -\mathcal{W}\cdot\otimes_{j=1}^{m} d\mu^j$ where $d\mu^j$ is the measure defined on $\mathbb{R}$ by $\exp -v(t)dt$.

(II)
If $\mu_1(m,h)$ is the largest eigenvalue of the operator

$$K^{(m)}(h)=\exp\,(-\frac{V^{(m)}(x)}{2})\cdot\exp\,(h^2\Delta^{(m)})\cdot\exp\,(-\frac{V^{(m)}(x)}{2}), \tag{1.2.2}$$

or of its "brother"

$$K^{(m)}(h)=\exp\,(-\frac{V^{(m)}(x)}{2h})\cdot\exp\,(h\Delta^{(m)})\cdot\exp\,(-\frac{V^{(m)}(x)}{2h}), \tag{1.2.3}$$

consider the asymptotic behavior of the quantity $-\dfrac{\ln\mu_1(m,h)}{m}$ as m tends to ∞ and control this limit with respect to h as h tends to $+0$. Here $\Delta^{(m)}$ is the Laplacian on $\mathbb{R}^m$. We shall call these operators transfer operators (or Kac operators or transfer matrices).
(III)
If $\lambda_1(m,h)$ is the smallest eigenvalue of the Schrödinger operator

$$S^{(m)}(h)=-h^2\Delta^{(m)}+V^{(m)}(x) \tag{1.2.4}$$

what is the asymptotic behavior of the quantity $\lambda_1(m,h)/m$ as m tends to ∞ and control this limit with respect to h as h tends to $+0$.

These three questions are of course strongly related and we shall analyze some of these links carefully in the next sections (see [He94e] for other links or any book in Field theory). If we think of a potential which is invariant by circular permutation of the variables and "near" in a suitable sense of the harmonic oscillator, all these questions are well analyzed for fixed m as h tends to zero. (I) can be treated by application of the stationary phase theorem (or more correctly of the Laplace method), (III) corresponds with a semiclassical analysis of the Schrödinger operator at the bottom (see for example [He88]) and the study of (II) can be considered as a pseudo-differential extension of (III) (See [BruHe91] or [He92b]). In particular this study gives for example that

$$-\ln(\mu_1(m,h)) = \lambda_1(m,h) + O_m(h^2). \tag{1.2.5}$$

It is also interesting to look at the asymptotic behavior of the quantity $\left[\ln\ \mathrm{Tr}\ (\exp\ -t(-h^2\Delta + V^{(m)}))\right]/m$ as m tends to ∞ and control (for fixed $t > 0$) this limit with respect to h as h tends to $+0$ (see [Sj92b] and [BaKo92]).

The new difficult problem is of course a good control with respect to m as m is large. Let us also mention that other interesting (and sometimes more difficult) problems appear in the same context.

(IV)
In the context of the Laplace integrals, the connected problem is to analyze the behavior as $|i-j| \to \infty$ of the pair correlation

$$\lim_{m\to\infty}\ \mathrm{Cor}^{\,(m)}(i,j) \tag{1.2.6}$$

where

$$\mathrm{Cor}^{\,(m)}(i,j) = \langle x_i.x_j\rangle_m - \langle x_i\rangle_m.\langle x_j\rangle_m\ , \tag{1.2.7}$$

and $\langle f\rangle_m$ is the mean value with respect to the measure $\exp -V^{(m)}(x)dx^{(m)}$ of the function f depending on a finite fixed number of variables:

$$\langle f\rangle_m = \frac{\int f(x_1,\cdots,x_k)\ \exp\ -V^{(m)}(x)\ dx^{(m)}}{\int \exp\ -V^{(m)}(x)\ dx^{(m)}}\ . \tag{1.2.8}$$

(V)
Study the lim inf and the lim sup of

$$m \mapsto \mu_2(m,h)/\mu_1(m,h)$$

as $m \to \infty$ where $\mu_2(m,h)$ is the second eigenvalue of $K^{(m)}(h)$.

(VI)
Study the lim inf and the lim sup of

$$m \mapsto (\lambda_2(m,h) - \lambda_1(m,h))$$

as $m \to \infty$ where $\lambda_2(m,h)$ is the second eigenvalue of $S^{(m)}(h)$.

The problem (VI) corresponds with the well known problem of the study of the splitting between the two first eigenvalues.

1.3 Our main toy models:

They correspond to a class containing the model "Kac" potential (K):

$$V^{(m)}(x;\nu) = (\frac{1}{4})\sum_{k=1}^{m}(x_k)^2 - \sum_{k=1}^{m}\ln\cosh\left((\frac{\nu}{2})^{\frac{1}{2}}(x_k + x_{k+1})\right) \ , \tag{1.3.1}$$

with the convention $(x_{m+1} = x_1)$.
But other connected potentials like

$$\Phi(X) = \sum_{j=1}^{p} V^{(m)}(x_j;\nu) + \frac{1}{2}|x_j - x_{j+1}|^2 \ , \tag{1.3.2}$$

with $x_j \in I\!R^m$, which depend on $n = mp$ variables arise very naturally in the lattice field theory and will be considered.
The Kac model was our initial toy model because we meet in this model all the difficulties of the problem of analyzing phase transition but we can also analyze as toy models other natural models coming from the field theory. We think in particular of the following models:

- Model of the field theory (DK) (see [DoKo93], [DoKo94] and [BaKo92]).

$$V^{(m)}(x) = \frac{a}{2}\sum_{k=1}^{m}(x_k - x_{k+1})^2 + \frac{b}{4}\sum_{k=1}^{m}(x_k - y)^2(x_k + y)^2 \tag{1.3.3}$$

  where $a > 0$, $b > 0$ and $y > 0$.

- More generally, we can consider :

$$V^{(m)}(x) = \frac{a}{2}\sum_{k=1}^{m}(x_k - x_{k+1})^2 + \sum_{k=1}^{m} v(x_k) \tag{1.3.4}$$

where v is a C^∞ potential with one or two symmetric non degenerate wells satisfying the inequality:

$$v(t) \geq \frac{1}{C}t^2 - C$$

for some strictly positive constant C. This model is a standard model occuring in the ϕ_2^4-field theory.

- Model of E.Brézin, S.Hikami (BH) (see [BreHi79]),

$$V^{(m)}(x) = \frac{a}{2}\sum_{k=1}^{m} x_k^2 \; + \; m^{1-\ell}(\sum_{k=1}^{m} x_k^2)^\ell \tag{1.3.5}$$

for some $\ell \in I\!N$, $\ell > 1$.

Acknowledgements :

I would like to thank all the students and colleagues who follow this course and make useful remarks and particularly: P. Kerdelhue, W.M. Wang, T. Bodineau and F. Nier.
The material which is presented here corresponds frequently to current research. I would also like to thank the colleagues which have worked or discussed with me on this subject in the recent years and particularly M. Brunaud, J. Sjöstrand and V. Sordoni.
Many thanks also to the ESI in Vienna where I find good conditions to improve the presentation of the notes.
Many thanks also to C. Albanese for explaining me in Vienna the properties of the Ising model with transverse field and V. Bach who organizes there this conference on the Heisenberg and Hubbard models.
Finally, P. Kerdelhue has accepted to read the final version and I am very grateful for all his useful comments.

1.4 CONTENTS

- Section 8: Decay of the eigenfunctions and applications
  - Subsection 8.1: Introduction
  - Subsection 8.2: Energy inequalities
  - Subsection 8.3: The Agmon distance
  - Subsection 8.4: Decay of eigenfunctions for the Schrödinger operator
  - Subsection 8.5: Splitting between the two first eigenvalues
  - Subsection 8.6: Decay for the eigenfunctions of the transfer operator
    * 8.6.1: Preliminary remarks
    * 8.6.2: Improved decay estimates, comparison with the semi-classical results
    * 8.6.3: The quadratic case
- Section 9: WKB constructions
  - Subsection 9.1: Introduction
  - Subsection 9.2: WKB for the Schrödinger operator, formal approach
    * 9.2.1: WKB, first approach
    * 9.2.2: The case of dimension $p = 1$
    * 9.2.3 The case of dimension $p \geq 1$
  - Subsection 9.3: WKB for the Laplace integral, formal approach
  - Subsection 9.4: WKB for the transfer integral, formal approach
    * 9.4.1: Eiconal and transport equation
    * 9.4.2: The analysis of the diffeomorphism in the quadratic case
  - Subsection 9.5: Around the stable manifold theorem
    * 9.5.1: Two theorems for solving eiconal and transport equations
    * 9.5.2: Around the proof
    * 9.5.3: The stable manifold for diffeomorphisms

2 Problems in statistical mechanics:

We discuss in this section various classical problems in statistical mechanics.

2.1 The Curie-Weiss model

The Curie-Weiss model is one of the simple models in statistical mechanics which plays an important role in the mean field theory. We consider a N-spins lattice $\sigma = (\sigma_1, \sigma_2, \cdots, \sigma_N)$ with $\sigma_j \in \{-1, +1\}$. In order to take into account of the magnetic field, we associate to any σ the energy $E_B(\sigma)$ defined by

$$E_B(\sigma) = -\frac{2J}{N} \sum_{1 \le i < j \le N} \sigma_i \cdot \sigma_j - B(\sum_{1 \le i \le N} \sigma_i) \tag{2.1.1}$$

The partition function Z_N is given by

$$\begin{aligned} Z_N &= 2^{-N} \left[\textstyle\sum_{\sigma \in \{-1,+1\}^N} \exp\ -E_B(\sigma)/kT \right] \\ &= 2^{-N} \cdot \exp -\nu \cdot \left[\textstyle\sum_{\sigma \in \{-1,+1\}^N} \exp\ \left(\nu (\sum_{i=1}^N \frac{\sigma_i}{\sqrt{N}})^2) + (kT)^{-1} B \sum_{1 \le i \le N} \sigma_i \right) \right] \end{aligned} \tag{2.1.2}$$

with $\nu = J/kT$.

A simple computation based on the easy identity

$$\exp\ a^2 = \frac{1}{\sqrt{2\pi}} \int_{I\!R} \exp\ (-\frac{\xi^2}{2} + \sqrt{2} a \xi) d\xi \tag{2.1.3}$$

gives the formula

$$Z_N(B) = \exp -\nu \cdot \sqrt{\frac{N}{2\pi}} \cdot \int_{I\!R} \exp\ -N \frac{\eta^2}{2} \left(\cosh(\eta \sqrt{2\nu} + \frac{B}{kT}) \right)^N d\eta \tag{2.1.4}$$

We rewrite this integral in the form:

$$Z_N(B) = \exp -\nu \cdot \sqrt{\frac{N}{2\pi}} \cdot \int_{I\!R} \exp\ -N \Phi_{\nu,B}(\eta) d\eta \tag{2.1.5}$$

with

$$\Phi_{\nu,B}(\eta) = \frac{\eta^2}{2} - \ln \cosh \left[\eta \sqrt{2\nu} + \frac{B}{kT} \right]\ . \tag{2.1.6}$$

We are first interested in the socalled thermodynamic limit

$$-\lim_{N\to\infty} N^{-1}\ln Z_N$$

and according to formula (2.1.5), this is easily analyzed as a Laplace integral. In particular, an easy computation gives:

$$-\lim_{N\to\infty} N^{-1}\ln Z_N = \inf_{\eta} \Phi_{\nu,B}(\eta)\ . \tag{2.1.7}$$

More precise information (asymptotic analysis of $N^{-1}\ln Z_N$ with respect to N as $N\to\infty$) can also be obtained by standard methods. We shall recall these results in Subsection 3.3. In particular we consider the minima of the phase $\Phi_{\nu,B}(\eta)$ and observe that the critical points are given by the equation

$$\eta = \sqrt{2\nu}\cdot\tanh\left[\eta\sqrt{2\nu}+\frac{B}{kT}\right]\ . \tag{2.1.8}$$

In the case $B=0$, the value $\nu=\frac{1}{2}$ of the parameter appears critical. We observe indeed:

- If $\nu>\frac{1}{2}$, the phase has two symmetric minima (double well situation),
- If $\nu=\frac{1}{2}$, the phase has a unique degenerate minimum,
- If $\nu<\frac{1}{2}$, the phase is strictly convex (single well situation) and has a unique nondegenerate minimum.

2.2 The 1-d Ising model

We consider now the following model

$$H_n(\sigma) = -J\sum_{1\le r\le n}\sigma_r\cdot\sigma_{r+1} - h\sum_{1\le r\le n}\sigma_r \tag{2.2.1}$$

where we identify σ_1 and σ_{1+n}. If one introduces

$$T(\sigma,\sigma') = \exp\ \beta\left(J\sigma\cdot\sigma'+\frac{h}{2}(\sigma+\sigma')\right)\ , \tag{2.2.2}$$

for $\sigma,\ \sigma'=\pm1$, we see immediately that we can write:

$$\exp\ -\beta H_n(\sigma) = T(\sigma_1,\sigma_2)\cdot T(\sigma_2,\sigma_3)\cdots T(\sigma_{n-1},\sigma_n)\cdot T(\sigma_n,\sigma_1) \tag{2.2.3}$$

We observe now that $T(\sigma_1, \sigma_1')$ with $\sigma_1, \sigma_1' = \pm 1$ can be considered as a 2×2-matrix

$$\mathbf{T} = \begin{pmatrix} \exp\ \beta(J+h) & \exp\ -\beta J \\ \exp\ -\beta J & \exp\ \beta(J-h) \end{pmatrix} \tag{2.2.4}$$

which is usually called transfer matrix and will appear very useful in order to express statistical quantities. Let us first consider the partition function

$$Z_n =_{def} \sum_{\sigma \in \{-1,+1\}^n} \exp\ -\beta H_n(\sigma)\ . \tag{2.2.5}$$

An immediate computation gives

$$Z_n = \sum_{\sigma_1} \mathbf{T}^n(\sigma_1, \sigma_1)\ , \tag{2.2.6}$$

or

$$Z_n = \ \mathrm{Tr}\ \ \mathbf{T}^n = \lambda_1^n + \lambda_2^n \tag{2.2.7}$$

where λ_1 and λ_2 are the two eigenvalues of $\mathbf{T}$

$$\begin{aligned} \lambda_1 &= \exp\ \beta J \cosh(\beta h) + \sqrt{\sinh^2(\beta h) \exp\ 2\beta J\ +\ \exp\ -2\beta J)}\ , \\ \lambda_2 &= \exp\ \beta J \cosh(\beta h) - \sqrt{\sinh^2(\beta h) \exp\ 2\beta J\ +\ \exp\ -2\beta J)}\ . \end{aligned} \tag{2.2.8}$$

We then compute the free energy

$$F_n = -kT \ln\ Z_n = -kT \ln\,(\lambda_1^n + \lambda_2^n) = -nkT \ln\,(\lambda_1) - kT \ln\,(1 + \lambda_2^n/\lambda_1^n)\ . \tag{2.2.9}$$

At the thermodynamic limit when $n \to \infty$, observing that $\lambda_1 > \lambda_2$ we get

$$f = \lim_{n \to \infty} F_n/n = -kT \ln \lambda_1\ . \tag{2.2.10}$$

We observe that the speed of convergence to the thermodynamic limit is immediately related to the comparison of λ_2/λ_1 with 1. More precisely, the strict inequality $\lambda_2/\lambda_1 < 1$ permits to get exponentially rapid convergence in (2.2.10). This will explain why we shall later be interested in estimates on the splitting in more general situations. We shall also compute in this very simple situation consider the correlation pair

$$\langle \sigma_s \cdot \sigma_{r+s} \rangle_n =_{def} Z_n^{-1} \sum_{\sigma \in \{-1,+1\}^n} \sigma_s \cdot \sigma_{s+r} \exp\ -\beta H_n(\sigma)\ . \tag{2.2.11}$$

An easy computation gives again:

$$\langle \sigma_s \cdot \sigma_{s+r} \rangle_n = Z_n^{-1} \sum_{\sigma,\sigma'=\pm 1} \sigma \mathbf{T}^r(\sigma,\sigma')\sigma' \mathbf{T}^{n-r}(\sigma',\sigma) \ . \tag{2.2.12}$$

If we now observe that the third Pauli matrix

$$\tau_3(\sigma,\sigma') = \sigma \delta_{\sigma,\sigma'}$$

satisfies:

$$(\tau_3 \circ \mathbf{A})(\sigma,\sigma') = \sigma \mathbf{A}(\sigma,\sigma') \ ,$$

we can rewrite (2.2.12) in the form

$$\langle \sigma_s \cdot \sigma_{s+r} \rangle_n = Z_n^{-1} \ \mathrm{Tr} \ (\tau_3 \circ \mathbf{T}^r \circ \tau_3 \circ \mathbf{T}^{n-r}) \ . \tag{2.2.13}$$

If we now denote by $|1\rangle$ and $|2\rangle$ the eigenvectors corresponding to λ_1 and λ_2, we finally obtain

$$\lim_{n\to\infty} \langle \sigma_s \cdot \sigma_{s+r} \rangle_n = |\langle 1|\tau_3|1\rangle|^2 + (\lambda_2/\lambda_1)^r |\langle 1|\tau_3|2\rangle|^2 \ . \tag{2.2.14}$$

We observe that if $h = 0$, then $|\langle 1|\tau_3|1\rangle| = 0$ and $|\langle 1|\tau_3|2\rangle| \neq 0$. In this case the correlation function decays exponentially with r :

$$\langle \sigma_s \cdot \sigma_{s+r} \rangle_\infty \approx \exp \ -r/\xi \tag{2.2.15}$$

with

$$\xi = (\ln(\lambda_1/\lambda_2))^{-1} \tag{2.2.16}$$

which is called the correlation length. In any case we observe that

$$\langle (\sigma_s - \langle \sigma_s \rangle_\infty) \cdot (\sigma_{s+r} - \langle \sigma_{s+r} \rangle_\infty) \rangle_\infty \approx \exp \ -r/\xi \ .$$

Again we observe that the splitting between the two eigenvalues λ_2 and λ_1 of the socalled transfer matrix T plays a very important role in the asymptotic behavior of the correlations.

2.3 The 2-d Ising model

We now review some facts concerning the two-dimensional Ising model. We consider a two-dimensional $n \times m$ lattice of m rows and n columns, with spins $\sigma_P = \pm 1$ occupying the vertices of the lattice. The interaction energy in a given configuration of spins is now given by

$$H_{n,m}(\sigma) = -J \sum^{*} \sigma_P \cdot \sigma_Q \ , \tag{2.3.1}$$

where the star on the sum denotes a sum over nearest-neighbor lattice points P and Q, and we have assumed that the coupling J between nearest neighbors is the same for spins in rows and columns. We assume also that $J > 0$, i.e. that the interaction is ferromagnetic, so that the ground state has all spins equal to $+1$ or -1. The partition function is now:

$$Z_{n,m} = \sum_{\sigma \in \{-1,+1\}^{\{\boldsymbol{Z}/n\boldsymbol{Z} \times \boldsymbol{Z}/m\boldsymbol{Z}\}}} \exp\ -H_{n,m}(\sigma)/kT = \sum_{(\sigma)} \exp\ \nu \sum^{*} \sigma_P \cdot \sigma_Q \ , \tag{2.3.2}$$

with

$$\nu = J/kT \ . \tag{2.3.3}$$

The free energy per spin ψ in the thermodynamic limit is defined [1] by

$$-\ \psi/kT = \lim_{m,n \to \infty} (mn)^{-1} \ln Z_{n,m} \ . \tag{2.3.4}$$

In order to evaluate $Z_{n,m}$, Kramers and Wannier relate this quantity to a spectral problem for the $2^m \times 2^m$ transfer matrix $\mathbf{T}$ defined by

$$T(\sigma, \sigma') = \exp\ \left(\frac{\nu}{2} \sum_{k=1}^{m} \sigma_k \cdot \sigma_{k+1}\right) \cdot \exp\ \left(\nu \sum_{k=1}^{m} \sigma_k \cdot \sigma'_k\right) \cdot \exp\ \left(\frac{\nu}{2} \sum_{k=1}^{m} \sigma'_k \cdot \sigma'_{k+1}\right) \ . \tag{2.3.5}$$

It is then a simple matter to get the following expression for the partition function:

$$Z_{n,m} = \ \mathrm{Tr}\ \mathbf{T}^n = \sum_{j=1}^{2^m} \mu_j^n \ , \tag{2.3.6}$$

[1] A precise definition of this limit is surely needed but we do not enter in the details (See for example [Ru69]). Here we shall choose an order by taking successively the limit $n \to \infty$ and then the limit $m \to \infty$.

where $\mu_1 > \mu_2 \geq \mu_3 \cdots \mu_{2^m}$ are the eigenvalues of the matrix $\mathbf{T}$. If we first take the limit as $n \to \infty$ we have immediately

$$\lim_{n\to\infty} n^{-1} \ln Z_{n,m} = \ln \mu_1(m) \tag{2.3.7}$$

and hence from (2.3.4)

$$-\psi/kT = \lim_{m\to\infty} m^{-1} \ln \mu_1(m) \tag{2.3.8}$$

The explicit computation of $\mu_1(m)$ was done by Onsager in 1944. This explicit computation permits to show that as $m \to \infty$ ther eigenvalue becomes asymptotically degenerate for T smaller than some critical temperature T_c. More precisely, for $T > T_c$, the spectrum of T is simple (this point is always true due to the Perron-Frobenius Theorem) and the spacing of the $\frac{\ln \mu_j(m)}{m}$ is of order $1/m$, in particular

$$\ln \mu_1(m) - \ln \mu_2(m) \geq 1/C \tag{2.3.9}$$

and below T_c there are two such spectra with spacings of $\frac{1}{m}\ln \mu_j$ of order $\frac{1}{m}$ but shifted with respect to each other by an amount of order exp $-cm$ for some $c > 0$, in particular:

$$\ln \mu_1 - \ln \mu_2 \leq \frac{1}{c} \exp\, -cm\ , \tag{2.3.10}$$

for some $c > 0$.
The basic idea suggested by M.Kac and illustrated by heuristic computations was to relate this properties to tunneling properties observed in quantum mechanics.

2.4 The Kac model A

The model we want to consider is called Model A in Section 7 of [Ka66]. We consider the following Hamiltonian:

$$E_{\Lambda(n,m)}(\sigma) = -\sum_{(P,Q)\in\Lambda(n,m)\times\Lambda(n,m)} v_{P,Q}\, \sigma_P\, \sigma_Q \tag{2.4.1}$$

with

$$\Lambda(n,m) = [1,...,n] \times (\mathbb{Z}/m\mathbb{Z})\ , \sigma_P \in \{-1,+1\}, J \in \mathbb{R}_+^\star, \gamma \in \mathbb{R}_+^\star \tag{2.4.2}$$

with

$$v_{P,P} = 0$$

and

$$v_{P,Q} = J\gamma \exp\left(-\gamma|k-k'|\right)\left(\delta_{\ell',\ell} + \frac{1}{2}(\delta_{\ell',\ell+1} + \delta_{\ell',\ell-1})\right)$$

if $P = (k,\ell) \neq Q = (k',\ell')$.

In this lattice, two spins interact if they are on the same column or nearest neighbors, but with exponential decay with respect to the distance between the lines. We are interested in the asymptotic behavior of this model when the boxes $\Lambda(n,m)$ tend to ∞ in a suitable sense. More precisely, let us first consider the partition function $Z_{\Lambda(n,m)} = Z_{n,m}$ which is defined by

$$Z_{n,m} = \sum_{\sigma\in\{-1,+1\}^{\Lambda(n,m)}} \exp\left(-\beta E_{\Lambda(n,m)}(\sigma)\right). \tag{2.4.3}$$

We get a natural probability $P^{(n,m)}$ on $\{-1,+1\}^{\Lambda(n,m)}$ such that

$$P^{(n,m)}(\{\sigma\}) = \exp\ -\beta(E_{\Lambda(n,m)}(\sigma))/Z_{n,m}\ . \tag{2.4.4}$$

We then consider the energy per site $-\beta\Psi$ in the thermodynamic limit

$$\beta\Psi := \lim_{m\to\infty}\left(\frac{1}{m}\cdot\left[\lim_{n\to\infty}\ln Z_{n,m}/n\right]\right)\ . \tag{2.4.5}$$

M.Kac remarks that this free energy per site can be computed by the formula:

$$-\beta\Psi = \ln 2 - \beta\gamma/2 + \lim_{m\to\infty}(\ln\mu_1^{(m)}/m) \tag{2.4.6}$$

where $\mu_1^{(m)}$ is the largest eigenvalue of a compact integral operator K defined by:

$$K = K_{Q^{(m)}} := \exp\left(-Q^{(m)}/2\right)\exp\left(\gamma\Delta^{(m)}\right)\exp\left(-Q^{(m)}/2\right) \tag{2.4.7}$$

with

$$Q^{(m)}(y) = (\tanh(\gamma/2)/2)\sum_{k=1}^{m} y_k^2 - \sum_{k=1}^{m}\ln\cosh(\sqrt{\nu\gamma/2}(y_k+y_{k+1})) \tag{2.4.8}$$

and

$$\nu = J\beta.$$

This operator is called Kac operator or transfer operator and its main properties will be studied later. We denote by $\mu_j^{(m)}$ the decreasing sequence of the eigenvalues of $K_{Q^{(m)}}$.
As γ tends to 0, the operator is in a certain sense well approximated by the operator $\exp\,(\gamma\Delta^{(m)} - Q^{(m)})$ (think of the Campbell-Hausdorff formula [2]) and it is consequently natural, after a scaling,

$$x_k = \gamma^{\frac{1}{2}} y_k \ ,$$

to study the limit as $m \to \infty$ of $\lambda_1(m; h, \nu)/m$ where $\lambda_1(m; h, \nu)$ is the smallest eigenvalue of the Schrödinger operator:

$$S^{(m)}(x, hD_x; \nu) = -h^2 \Delta^{(m)} + V^{(m)}(x; \nu) \tag{2.4.9}$$

with:

$$V^{(m)}(x, \nu) = \frac{1}{4} \sum_{k=1}^{m} x_k^2 - \sum_{k=1}^{m} \ln \cosh(\sqrt{\nu/2}(x_k + x_{k+1})), \tag{2.4.10}$$

where $x_{m+1} = x_1$.
The parameter h is essentially equivalent to γ as γ tends to 0 and we arrive to a more traditional semiclassical problem for the Schrödinger operator.
This potential has different properties according to the different values of ν and has to be compared with the potential in the Curie-Weiss model. In particular it is convex and has a unique minimum for $\nu \le \nu^c$ and has two symmetric minima for $\nu > \nu^c$, where ν^c is m-independent. Theorems corresponding to the study of all the statistical limit as $\gamma \to 0$ are related to the socalled mean field approximation and to the famous theorem of Lebowitz-Penrose (see for example [Tho72] and the more recent [Si93]).
In this context, two natural correlations appear in statistical mechanics. We follow here the course by M.Kac [Ka66]. We can first consider the correlation between two spins in a column separated by a distance r:

$$\mathrm{Cor}_{\,\mathrm{row}}(r) = \lim_{m \to \infty} \ \mathrm{Cor}_{\,\mathrm{row}}^{\,(m)}(r) \tag{2.4.11}$$

where

$$\mathrm{Cor}_{\,\mathrm{row}}^{\,(m)}(r) = \lim_{n \to \infty} \langle \sigma_{k,\ell} . \sigma_{(k+r,\ell)} \rangle_{n,m} \tag{2.4.12}$$

[2]The Campbell-Hausdorff is a formula expressing in a Lie Algebra (think of matrices) C such that $\exp A \exp B = \exp C$ as a suitable sum of A, B and successive brackets of A and B.

and $\langle \quad . \quad \rangle_{n,m}$ corresponds to the mean value for the probability measure $P^{(n,m)}$. The computation of $\mathrm{Cor}\,^{(m)}_{\mathrm{row}}(r)$ gives:

$$\mathrm{Cor}\,^{(m)}_{\mathrm{row}}(r) = \sum_{j=2}^{\infty}(\frac{\mu_j^{(m)}}{\mu_1^{(m)}})^r \left[\int_{I\!R^m} u_1^{(m)}(x)u_j^{(m)}(x)\tanh(\sqrt{\nu\gamma/2}(x_1+x_2))dx\right]^2 . \tag{2.4.13}$$

Its asymptotic behavior as r tends to ∞ is immediately related to the behavior as $m \to \infty$ of $\mu_2^{(m)}/\mu_1^{(m)}$.
Note that if one thinks of the correspondence Kac-Schrödinger this quotient corresponds to exp $-(\lambda_1 - \lambda_2)$ where λ_1 and λ_2 correspond to the two first eigenvalues of the Schrödinger operator.
Let us now consider the correlation of two spins in a row separated by a distance t:

$$\mathrm{Cor}\,_{\mathrm{col}}(t) = \lim_{m\to\infty} \mathrm{Cor}\,^{(m)}_{\mathrm{col}}(t) \tag{2.4.14}$$

where

$$\mathrm{Cor}\,^{(m)}_{\mathrm{col}}(t) = \lim_{n\to\infty}\langle\sigma_{k,\ell}\cdot\sigma_{(k,\ell+t)}\rangle_{n,m}. \tag{2.4.15}$$

The computation [3] of $\mathrm{Cor}\,^{(m)}_{\mathrm{col}}(t)$ (cf formula (7.36) in [Ka66]) gives:

$$\mathrm{Cor}\,^{(m)}_{\mathrm{col}}(t) = \int_{I\!R^m} u_1^{(m)}(x)^2.\tanh(\sqrt{\nu\gamma/2}(x_1+x_2)).\tanh(\sqrt{\nu\gamma/2}(x_{1+t}+x_{2+t}))dx. \tag{2.4.16}$$

This appears as the mean value of the function:

$$x \to \tanh(\sqrt{\nu\gamma/2}(x_1+x_2)).\tanh(\sqrt{\nu\gamma/2}(x_{1+t}+x_{2+t}))$$

with respect to the probability measure $u_1^{(m)}(x)^2\, dx$.

2.5 The Ising model with a transverse field

We learned about this model from C. Albanese[4] [Alb] only quite recently but this model is really good to understand what one could hope to prove in the double well problem for the (DK) model or the Kac (K) model, which was mentioned in the preceding subsection and the introduction.

[3]The computation is not difficult but rather long if one uses elementary techniques. M.Kac uses the probability theory.

[4]After this course was given.

C. Albanese has proposed to us the following model where the Hamiltonian is defined, instead of taking $\otimes^{2L+1}L^2(\mathbb{R})$ $(m = 2L+1)$ in the case of the Schrödinger, on the Hilbert space $\otimes^{2L+1}\mathbb{C}^2$.
So we denote by $\mathcal{H}$ our Hilbert space

$$\mathcal{H} = \bigotimes_{i=-L}^{+L} \mathbb{C}^2 , \tag{2.5.1}$$

where our line lattice is

$$\Lambda = [-L, +L] \cap \mathbb{Z} .$$

Let us now describe the Hamiltonian with help of the Pauli matrices

$$\sigma^{(3)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} , \ \sigma^{(1)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} .$$

The tunneling parameter is denoted[5] by λ . The Hamiltonian is then

$$\mathbf{H}_\lambda = \sum_{i\sim j} \frac{1}{2}(1 - \sigma_i^{(3)}\sigma_j^{(3)}) + \lambda \sum_i \sigma_i^{(1)} . \tag{2.5.2}$$

We shall also write it in the form

$$\mathbf{H}_\lambda = S + \lambda K , \tag{2.5.3}$$

with

$$S = \sum_{i\sim j} \frac{1}{2}(1 - \sigma_i^{(3)}\sigma_j^{(3)}) := \sum_{i\sim j} S_{ij} , \tag{2.5.4}$$

and

$$K = \sum_i \sigma_i^{(1)} . \tag{2.5.5}$$

Here $i \sim j$ means $i \neq j$ and i nearest neighbour of j (that is, in $\mathbb{Z}/(2L+1)\mathbb{Z}$, $i = j \pm 1$). Here the convention is that $\sigma_j^{(\ell)}$ acts only on the j component:

$$\sigma_j^{(\ell)}(e_{-L} \otimes \cdots \otimes e_j \otimes \cdots \otimes e_L) = e_{-L} \otimes \cdots \otimes \sigma^{(\ell)} e_j \otimes \cdots \otimes e_L .$$

[5]This corresponds indeed to the modelization of the tunneling effect for the one dimensional double well problem (say for $-h^2 \frac{d^2}{dx^2} + v(x)$) and you have to think of λ as corresponding to the splitting which is of order $\exp -\frac{S}{h}$.

The statement of Albanese [6] [Alb] is

Theorem 2.5.1 *:*
If we denote by $E_\pm$ the two lowest levels, we have

$$\frac{E_\pm}{2L+1} = c\lambda^2 + \sum_{k>2} c_{k,\pm}\lambda^k \ , \tag{2.5.6}$$

and there exists C such that, for all L,

$$|E_+ - E_-| \leq (2L+1)C^{(2L+1)} \exp[(\ln \lambda)(2L+1)] \ . \tag{2.5.7}$$

In particular, the splitting between the two lowest eigenvalues as the dimension $m = 2L+1$ tends to ∞. The proof explained to us by C. Albanese gives actually a convergent series in λ for small λ. The second part is actually a consequence of the non trivial property that the coefficients $c_{k,\pm}$ are equal for $k \leq 2L+1$. What is quite important will be of course to have a control with respect to the dimension. The standard perturbation theory (for finite matrices) will give of course a result for λ small because we can see that the Hamiltonian commutes with the operator

$$P := \bigotimes_{i=-L}^{+L} \sigma_i^{(1)} \ , \tag{2.5.8}$$

and we can consequently consider the two lowest eigenvalues as simple if we restrict $\mathbf{H}_\lambda$ to the eigenspaces of $P\ \mathcal{H}_\pm$ attached to the eigenvalues ± 1. We observe also that the norm of $\sum_i \sigma_i^{(1)}$ is a priori of order L and this makes the usual argument of perturbation true only for $|\lambda| \leq C/L$. This means that we have to do something more tricky. This tricky method is called "cluster expansion" technique and explained in the Field theory context in [GlJa87]. We have no place here to explain all the details. We just sketch some scheme of the proof.

[6] The proof is given actually given for a slightly more complicate model, called the Quantum Heisenberg model. An alternative proof was obtained by Kirkwood-Thomas [KiTho] and simplified by T. Kennedy [Ken] who seems however to look for the regime λ large.

We recall first that the Pauli matrices satisfy the following anticommutation relation

$$\sigma^{(1)}\,\sigma^{(3)} = -\sigma^{(3)}\,\sigma^{(1)}\,. \tag{2.5.9}$$

We observe also that

$$P^2 = Id \tag{2.5.10}$$

We now decompose $\mathcal{H}$ as

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-\,, \tag{2.5.11}$$

where $\mathcal{H}_\pm$ is the eigenspace of P attached to ± 1.
For $\lambda = 0$, the minimal energy is 0 and a basis of the corresponding two-dimensional 0 eigenspace is given by

$$|0\rangle_\pm = \frac{1}{\sqrt{2}}\left(\bigotimes_{i=-L}^{+L} |+1\rangle_i \pm \bigotimes_{i=-L}^{+L} |-1\rangle_i \right)\,.$$

Here $|\pm 1\rangle$ is the eigenvector in $\mathbb{C}^2$ of $\sigma^{(3)}$ attached to ± 1. This choice is done in order to have the property

$$|0\rangle_\pm \in \mathcal{H}_\pm\,. \tag{2.5.12}$$

We observe also that in $\mathbb{C}^2$ (this corresponds to $L = 0$)

$$\sigma_0^{(1)}|0\rangle_\pm = \pm|0\rangle_\pm\,. \tag{2.5.13}$$

We now introduce the cluster technique (this seems to be also called the "dressing technique"). For any subset[7] $\gamma \subset \Lambda$, we introduce

$$\tau_\gamma = \Pi_{i\in\gamma}\sigma_i^{(1)}\,. \tag{2.5.14}$$

We observe that $\mathcal{H}_\pm$ is stable by τ_γ and that $\mathcal{H}_\pm$ is generated from $|0\rangle_\pm$ by the τ_γ. We observe also that

$$[\tau_\gamma, \tau_{\gamma'}] = 0\,, \tag{2.5.15}$$

for any subsets γ, γ' in Λ. We want to find an operator $\mathbf{R}(\lambda)$ (commuting with P) such that

$$\mathbf{H}_\lambda \exp \mathbf{R}(\lambda)|0\rangle_\pm = E_0^\pm(\lambda)\exp \mathbf{R}(\lambda)|0\rangle_\pm\,. \tag{2.5.16}$$

[7] or cluster,

We shall sometimes denote by $\mathbf{H}_\lambda^\pm$ the restriction of $\mathbf{H}_\lambda$ to $\mathcal{H}_\pm$.
We are looking for an operator of the form

$$\mathbf{R}(\lambda) = \sum_{n=1}^{+\infty} \lambda^n \mathbf{R}_n \ , \tag{2.5.17}$$

with

$$\mathbf{R}_n = \sum_{\gamma \subset \Lambda} r_{\gamma,n} \tau_\gamma \ .$$

The basic estimates to prove are

$$\sup_{i \in \lambda} \sum_{\gamma \ni i} |r_{n,\gamma}| \leq C^n \ , \tag{2.5.18}$$

and the estimate

$$|E_{0,n}^\pm| \leq (2L+1) C^n \ , \tag{2.5.19}$$

for a suitable L-independent constant C.
Actually, because we are working on the periodic model, $\sum_{\gamma \ni i} |r_{n,\gamma}|$ is independent of i.
If (2.5.18) is satisfied, we deduce immediately that

$$\begin{array}{ll} ||\mathbf{R}_n|| & \leq \sum_\gamma |r_{n,\gamma}| \ ||\tau_\gamma|| \\ & \leq \sum_i \sum_{\gamma \ni i} |r_{n,\gamma}| \ ||\tau_\gamma|| \\ & \leq (2L+1) C^n \sup_\gamma ||\tau_\gamma|| \ . \end{array}$$

But for the natural ℓ^2-norm on $\mathcal{H}$, we have

$$||\tau_\gamma|| = 1 \ .$$

We finally obtain

$$||\mathbf{R}_n|| \leq (2L+1) C^n \ , \tag{2.5.20}$$

and this makes the series $\sum_n \lambda^n \mathbf{R}_n$ convergent for $|\lambda| < \frac{1}{C}$ that is in a ball whose radius is independent of L.
What is actually announced by C. Albanese is that we have by restriction to $\mathcal{H}_\pm$ the identity

$$\mathbf{H}_\lambda^{Mod,\pm} := \exp -\mathbf{R}(\lambda) \ \ \mathbf{H}_\lambda^\pm \ \ \exp \mathbf{R}(\lambda) = S + V_\pm(\lambda) + E_0^\pm(\lambda) \ ,$$

with the property that

$$V_\pm(\lambda)|0\rangle_\pm = 0 \ ,$$

and

$$||V_\pm(\lambda)S^{-1}|| \leq c\lambda \ .$$

We have so replaced λK by $V(\lambda)$ for which the standard perturbation theory will prove the existence of a gap independent of L between $E_{0,\pm}(\lambda)$ and the remainder of the spectrum of $\mathbf{H}_\lambda$ restricted to $\mathcal{H}_\pm$.
The estimate on the splitting is then reduced to a purely algebraic consideration about the independence of the first coefficients of $E_0^\pm(\lambda)$ with respect to $\pm$. More precisely, the following properties can be verified

$$r_{n,\gamma} = 0 \ , \ \text{if } d(\gamma) > n \ , \tag{2.5.21}$$

and

$$E_{0,n}^+ = E_{0,n}^- \ , \ \text{if } 2L \geq n \ \ , \tag{2.5.22}$$

and we obtain the final estimate through (2.5.19).

2.6 Comments

In all these models we have met through various ways the different problems which were mentioned in the introduction. For two models, it appears a semiclassical problem through the introduction of a semiclassical parameter γ. In the last model, one has to think of the correspondence: $\lambda \sim \exp -\frac{S}{h}$ where h is the semiclassical parameter. We emphasize that the semiclassical limit

$$\gamma \to 0$$

is considered **after** the thermodynamic limit

$$m \text{ or } n \to \infty \ .$$

This is actually the crucial difficulty: we have indeed our semi-classical expansions uniformly with respect to the dimension m (which has to be interpreted in the case of these spin models as a volume).
Anyway the semiclassical study for fixed m can be considered as a first step to understand the situation.

3 Laplace integrals:

3.1 Introduction

This section is devoted to the study of statistical quantities associated with a family (indexed by the dimension m) of measures

$$\exp -\frac{1}{h}\Phi^{(m)}(x)dx^{(m)}$$

on $I\!R^m$, where $\Phi^{(m)}(x)$ is a phase (or potential) and h is as possibly small parameter. Although the case when the space $I\!R^m$ is replaced by a more general measured space and the corresponding measure by a more general one (this permits in some case to treat simultaneously spin systems and classical integrals) is quite interesting, the techniques we shall present in this course are adapted only to this special form and we shall limit our presentation to this situation (or to cases leading to this situation as it is the case in the next subsection). We refer to the book of Ellis [El85] for a more general point of view.

3.2 From spin models to Laplace integrals:

This subsection is in some sense a transition. As a consequence we shall obtain expansions in the large temperature regime but other techniques (where one looks directly to the spin systems) as it is said in Chapter 4 in [Ru69] seem to give the way to obtain a convergent expansion in power of β for the thermodynamic limit. We will only get a weaker result by justifying the approach which follows. Let us look at :

$$Z_n(\beta) = \sum_{\sigma\in\{-1,+1\}^n} \exp\,(\frac{\beta}{2} \sum_{\substack{i=1,\cdots,n\\ j=1,\cdots,n}} \sigma_i \cdot J_{ij} \cdot \sigma_j) \tag{3.2.1}$$

and at its behavior as $\beta \to 0$ with control with respect to n (we are actually working with a family of matrix $J^{(n)}$, $n \in I\!N$). We use the Laplace transform and get :

$$\begin{aligned} &Z_n(\beta)\\ &= (2\pi)^{-n/2}(\det \beta\mathbf{J})^{-1/2} \textstyle\int_{I\!R^n} \exp\left(-\frac{\beta}{2}\sum_{ij} x_i \cdot (\mathbf{J}^{-1})_{ij}\cdot x_j + \sum_i \ln\cosh x_i\right)\, dx \end{aligned} \tag{3.2.2}$$

This is only true if the $n \times n$ matrix J_{ij} is positive definite (and consequently its inverse). If this property is not satisfied, one can use the following classical trick (see formula (2.1.3)). We rewrite :

$$\begin{aligned} \exp & \left(\frac{\beta}{2} \sum_{i,j=1,\cdots,n} \sigma_i \cdot J_{ij} \cdot \sigma_j \right) \\ & = \exp \left(\frac{\beta}{2} \sum_{i,j=1,\cdots,n} \sigma_i \cdot \tilde{J}_{ij} \cdot \sigma_j \right) \cdot \exp(-\beta \lambda n/2) \end{aligned} \tag{3.2.3}$$

with

$$\tilde{J}_{ij} = J_{ij} + \lambda \delta_{ij} \ .$$

If one knows for example that $\sup_j \sum_i |J_{ij}|$ is finite (as it is the case when for example $J_{ij} = J(i-j)$ with J in $\ell^1(\mathbb{Z})$, J symmetric), the existence of λ is evident. But we always put this type of condition in order to obtain the existence of the thermodymamic limit.
In the case of the exponential interaction, we have

$$J_{ij} = -J\tau \exp -\tau |i-j|$$

and its inverse is given (see [Ka66] p.254) by :

$$\sum_{ij} (J_\tau^{-1})_{ij} \xi_i \cdot \xi_j = (\frac{1}{J\tau}) \left(\xi_1^2 + (\sum_{j=1}^{n-1} (\xi_{j+1} - \xi_j \exp -\tau)^2 / (1 - \exp -2\tau)) \right) \ .$$

In this last case, we do not need the trick. In the Ising case, we have

$$J_{ij} = \delta_{i,j\pm 1} \ .$$

The eigenvalues are symmetric around 0 and we need the trick. We observe also that this choice of λ has to be independent of n if we want to take later the thermodynamic limit $n \to \infty$. Hence we have to calculate

$$\begin{aligned} Z_n(\beta) &= \exp(-(\beta\lambda n/2).(2\pi)^{-n/2} (\det \beta \tilde{J}^{(n)})^{-1/2} \times \\ & \int_{\mathbb{R}^n} \exp\{(-1/2\beta) \textstyle\sum_{ij} x_i ((\tilde{J}^{(n)})^{-1})_{ij} x_j + \sum_i \ln\cosh x_i\} dx \end{aligned}$$

with

$$\tilde{J}_{ij} = J_{ij} + \lambda \delta_{ij}$$

We find again a Laplace integral and we shall perhaps see later that it enters inside a general theory. We possibly have to play with λ in order to apply the theory. In this direction, we remark that

$$\tilde{J}_{ij} = J_{ij} + \lambda\delta_{ij} = \lambda(I + (\mathbf{J}/\lambda))$$

and that consequently

$$\tilde{J}_{ij}^{-1} = \lambda^{-1}(I + (\mathbf{J}/\lambda))^{-1} \ .$$

If we introduce $h = \beta\lambda$, we then have to analyze the behavior as h tends to 0 of :

$$\begin{aligned} Z_n(\beta) &= \exp(-(\beta\lambda n/2).(2\pi h)^{-n/2}(\det A^{(n)})^{1/2} \times \\ &\quad \textstyle\int_{I\!R^n} \exp\left\{-\frac{1}{2h}\sum_{ij} x_i \cdot A_{ij}^{(n)} \cdot x_j + \sum_i \ln\cosh x_i\right\} dx \ , \end{aligned}$$

with

$$A^{(n)} = (I + (J^{(n)}/\lambda))^{-1} \ .$$

When λ is large enough, $||J^{(n)}/\lambda||_{\mathcal{L}(\ell^2)}$ can be made as small [8] as we need.

More details for the exponential model:
In this particular case

$$J_{ij} = -J\tau \exp -\tau|i-j|$$

and as we have seen, we can write using formula (3.2.2) and with $\nu = J\beta$

$$\begin{aligned} &Z_n(\tau,\beta) = \\ &(2\pi)^{-\frac{n}{2}} \exp -\nu\tau\tfrac{n}{2} \cdot \textstyle\int_{I\!R^n} \exp -\frac{1}{\tau}\left(\xi_1^2 + (\sum_{j=1}^{n-1}(\xi_{j+1} - \xi_j \exp -\tau)^2/(1 - \exp -2\tau))\right) \cdot \\ &\exp \textstyle\sum_i \ln\cosh\xi_i \ d\xi \ . \end{aligned}$$

We now observe that this can be seen as

$$Z_n(\tau,\beta) = \exp -\nu\tau\frac{n}{2} \cdot \int_{I\!R^n} h(\xi_1)\prod_{k=1}^{n-1} K_\tau(\xi_k,\xi_{k+1})h(\xi_n) \ d\xi \ ,$$

[8]Note here that the choice of the norm which is not important if we do not want to control with respect to n can be very important if we want to take the thermodynamic limit.

with

$$
\begin{aligned}
h(t) \quad &= \left[\tfrac{1}{(2\pi)^{\frac{1}{2}}} \exp -\tfrac{t^2}{\nu\tau} \ \cosh t\right]^{\frac{1}{2}} \\
K_\tau(t,s) \quad &= c(\tau) \exp - \left[\tfrac{1}{2\nu\tau} \tanh \tau (s^2+t^2)\right] \\
&\qquad \exp\left[\tfrac{1}{2\nu\tau \sinh\tau}(s-t)^2 + \ln\cosh t + \ln\cosh s\right]
\end{aligned}
$$

where $c(\tau)$ is a possible (?) normalization constant.
We observe that there is no uniqueness in the choice of K but the guide line is here to find a compact symmetric operator. We now observe that

$$
Z_n(\tau,\beta) = \exp -\nu\tau\frac{n}{2} \cdot \langle K^{n-1}h|h\rangle \ ,
$$

or

$$
Z_n(\tau,\beta) = \exp -\nu\tau\frac{n}{2} \cdot \sum_j \mu_j^{n-1} |\langle h|\phi_j\rangle|^2
$$

We get for the thermodynamic limit

$$
\lim_{n\to\infty} \ln Z_n(\tau,\beta)/n = -\frac{\nu}{2}\tau + \ln\mu_1 \ ,
$$

and we can if we want control the speed of convergence which appears to be in $\mathcal{O}(\frac{1}{n})$.

In order to have a more standard semiclassical problem we perform the change of variable $t = [\frac{\nu \sinh\tau}{\tau}]^{\frac{1}{2}} \ \tilde{t}$ and get as a new kernel

$$
\begin{aligned}
&\tilde{K}(\tilde{t},\tilde{s}) = \tilde{c}(\tau) \\
&\exp - \left[\tfrac{\tanh\tau\cdot\sinh\tau}{2\tau^2}(\tilde{t}^2+\tilde{s}^2) + \tfrac{1}{2\tau^2}(\tilde{t}-\tilde{s})^2 \right. \\
&\quad \left. - \ln\cosh\left(\nu^{\frac{1}{2}} \ (\tfrac{\sinh\tau}{\tau})^{\frac{1}{2}} \ \tilde{t}\right) - \ln\cosh\left(\nu^{\frac{1}{2}} \ (\tfrac{\sinh\tau}{\tau})^{\frac{1}{2}} \ \tilde{s}\right)\right] \ .
\end{aligned}
$$

This explains why we have met as a first approximation (when $\tau \to 0$) the potential

$$
V(t) = t^2 - \ln\cosh(\nu^{\frac{1}{2}} t) \ ,
$$

and the transfer operator

$$
K_V(t,s) = \exp -\frac{V}{2} \ \exp \tau^2 \Delta \ \exp -\frac{V}{2} \ .
$$

The computations for the model (A) which we have mentioned in the preceding section are of the same type.

3.3 Classical Laplace methods

Before to enter in more general questions it is perhaps better to recall very simple results concerning Laplace integrals. The first one is modelled on the stationary phase theorem:

Theorem 3.3.1 *:*
Let Φ be a real C^∞ phase defined in a neighborhood $\mathcal{V}$ of the closure of the ball $B(0,1)$ in $\mathbb{R}^m$ such that

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

Let a be a C^∞ function defined in $\mathcal{V}$ and let us consider the Laplace integral

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

where $h \in]0,h_0]$. Then, as h tends to 0, $I(a,\Phi;h)$ has the following asymptotic behavior

$$I(a,\Phi;h) \sim h^{\frac{m}{2}} \sum_j \alpha_j \cdot h^j\ , \tag{3.3.1}$$

with

$$\alpha_0 = (2\pi)^{\frac{m}{2}} \cdot a(0)\ (\det\ \mathit{Hess}\ \Phi(0))^{-\frac{1}{2}}\ . \tag{3.3.2}$$

The proof is rather simple (and actually simpler than for an oscillatory integral). The assumptions permit to reduce modulo exponentially small contributions (in $\mathcal{O}(\exp -\epsilon_0/h)$) to an arbitrarily small neighborhood of 0. We can then use the Morse Lemma in order to write in new coordinates: $\Phi(x) = \sum y_j^2 =: \hat{\Phi}(y)$. We are then reduced to the study of $I(b,\hat{\Phi};h)$ which is easy by taking the Taylor expansion of b at 0. We are then reduced to the computation of very explicit integrals associated with gaussian measures on $\mathbb{R}^m$.

Lemma 3.3.2 *The Morse Lemma :*
Let $f(x,y)$ ($x \in \mathbb{R}^n, y \in \mathbb{R}^N$) be a real valued C^∞ function in a neighborhood

of $(0,0)$. *Assume that* $(\nabla_x f)(0,0) = 0$ *and that* $A = (\text{ Hess }_{xx} f)(0,0)$ *is non-singular. Then the equation* $f'_x(x,y) = 0$ *determines in a neighborhood of* 0 *a* C^∞ *function* $x(y)$ *with* $x(0) = 0$ *and we have in a neighborhood of* 0

$$f(x,y) = f(x(y),y) + \langle Az|z\rangle/2$$

where $z = x - x(y) + \mathcal{O}(|x - x(y)|)(|x| + |y|)$ *is a* C^∞ *function of* (x,y) *at* $(0,0)$.

The proof is standard and can be found for example in Hörmander's book (Tome III p.502).
One of the basic problems later will be to control all this procedure with respect to the dimension. There is also an analog of the above theorem for a phase with more than one minimum and under suitable assumptions at ∞ one can also consider Laplace integrals over $I\!R^m$. The assumption that Φ is real can be made weaker if one assume holomorphy of a and Φ and we then enter in the world of the saddle point method (see J.Sjöstrand [Sj82], Chapter 2 for a sophisticated and general presentation of the method).
We shall also have to discuss problems with parameter when the phase is deformed from a convex phase into a double well. The most simple case of such a situation (see for example [He92a]) is the phase defined on $I\!R$

$$x \mapsto \phi(x,\theta) = (1-\theta)x^2 + x^4 \ ,$$

and, for $a \in C_0^\infty(I\!R)$, one can consider the integral $I(a, \phi(\cdot,\theta); h)$ over $I\!R$ and it is interesting to follow the behavior of this integral with respect to $\theta \in]0,\infty[$. For fixed θ, we can distinguish three cases

- For $\theta = 1$,
  $I(\theta;h) = a(0)\, h^{\frac{1}{4}} \, \left(\int_{I\!R} \exp -x^4\, dx + \mathcal{O}(h^{\frac{1}{2}})\right)$
- For $\theta < 1$,
  $I(\theta;h) = \pi^{\frac{1}{2}}\, a(0)\, h^{\frac{1}{2}}(1 + \mathcal{O}(h))$,
- For $\theta > 1$,
  $I(\theta;h) = (2(\theta-1))^{-\frac{1}{2}} \exp \frac{(\theta-1)^2}{4h} h^{\frac{1}{2}} \times$
  $\left(a(+((\theta-1)/2)^{\frac{1}{2}}) + a(-((\theta-1)/2)^{\frac{1}{2}}) + \mathcal{O}(h)\right)$.

As $\theta \sim 1$, one has to be more precise in order to get a behavior in h uniform with respect to θ. This can be done by using as a reference $J(\alpha) = \int_{\mathbb{R}} \exp -(\alpha x^2 + x^4)\, dx$ where α is a new parameter $\alpha = h^{-\frac{1}{2}}(\theta - 1)$. We observe that

- For $\alpha \to \infty$, $J(\alpha) \sim \alpha^{-\frac{1}{2}}$,
- For $\alpha = 0$, $J(0) = \int_{\mathbb{R}} \exp -x^4 dx$,
- For $\alpha = -\infty$, $J(\alpha) \sim \sqrt{2\pi} \cdot \exp \frac{\alpha^2}{4} \cdot \alpha^{-\frac{1}{2}}$.

It is then possible to prove that

$$I(\theta; h) = \frac{1}{2} h^{\frac{1}{4}} \cdot J(\alpha) \cdot \left(a(+((\theta-1)_+/2)^{\frac{1}{2}}) + a(-((\theta-1)_+/2)^{\frac{1}{2}}) + \mathcal{O}(h^{\frac{1}{2}}) \right) .$$

In a very simple situation this explains what is going on near the transition of phase.

4 From statistical mechanics to quantum mechanics

4.1 Introduction

Our initial problem was to find a rather general approach for the estimate of the decay of correlations attached to "gaussian like" measures of the type

$$\exp -\Phi(X) dX \tag{4.1.1}$$

on $\mathbb{R}^n$ with Φ convex. One proof of this estimate (in the case when Φ has a particular structure) is based on the analysis of the transfer matrix method, originally due to Kramers-Wannier, that we have already seen for the study of the Ising model (see for example the book of Thompson [Tho72]). We present here briefly the technique. In order to present this approach (other cases are considered in Section 12.4 of the book by Parisi [Pa84]), we consider a particular case when $n = mp$ and we then take a matrix notation for the variable X:

$$X = x_j^i$$

where the index $i = 1, ..., m$ corresponds to the row and the index $j = 1, ..., p$ corresponds to the column. We use alternatively the notation $X = (x_1, ..., x_p)$ with $x_j \in \mathbb{R}^m$ or $X = (x^1, ..., x^m)$ with $x^i \in \mathbb{R}^p$. We now consider the particular potential Φ

$$\Phi^{(p)}(X) \equiv \Phi(X) \equiv \sum_{j=1}^{p} V(x_j) + \frac{|x_j - x_{j+1}|^2}{4h^2} \tag{4.1.2}$$

where we take the convention that $x_{p+1} = x_1$ and where h is possibly a semiclassical parameter which is sometimes chosen equal to one if we are not interested in the "semiclassical" aspects. More generally, we could more generally consider examples of the form:

$$\Phi(X) = \sum_{j=1}^{p} (V(x_j) + I(x_j, x_{j+1})) \tag{4.1.3}$$

where I is a symmetric "interaction" potential on $\mathbb{R}^m \times \mathbb{R}^m$. Let us mention however that the example (4.1.2) appears naturally in quantum field theory when the so called "lattice approximation" is introduced. For this special class of potentials, we shall demonstrate that the informations given by the transfer operator method is complementary to the other approachs we have explained before. We shall present the "dictionary" between the properties of the measure $\exp -\Phi(X) dX$ and the spectral properties of the transfer operator (which is also called Kac operator in other references)

$$K_V(x,y) = (2\pi h)^{-\frac{m}{2}} \exp -\frac{V(x)}{2} . \exp -\frac{|x-y|^2}{4h^2} . \exp -\frac{V(y)}{2} \,. \tag{4.1.4}$$

(We shall forget sometimes the coefficient $(2\pi h)^{-\frac{m}{2}}$ which is simply a normalization and appears only in the problem of the thermodynamic limit).
This dictionary permits to obtain interesting connections between estimates for the quotient μ_2/μ_1 of the two first largest eigenvalues of the transfer operator and corresponding estimates controlling the speed of convergence of thermodynamic quantities or the decay of the correlations. In particular, for fixed m and h, this speed of convergence can be exponentially rapid as $p \to \infty$. For this we do not need convexity of the potential. The phenomenon is here similar to what we have observed for the one-dimensional Ising model. In particular there is apparently no phase transition. But, as will be later discussed on an example all these problems reappear in the semiclassical context $h \to 0$ or in the limit $m \to \infty$.

4.2 A link between statistical mechanics and quantum mechanics.

4.2.1 Elementary properties of the Kac operator.

We first recall some properties of the Kac operator (or transfer operator). This operator is associated with a potential V. We do not try to give the minimal assumptions which are needed for V and we assume in order to simplify the discussion the two following conditions

$$V(y) \geq \frac{1}{C}|y|^2 - C \tag{4.2.1}$$

for some strictly positive constant C, and

$$\forall \alpha \in \mathbb{Z}^m \,,\ \exists C_\alpha \ s.t.\ |D_y^\alpha V(y)| \leq C_\alpha < y >^{(2-|\alpha|)_+} \,. \tag{4.2.2}$$

Under these assumptions, K_V is a compact strictly positive selfadjoint operator with strictly positive kernel. In particular it satisfies the assumptions of the extended Perron-Frobenius Theorem (see for example Theorem 3.3.2 in Glimm-Jaffé [GlJa87]) also called Krein-Rutman Theorem and K_V admits consequently a largest eigenvalue μ_1 equal to $||K_V||$ which is simple and corresponds to a unique strictly positive normalized eigenfunction which we denote by u_1. Let μ_j the sequence of eigenvalues that we order as a decreasing sequence tending to 0:

$$0 \leq \mu_{j+1} \leq \mu_j \leq .... \leq \mu_2 < \mu_1. \tag{4.2.3}$$

We shall denote by u_j a corresponding orthonormal basis of eigenvectors with

$$K_V u_j = \mu_j u_j \ , \ ||u_j|| = 1 \ . \tag{4.2.4}$$

Let us recall the proof and the statements:

Definition 4.2.1 *:*
Let A be a bounded operator on a Hilbert space $\mathcal{H} = L^2(X, d\nu)$ where (X, ν) is a measured space. Then we say that A has a strictly positive kernel if for each choice of a non negative function $\theta \in \mathcal{H}$ ($||\theta|| \neq 0$),

$$0 < A\theta$$

almost everywhere.

Example 4.2.2 *:*

- *In the finite dimensional case, the matrices with strictly positive coefficients,*
- *On $L^2(I\!R^m)$, the kernel $(2\pi)^{-\frac{m}{2}} \ \exp -\frac{V(x)}{2} \exp -\frac{1}{4}|x-y|^2 \exp -\frac{V(y)}{2}$,*
- *The kernel of the heat equation.*

The theorem generalizing the Perron-Frobenius theorem is then the following:

Theorem 4.2.3 *:*
Let A be a bounded compact symmetric [9] *operator on $\mathcal{H}$ having a strictly positive kernel and let $||A|| = \lambda$ be the largest eigenvalue of A. Then λ has multiplicity 1 and the corresponding eigenvector Ω can be chosen to be a strictly positive function.*

Proof:

Since A maps real functions into real functions, we may assume that Ω is real.
We now prove that

$$\langle A\Omega, \Omega\rangle \leq \langle A|\Omega|, |\Omega|\rangle.$$

This is an immediate consequence of the strict positivity of the kernel. We just write:

$$\Omega = \Omega_+ - \Omega_-$$

and

$$|\Omega| = \Omega_+ + \Omega_-$$

and the above inequality is then a consequence of

$$\langle A\Omega_+, \Omega_-\rangle \geq 0 \ ,$$

and

$$\langle \Omega_+, A\Omega_-\rangle \geq 0 \ .$$

We then obtain

$$\lambda||\Omega||^2 = \langle A\Omega, \Omega\rangle \leq \langle A|\Omega|, |\Omega|\rangle \leq ||A||||\Omega||^2 = \lambda||\Omega||^2 \ .$$

This implies

$$\langle A\Omega, \Omega\rangle = \langle A|\Omega|, |\Omega|\rangle \ .$$

This equality means

$$\langle \Omega_+, A\Omega_-\rangle + \langle \Omega_-, A\Omega_+\rangle = 0 \ .$$

[9] We put this condition of symmetry in order to simplify and to work directly with real eigenvalues (See [El85], Lemma IX.4.1, p. 280, for generalizations).

We then get a contradiction unless $\Omega_+ = 0$ or $\Omega_- = 0$. We can then assume $\Omega \geq 0$ and the assumption gives again

$$O < \langle \theta, A\Omega \rangle = \lambda \langle \theta, \Omega \rangle \ ,$$

for any positive θ. This gives

$$\Omega \geq 0 \quad a.e \ .$$

But

$$\Omega = \lambda^{-1} A \Omega$$

and this gives

$$K > 0 \quad a.e \ .$$

Finally if there was two linearly independent eigenvectors Ψ and Ω corresponding to λ, we would obtain the same property for Ψ by considering as new Hilbert space the orthogonal of Ω in $\mathcal{H}$. But it is impossible to have two orthogonal vectors which are strictly positive.
q.e.d.

4.2.2 The transfer matrix method

Thermodynamic limit

Let us first look at the thermodynamic limit. We start from the decomposition:

$$\exp -\Phi(X) = K_V(x_1, x_2) \cdot K_V(x_2, x_3) \cdots K_V(x_{p-1}, x_p) \cdot K_V(x_p, x_1) \quad (4.2.5)$$

and we observe that

$$\int_{\mathbb{R}^{mp}} \exp -\Phi(X) \ dX = \int_{\mathbb{R}^m} K_V^{(p)}(y, y) \ dy \qquad (4.2.6)$$

where $K_V^{(p)}(x, y)$ is the distribution kernel of $(K_V)^p$. Our assumption on V

permits to see that $(K_V)^p$ is trace class [10] and we rewrite (4.2.6) in the form:

$$\int_{I\!R^{mp}} \exp -\Phi(X)\; dX = \text{ Tr } [(K_V)^p] = \sum_j \mu_j^p \; , \tag{4.2.7}$$

where the μ_j are introduced in (4.2.3).
We note also for future use that

$$K_V^{(p)}(x,y) = \sum_j \mu_j^p u_j(x) u_j(y) \; . \tag{4.2.8}$$

In particular we get :

$$\lim_{p\to\infty} \frac{\ln \int_{I\!R^{mp}} \exp -\Phi(X)\, dX}{p} = \ln \mu_1 \tag{4.2.9}$$

and the speed of the convergence is easily estimated by:

$$-\ln \left| \frac{\ln \int_{I\!R^{mp}} \exp -\Phi(X)\, dX}{p} - \ln \mu_1 \right| = -p \ln(\frac{\mu_2}{\mu_1}) - \ln k_2 + \ln p + \mathcal{O}(\exp -\delta_2 p) \; , \tag{4.2.10}$$

where k_2 is the multiplicity of μ_2.

Mean value

Let us continue the dictionary. We consider now the mean value with respect to our measure of some cylindrical functions. More precisely, if f is a function of x_1 in $C_0^\infty(I\!R^m)$, let us introduce

$$\langle f^{(1)} \rangle_p = \frac{\int f(x_1) \exp -\Phi(X)\, dX}{\int \exp -\Phi(X) dX} \; . \tag{4.2.11}$$

An immediate computation using (4.2.8) gives

$$\langle f^{(1)} \rangle_p = \frac{\sum_j \mu_j^p (\int f(y)\, u_j(y)^2\, dy)}{\sum_j \mu_j^p} \; . \tag{4.2.12}$$

[10] See [ReSi78] or [Ro87] for the properties of the trace class operator. For positive compact symmetric operators T on $\mathcal{H} = L^2(I\!R^m)$, it is sufficient to say that the eigenvalues λ_j satisfy $\sum_j \lambda_j < +\infty$ and the trace is simply, as in the finite dimensional case, $\text{Tr } T = \sum_j \lambda_j$. If the operator has a nice regular distribution kernel $K_T(x,y)$ (we shall work actually with kernels in $\mathcal{S}(I\!R^m \times I\!R^m)$), then the trace is also obtained as $\text{Tr } T = \int_{I\!R^m} K_T(x,x) dx$.

In particular, we get the following convergence

$$\lim_{p\to\infty}\langle f^{(1)}\rangle_p = \int f(y)\,u_1(y)^2\,dy\;, \tag{4.2.13}$$

and we have moreover the following control of the convergence

$$\langle f^{(1)}\rangle_p - \int f(y)\,u_1(y)^2\,dy = \mathcal{O}((\frac{\mu_2}{\mu_1})^p) \tag{4.2.14}$$

Pair correlation
Let us consider the correlation functions. If f and g are two functions in $C_0^\infty(I\!R^m)$, we denote by $f^{(j)}$ the corresponding function on $I\!R^{mp}$:

$$X \to f(x_j)\;.$$

We shall now compute the pair correlation

$$\mathrm{Cor}^{(p)}(f^{(i)}, g^{(j)}) = \langle (f^{(i)} - \langle f^{(i)}\rangle_p)(g^{(j)} - \langle g^{(j)}\rangle_p)\rangle_p\;.$$

(If $f(x) = g(x) = x$, we write more simply $\mathrm{Cor}^{(p)}(i,j)$.) Because everything is invariant by circular permutation we can take $i = 1$. We first have

$$\langle f^{(1)} g^{(j)}\rangle_p \;=\; \frac{\sum_{k,\ell}\mu_k^{j-1}\mu_\ell^{p-j+1}[\int f(y)u_k(y)u_\ell(y)dy][\int g(y)u_k(y)u_\ell(y)dy]}{\sum_i \mu_i^p}\;.$$

In particular, if $f = g$ (and this will be the interesting case for us), we get

$$\langle f^{(1)} f^{(j)}\rangle_p = \frac{\sum_{k,\ell}\mu_k^{j-1}\mu_\ell^{p-j+1}[\int f(y)\,u_k(y)\,u_\ell(y)\,dy]^2}{\sum_i \mu_i^p}\;,$$

and

$$\begin{aligned}
&(\textstyle\sum_i \mu_i^p)^2.\ \mathrm{Cor}^{(p)}(f^{(1)}, f^{(j)})\\
&\quad= \left[\textstyle\sum_k \mu_k^p\,(\int f(y)\,u_k(y)^2\,dy)^2\right](\textstyle\sum_i \mu_i^p)\\
&\qquad - [\textstyle\sum_k \mu_k^p(\int f\,u_k^2\,dx)]^2\\
&\qquad + \left[\textstyle\sum_{k\neq\ell}\mu_k^{-1+j}\mu_\ell^{p-j+1}\,(\int f(y)\,u_k(y)\,u_\ell(y)\,dy)^2\right](\textstyle\sum_i \mu_i^p)
\end{aligned}$$

and, taking the limit as $p\to\infty$, we finally obtain the following identity

$$\lim_{p\to\infty}\ \mathrm{Cor}^{(p)}(f^{(1)}, f^{(j)}) = \sum_{k>1}(\frac{\mu_k}{\mu_1})^{j-1}[\int f(y)\,u_k(y)\,u_1(y)\,dy]^2\;. \tag{4.2.15}$$

From this we get the inequality

$$(\frac{\mu_2}{\mu_1})^{j-1} \text{ var } (f) \geq \lim_{p\to\infty} \Big[\text{ Cor }^{(p)}(f^{(1)}, f^{(j)})\Big] \geq (\frac{\mu_2}{\mu_1})^{j-1}[\int f(y)\, u_2(y)\, u_1(y)\, dy]^2 \ , \tag{4.2.16}$$

where

$$\text{var}(f) = \int_{I\!R^m} u_1^2\, f^2\, dx - (\int_{I\!R^m} u_1^2\, f\, dx)^2 \tag{4.2.17}$$

is thevariance variance of f with respect to the measure $u_1^2(x)\, dx$.
For the first inequality, we have used the property that, by the Parseval equality, we have

$$\int (f u_1)^2 dx = \sum_j \Big(\int f(x) u_1(x) u_j(x)\, dx\Big)^2 \ ,$$

remembering that u_j is an orthonormal basis.

If we know by other means how to control the decay with respect to j uniformly with respect to p ($p \gg j$), and if we can choose f such that $\int f(y)\, u_2(y)\, u_1(y)\, dy \neq 0$, then we shall find a way to get a new estimate for $\frac{\mu_2}{\mu_1}$. Conversely, a good estimate for $\frac{\mu_2}{\mu_1}$ will give a very precise estimate for the corresponding correlation. Suppose indeed that we prove as a first step that

$$\begin{array}{l} \exists\, \kappa \text{ s.t. } \forall \epsilon > 0 \ , \ \exists\, j_0 \ \text{ and } \ C_\epsilon \text{ s.t } \forall j \geq j_0 \ , \ p > 2j \ , \\ \Big[\text{ Cor }^{(p)}(f^{(1)}, f^{(j)})\Big] \leq C_\epsilon \exp -(\kappa - \epsilon)(j-1) \ , \end{array} \tag{4.2.18}$$

with $[\int f(y)\, u_2(y)\, u_1(y)\, dy] \neq 0$, then we get, taking successively the limit $p \to \infty$, the limit $j \to \infty$ for $\frac{1}{j} \ln \Big(\text{ Cor }^{(p)}(f^{(1)}, f^{(j)})\Big)$ and then the limit $\epsilon \to 0$ in the upper bound obtained by combining the r.h.s inequality in (4.2.16) and (4.2.18)

$$\frac{\mu_2}{\mu_1} \leq \exp -\kappa \ . \tag{4.2.19}$$

But using now the l.h.s in (4.2.16), we get the improved estimate replacing (4.2.18) and establishing the existence of κ and C s.t. for all j,

$$\lim_{p\to\infty} \Big[\text{ Cor }^{(p)}(f^{(1)}, f^{(j)})\Big] \leq C \exp -\kappa(j-1) \ . \tag{4.2.20}$$

Let us now recall that estimates for the correlations were obtained in the case where f is C^∞ but with bounded gradient, and a possible choice for f is $f = u_2$. Here we observe that if μ_2 is not of multiplicity one u_2 is not uniquely determined but corresponds to some arbitrary choice of a second eigenvector. Another natural choice was $f(y) = y^\ell$ for some ℓ, but it is not always true that

$$\int y^\ell \, u_2(y) \, u_1(y) \, dy \neq 0 \tag{4.2.21}$$

is satisfied for some ℓ and for some choice of u_2 (remember the case when μ_2 has multiplicity larger than 1).

On the other hand, one is usually interested in the correlation associated to $f(y) = y^\ell$ and we can not avoid in this case the question of the validity of (4.2.21). Note that in the case when V is a non degenerate quadratic form this condition (4.2.21) can be explicitely verified. Under this condition we get that the logarithm of the correlation is effectively asymptotic to $j \ln(\frac{\mu_2}{\mu_1})$ and the correlation length is $\ln(\frac{\mu_2}{\mu_1})$.
This argument is used in the proof [11] by Helffer [He94b] of the following

Theorem 4.2.4 *:*
If for some $\sigma > 0$

$$\textit{Hess } V(x) \geq \sigma \ , \ \forall \, x \in I\!R^m \tag{4.2.22}$$

then

$$\frac{\mu_2}{\mu_1} \leq \exp - \left[\cosh^{-1}[h^2\sigma + 1]\right] \tag{4.2.23}$$

Remark 4.2.5 *:*
The result is optimal in the sense that the quadratic case when $V(y) = \sum_{j=1}^m \sigma_j y_j^2/2$ *gives for* $\sigma = \inf \sigma_j$ *the equality:*

$$\frac{\mu_2}{\mu_1} = \exp - \left[\cosh^{-1}[h^2\sigma + 1]\right] \tag{4.2.24}$$

[11] This result was also motivated by the corresponding result on the splitting for the Schrödinger operator obtained by J. Sjöstrand [Sj93b] (cf also [HeSj92a]) saying under basically the same assumptions that

$$\lambda_2 - \lambda_1 \geq \sqrt{2\sigma} \ .$$

Remark 4.2.6 :
In the semiclassical limit, the semiclassical techniques[12] *permit to prove that:*

$$\frac{\mu_2(h)}{\mu_1(h)} = \exp(\lambda_1(h) - \lambda_2(h)) + \mathcal{O}(h^2)\ . \tag{4.2.25}$$

An easy computation shows that the results on the splitting for Kac and the result on the splitting for Schrödinger are coherent.

4.3 Explicit computations for the harmonic oscillator:

As will be seen in all this course, the harmonic oscillator

$$H^h = -h^2 d^2/dx^2 + x^2$$

plays a central role in the theory. We recall that its spectrum is given by a sequence of eigenvalues $\lambda_n(h)$ $(n \in I\!N)$

$$\lambda_n(h) = (2n-1)h\ .$$

In particular the fundamental level is

$$\lambda_1(h) = h$$

and the splitting between the two first eigenvalues is $2h$. The first eigenfunction is given by

$$\phi_1(x,h) = c_1\, h^{-\frac{1}{4}} \exp -\frac{x^2}{2h}$$

and the other eigenvectors are obtained by applying the creation operator

$$L^+ = -h\partial_x + x\ .$$

We observe indeed that

$$H^h = L^+ \cdot L^-\ +\ h$$

where

$$L^- = h\partial_x + x = (L^+)^*$$

and has the property

$$L^-\phi_1 = 0.$$

The $n^t h$-eigenfunction is then given by

$$\phi^n = c_n (L^+)^{n-1} \phi^1\ .$$

[12] This is for example analyzed in [BruHe91].

4.4 Explicit computations for the harmonic Kac operator:

In the context of the transfer operator the harmonic oscillator is replaced by the harmonic Kac operator

$$\exp -\frac{x^2}{2} \cdot \exp h^2 \frac{d^2}{dx^2} \cdot \exp -\frac{x^2}{2} \,. \tag{4.4.1}$$

and there are good reasons to think (use the formal Campbell-Hausdorff formula) that the spectrum is quite near the spectrum of the operator $\exp -H^h$ as $h \to 0$. The point is that this can be done quite explicitely in the case of the harmonic potential. We want to compare :

$$\exp(-x^2/2).\exp(t(d/dx)^2).\exp(-x^2/2) \,, \tag{4.4.2}$$

with

$$\exp -(-t(d/dx)^2 + x^2) \text{ for } t > 0 \,. \tag{4.4.3}$$

We have by explicit computations (see the book of Simon [Si79] p. 36-38) the so called Mehler's Formula, expressing that the kernel of

$$\exp -t(-\frac{1}{2}d^2/dx^2 + \frac{1}{2}x^2 - \frac{1}{2})$$

is given by

$$\begin{aligned} K_t(x,y) = {} & \pi^{-1}(1-\exp -2t)^{-\frac{1}{2}} \\ & \exp[-(1-\exp -2t)^{-1}(\tfrac{1}{2}(1+\exp -2t)(x^2+y^2) - 2\exp -t\, xy)] \,. \end{aligned} \tag{4.4.4}$$

or

$$\begin{aligned} & K_t(x,y) = \\ & \pi^{-1}(1-\exp -2t)^{-\frac{1}{2}} \exp[-(\tfrac{1}{2\tanh t})(x^2+y^2) - \tfrac{1}{\sinh t}\, xy] \,, \end{aligned} \tag{4.4.5}$$

One can verify the coherence of the result by verifying

$$\int_y K_t(x,y) \exp -\frac{y^2}{2} dy = \exp -\frac{x^2}{2} \,, \tag{4.4.6}$$

or

$$\partial_t K(x,y;t) + (-\frac{1}{2}\partial^2/\partial x^2 + \frac{1}{2}x^2 - \frac{1}{2})K(x,y;t) = 0 \,, \tag{4.4.7}$$

and

$$\lim_{t\to 0} K(x,y;t) = \delta(x-y)\ . \tag{4.4.8}$$

Let us just sketch (the proof is not complete) what we get from the second point of view. If we look for a kernel of the form

$$K(x,y;t) = c(t)\exp - \Big[a(t)(x^2+y^2) - 2b(t)\,xy\Big] \tag{4.4.9}$$

we get plugging inside (4.4.7)

$$-a'(t)(x^2+y^2) + 2b'(t)\,xy\ +\ \frac{1}{2}x^2 - 2(a(t)\,x - b(t)\,y)^2 = 0\ .$$

This is decomposed in three equations

$$\begin{array}{l} -a'(t) + \frac{1}{2} - 2a^2(t) = 0 \\ -a'(t) - 2b(t)^2 = 0 \\ 2b'(t) + 4a(t)b(t) = 0 \end{array}$$

One finds effectively that $a(t) = \frac{1}{2}\tanh t^{-1}$ is a solution of the first equation. The second equation then determines essentially $b(t)^2$ by

$$b^2(t) = -\frac{1}{4} + a^2(t) = \frac{1}{4}[1/\sinh^2(t)]\ .$$

The choice of the sign for b can probably be determined by looking at the limit $t\to 0$ and we take $b(t) = \frac{1}{2\sinh t}$. The function c is then easy to determine as a normalization constant.

The proof given in [Si79] is based on the Feynman-Kac formula (or its simpler version : the Trotter-Kato formula that we shall recall in the next subsection). We then obtain by identification of the coefficients

$$\begin{array}{l} \exp(-x^2/2).\exp(t(d/dx)^2).\exp(-x^2/2) = \\ \exp\Big[-[\ln(z+\sqrt{z^2-1})/4K\sqrt{z^2-1}].[-d^2/dx^2 + 4K^2(z^2-1)x^2]\Big] \end{array} \tag{4.4.10}$$

with $K = 1/4t$ and $z = (2t+1)$.
We then obtain the explicit computation of the eigenvalues of

$$\exp(-x^2/2).\exp(t(d/dx)^2)\cdot\exp(-x^2/2)$$

as:

$$\exp(-(n-(1/2))\ln(z+\sqrt{z^2-1}))\ (n\geq 1, n\in I\!N)\ .$$

In order to come back to our notation above we compute the formula for the operator $\exp(-\sigma x^2/4).\exp((d/dx)^2)\cdot\exp(-\sigma x^2/4)$ and we get for the eigenvalues μ_n:

$$\mu_n=\exp(-((2n-1)/2)\cosh^{-1}(\sigma+1))\ , \tag{4.4.11}$$

and the splitting is given by:

$$\mu_2/\mu_1=\exp-\cosh^{-1}(1+\sigma). \tag{4.4.12}$$

4.5 The Trotter's product formula

The Trotter-Kato Formula plays a role in many different contexts in mathematics and physics: in particular in Quantum mechanics but also in numerical analysis.

Theorem 4.5.1 *:*
Let A and B be selfadjoint operators on a separable Hilbert-space so that $A+B$, defined on $D(A)\cap D(B)$, is selfadjoint. Then

$$\exp it(A+B)=s-\lim_{n\to\infty}(\exp itA/n\exp itB/n)^n\ . \tag{4.5.1}$$

If, moreover, A and B are bounded from below, then

$$\exp -t(A+B)=s-\lim_{n\to\infty}(\exp -tA/n\exp -tB/n)^n\ . \tag{4.5.2}$$

and

$$\exp -t(A+B)=s-\lim_{n\to\infty}(\exp -tB/2n\ \exp -tA/n\ \exp -tB/2n)^n\ . \tag{4.5.3}$$

Proof:
Let us prove (4.5.2). It is actually sufficient to prove it on a dense set and we can also assume after translation that A and B are positive. As dense set, we shall choose at the end $D(A)\cap D(B)$. Let $S_t=\exp -t(A+B)$, $V_t=\exp -tA$, $W_t=\exp -tB$ and $U_t=V_tW_t$. Let $\Psi_t=S_t\psi$ for some ψ in $\mathcal{H}$ the underlying Hilbert space. Then

$$\begin{aligned} ||(S_t-U^n_{\frac{t}{n}})\psi|| &= ||\textstyle\sum_{j=0}^{n-1}U^j_{\frac{t}{n}}(S_{\frac{t}{n}}-U_{\frac{t}{n}})S^{n-j-1}_{\frac{t}{n}}\psi|| \\ &\leq n\sup_{0\leq s\leq t}||(S_{\frac{t}{n}}-U_{\frac{t}{n}})\psi_s|| \end{aligned} \tag{4.5.4}$$

Let $\phi \in D(A) \cap D(B)$. Then

$$s^{-1}(S_s - 1)\phi \to -(A+B)\phi$$

as $s \to 0$ $(s > 0)$ and

$$\begin{aligned} s^{-1}(U_s - 1)\phi \ &= V_s(-B\phi) + V_s[s^{-1}(W_s - 1) + B]\phi + s^{-1}(V_s - 1)\phi \\ &\to -B\phi + 0 - A\phi\ . \end{aligned}$$

So

$$\lim_{n\to\infty}[n||(S_{\frac{t}{n}} - U_{\frac{t}{n}})\phi||] \to 0\ , \forall\phi \in D(A)\cap D(B)\ . \tag{4.5.5}$$

Let D denote $D(A) \cap D(B)$ with the norm $||(A+B)\phi|| + ||\phi|| \equiv |||\phi|||$. By hypothesis, D is a banach space. By the above calculations, $\{n(S_{\frac{t}{n}} - U_{\frac{t}{n}})\}$ is a family of bounded operators from D to $\mathcal{H}$ with $\sup_n\{n(S_{\frac{t}{n}} - U_{\frac{t}{n}})\phi\} < \infty$ for each ϕ. Using the Banach-Steinhaus theorem, we get the existence of a constant C such that

$$||n(S_{\frac{t}{n}} - U_{\frac{t}{n}})\phi|| \leq C\,|||\phi|||\ . \tag{4.5.6}$$

But (4.5.6) implies that the limit in (4.5.5) is uniform over compact subsets of D. Let $\psi \in D$. Then $s \mapsto \psi_s$ is a continuous map from $[0,t]$ into D, so that $\{\psi_s | 0 \leq s \leq t\}$ is compact in D. Thus the right-hand side of (4.5.4) goes to 0 as $n \to \infty$. We have consequently proved (4.5.2) for $\psi \in D$ and conclude for the general case by density.

Remark 4.5.2 *:*
Using the Trotter-Kato formula, one can see easily understand why we can look a priori for a quadratic phase for the kernel of $K_t(x,y)$ (in formula (4.4.5)). This is indeed the weak limit of the kernel $K_n(x,y;t)$ of

$$(\exp -tB/2n\ \exp -tA/n\ \exp -tB/2n)^n$$

(with $A = -\frac{1}{2}\Delta$, $B = \frac{1}{2}x^2 - \frac{1}{2}$) which can be immediatly seen as log-quadratic.

5 Basic facts in spectral theory and on the Schrödinger operator

We summarize without proof the properties which are needed in spectral theory for the comprehension of these lectures with a particular emphasis on the Schrödinger operator. There are many books where this material is presented [CFKS87], [He84], [Hu], [ReSi72], [ReSi75], [Ro87]... to mention some.
We illustrate the theory by a careful study of the harmonic oscillator and of the Schrödinger operator with a Coulomb potential.

5.1 Selfadjoint operators, spectrum and spectral decomposition

We consider an Hilbert space $\mathcal{H}$ and a dense vector subspace $\mathcal{H}_0$ of $\mathcal{H}$. An unbounded operator L is determined by a given domain $D(L) = \mathcal{H}_0$ and by an operator mapping $\mathcal{H}_0$ into $\mathcal{H}$.
The operator is called **closed** if the graph of L is closed in $\mathcal{H} \times \mathcal{H}$.
The operator is called **closable** if the closure of the graph is a graph.
We can then define the closure of the operator by a limit procedure.
If $\mathcal{H}_0 = \mathcal{H}$, the closed graph Theorem says that a closed operator L is continuous.
We shall say that $L : \mathcal{H}_0 \mapsto \mathcal{H}$ is **symmetric** if it satisfies

$$\langle Lu, v\rangle_{\mathcal{H}} = \langle u, Lv\rangle_{\mathcal{H}}\ , \forall u, v\ \in \mathcal{H}_0\ .$$

It is easy to see that a symmetric operator is closable.
Let us now recall the definition of the adjoint of an unbounded operator. If L is an unbounded operator whose domain $D(L)$ is dense in $\mathcal{H}$, we define L^* by

$$\begin{aligned} D(L^*) \ &= \{u \in \mathcal{H}, D(L) \ni v \mapsto \langle u, Lv\rangle, \\ &\quad \text{can be extended as an antilinear continuous form on } \mathcal{H}\}\ . \end{aligned}$$

Using the Riesz Theorem, there exists $f \in \mathcal{H}$ such that

$$(f, v) = (u, Lv)\ ,\ \forall u \in D(L^*), v \in D(L)$$

and we can then define L^* by

$$L^* u = f \ .$$

It is then easy to see that L^* is a closed operator. If L is symmetric it is easy to see that

$$D(L) \subset D(L^*)$$

and that

$$Lu = L^* u \ , \ \forall u \in D(L) \ .$$

We say in this case that $(L^*, D(L^*))$ is an extension of $(L, D(L))$.
We shall say that L is **selfadjoint** if $L^* = L$, i. e.

$$D(L) = D(L^*) \ , \ \text{ and } \ Lu = L^* u \ , \quad \forall u \in D(L) \ .$$

For a symmetric operator, we have consequently two natural closed extensions:

- The **minimal** one denoted by L_{min} which is obtained by taking the closure of the graph of L,
- The **maximal** one denoted by L_{max} the adjoint of L.

If L^{sa} is a selfadjoint extension of L, then L^{sa} is automatically an extension of L_{min} and admits as an extension L_{max}. A natural way to verify the uniqueness of the selfadjoint extension (see Subsection 5.3) is to prove the equality between L_{min} and L_{max}.
Once we have a selfadjoint operator we can apply the following basic spectral decomposition lemma (see for example K.Yosida, Functional Analysis p.309-316, D.Huet [Hu]).

Definition 5.1.1 *:*
A family of projectors $E(\lambda)$, $-\infty < \lambda < \infty$ in an Hilbert space $\mathcal{H}$ is called a resolution of the identity if it satisfies:

$$E(\lambda)E(\mu) = E(\min(\lambda, \mu)) \ , \tag{5.1.1}$$

$$E(-\infty) = 0, E(+\infty) = I, \tag{5.1.2}$$

where $E(\pm\infty)$ *is defined* [13] *by*

$$E(\pm\infty)x = \lim_{\lambda\to\pm\infty} E(\lambda)x$$

for all x *in* $\mathcal{H}$.

$$E(\lambda+0) = E(\lambda)\ , \tag{5.1.3}$$

where $E(\lambda+0)$ *is defined by*

$$E(\lambda+0)x = \lim_{\mu\to\lambda\ ,\ \mu>\lambda} E(\mu)x\ .$$

We now observe that for all x and y in $\mathcal{H}$ the function $\lambda \mapsto \langle E(\lambda)x, y\rangle$ is with bounded variation and one can then show the existence of $E(\lambda+0)$ and $E(\lambda-0)$. It is then classical (Stieltjes integrals) that one can define for any continuous complex valued function $\lambda \mapsto f(\lambda)$ the integrals $\int_a^b f(\lambda)d\langle E(\lambda)x, y\rangle$ as a limit of Riemann sums. The theory works more generally for any borelian function. We can then define an unbounded operator L_f whose domain is defined by

$$D(L_f) = \{x \in \mathcal{H}, \int_{-\infty}^{+\infty} |f(\lambda)|^2\ d\langle E(\lambda)x, y\rangle\ <\ \infty\ ,\ \forall y \in \mathcal{H}\}$$

and

$$\langle L_f x, y\rangle\ =\ \int_{-\infty}^{+\infty} f(\lambda)d\langle E(\lambda)x, y\rangle$$

for all x in $D(L_f)$ and y in $\mathcal{H}$.

We observe that for $f_0 = 1$ we have $L_{f_0} = I$ and for $f_1(\lambda) = \lambda$, we obtain a selfadjoint operator $L_{f_1} := L$.
In this case we say that

$$L = \int_{-\infty}^{+\infty} \lambda\ dE(\lambda)$$

is a spectral decomposition of L and we shall note that

$$||Lx||^2 = \int_{-\infty}^{+\infty} \lambda^2 d\,\langle E(\lambda)x, x\rangle\ =\ \int_{-\infty}^{+\infty} \lambda^2 d\,||E(\lambda)x||^2\ ,$$

[13] (5.1.1) gives the existence of the limit.

for $x \in D(L)$.
More generally

$$||L_f x||^2 = \int_{-\infty}^{+\infty} |f(\lambda)|^2 d((E(\lambda)x, x)) = \int_{-\infty}^{+\infty} |f(\lambda)|^2 d(||E(\lambda)x||^2)$$

for $x \in D(L_f)$.

The spectral decomposition theorem explicits that the preceding situation is the general one

Theorem 5.1.2 *:*
Any selfadjoint operator L in an Hilbert space $\mathcal{H}$ admits a spectral decomposition.

We now recall that the spectrum of a closed operator L is defined as the complementary set [14] of the set of the $\lambda \in \mathbb{C}$ such that $(L - \lambda)$ is invertible from $D(L)$ onto$\mathcal{H}$ and admits a continuous inverse.
The spectrum $\sigma(L)$ is closed in $\mathbb{C}$ and real if L is selfadjoint. Note the following characterization[15]

Proposition 5.1.3 *:*

$$\sigma(L) = \{\lambda \in \mathbb{R},\ s.t.\ \forall \epsilon > 0, E(]\lambda - \epsilon, \lambda + \epsilon[) \neq 0\}$$

Applications of the spectral theorem:

One of the first applications of the spectral theorem is the following property which plays a crucial role

Proposition 5.1.4 *:*

$$d(\lambda, \sigma(L))||x|| \leq ||(L - \lambda)x|| \ , \tag{5.1.4}$$

for all x in $D(L)$.

[14] The complementary of the spectrum of an unbounded L is usually called the resolvent set. It is more precisely described as the set of the λ in $\mathbb{C}$ such that the range of $(L - \lambda)$ is dense in $\mathcal{H}$ and such that $(L - \lambda)$ admits a continuous inverse from Im $(L - \lambda)$ into $D(L)$. If L is closed this implies that Im $(L - \lambda) = H$. (See the discussion in Yosida p.209)

[15] cf appendix 2 in the book of D.Robert [Ro87],

This theorem is frequently used in the following context. It is usually difficult to get explicitely the values of the eigenvalues of an operator. One consequently tries to localize these eigenvalues by using approximations. Let us suppose for example that one has found λ_0 and y in $D(L)$ such that

$$||(L-\lambda_0)y|| \leq \epsilon \tag{5.1.5}$$

and $||y|| = 1$ then we deduce the existence of λ in the spectrum of L such that $|\lambda - \lambda_0| \leq \epsilon$.
Standard examples are the case of hermitian matrices or the case of the anharmonic oscillator $L := -h^2 \frac{d^2}{dx^2} + x^2 + x^4$. In the second case the first eigenfunction of the harmonic oscillator $-h^2 \frac{d^2}{dx^2}$ can be used as y in (5.1.5) with $\lambda_0 = h$. We then find (5.1.5) with $\epsilon = \mathcal{O}(h^2)$.
Another application is, using the property that the spectrum is real, the following inequality

$$|\operatorname{Im} \lambda| ||x|| \leq ||(L-\lambda)x|| \tag{5.1.6}$$

and this gives an upper bound on the norm of $(L-\lambda)^{-1}$ in $\mathcal{L}(\mathcal{H})$ by $1/|\operatorname{Im} \lambda|$.

Examples of functions of a selfadjoint operator :

We shall for example meet usually in spectral theory the functions

1. f is the characteristic function of $]-\infty, \lambda]$, $Y_{]-\infty,\lambda]}$; $f(L)$ is then $L_{Y_{]-\infty,\lambda]}} = E(\lambda)$.

2. f is the characteristic function of $]-\infty, \lambda[$, $Y_{]-\infty,\lambda[}$; $f(L)$ is then $L_{Y_{]-\infty,\lambda[}} = E(\lambda - 0)$.

3. f is a compactly supported continuous function. $f(L)$ will be an operator whose spectrum is localized in the support of f.

4. $f_t(\lambda) = \exp(it\lambda)$ with t real.
   $f_t(L)$ is then a solution of the functional equation

$$\begin{array}{ll} (\partial_t - iL)(f(t,L)) & = 0 \\ f(0,L) & = Id \end{array}$$

   We note here that, for all real t, $f_t(L) = \exp(itL)$ is a bounded unitary operator .

5. $g_t(\lambda) = \exp(-t\lambda)$ with t real positive. $g_t(L)$ is then a solution of the functional equation

$$\begin{array}{ll} (\partial_t + L)(g(t,L)) & = 0 \ , \text{ for } t \leq 0 \\ g(0,L) & = Id \ . \end{array}$$

Compact operators:

Operators with compact resolvent:
We know that, if the operator L (which will be assumed left semi-bounded) is with compact resolvent, then its spectrum is a sequence of eigenvalues λ_j tending to ∞ (each eigenvalue being with finite multiplicity). There are two conventions for the notation of the eigenvalues. The first one is to classify them into an increasing sequence

$$\lambda_j \leq \lambda_{j+1}$$

counting each eigenvalue according to its multiplicity. The second one is to describe them as a strictly increasing sequence μ_k with μ_k eigenvalue of multiplicity m_k.

Examples :

1. The Dirichlet problem in an open bounded set Ω.
   One can for example explicitely compute the spectrum of the Dirichlet realization of a Laplacian in a square.

2. Laplace Beltrami operators on a Riemannian manifolds (See [BGM]).
   The simplest model is the operator $-d^2/d\theta^2$ on the circle of radius one whose spectrum is $\{(2\pi n^2 \ , \ n \in I\!N\}$. For $n > 0$ the multiplicity is 2. An orthonormal basis is given by the functions $\theta \mapsto (2\pi)^{-\frac{1}{2}} \exp in\theta$ for $n \in Z\!\!Z$.

3. The harmonic oscillator on $I\!R^n$.
   In this case we have already given a description of the eigenvalues and of the corresponding eigenvectors.

For the description of the spectral decomposition, it is better to take the second convention but we shall most of the time use the first one.
If Π_{μ_k} denotes the projector on the spectral space attached to the eigenvalue μ_k of dimension m_k, one can then describe $E(\lambda)$ as

$$\sum_{\mu_k \leq \lambda} \Pi_{\mu_k} \ .$$

The measure $d\langle E(\lambda)x, y\rangle$ is then equal to

$$d\langle E(\lambda)x, y\rangle = \sum_k \delta(\lambda - \mu_k) \cdot \Pi_{\mu_k}$$

We can also write $f(L)$ as

$$f(L) = \sum_k f(\mu_k) \cdot \Pi_{\mu_k} \ .$$

The other case to understand for the beginner is of course the case of the free Laplacian $-\Delta$ on $I\!R^n$.
Another interest of the spectral theorem is to permit the study of the different properties of the spectrum according to the nature of the spectral measure (using the natural decomposition of the measure (Radon Nikodym Theorem)) and this leads to the definition of the continuous spectrum and of the pure point spectrum. Let us also observe that the spectrum corresponds to the support of the spectral measure $d\,E(\lambda)$.

5.2 Discrete spectrum, essential spectrum

We have already recalled in Proposition 5.1.3 a characterization of the spectrum. Let us now complete this characterization by introducing different spectra.

Definition 5.2.1 *:*
If L is a selfadjoint operator, we shall call discrete spectrum of L the set

$$\sigma_{disc}(L) = \{\lambda \in \sigma(L) s.t. \exists \epsilon > 0, \dim range\,(E(]\lambda - \epsilon, \lambda + \epsilon[)) < +\infty\} \ .$$

With this new definition, we get the following:
For a selfadjoint operator with compact resolvent, the spectrum is reduced

to the discrete spectrum.
Equivalently, we shall observe that λ is in the discrete spectrum iff λ is an isolated point in $\sigma(L)$ and if λ is an eigenvalue of finite multiplicity.

Definition 5.2.2 :
The essential spectrum is by definition the complementary of the discrete spectrum.

Intuitively, a point of the essential spectrum corresponds

- either to a point in the continuous spectrum,
- or to a limit point of a sequence of eigenvalues with finite multiplicity,
- or to an eigenvalue of infinite multiplicity.

Basic examples:

1. The Laplacian on $I\!R^n$ $-\Delta$ is a selfadjoint operator on $L^2(I\!R^n)$ whose domain is the Sobolev space $H^2(I\!R^n)$. The spectrum is continuous and equal to $\overline{I\!R^+}$. The essential spectrum is also $\overline{I\!R^+}$ and the operator has no discrete spectrum.

2. The Schrödinger operator with constant magnetic field in $I\!R^2$:
$$(D_{x_1} - \frac{Bx_2}{2})^2 + (D_{x_2} + \frac{Bx_1}{2})^2 \,,$$
with
$$D_{x_j} := \frac{1}{i}\partial_{x_j} = \frac{1}{i}\frac{\partial}{\partial x_j}\,.$$
The spectrum is formed with eigenvalues $(2k+1)|B|$ but the spectrum is not discrete because each eigenvalue is with infinite multiplicity.

It is clear that the essential spectrum is a closed set. In order to determine the essential spectrum it is useful to have theorems proving the invariance by perturbation. The following characterization is in this spirit quite useful.

Theorem 5.2.3 :
Let L be a selfadjoint operator. Then λ belongs to the essential spectrum iff there exists a sequence u_n in $D(L)$ with $||u_n|| = 1$ such that u_n tends weakly to 0 and such that $||(L-\lambda)u_n|| \to 0$ as $n \to \infty$.

Example 5.2.4 *:*
The operator $-h^2\Delta + V$ with V tending to 0 as $|x| \to \infty$ ($x \in I\!R^D$) has $\bar{I\!R}^+$ as essential spectrum.

For proving the inclusion of $\bar{I\!R}^+$ in the essential spectrum, we can indeed consider the sequence

$$u_n(x) = \exp(ix.\xi) n^{-(D/2)}.\chi((x - R_n)/n)$$

with $\chi \geq 0$ and supported in the ball $B(0,1)$ and equal to one on say $B(0, \frac{1}{2})$. The sequence R_n is chosen such that $|R_n|$ tends to ∞ and such that the support of the u_n are disjoints.
The converse can be obtained by abstract analysis and the fact that we know the essential spectrum of $-\Delta$.
Another way to localize the essential spectrum is to use the relative compacity. If L is a closed operator with a dense domain D_L, we shall say that the operator V is relatively compact with respect to L or L-compact if $D_V \subset D_L$ and if the image by V of a closed ball in D_L (for the graph-norm $u \mapsto \sqrt{||u||^2 + ||Lu||^2}$) is relatively compact in $\mathcal{H}$.
In other words, we shall say that V is L-compact, if , from each sequence u_n in D_L bounded in $\mathcal{H}$ and such that Lu_n is bounded in $\mathcal{H}$, one can extract a subsequence u_{n_i} such that Vu_{n_i} is convergent in $\mathcal{H}$. The Weyl's Theorem says

Theorem 5.2.5 *:*
Let L be a selfadjoint operator, and V be symmetric and L-compact, then $L + V$ is selfadjoint and the essential spectrum of $L + V$ is equal to the essential spectrum of L.

The first part will be discussed in the next subsection. For the second part we can use the preceding criterion.

5.3 Essentially selfadjoint operators

In most of the examples we have met, the abstract operators are associated with differential operators. These differential operators are naturally defined on $C_0^\infty(\Omega)$ or $\mathcal{D}'(\Omega)$. Most of the time (for suitable potentials increasing slowly at ∞) they are also defined (when $\Omega = I\!R^m$) on $\mathcal{S}(I\!R^m)$ or $\mathcal{S}'(I\!R^m)$.

It is important to understand how the abstract point of view can be related to the PDE point of view. The theory of the essential selfadjointness gives a clear understanding of the problem. The question is to decide if, starting from a symmetric operator L , whose domain $D(L)=\mathcal{H}_0$ is dense in $\mathcal{H}$, there exists a unique selfadjoint extension L^{ext} of L (that is $D(L)\subset D(L^{ext})$ and $L^{ext}u = Lu$, $\forall u\in D(L)$). This leads to

Definition 5.3.1 *:*
A symmetric operator L with domain $\mathcal{H}_0$ is called essentially selfadjoint if it admits a unique selfadjoint extension as unbounded operator on $\mathcal{H}$.

Examples:

1. The differential operator $-\Delta$ with domain $\mathcal{H}_0 = C_0^\infty(\mathbb{R}^m)$ is essentially selfadjoint and admits consequently a unique selfadjoint extension L^{ext} whose domain is the Sobolev space $H^2(\mathbb{R}^m)$. L^{ext} is simply defined as
$$L^{ext}u = -\Delta u\ ,\ \forall u \in H^2$$
where the r.h.s is defined in the sense of the distribution theory.

2. The differential operators $-\Delta + |x|^2$ with domain $\mathcal{H}_0 = C_0^\infty(\mathbb{R}^m)$ or $H_1 = \mathcal{S}(\mathbb{R}^m)$ are essentially selfadjoint and admit consequently a unique selfadjoint extension. This extension is the same for the two operators. The domain can be explicitely described as
$$\begin{aligned}&B^2(\mathbb{R}^m) = \\ &\quad \{u\in L^2(\mathbb{R}^m)\mid x^\alpha D_x^\beta u \in L^2(\mathbb{R}^m)\ ,\ \forall \alpha,\beta\in \mathbb{N}^m \text{ with } |\alpha|+|\beta|\leq 2\}\ .\end{aligned}$$

3. The differential operator $-\Delta$ with domain $C_0^\infty(\Omega)$ (where Ω is an open bounded set with smooth boundary) is not essentially selfadjoint. There exists a lot of selfadjoint extensions related to the choice of a boundary problem. We just mention here
   - the Dirichlet realization whose domain is $H_0^1(\Omega)\cap H^2(\Omega)$ (where H_0^1 is the closure [16] of $C_0^\infty(\Omega)$ in $H^1(\Omega)$),

[16] We recall that if $u\in H^1(\Omega)$ the restriction of u to $\partial\Omega$ is well defined and belongs to the Sobolev space $H^{\frac{1}{2}}(\partial\Omega)$. The space $H_0^1(\Omega)$ can also be characterized as $H_0^1(\Omega)=\{u\in H^1(\Omega)\ s.t.\ u_{/\partial\Omega}=0\}$.

- the Neumann realization whose domain[17] is $\{u \in H^2(\Omega) \mid (\partial u/\partial \nu)_{/\partial\Omega} = 0\}$

4. The Laplace Beltrami operator on a compact manifold M with domain $C^\infty(M)$ is essentially selfadjoint on $L^2(M)$. The domain of the selfadjoint extension can be described as $H^2(M)$ (which can be described using local charts).

We now give some criteria in order to verify that an operator is essentially selfadjoint. As already mentioned, one can prove essential selfadjointness by proving that the minimal closed extension coincides with the maximal closed extension:

$$L_{min} = L_{max} \; .$$

Here we recall that the minimal extension of a symmetric operator L of domain $\mathcal{H}_0$ is the operator L_{min} whose graph is the closure of the graph of L. L_{max} can be seen as the adjoint operator L^*.
The second criterion is to establish the injectivity of $L_{max} \pm i$. We shall see in the next subsection how to apply it in simple cases. A more sophisticated criterion is the following

Lemma 5.3.2 *:*
Let $L : \mathcal{H}_0 \mapsto \mathcal{H}$ a symmetric operator, whose associate minimal operator is L_{min}. Then L is essentially selfadjoint iff there exists $t \in I\!R$, $t > 0$ and for linear operators $B_\pm$, $R_\pm$ such that:

- *(i) $B_\pm$ maps $\mathcal{H}_0$ into $D(L_{min})$,*
- *(ii) $R_\pm \in \mathcal{L}(\mathcal{H})$ and $||R_\pm||_{\mathcal{L}(\mathcal{H})} < 1$,*
- *(iii) $(L_{min} \pm it)B_\pm = Id + R_\pm$.*

Remark 5.3.3 *:*
In the case when L is semibounded it is sufficient to consider $(L_{min} + t)$ for some large enough $t > 0$.

The theory of pseudodifferential operators[18] is very well adapted to the verification of this criterion. This theory permits indeed to construct pseudo-inverses or parametrices.

[17] We recall that if $u \in H^2(\Omega)$ the restriction of $\partial u/\partial \nu$ to $\partial\Omega$ is well defined and belongs to the Sobolev space $H^{\frac{1}{2}}(\partial\Omega)$.

[18] See for example [He84] for a detailed presentation of this approach.

5.4 Examples

5.4.1 The free Laplacian

In this spirit let us treat first $L_0 = -\Delta$ with domain $\mathcal{H}_0 = C_0^\infty(I\!R^m)$. It is immediate to verify that $-\Delta$ is symmetric (we say also formally selfadjoint) and we recall that $C_0^\infty(I\!R^m)$ is dense in $\mathcal{H} = L^2(I\!R^m)$. The domain of the smallest closed extension appears as the subset of the u's in $L^2(I\!R^m)$ such that there exists a sequence $u_j \in C_0^\infty(I\!R^m)$ such that $u_j \to u$ in L^2 and such that $-\Delta u_j$ converges in L^2. We then define $L_{min}u$ as $\lim_{j\to\infty} -\Delta u_j$. The theory of distributions says actually that $L_{min}u = -\Delta u$ in the sense of the distribution theory.
The adjoint $L^* = L_{max}$ (which is also equal to L_{min}^*) is by definition the operator whose domain is

$$D(L_{max}) = \{u \in L^2(I\!R^m) \mid -\Delta u \in L^2(I\!R^m)\}$$

and which is defined by

$$D(L_{max}) \ni u \mapsto -\Delta u \ .$$

Here we have used the Riesz Theorem, characterizing the dual of L^2. It is clear that $L_{min} = L_{max}$ using easy Fourier analysis. It is sufficient indeed to prove a result of density, that is to prove that if $\{u \in L^2 \ , \ -\Delta u \in L^2\}$ then there exists a sequence u_j in C_0^∞ such that $u_j \to u$ in L^2 and such that $-\Delta u_j$ converges in L^2. If one first recognizes $D(L_{max})$ as H^2 (which is immediate via Fourier), this is simply a consequence of the density of $C_0^\infty(I\!R^m)$ in $H^2(I\!R^m)$.
Of course this example is in some sense too simple for seeing really the problems which may occur.

5.4.2 The Schrödinger operator with Coulomb potential

We now consider $L_0 = -\Delta - \frac{1}{r}$ a priori defined on $C_0^\infty(I\!R^3)$. This is well defined because $\frac{1}{r}$ belongs to $L^2_{loc}(I\!R^3)$. The proof of the essential selfadjointness is based on the application of Lemma 5.3.2.
We first observe a Sobolev type inequality.

Lemma 5.4.1 *:*
There exists a constant C such that for all $u \in H^2(I\!R^3)$, all $a > 0$ and all $x \in I\!R^3$, we have

$$|u(x)| \leq C(a||\Delta u||_0 + a^{-3}||u||_0) \ .$$

(Prove first the inequality for all u with $x = 0$ and $a = 1$, then use translation and dilation.)
In the second step, we show that the potential $V = -\frac{1}{r}$ is a perturbation of the Laplacian.
There exists indeed a constant C such that for all $u \in H^2(I\!R^3)$ and all $b > 0$, we have

$$||Vu||_0 \leq C(b||\Delta u||_0 + b^{-1}||u||_0) \ .$$

For this proof we observe that, for any $R > 0$,

$$\int V(x)|u(x)|^2 dx = \int_{|x|\leq R} V(x)|u(x)|^2 dx + \int_{|x|\geq R} V(x)|u(x)|^2 dx \ ,$$

and treat the first term of the left hand side using the Sobolev's type inequality and the second term by the trivial estimate $|V(x)| \leq \frac{1}{R}$.

In order to apply Lemma 5.3.2, we can take as approximate inverse $B_t = (-\Delta + t)^{-1}$ with $t > 0$ large enough. We have also obtained in this proof that the domain of the selfadjoint extension is $H^2(I\!R^3)$.
This example is typical of the case when V can be considered as a perturbation of the Laplacian. We have followed in a particular case the proof of a general theorem due to Kato-Rellich.

Theorem 5.4.2 *:*
Let A be a selfadjoint operator, B be a symmetric operator whose domain contains $D(A)$. Let us assume the existence of a and b such that $0 \leq a < 1$ and $b \geq 0$ such that

$$||B\phi|| \leq a\,||A\phi|| + b\,||\phi||$$

for all $\phi \in D(A)$. Then $A + B$ is selfadjoint on $D(A)$. If A is essentially selfadjoint on $D \subset D(A)$, then $A + B$ has the same property.

But other cases are interesting and not contained in the preceding theory like the harmonic oscillator. We shall consider it in the next subsection.

5.4.3 The harmonic oscillator revisited

Before to treat this example, let us first recall a quite general theorem due to Kato.

Theorem 5.4.3 *:*
Let V in $L^2_{loc}(I\!R^m)$ such that $V \geq 0$ almost everywhere on $I\!R^m$. Then $-\Delta+V$ with domain $C_0^\infty(I\!R^m)$ is essentially selfadjoint.

We now consider the case $V = |x|^2$. Of course the above criterion can be applied. A pseudodifferential proof [19] can also be given which will give that the domain of the operator is

$$B^2(I\!R^m) = \{u \in L^2(I\!R^m) \mid x^\alpha D_x^\beta u \in L^2(I\!R^m), \forall (\alpha, \beta) \text{ with } |\alpha| + |\beta| \leq 2 \} \,.$$

Let us sketch, a more elementary proof. Following the scheme of the proof given for the free Laplacian, it is sufficient to prove that if $u \in L^2$ and $(-\Delta+V)u \in L^2$ then $u \in B^2$ and we then use the well known density of C_0^∞ in B^2.
We first remark that the local regularity theorems concerning elliptic operators give that $u \in H^2_{loc}$. We then obtain for a suitable cutoff sequence χ_n

$$\mathrm{Re}\,((-\Delta+V)u, \chi_n u) = \int \chi_n |\nabla u|^2 dx + \int V \cdot \chi_n |u|^2 dx - \frac{1}{2} \int (\Delta \chi_n)|u|^2 \,.$$

This gives that $u \in B^1$ and a meaning to

$$\mathrm{Re}\,((-\Delta+V)u, u) = \int |\nabla u|^2 dx + \int V \cdot |u|^2 dx \,.$$

In order to get the regularity in B^2 we can use the method of the differential quotients, that is apply the inequality to the family $\frac{(\tau_{he_j}-I)}{h} u$ (where τ_{he_j} is the translation by he_j with e_j, $j-$th vector of an orthonormal basis in $I\!R^m$) and to the family $\frac{\exp ih x_j - 1}{h} u$

[19]Let us consider the harmonic oscillator as a pseudodifferential operator $p(x, D_x)$ whose symbol is $p(x,\xi) = \xi^2 + x^2$. Consider the pseudodifferential operator $q(x, D_x)$ whose symbol is

$$q(x,\xi) = 1/(x^2 + \xi^2 + 1)$$

Then

$$q(x,D) \circ p(x,D) = Id + r(x,D)$$

and $r(x,D)$ and $q(x,D)$ can be seen as continuous from B^k into B^{k+2} for any k.

Remark 5.4.4 :
What is said here for the harmonic oscillator can be extended to C^∞ potentials V satisfying in $I\!R^m$

$$V(x) \geq \frac{1}{C}|x|^2 - C \;,$$

for some constant $C > 0$, and

$$|D_x^\alpha V(x)| \leq C_\alpha \langle x \rangle^{(2-|\alpha|)_+} \;.$$

5.5 The minimax principle

We first recall the following general theorem [20]

Theorem 5.5.1 :
A symmetric semibounded operator admits a selfadjoint extension.

Example 5.5.2 :
The realization of the Dirichlet problem for the Laplacian in an open set Ω is obtained by this way. In the case of the Schrödinger operator with a bounded from below C^∞ potential on $\bar{\Omega}$, the domain D of the extension will be described as

$$D = \{u \in H_0^1(\Omega) \;,\; (V+C)^{\frac{1}{2}} u \in L^2 \;\; and \;\; (-\Delta + V)u \in L^2\} \;.$$

They are many cases where one can prove a regularity theorem giving that if $u \in D$ then $-\Delta u \in L^2$ and $Vu \in L^2$.

We now give two criteria for the determination of the bottom of the spectrum (see Reed-Simon Tome 3, [ReSi]) and for the bottom of the essential spectrum.

Theorem 5.5.3 :
Let A be a selfadjoint semibounded operator and $Q(A)$ its form domain [21] . *Let us introduce*

$$e\mu_n(A) = \max_{\psi_1, \psi_2, \ldots, \psi_{n-1}} \; \min_{\left\{ \begin{array}{l} \phi \in [span(\psi_1, \ldots, \psi_{n-1})]^\perp ; \\ \phi \in Q(A) \;\; and \;\; ||\phi|| = 1 \end{array} \right\}} \langle A\phi \mid \phi \rangle \;.$$

[20] See for example Yosida [Yos] p.317.

[21] associated by completion with the form $u \mapsto \langle u | Au \rangle$

Then either
(a) $\mu_n(A)$ is the n-th eigenvalue when ordering the eigenvalues in increasing order (and counting the multiplicity) and A has a discrete spectrum in $]-\infty, \mu_n(A)[$
or
(b) $\mu_n(A)$ corresponds to the bottom of the essential spectrum.

Remarks

- It is very often useful to apply the minimax by taking the " min" over a dense set in $Q(A)$.
- For the first eigenvalue the criterion gives
$$\mu_1(A) = \inf_{\phi \in Q(A) \text{ and } ||\phi||=1} \langle A\phi \mid \phi \rangle \, .$$
- The mini-max principle permits to control the continuity of the eigenvalues with respect to parameters.
- The mini-max permits to give an upperbound on the bottom of the spectrum and the comparison between the spectrum of two operators.

The essential spectrum:

Criteria in the case of the Schrödinger operator are given for example in the book of Agmon [Ag]. We have for example the following result

Theorem 5.5.4 *:*
Let us consider a Schrödinger operator $P = -\Delta + V$ with V C^0 and semibounded. Then the bottom of the essential spectrum is characterized as
$$\inf \sigma^{ess}(P) = \sup_{K \in \mathcal{K}} \inf_{\{\phi \in C_0^\infty(I\!\!R^m \setminus K), ||\phi||=1\}} \langle P\phi \mid \phi \rangle \, ,$$
where $\mathcal{K}$ is the set of the compacts of $I\!\!R^m$.

Remark 5.5.5 *:*
This gives in particular that the spectrum of the Schrödinger operator is discrete in $]-\infty, \inf \lim_{|x|\to\infty} V(x)[$. The mini-max principle gives also immediately
$$\sigma(P) \subset [\inf V, +\infty[\, . \tag{5.5.1}$$

5.6 Compactness

We have already discussed the notion of compactness in the preceeding section. We recall that an operator T is compact if the range of the unit ball B of $\mathcal{H}$ by T is relatively compact in $\mathcal{H}$. In the Hilbertian context, another characterization is that T is compact if from each weakly convergent sequence $x_n \in \mathcal{H}$ one can extract a subsequence such that Tx_{n_i} is strongly convergent. We shall denote by $\mathcal{C}(\mathcal{H})$ the subspace of the compact operators.
Let us recall the following properties

- If $T \in \mathcal{C}(\mathcal{H})$ and $A \in \mathcal{L}(\mathcal{H})$, then $TA \in \mathcal{C}(\mathcal{H})$ and $TA \in \mathcal{C}(\mathcal{H})$.
- If $T \in \mathcal{C}(\mathcal{H}))$, then $T^* \in \mathcal{C}(\mathcal{H})$.

There are stronger subclasses of compact operators which can be useful like Hilbert-schmidt and Trace-class operators. We refer to Reed-Simon [ReSi78], Robert [Ro87] or to [GlJa87] (Appendix A.3, p. 132).
We just recall some criteria of compactness for the resolvent of the Schrödinger operator. In the case of the Schrödinger equation on $I\!R^m$ and if V is C^∞ and bounded from below, the domain of the selfadjoint extension is always contained in the form domain that is

$$Q(P) := H^1_V(I\!R^m) = \{u \in H^1(I\!R^m) | (V + C)^{\frac{1}{2}} u \in L^2(I\!R^m)\} \,.$$

It is then easy to see that if V tends to ∞ then the injection of H^1_V in L^2 is compact (use a criterion of precompactness). We then obtain that the resolvent $(P + \lambda)^{-1}$ is compact for $\lambda \notin \sigma(P)$.
In the case of a compact manifold M and if we consider the Laplace-Beltrami operator on M (see Berger-Gauduchon-Mazet [BGM]), then the compactness of the resolvent is obtain without additional assumption on V. The domain of the operator is $H^2(M)$ and we have compact injection from $H^2(M)$ into $L^2(M)$.
The condition that $V \to \infty$ as $|x| \to \infty$ is not a necessary condition. The Schrödinger operator on $I\!R^2$: $-\Delta + x^2 \cdot y^2$ is with compact resolvent.

5.7 Comparison between closed subspaces in an Hilbert space

We have given in the presentation of the spectral representation of a selfadjoint a lemma permitting to deduce from the existence of an approximate

solution attached to an approximate eigenvalue the presence of spectrum in a measured neighborhood of this approximate eigenvalue. We present here a more precise result which appears to be quite useful, for example in the comparison of the approximate eigenspace and of the actual eigenspece. We first introduce a notion of distance between closed subspaces of an Hilbert space.
Let E an F be closed subspaces in a Hilbert space $\mathcal{H}$. Let Π_E and Π_F the corresponding orthogonal projection on E and F respectively. We then define the non-symmetric distance $\vec{d}(E,F)$ as

$$\vec{d}(E,F) = ||\Pi_E - \Pi_F\Pi_E|| = ||\Pi_E - \Pi_E\Pi_F|| \,. \tag{5.7.1}$$

Note that

$$\vec{d}(E,F) = 0 \text{ iff } E \subset F \,. \tag{5.7.2}$$

Note also that if $\vec{d}(E,F) \leq \epsilon$ and if $u \in E$ then

$$||u - \Pi_F u|| \leq \epsilon ||u|| \,,$$

and this expresses the property that u is then near a vector in F.
We observe now that a triangular inequality is satisfied

$$\vec{d}(E,G) \leq \vec{d}(E,F) + \vec{d}(F,G) \,,$$

if G is a third closed space of $\mathcal{H}$.
We have also the following property that if $\vec{d}(E,F) < 1$ then Π_F/E which maps E into F is injective and Π_E/F has a continuous right inverse.
In the case when $\vec{d}(E,F) < 1$ and $\vec{d}(F,E) < 1$, then Π_F/E and Π_E/F are bijective with continuous inverse. Moreover we have in this case $\vec{d}(E,F) = \vec{d}(F,E)$.
The following result is quite useful in order to compare different spectra of selfadjoint operators

Proposition 5.7.1 *:*
Let A be a selfadjoint operator in a Hilbert space $\mathcal{H}$. Let $I \subset I\!R$ be a compact interval, $\Psi_1, \cdots, \Psi_N$, N independent vectors in $D(A)$ and $\mu_1, \cdots, \mu_N$ such that

$$A\Psi_j = \mu_j \Psi_j + r_j \,, \tag{5.7.3}$$

with

$$||r_j|| \leq \epsilon \ .$$

Let $a > 0$ and assume that $\sigma(A) \cap (I + B(0, 2a) \setminus I) = \emptyset$.
Then if E is the space spanned by $\Psi_1, \cdots, \Psi_N$ and if F is the space associated to $\sigma(A) \cap I$, we have

$$\vec{d}(E, F) \leq \frac{N^{\frac{1}{2}} \ \epsilon}{a \, (\lambda_{min}(S))^{\frac{1}{2}}} \ , \tag{5.7.4}$$

where $\lambda_{min}(S)$ is the smallest eigenvalue of the Gram matrix

$$S = (\langle \Psi_j | \Psi_k \rangle) \ .$$

Remark 5.7.2 *:*
If we know by other means that $\sigma(A) \cap I$ is discrete of finite multplicity and if the r.h.s of (5.7.4) is strictly smaller than 1, then we conclude that F is at least of dimension N and consequently that A has at least N eigenvalues in I.

6 Thermodynamic Limit

6.1 Introduction

If the potential $V^{(m)}$ on $\mathbb{R}^m$ is a sum

$$V(x) = \sum_{j=1}^{m} v(x_j)$$

then it is immediate to see that the first eigenvalue $\lambda_1(m)$ of the Schrödinger operator $-\Delta + V^{(m)}(x)$ divided by m is constant and equal to $\lambda_1(1)$.
Similarly the logarithm of the Laplace integral $\ln \int \exp -V^{(m)}(x)dx$ divided by m is constant and equal to $\ln \int \exp -V^{(1)}(x)dx$. It is natural to ask if this property remains true asymptotically as $m \to +\infty$, when some interaction like $\sum_j w(x_j, x_{j+1})$ is added. This is the object of this section to present simple results of this type. We refer to the books by Ruelle [Ru69] or Ellis [El85] for general references on this subject. Finally, we mention that a similar result can be obtained for the transfer operator by considering the limit of $\frac{\ln \mu_1(m)}{m}$ as $m \to +\infty$. Under the same assumptions as for the Schrödinger case, it is possible [He93b] to prove the existence of the thermodynamic limit. This will not be detailed in these notes.

6.2 The crucial lemma

Lemma 6.2.1 *:*
Let C be some fixed constant ($C \geq 0$). Let $\lambda(m)$ ($m \in \mathbb{N}^*$) be a sequence of real numbers such that

$$|\lambda(m+p) - \lambda(m) - \lambda(p)| \leq C \ , \ \forall m, p \ , \tag{6.2.1}$$

then the limit of the sequence $\lambda(m)/m$ exists and :

$$|(\lambda(m)/m) - \lim_{m\to\infty}(\lambda(m)/m)| \leq C/m \ . \tag{6.2.2}$$

Proof:
Let $\mu(m) = \lambda(m)/m$. Let us rewrite (6.2.1) on the form :

$$|\mu(m+p) - ((m/(m+p))\mu(m)) - ((p/(m+p))\mu(p))| \leq C/(m+p) \tag{6.2.3}$$

In particular, for $p = m$, we get :

$$|\mu(2m) - \mu(m)| \leq C/2m \tag{6.2.4}$$

and by iteration :

$$|\mu(2^{k+1}m) - \mu(2^k m)| \leq C/(2^k m) .$$

In particular $\bar{\mu}(m) := \lim_{k\to\infty} \mu(2^k m)$ exists and

$$|\bar{\mu}(m) - \mu(m)| \leq C/m . \tag{6.2.5}$$

Replacing m and p in (6.2.3) by $2^k m$ and $2^k p$ and taking the limit in k, we get

$$\bar{\mu}(m+p) = ((m/(m+p))\bar{\mu}(m)) + ((p/(m+p))\bar{\mu}(p)) . \tag{6.2.6}$$

We now define $\bar{\lambda}(m)$ by

$$\bar{\lambda}(m) = m\bar{\mu}(m) ,$$

and rewrite (6.2.5) as

$$\bar{\lambda}(m+p) = \bar{\lambda}(m) + \bar{\lambda}(p) . \tag{6.2.7}$$

This implies in particular that

$$\bar{\lambda}(m) = m\bar{\lambda}(1)$$

and then

$$\bar{\mu}(m) = \bar{\mu}(1) . \tag{6.2.8}$$

(6.2.5) and (6.2.8) give the lemma.

6.3 Laplace integrals in large dimension: the thermodynamic limit

In this section we shall analyze more precisely the existence of the thermodynamic limit for Laplace integrals.

Proposition 6.3.1 *:*
Let C_1, C_2, C_3 be positive constants and let us consider the following family of potentials indexed by $m \in I\!N$

$$\Phi^{(m)}(x) = \frac{x^2}{2} + \Psi^{(m)}(x) \tag{6.3.1}$$

satisfying the following properties

$$\Psi^{(m)}(0) = 0 \ , \tag{6.3.2}$$

$$|\nabla\Psi^{(m)}(x)|_{\ell^\infty} \leq C_1 \ , \tag{6.3.3}$$

$$|\left(\nabla\left(\Psi^{(m+n)} - (\Psi^{(m)}\tilde{\oplus}\Psi^{(n)})\right)\right)(x)|_{\ell^1} \leq C_2 \ , \tag{6.3.4}$$

$$|\left(\Delta(\Psi^{(m+n)} - (\Psi^{(m)}\tilde{\oplus}\Psi^{(n)}))\right)(x)| \leq C_3 \ . \tag{6.3.5}$$

Then the thermodynamic limit

$$\lambda_\infty =: -\lim_{m\to\infty}(\ln\int_{I\!R^m} \exp -\frac{1}{h}\,\Phi^{(m)}(x)\ dx^{(m)})/m) \ ,$$

exists and the speed of the convergence to the limit is controlled in the following manner

$$|\lambda_\infty + (\ln\int_{I\!R^m} \exp -\frac{1}{h}\ \Phi^{(m)}(x)\ dx^{(m)})/m)| \leq D/m \ , \tag{6.3.6}$$

with $D = C_3 \ + \ C_1 \cdot C_2/h$.

Here we have used the notation

$$(\Phi^{(m)}\tilde{\oplus}\Phi^{(n)})(x) = \Phi^{(m)}(x') + \Phi^{(n)}(x") \ .$$

Remark 6.3.2 *:*
Let W be a C^2- function on $I\!R^2$ such that ∇W and ΔW are bounded. Then the assumptions of Proposition 6.3.1 are satisfied for

$$\Psi^{(m)}(x) = \Sigma_{i=1}^{m}\ W(x_i, x_{i+1}) \tag{6.3.7}$$

with the convention that $m+1 = 1$.

Similar results are of course older (see for example [Ru69]). Due to the particular structure of the interaction in the corollary, it can also be obtained by the technique of the transfer operator (See Section 4).

Example 6.3.3 *:*

$$W(u,v) = -\ln\cosh(\sqrt{\nu}(u+v))$$

The corresponding family of potentials is convex for $\nu \leq \frac{1}{4}$.

Proof of the proposition:
In order to get the existence of the thermodynamic limit and the control of the speed of convergence (6.3.6), it is sufficient to prove a result of "approximative additivity", that is to prove that

$$|a(m+n) - a(m) - a(n)| < D \, , \tag{6.3.8}$$

for some D where we recall that :

$$a(m) = -\ln\left(\int \exp(-\Phi^{(m)}(x)/h)dx\right) \, .$$

We introduce the interpolating family :

$$\Phi^{(m,n)}(x,s) = (1-s)\Phi^{(m+n)}(x) + s(\Phi^{(m)}(x') + \Phi^{(n)}(x"")) \tag{6.3.9}$$

with $x = (x', x") \in I\!R^{n+m}$, $s \in [0,1]$ and the corresponding $a(m,n;s)$. We observe that

$$a(m,n;1) = a(m) + a(n) \; ; \; a(m,n;0) = a(m+n) \, .$$

We consider the derivative $(\partial_s a)(m,n;s)$ of $a(m,n;\cdot)$ with respect to s which is given by :

$$-\frac{1}{h}\frac{\left(\int_{I\!R^{m+n}} \partial_s\Phi^{(m,n)}(x,s) \exp-(\Phi^{(m,n)}(x,s)/h)\; dx^{(m+n)}\right)}{\left(\int_{I\!R^{m+n}} \exp-(\Phi^{(m,n)}(x,s)/h)\; dx^{(m+n)}\right)} \, . \tag{6.3.10}$$

We have just to prove a uniform bound of this derivative with respect to $s \in [0,1], m, n$. We have

$$\partial_s\Phi^{(m,n)}(x,s) = \Psi^{(m+n)} - \left(\Psi^{(m)}\tilde{\oplus}\Psi^{(n)}\right)$$

and

$$\begin{array}{l}(\Psi^{(m+n)} - (\Psi^{(m)}\tilde{\oplus}\Psi^{(n)}))(x) = \\ \sum_{\ell=1}^{m+n} \left[x_\ell \int_0^1 \left(\partial_{x_\ell}(\Psi^{(m+n)} - (\Psi^{(m)}\tilde{\oplus}\Psi^{(n)}))(tx)\right) dt\right]\end{array} \quad (6.3.11)$$

An integration by part gives

$$\begin{array}{l}-\frac{1}{h}\left(\int_{I\!R^{m+n}} (\partial_s \Phi^{(m,n)}). \exp -(\Phi^{(m,n)}(x,s)/h) dx\right) = \\ \quad -\left(\int_{[0,1]} \int_{I\!R^{m+n}} \Delta(\Psi^{(m+n)} - (\Psi^{(m)}\tilde{\oplus}\Psi^{(n)}))(tx) \exp -(\Phi^{(m,n)}(x,s)/h) t dx dt\right) \\ \quad +\frac{1}{h}(\int_{[0,1]} \int_{I\!R^{m+n}} (\nabla(\Psi^{(m+n)} - (\Psi^{(m)}\tilde{\oplus}\Psi^{(n)}))(tx)) \times \\ \quad \times \left(((1-s)\nabla\Psi^{(m+n)} + s\nabla(\Psi^{(m)}\tilde{\oplus}\Psi^{(n)}))(x) \exp -(\Phi^{(m,n)}(x,s)/h) dx\, dt\right) .\end{array}$$

We can then compute explicitely D from the C_j by direct estimate. The fact that D is controlled with respect to h (polynomial function of $\frac{1}{h}$ is sufficient for what follows) is very important for the control of the semiclassical expansion of the thermodynamic limit. ∎

Remark 6.3.4 *The model of Brézin-Hikami:*
There are other examples which do not fit completely with the preceding proof. Let us mention [22] *for example the model of Brézin-Hikami (BH)*

$$\Phi^{(m)}(x) = \mu \sum_{j=1}^{m} x_j^2 + g m^{1-n} (\sum_{j=1}^{m} x_j^2)^n \quad (6.3.12)$$

with $\mu \in I\!R$, $g \in I\!R^+$ and $n > 1$. We observe here that due to the invariance by rotation a direct aproach is available. We get indeed that

$$\int_{I\!R^m} \exp -\Phi^{(m)}(x)\, dx^{(m)} = Vol(S^{(m-1)}) \int_0^\infty r^{m-1} \exp -[\mu r^2 + g m^{1-n} r^{2n}]\, dr$$

that we compare with the harmonic case

$$\int_{I\!R^m} \exp -|x|^2\, dx^{(m)} = Vol(S^{(m-1)}) \int_0^\infty r^{m-1} \exp -r^2\, dr = \pi^{\frac{m}{2}} .$$

We now introduce the change of variables $r = m^{\frac{1}{2}} t$ which leads to the study of

$$\pi^{\frac{m}{2}} \frac{\int_0^\infty \exp -m[\mu t^2 + g t^{2n} - \frac{m-1}{m} \ln t]\, dt}{\int_0^\infty \exp -m[t^2 - \frac{m-1}{m} \ln t]\, dt}$$

[22] confer [BreHi79], [Sor93a] and [Sor93b].

which can be analyzed by the standard Laplace integral method (see Subsection 3.3) by looking at the minimas of the functions

$$t \mapsto \mu t^2 + g t^{2n} - \ln t$$

and

$$t \mapsto t^2 - \ln t \ .$$

Here we observe that the role of the semiclassical parameter is played by $m = \frac{1}{h}$. *We observe also that*

$$\lim_{m \to \infty} \left(\ln \int_{I\!R^m} \exp -\Phi^{(m)}(x) \; dx^{(m)} \right) / m \ ,$$

exists and the speed of convergence is $\mathcal{O}(\frac{1}{m})$ *if the second term in the expansion of the Laplace integral does not vanish.*

Remark 6.3.5 *Other examples:*
Other classical examples appear in [BeBru90](Section I) where the potential has the more general form

$$\phi^{(m)}(x) = \sum_{j=1}^{m} v(x_j) + \sum_{k=2}^{r} \ m^{-(k-1)} \sum_{1 \leq i_1, \cdots, i_k \leq m} V_k(x_{i_1}, \cdots, x_{i_k}) \tag{6.3.13}$$

where

- $\exp -v(t)dt$ *is a probability measure on* $I\!R$,
- r *is an integer* ≥ 2,
- V_k *is a continuous bounded symmetric function from* $I\!R^k$ *into* $I\!R$ *for* $k \in \{2, \cdots, r\}$.

This model is an extension of the Curie-Weiss model (cf Section 2.1).

6.4 The thermodynamic limit for the Schrödinger operator

Theorem 6.4.1 *:*
If we assume that $V^{(m)}$ is one of the three models (K), (DK) or (BH) introduced in Subsection 1.3, then the limit,

$$\Lambda(h) = \lim_{m\to\infty}(\lambda_1(m;h)/m) \tag{6.4.1}$$

exists.

Preliminary comments:
This is not surprising if one first looks at the simple case of the harmonic oscillator. We shall prove it following the same ideas of statistical mechanics as we used in the corresponding study of the Laplace integrals (see Proposition 6.3.1 and (6.3.8)). Another ingredient is some a priori estimate for the Schrödinger operator. Let us also observe that the proof giving an approximate additivity property (modulo $\mathcal{O}(h)$) gives simultaneously

$$|\Lambda(h) - (\lambda_1(m;h)/m)| = h\mathcal{O}(1/m) \tag{6.4.2}$$

in the convex case and in the general case

$$|\Lambda(h) - (\lambda_1(m;h)/m)| = \mathcal{O}(1/m) \tag{6.4.3}$$

by easy arguments (see at the end of this subsection). We have consequently the analog of (6.3.6) for the Laplace integrals.

Proof of Theorem 6.4.1:
We just sketch the proof of Theorem 6.4.1 in the case $h = 1$ and for the model (DK). The proof for the (BH) model is left as a possible problem[23]. Let us prove the approximate additivity:

$$|\lambda_1(m+p) - \lambda_1(m) - \lambda_1(p)| \leq D\ .$$

We start from the following decomposition of $S^{(m+p)}$

$$S^{(m+p)} = S^{(m)}+\hat{S}_p^{(m+1)}-W(x_m,x_1)+W(x_m,x_{m+1})-W(x_{m+p},x_{m+1})+W(x_{m+p},x_1)$$

[23]See [Sor93b]

with

$$\hat{S}_p^{(m+1)} = -\hat{\Delta}_p^{(m+1)} + \sum_{k=m+1}^{m+p-1} W(x_k, x_{k+1}) + W(x_{m+p}, x_{m+1}),$$

$$W(x,y) = a|x-y|^2,$$

and

$$\hat{\Delta}_p^{(m+1)} = \sum_{k=m+1}^{m+p} \partial_{x_k}^2 \, .$$

It is then clear that the infimum of the spectrum of $S_p^{(m+1)}$ is the same as the infimum of $S^{(p)}$. For the lower bound on $\lambda_1(m+p)$, one writes

$$\begin{array}{ll}\lambda_1(m+p) & = \langle S^{(m+p)} u_1^{(m+p)} | u_1^{(m+p)} \rangle \\ & \geq \langle S^{(m)} u_1^{(m+p)} | u_1^{(m+p)} \rangle + \langle \hat{S}_p^{(m+1)} u_{m+p} | u_{m+p} \rangle \\ & -||W^{\frac{1}{2}}(x_m, x_1) u_1^{(m+p)}||^2 - ||W^{\frac{1}{2}}(x_{m+p}, x_{m+1}) u_1^{(m+p)}||^2 . \end{array}$$

We now observe that, under the assumption on v

$$v(t) \geq \frac{t^2}{C} - C \, ,$$

and, using the invariance by permutation,

$$\begin{array}{ll}\lambda_1(m) & = \langle S^{(m)} u_1^{(m)} | u_1^{(m)} \rangle \\ & \geq \sum_{j=1}^m \int_{\mathbb{R}^m} v(x_j) |u_1^{(m)}|^2 dx \\ & = m \int_{\mathbb{R}^m} v(x_1) |u_1^{(m)}|^2 dx \\ & \geq \frac{m}{C} \int_{\mathbb{R}^m} x_1^2 |u_1^{(m)}|^2 dx - Cm \, . \end{array}$$

From this we deduce [24]

$$\int x_j^2 |u_1^{(m)}|^2 dx \leq C^2 + C \frac{\lambda_1(m)}{m} \leq D_1 \, .$$

It is then easy to get:

$$\lambda_1(m+p) \geq \lambda_1(m) + \lambda_1(p) - D$$

for some new D independent of m, p and well controlled with respect to the semiclassical parameter if necessary.
For the upper bound we proceed similarly using the fonction:

$$\hat{u}_{p,m} = u_1^{(m)}(x_1, ..., x_m) \cdot u_1^{(p)}(x_{m+1}, ..., x_{m+p}) \, .$$

[24] In the convex case, if $v"(t) \geq \sigma > 0$ and $v(0) = v'(0) = 0$, this can be improved and we can get a good control of the constants with respect to h, for example: $D_1 = \mathcal{O}(h)$.

7 Harmonic approximation

7.1 Introduction

The harmonic oscillator plays a uniform role in Quantum Mechanics. This is not only the fact that its spectrum can be computed explicitely. As we shall see here, it gives the more natural approximation in order to analyze the spectrum of the Schrödinger near the bottom in the generic situation where there is a unique non degenerate minimum. We shall analyze in this section this approximation, some large dimension aspects and also high order approximations. We refer for this sections to the books of Cycon-Froese-Kirsch-Simon [CFKS87] and to [He88].

7.2 The case of dimension 1

We start with the simplest one-well problem:

$$S_v^h := -h^2 d^2/dx^2 + v(x) \ , \tag{7.2.1}$$

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

$$v''(0) > 0 \ . \tag{7.2.2}$$

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

$$-h^2 d^2/dx^2 + \frac{1}{2} v''(0) x^2 \ . \tag{7.2.3}$$

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

$$h \left[-d^2/dy^2 + \frac{1}{2} v''(0) y^2 \right] \ . \tag{7.2.4}$$

Consequently, the eigenvalues are given as

$$\lambda_n(h) = h \cdot \lambda_n(1) = (2n+1) h \cdot \sqrt{\frac{v''(0)}{2}} \ , \tag{7.2.5}$$

and the corresponding eigenfunctions are

$$u_n^h(x) = h^{-\frac{1}{4}} u_n^1(\frac{x}{h^{\frac{1}{2}}}) \tag{7.2.6}$$

with [25]

$$u_n^1(y) = P_n(y) \exp -\sqrt{\frac{v''(0)}{2}} \frac{y^2}{2} \tag{7.2.7}$$

We are just looking for simplification 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. We now get

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

The coefficients corresponding to the commutation of S_v^h 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 as $\mathcal{O}(h^{\frac{3}{2}})$. Then the spectral theorem gives the existence for S_v^h of an eigenvalue $\lambda(h)$ such that

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

In particular, we get the inequality

$$\lambda_1(h) \leq h \cdot \sqrt{\frac{v''(0)}{2}} + C h^{\frac{3}{2}} . \tag{7.2.8}$$

[25] We normalize by assuming that the L^2-norm is one. For the first eigenvalue, we have seen that, by assuming in addition that the function is strictly positive, we determine completely $u_1^h(x)$.

Remark 7.2.1 *:*
At this level, we have only an inequality in one direction. If we analyze, what we have done we have used that $u_1^h(x)$ and its first derivative are exponentially decreasing like $\mathcal{O}(\exp -\epsilon/h)$ in L^2 outside of 0 and the finer $||x^3 \cdot u_1^h(x)||_{L^2} = \mathcal{O}(h^{\frac{3}{2}})$. If we want to exchange in the proof the roles of the harmonic oscillator and of S_v^h, we have to prove the same properties for the first eigenfunction of S_v^h without to use the explicit expression of the first eigenfunction which is unknown for a general v. This will be done in the next section.

Exercise 7.2.2 *:*
Verify that it works in the case of a potential with more than one minimum. Observe that with the introduction of χ, we have used only the behavior of v near one minimum.

Exercise 7.2.3 *:*
Study the case when, for some $k_0 > 1$,

$$v^{(k)}(0) = 0\ ,\ \forall k < 2k_0$$

and

$$v^{(2k_0)}(0) > 0\ .$$

Exercise 7.2.4 *:*
Using the mini-max principle and the Laplace integral method, prove that we have actually

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

Complete expansions.

We now sketch one way for getting a complete expansion for the eigenvalue (This type of expansions will be also obtained as a consequence of WKB expansions which will be described later). We will prove the following

Proposition 7.2.5 *:*
Under assumptions (7.2.1)-(7.2.2), there exists, for any m, a normalized quasimode $u_1^{h,app.,m}$ and $\mu_1^{h,m}$ such that

$$(S_v^h - \mu_1^{h,m})u_1^{h,app.,m} = \mathcal{O}(h^{1+\frac{m+1}{2}})\ .$$

We start with a completely formal expansion in powers of $h^{\frac{1}{2}}$ and x. For this we consider the Taylor expansion of v at 0 :

$$v(x) \sim \sum_{k\geq 2} v_k x^k \ .$$

One will make more precise the feeling that everything depends only of this Taylor's expansion at the origin (modulo an error of order $\mathcal{O}(h^\infty)$).
Let us consider the formal operator

$$-h^2 d^2/dx^2 + \sum_{k\geq 2} v_k x^k \ .$$

Following what we have done for the harmonic approximation, we consider the dilation associated with the change of variables

$$x = h^{\frac{1}{2}} y \ .$$

In the new variables, we get the new formal operator

$$h \left(-d^2/dy^2 + \sum_{k\geq 2} h^{\frac{k}{2}-1} v_k y^k \right) \ ,$$

that we write in the form

$$h \left(\sum_{\ell \in \mathbb{N}} h^{\frac{\ell}{2}} T_\ell \right) \ ,$$

with

$$\begin{aligned} T_0 \ &= -d^2/dy^2 + v_2 y^2 \\ T_\ell \ &= v_\ell \ y^{\ell+2} \ \text{ for } \ \ell \geq 1 \ . \end{aligned}$$

The formal problem consists in looking for a family $(w_j, \mu_{1,j})$ in $\mathcal{S}(\mathbb{R}) \times \mathbb{R}$ such that

$$\left(\sum_{\ell \in \mathbb{N}} h^{\frac{\ell}{2}} (T_\ell - \mu_{1,\ell}) \right) \left(\sum_\ell h^{\frac{\ell}{2}} w_\ell \right) \sim 0 \ ,$$

when identifying the different powers of $h^{\frac{1}{2}}$.
The first equation is

$$(T_0 - \mu_{1,0}) w_0 = 0 \ .$$

This is solved by taking for $\mu_{1,0}$ the first eigenvalue of the harmonic oscillator T_0 and for w_0 the first eigenfunction. Until now we have just reproduced the

preceding construction.
Let us now consider the second equation. We find

$$(T_0 - \mu_{1,0})w_1 = T_1 w_0 - \mu_{1,1} w_0 \ .$$

This new equation can only be satisfied if the right hand side is orthogonal to w_0. The range of $(T_0 - \mu_{1,0})$ is indeed the orthogonal of the kernel (according to the standard Fredhom theory). This condition gives

$$\mu_{1,1} = \langle T_1 w_0, w_0 \rangle$$

that is, using the property that w_0 is even,

$$\mu_{1,1} = 0 \ .$$

Then we can solve the equation by adding the condition that w_1 is orthogonal to w_0. We write

$$\begin{aligned} w_1 &= R'(\mu_{1,0})(T_1 w_0 - \mu_{1,1} w_0) \\ &= R'(\mu_{1,0})(T_1 w_0) \ , \end{aligned}$$

where

$$R'(\mu_{1,0}) = (T_0 - \mu_{1,0})^{-1} \ ,$$

on the orthogonal of $I\!R \cdot w_0$ and

$$R'(\mu_{1,0}) w_0 = 0 \ .$$

w_1 is a priori[26] in B^2 but, using the regularity of the harmonic oscillator (cf Subsection 5.3), it is clear that w_0 being in $\mathcal{S}(I\!R) = \cap_{k \in I\!N} B^k$, the same is true for w_1.

The next equations can be solved in the same way. The general equation is

$$(T_0 - \mu_{1,0}) w_\ell = \sum_{k=0}^{\ell-1} (T_{\ell-k} - \mu_{1,\ell-k}) w_k \ .$$

[26]We recall from this subsection that

$$\begin{aligned} &B^k(I\!R^m) = \\ &\quad \{u \in L^2(I\!R^m) \mid x^\alpha D_x^\beta u \in L^2 \ , \ \forall \alpha, \beta \in I\!N^m \text{ with } |\alpha| + |\beta| \leq k\} \ . \end{aligned}$$

and $\mu_{1,\ell}$ is obtained by

$$\mu_{1,\ell} = \sum_{k=1}^{\ell-1} \langle (T_{\ell-k} - \mu_{1,\ell-k}) w_k, w_0 \rangle + \langle T_\ell w_0, w_0 \rangle \ .$$

Remark 7.2.6 *:*
If we observe that w_0 is even and that the operators T_ℓ conserve the parity for ℓ even and inverse the parity for ℓ odd, then we get that

$$\mu_{1,\ell} = 0$$

for odd ℓ.

Remark 7.2.7 *:*
If we have refered to functional analysis and to the regularity for the harmonic oscillator, it was just to present relatively general arguments working in a more general situation. In the particular case, we can work much more explicitely using the Hermite polynomials. If one for example looks at the equation corresponding to $\ell = 1$, one has just to express $y^3 w_0$ as a linear combination of the second eigenvector and of the forth eigenvector of T_0 and we have an explicit expression for w_1 as a new combination of these two eigenvectors. It is then clear on this explicit expression that w_1 is in $\mathcal{S}(I\!R)$ and actually of gaussian type.

From the formal construction to an approximate solution

For a given m, we now take for candidate for our approximate solution

$$u_1^{h,app.,m}(x) = h^{-\frac{1}{4}} \, \chi(x) \, \sum_{\ell=0}^{m} h^{\frac{\ell}{2}} \, w_\ell(x \cdot h^{-\frac{1}{2}}) \ .$$

and one get easily the announced properties. This proves the proposition.

Decomposition by partition of unity:

The first remark is valid for any partition of unity:

$$(-\Delta u, u) = \sum_j (-\Delta \phi_j u, \phi_j u) - \sum_j || \, |\nabla \phi_j| \, u \, ||^2 \qquad (7.2.9)$$

for all u in C_0^∞ if
$$\sum_j \phi_j^2 = 1 \;. \tag{7.2.10}$$

Hint:
We use (7.2.10) and differentiate it. We first get
$$\sum_j \nabla\phi_j \cdot \phi_j = 0 \;,$$
and then taking the divergence
$$\sum_j |\nabla\phi_j|^2 + \sum_j \Delta\phi_j \cdot \phi_j = 0 \;.$$
This formula permits, modulo a remainder term, to control the lower bound of $-h^2\Delta + V$ by examining separately the Schrödinger operator in the support of a fixed ϕ_j. In our special case, the best is to use a h-dependent partition of unity constructed with (around the wells) functions of the form $\phi(x\cdot h^{-\frac{2}{5}})$.

Remark 7.2.8 *:*
The case when we get eigenvalues with multiplicity larger than one for the harmonic oscillator (and this can only occur in dimension larger than one) can also be analyzed using the abstract proposition 5.7.1 recalled in Section 5.

7.3 Quadratic models

We look in this subsection at the quadratic case and more specifically for the following model
$$y \mapsto Q(y) = \frac{b}{2}\sum_j y_j^2 + \frac{a}{2}\sum_{j\in\mathbb{Z}/m\mathbb{Z}} (y_j - y_{j+1})^2 \;. \tag{7.3.1}$$
This potential is sometimes called the harmonic spin-chain potential (see for example Roepstorff, Section 2.8, p.85-86 in [Roe94], Section 4.4, p.258 in Gallavotti [Ga83]). The corresponding matrix can be written as
$$(b+2a)Id - a(\tau_{+1} + \tau_{-1}) \;,$$

where $(\tau_1 u)_k = u_{k-1}$ for $k = 1, \cdots, m$. The spectrum of this matrix is well known. One way to prove that these eigenvalues are

$$\omega_i(m) = b + 2a\left(1 - \cos(2\pi\frac{(i-1)}{m})\right) \ , \ i = 1, \cdots, m \ ,$$

is to use the discrete Fourier transform defined on $\mathbb{C}^m$ by

$$a \mapsto \hat{a}_k = \frac{1}{\sqrt{m}} \sum_{n=1}^{m} \exp -2i\pi \frac{kn}{m} a_n \ .$$

The first eigenvalue of the corresponding harmonic oscillator is then given by

$$\lambda^{osc}(m) = \sum_{i=1}^{m} \sqrt{\frac{b}{2} + a\left(1 - \cos(2\pi\frac{(i-1)}{m})\right)} \tag{7.3.2}$$

The thermodynamic limit is then

$$\lim_{m\to\infty} \frac{\lambda^{osc}(m)}{m} = \int_0^1 \sqrt{\frac{b}{2} + a\left(1 - \cos(2\pi\theta)\right)} d\theta \ .$$

Exercise 7.3.1 *:*
Prove that the convergence is exponentially rapid. A possible reference is Dieudonné [Die] where a Poisson relation is proved which permits to get the result. Another proof is given in 7.5.

7.4 An instructive model:

In order to understand what is going on, it is perhaps useful to analyze in detail an "almost" solvable model. Let us consider [27]

[27] This model was inspired by the limit $\nu \to \infty$ of the Kac model which gives after rescaling the model

$$- h^2 \Delta_x + \frac{1}{2}|x|^2 - \frac{1}{2}\sum_{i=1}^{m} |x_i + x_{i+1}| \ , \tag{7.4.1}$$

which seems less easy to analyze.
In this model, the "one well" problems are (at least in small neighborhoods of these wells) attached to harmonic oscillators.

$$S^{(m)}(x,hD_x) = -h^2\Delta_x + \frac{1}{2}|x|^2 - |\sum_{i=1}^{m} x_i| \,, \tag{7.4.2}$$

and look for an estimate of the splitting. We first perform an orthonormal change of variables $x \mapsto y = (y_1, y'')$ s.t.

$$y_1 = m^{-\frac{1}{2}} \sum_{i=1}^{m} x_i \;.$$

We get in the new coordinates the following operator with separate variables

$$-h^2\Delta_y + \frac{1}{2}|y|^2 - \sqrt{m}\,|y_1| \;.$$

We now perform a new dilation $y = m^{\frac{1}{2}}\tilde{y}$ and get

$$m(-(\frac{h}{m})^2\Delta_{\tilde{y}} + \frac{1}{2}|\tilde{y}|^2 - |\tilde{y}_1|) \,,$$

and this permits to reduce the analysis of the splitting between the two first lowest eigenvalues to a corresponding analysis of the one dimensional model

$$m(-(\frac{h}{m})^2\partial_t^2 + v(t)) \,,$$

with

$$v(t) := \frac{1}{2}t^2 - |t| \;.$$

This potential $v(t)$ admits a minimum at $|t| = \pm 1$,

$$\inf v = -\frac{1}{2} \;.$$

The new semiclassical parameter is $\tilde{h} = \frac{h}{m}$ and the splitting can almost be analyzed by standard one dimensional classical [28] techniques which we shall

[28] There is actually a small difficulty due to the fact that the potential is only Lipschitz, but this does not affect the optimal result. One can indeed observe, in order to eliminate the problem relative to the discontinuity of the derivative at 0, that this splitting is also the splitting between the first eigenvalue of the Neumann problem in $]0,+\infty[$ and the first eigenvalue for the Dirichlet problem in $]0,\infty[$ for the harmonic oscillator $-\tilde{h}^2\partial_t^2 + \frac{1}{2}t^2 - t$. But this is also the splitting between the first eigenvalue of the Neumann problem and the first eigenvalue for the Dirichlet problem in $]-1,\infty[$ for the harmonic oscillator $-\tilde{h}^2\partial_s^2 + \frac{1}{2}s^2$. This problem is treated in [BoHe93]

discuss (see for the upper bound in Section 8).

It is indeed possible to get

$$\lambda_2(m,h) - \lambda_1(m,h) \sim (hm)^{\frac{1}{2}} a(\tilde{h}) \exp -mS/h \;, \tag{7.4.3}$$

where S is given by

$$S = 2\int_0^1 \sqrt{v(t) - \inf v}\; dt = 2\int_0^1 \sqrt{v(t) + \frac{1}{2}}\; dt = 1/\sqrt{2}\;.$$

One can also observe that $\lambda_1(m,h)/m$ is the sum of the smallest eigenvalue of

$$\mathcal{S}(t, \tilde{h}D_t) = -(\frac{h}{m})^2 \partial_t^2 + \frac{1}{2}t^2 - |t|\;,$$

and of the smallest eigenvalue of the Schrödinger operator

$$\frac{1}{m}\left(-h^2 \Delta_{y''} + \frac{1}{2}|y''|^2\right)\;,$$

which can be computed as equal to

$$\lambda_1''(m,h) = \frac{m-1}{m}\,\frac{h}{\sqrt{2}}\;.$$

Taking the limit $m \to \infty$ corresponds to taking the limit $\tilde{h} \to 0$ and we get

$$\lim_{m\to\infty} \lambda_1^{(m)}(h)/m = -\frac{1}{2}\; + \frac{h}{\sqrt{2}}. \tag{7.4.4}$$

A superficial analysis could lead to think that we have an error in $m\mathcal{O}(\tilde{h}^2) = \frac{1}{m}\mathcal{O}(h^2)$ but, near $t = 1$, (and modulo an exponentially small error in $m\;\exp -(S-\epsilon)\frac{m}{h}$ for any $\epsilon > 0$), the first eigenvalue of $\mathcal{S}(t, \tilde{h}D_t)$ is the same as the first eigenvalue of

$$\hat{\mathcal{S}}(t, \tilde{h}D_t) = -(\frac{h}{m})^2 \partial_t^2 + \frac{1}{2}t^2 - t\;.$$

which is exactly $-\frac{1}{2}\; + \frac{h}{\sqrt{2}}$.
We recover what we were waiting for this model, that is a convergence to

the thermodynamic limit which is exponentially rapid and directly related to the tunneling effect. The operator $\hat{\mathcal{S}}$ corresponds indeed to a "right" approximation of the double well problem which appears to be an exact harmonic oscillator. The same is of course true for the "left" approximation. It is also interesting to consider more generally the family of operators

$$\nu \mapsto S^{(m)}(x, hD_x, \nu) = -h^2\Delta_x + \frac{1}{2}|x|^2 - \nu|\sum_{i=1}^{m} x_i| \,. \tag{7.4.5}$$

Playing with ν could permit to understand the transition procedure around $\nu = 0$ for this model. The case $\nu = 0$ gives a splitting of order $m \cdot \sqrt{2}\ \tilde{h} = \sqrt{2}\ h$. In the case $\nu < 0$, the splitting is obtained (for $\frac{h}{m}$ small enough) by the splitting of $m\left(-\frac{h}{m}^2\Delta_{\tilde{y}'} + \frac{1}{2}|\tilde{y}'|^2\right)$ on $L^2(I\!R^{m-1})$ that is $\frac{h}{\sqrt{2}}$.
We have finally obtained the following lemma

Lemma 7.4.1 *:*
If $\lambda_j(m,h,\nu)$ are the eigenvalues of $S^{(m)}(x,hD_x,\nu)$ then we have

$$\lim_{m\to\infty} \lambda_1(m,h,\nu)/m = -\frac{\nu_+^2}{2} + \frac{h}{\sqrt{2}} \,, \tag{7.4.6}$$

and

$$\begin{aligned} \lim_{m\to\infty}(\lambda_2(m,h,\nu) - \lambda_1(m,h,\nu)) \ &= 0 \ \ \textit{if} \ \ \nu > 0 \,, \\ &= \tfrac{h}{\sqrt{2}} \ \ \textit{if} \ \ \nu < 0 \,. \end{aligned} \tag{7.4.7}$$

The model presents clearly a transition of phase at $\nu = 0$. We can see also that the speed of the convergence of the thermodynamic limit is exponential in the case $\nu \geq 0$. This does not seem the case for $\nu < 0$. The study of the transition around $\nu = 0$ is interesting .

7.5 The harmonic approximation, analysis in large dimension

There are different proofs for the harmonic approximation. We follow here a version due to B. Simon [Si84] but control with respect to the dimension and we focuse on the model (DK)

$$V^{(m)} = \sum_j v(x_j) + \frac{a}{2}|x_j - x_{j+1}|^2 \,.$$

We first observe that

Lemma 7.5.1 *:*
If v is the above defined single well potential on $I\!R$, the minimum of $V^{(m)}$ is equal to $m \cdot \min v$ and is only attained at $x_c(m) = 0$.
If v is the above defined double well potential on $I\!R$, the minimum of $V^{(m)}$ is equal to $m \cdot \min v$ and is only attained at the following two points:

$$x_{c\pm}(m) = \pm x_c(m) \quad \textit{with} \quad x_c = s\ (1, 1, 1, ..., 1). \tag{7.5.1}$$

At x_c, the Hessian corresponds [29] to

$$Q_0(\bar{x}) = \frac{1}{2} v''(s) \sum_{k=1}^{m} \bar{x}_k^2 + \frac{a}{2} \sum_{k=1}^{m} (\bar{x}_k - \bar{x}_{k+1})^2 \tag{7.5.2}$$

where we have written :

$$x = \bar{x} + x_c \tag{7.5.3}$$

The harmonic approximation consists in replacing S_h by

$$H_h = -h^2 \Delta_{\bar{x}} + Q_0(\bar{x}) \ ,$$

and we have

Proposition 7.5.2 *:(the convex case)*
Let us assume that

- $\min v = v(0) = 0$,
- $v''(x) \geq v''(0)$,
  and
- $0 \leq v(x) \leq C \cdot \langle x \rangle^{N_1}$.

Then, there exists a constant C such that, for all $h \in]0, h_0]$ and all $m \geq m_0$, we have :

$$h\lambda^{app.}(m) \leq \lambda_1(m, h) \leq h\lambda^{app.}(m) + C \cdot m \cdot h^{\frac{3}{2}} \tag{7.5.4}$$

where $\lambda^{app.}(m)$ is the first eigenvalue of the harmonic approximating oscillator

$$H_1 = -\Delta_{\bar{x}} + Q_0(\bar{x}) \ . \tag{7.5.5}$$

[29] we take $s = 0$ in the one well case.

Remark 7.5.3 :
The existence of the harmonic approximation was already explained. What is analyzed in detail here is the control of the remainder with respect to m. At least in the case when v is even, this can be improved in $C \cdot m \cdot h^2$ instead of $C \cdot m \cdot h^{\frac{3}{2}}$.

Proof:
The lower bound is evident by assumption using the minimax Principle.
For the converse we shall use the first eigenfunction of the harmonic oscillator H as a quasi-mode. We have already analyzed the change of variable diagonalizing the quadratic form.

$$x_\ell = \sum_{r=1}^{m} a_{\ell r} y_r \tag{7.5.6}$$

with

$$\sum_{r=1}^{m} a_{\ell r}^2 = 1 \tag{7.5.7}$$

In these new coordinates we have seen that

$$\tilde{Q}(y) = \sum_{i=1}^{m} \omega_i(m) y_i^2 \tag{7.5.8}$$

with,

$$\omega_i(m) = \frac{1}{2} v''(0) + a(1 - \cos 2(i-1)\frac{\pi}{m}) \ , \ i = 1, \ldots, m \ . \tag{7.5.9}$$

In the following proof, C is a constant (possibly changed from line to line) but independent of m.
Let us define

$$\phi(y,h) = \psi(x,h)$$

where $\psi(\cdot, h)$ is the normalized first eigenfunction of H_h.
We observe that

$$\begin{aligned} \phi(y,h) &= h^{-\frac{m}{4}} \phi(h^{-\frac{1}{2}} y, 1) \\ \psi(x,h) &= h^{-\frac{m}{4}} \psi(h^{-\frac{1}{2}} x, 1) \end{aligned}$$

We have

$$| - v(s) + v''(0)s^2/2| \leq C \cdot (|s|^3 + |s|^{N_1})$$

where the second term in the right hand side is put in order to control v at ∞ (we forget later this term which produces smaller error terms). In order to prove the lemma we have mainly to estimate (taking account of the min-max Principle) m terms of the form:

$$\int x_k^6 \, \psi(x,h)^2 \, dx \, ,$$

and to prove that

$$\int x_k^6 \psi(x,h)^2 \, dx \leq C \cdot h^3 \, .$$

An argument of homogeneity permits to analyze the case $h = 1$ and using the invariance by permutation of the problem we have only to analyze

$$\int x_1^6 \psi(x,1)^2 \, dx \leq C \, .$$

Coming back to the new coordinates, it is sufficient to consider

$$\int (\sum_{r=1}^{m} a_{1r} y_r)^6 \phi(y,1)^2 \, dy \leq C \, .$$

We observe that there are a lot of cancellations in the above integrals (using the property of symmetry of ϕ) . We have finally to analyze only

$$\sum_{r,s,t} \int (a_{1r} y_r)^2 (a_{1s} y_s)^2 (a_{1t} y_t)^2 \phi(y)^2 \, dy \, .$$

We observe now that

$$\frac{1}{2} v''(0) \leq \omega_r(m) \leq \frac{1}{2} v''(0) + 2a \, , \tag{7.5.10}$$

and we get an upper bound by

$$C(\sum_{r,s,t} a_{1r}^2 \cdot a_{1s}^2 \cdot a_{1t}^2) \ \ ,$$

observing that

$$\frac{\int y_{i_1}^2 \, y_{i_2}^2 \, y_{i_3}^2 \phi(y)^2 \, dy}{\int \phi(y)^2 \, dy}$$

is bounded independently of i_1, i_2, i_3, m, by using integration by parts and the control of $\omega_r(m)$ given in (7.5.10).
Using finally (7.5.7), we are done.

Remark 7.5.4 :
When v is simply strictly convex without the property $v''(t) \geq v''(0)$, we shall only have a lower bound by $h \cdot \lambda^{app.}(m) - C \cdot m \cdot h^{\frac{6}{5}}$. The proof is a simplified version of the proof for the non convex case.

We now look at the non convex case.

Proposition 7.5.5 : *(the non convex case)*
Let us assume that v is a double well potential with two nondegenerate minima at $\pm s$, with $v(\pm s) = 0$. Then there exists a constant C such that for all $h \in]0, h_0]$ and all $m \geq m_0$, we have :

$$h\lambda^{app.}(m) - C \cdot m \cdot h^{\frac{6}{5}} \leq \lambda_1(m,h) \leq h\lambda^{app.}(m) + Cmh^{\frac{3}{2}} . \tag{7.5.11}$$

Proof:
The lower bound on the first eigenvalue is no more evident because the lower bound by the quadratic approximation is no more true. The proof given by B.Simon [Si84] does not give a satisfactory result and introduces a bad behavior of the remainder with respect to m at least if one takes the initial partition of the unity. The proof of the upper bound, on the contrary, does not introduce new problems (we have just to compose the quasimode with a suitable cylindrical cut off function independent of h which in the new coordinates around one critical point takes the form $\chi(y) = \prod_{i=1}^{m} \theta(y_i)$). This creates an error whose order is $m \exp -\epsilon/h$. Using this point we see that the condition we put on v at ∞ can be very weak.

Proof of the lower bound
The idea is to construct an adapted partition of unity. We treat here the case of the Dobrokhotov-Kolokoltsov model but everything works analogously for the Kac model.
Let us remember that we consider the operator

$$S^{(m)}(h) = -h^2 \sum_{k=1}^{m} \partial_{x_k}^2 + \frac{a}{2} \sum_{k=1}^{m} (x_k - x_{k+1})^2 + \sum_{k=1}^{m} v(x_k) ,$$

(We recall the convention $x_{m+1} = x_1$).

The inequality we want to prove can be rewritten in the form

$$- C \cdot m \cdot h^{\frac{6}{5}} \leq \lambda_1(m,h) - h \cdot \lambda^{app.}(m) , \tag{7.5.12}$$

where $\lambda^{app.}(m)$ is the already computed first eigenvalue of

$$-\sum_{k=1}^{m} \partial_{x_k}^2 + \frac{a}{2}\sum_{k=1}^{m}(x_k - x_{k+1})^2 + \frac{v''(s)}{2}|x|^2 \, ,$$

which is directly obtained as Tr $Q^{\frac{1}{2}}$ where $Q^{\frac{1}{2}}$ is the positive square root of the matrix Q attached to the quadratic form

$$\langle x|Q|x\rangle = \frac{a}{2}\sum_{k=1}^{m}(x_k - x_{k+1})^2 + \frac{v''(s)}{2}|x|^2 \, .$$

A partition of unity

Let θ be a function in $C_0^\infty(]-1,+1[)$ such that

$$0 \leq \theta \leq 1 \text{ with } \theta = 1 \text{ on }]-1/2, 1/2[\, .$$

We now introduce for $j \in \{-1, 1\}$, $k \in \{1, \ldots.., m\}$

$$\phi_j(t,h) = \theta((t - js)/h^{\frac{2}{5}}) \, , \tag{7.5.13}$$

and we choose θ and ϕ_0 such that the following relation is satisfied

$$\sum_{j\in\{-1,0,1\}} \phi_j(t,h)^2 = 1 \, . \tag{7.5.14}$$

We now introduce a multiindex α with

$$\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_m) \text{ with } \alpha_k \in \{-1, 0, 1\} \, .$$

We now introduce

$$\phi_\alpha(x,h) = \prod_{k=1}^{m} \phi_{\alpha_k}(x_k, h) \, .$$

We deduce from (7.5.13) and (7.5.14) the following properties:

$$\sum_\alpha \phi_\alpha(x,h)^2 \; = \; 1 \tag{7.5.15}$$

and

$$\sum_\alpha ||\nabla\phi_\alpha(x,h)||^2 \leq C \cdot m \cdot h^{-\frac{4}{5}} \tag{7.5.16}$$

where C is independent of h and m. The first step is a very elementary and old formula called in some context "IMS localization formula" (already presented in (7.2.9))

$$S(h) = \sum_\alpha \phi_\alpha S(h)\phi_\alpha - h^2 \sum_\alpha ||\nabla\phi_\alpha||^2 . \tag{7.5.17}$$

According to (7.5.16), Formula (7.5.17) permits to reduce the proof of (7.5.12) to the proof of the existence of C s.t for all α, m, we have

$$-Cmh^{\frac{6}{5}} + h\cdot\lambda^{app.}(m) \leq \inf_{\substack{u\in C_0^\infty(E_\alpha)\ ,\\ ||u||=1}} \langle S(h)u\ ,\ u\rangle_{L^2}\ , \tag{7.5.18}$$

where E_α is defined as

$$E_\alpha = \prod_{k=1}^m B_{\alpha_k}\ ,$$

where,

- for $j=\pm 1$,

  $$B_j = \{t\ ,\ |t-j.s| \leq h^{\frac{2}{5}}\}\ ,$$

  and

- for $j=0$, by

  $$B_0 = \{t\ ,\ |t-\ell.s| \geq \frac{1}{2}h^{\frac{2}{5}}\ \text{ for } \ell=\pm 1\}\ .$$

We now observe that, if

$$|z-\ell\cdot s| \geq \frac{1}{2}h^{\frac{2}{5}} \text{ for } \ell=\pm 1\ ,$$

there exists $\delta>0$ s.t

$$v(z) \geq \delta\cdot h^{\frac{4}{5}}\ , \tag{7.5.19}$$

and we get consequently, for $x\in B_k^0$,

$$v(x_k) \geq \delta\cdot h^{\frac{4}{5}}\ . \tag{7.5.20}$$

We have now localized the problem in a box E_α. Of course all our constants have to be found independently of α, m and h. We now introduce

$$\mathcal{C}_\alpha = \{k \mid \alpha_k = 0\} \tag{7.5.21}$$

In order to prove (7.5.18), we can, according to (7.5.20), minorize $S(h)$ in E_α by $S'(h, \mathcal{C}_\alpha)$ where $S'(h, \mathcal{C})$ is

$$S'(h, \mathcal{C}) = -h^2\Delta \ + \ \frac{a}{2}\sum_{k=1}^{m}(x_k - x_{k+1})^2 + \sum_{k \notin \mathcal{C}} v(x_k) \ + \ \delta \cdot n_{\mathcal{C}}.h^{\frac{4}{5}} \ , \tag{7.5.22}$$

and

$$n_{\mathcal{C}} = \ \text{Cardinal}\, \mathcal{C} \ . \tag{7.5.23}$$

We have now to prove

$$-\,C \cdot m \cdot h^{\frac{6}{5}} + h \cdot \lambda^{app.}(m) \leq \inf_{\substack{u \in C_0^\infty(E_\alpha),\\ ||u|| = 1}} \langle S'(h, \mathcal{C}_\alpha) u \mid u \rangle_{L^2} \tag{7.5.24}$$

Now in each E_α, we can approach $v(x_k)$, for $k \notin \mathcal{C}_\alpha$, by its quadratic approximation $\frac{v''(s)}{2}.(x_k - \alpha_k\, s)^2$ with, for each term, an error of order $C \cdot (x_k - \alpha_k\, s)^3$, that is in E_α of order $C.h^{\frac{6}{5}}$. But there are $(m - n_{\mathcal{C}_\alpha})$ terms of this type and this error is consequently majorized by $C\ m\ h^{\frac{6}{5}}$ in this quadratic approximation.
We are now reduced to the study of a family of harmonic oscillators. We introduce

$$S(h, \alpha) = -h^2\Delta + \frac{a}{2}\sum_{k=1}^{m}(x_k - x_{k+1})^2 + \frac{v''(s)}{2}\sum_{k \notin \mathcal{C}_\alpha}(x_k - \alpha_k\, s)^2 \ + \ \delta \cdot n_{\mathcal{C}_\alpha} \cdot h^{\frac{4}{5}} \tag{7.5.25}$$

and it is sufficient to prove the existence of h_0 such that for all $0 < h \leq h_0$, for all m and for all α s.t $\mathcal{C}_\alpha = \mathcal{C}$, we have

$$h.\lambda^{app.}(m) \leq \inf_{\left\{\substack{u \in C_0^\infty(I\!\!R^m),\\ ||u|| = 1}\right\}} \langle S(h, \alpha) u \ , \ u \rangle_{L^2} \tag{7.5.26}$$

We observe that the left hand side corresponds by definition to the right hand side with $\mathcal{C} = \emptyset$ and $\{\alpha_k = 1 \ , \ \forall k\}$ or $\{\alpha_k = -1 \ , \ \forall k\}$.
Let us consider the operator $S(h, \alpha)$. The potential

$$V_\alpha(x) = \frac{a}{2} \sum_{k=1}^{m} (x_k - x_{k+1})^2 + \frac{v''(s)}{2} \sum_{k \notin \mathcal{C}_\alpha} (x_k - \alpha_k \, s)^2$$

admits, if $\mathcal{C}_\alpha$ is different of $\{1, ..., m\}$, a unique minimum and its Hessian is independent of α. If $\mathcal{C}_\alpha = \{1, ..., m\}$, the minimum is given by $x_k = x_{k+1} \ , \ k = 1, ..., m$.
After a translation the operator $S(h, \alpha) - \delta \cdot n_{\mathcal{C}_\alpha} \cdot h^{\frac{4}{5}}$ becomes unitary equivalent to:

$$\begin{array}{l} -h^2 \Delta_y + \min V_\alpha + \frac{a}{2} \sum_{k=1}^{m} (y_k - y_{k+1})^2 + \frac{v''(s)}{2} \sum_{k \notin \mathcal{C}} y_k^2 \\ \quad \geq -h^2 \Delta_y + \frac{a}{2} \sum_{k=1}^{m} (y_k - y_{k+1})^2 + \frac{v''(s)}{2} \sum_{k \notin \mathcal{C}} y_k^2 \ , \end{array}$$

with $\mathcal{C} = \mathcal{C}_\alpha$.
We are now reduced to a problem which depends only on α through $\mathcal{C} = \mathcal{C}_\alpha$.
The last step is in the proof of the following

Lemma 7.5.6 *:*
There exists h_0, such that, for all m and all $\mathcal{C}$, for all $u \in C_0^\infty(I\!R^m)$, we have

$$\begin{array}{l} \langle \left(-h^2 \Delta_y \ + \ \frac{a}{2} \sum_{k=1}^{m} (y_k - y_{k+1})^2 + \frac{v''(s)}{2} \sum_{k \notin \mathcal{C}} y_k^2 \ + \ \delta . n_{\mathcal{C}} . h^{\frac{4}{5}} \right) u \mid u \rangle \\ \quad \geq h . \lambda^{app.}(m) ||u||^2 \end{array} \tag{7.5.27}$$

Proof:
Because we know explicitly the spectrum of the harmonic oscillator, we have to prove:

$$h \ \text{Tr} \ (Q_{\mathcal{C}}^{\frac{1}{2}}) + \delta \cdot n_{\mathcal{C}} \cdot h^{\frac{4}{5}} \geq h \ \text{Tr} \ (Q^{\frac{1}{2}}) \tag{7.5.28}$$

where $Q_{\mathcal{C}}$ is the matrix attached to the quadratic form

$$Q_{\mathcal{C}}(y) = \frac{a}{2} \sum_{k=1}^{m} (y_k - y_{k+1})^2 + \frac{v''(s)}{2} \sum_{k \notin \mathcal{C}} y_k^2 \ .$$

The problem is of course to control the uniformity with respect to m. We shall now prove the existence of C_0, such that, for all m and $\mathcal{C}$

$$\text{Tr} \ (Q_{\mathcal{C}}^{\frac{1}{2}}) + n_{\mathcal{C}} \cdot C_0 \geq \ \text{Tr} \ (Q^{\frac{1}{2}}) \ , \tag{7.5.29}$$

It is then not difficult to deduce that (7.5.24) is satisfied for $h \leq (\frac{\delta}{C_0})^5$.

We give an indirect proof of (7.5.29) by coming back to the corresponding harmonic oscillators. We recall that, for every quadratic form $\mathcal{Q}$, we have

$$\text{Tr } (\mathcal{Q}^{\frac{1}{2}}) = \inf_{||u||=1} \langle (-\Delta + \mathcal{Q})u \mid u \rangle \tag{7.5.30}$$

where the norms and the scalar products are taken in L^2.
We now work on $\mathbb{Z}/m \cdot \mathbb{Z}$ identified with $\{1, ..., m\}$. We have a natural notion of interval induced by $\mathbb{R}/m \cdot \mathbb{Z}$. We now write $\{1, ..., m\} \setminus \mathcal{C}$ as a union of disjoint maximal intervals I_ℓ

$$\{1, ..., m\} \setminus \mathcal{C} = \cup I_\ell \; . \tag{7.5.31}$$

We shall minorize by a decoupled potential where there are no interaction between the intervals I_ℓ. We have

$$\text{Tr } (Q_{\mathcal{C}}^{\frac{1}{2}}) \geq \sum_\ell \text{ Tr } (\tilde{Q}_{I_\ell}^{\frac{1}{2}}) \tag{7.5.32}$$

where for all interval I we have defined

$$\tilde{Q}_I(x) = \sum_{k \in \tilde{I}} \frac{a}{2}(x_k - x_{k+1})^2 \; + \; \frac{v''(s)}{2} \sum_{k \in I} x_k^2 \tag{7.5.33}$$

with $\tilde{I} = \{k \in I \; , \; s.t \quad k+1 \in I\}$.
Let us admit for a moment the following lemma

Lemma 7.5.7 *:*
There exists a constant C_1 such that, for all I, we have

$$| \;\; Tr \; (\tilde{Q}_I^{\frac{1}{2}}) - \lambda^{app.}(n_I)| \leq C_1 \; . \tag{7.5.34}$$

We recall also the lemma

Lemma 7.5.8 *:*
There exists $\lambda_0 > 0$ such that

$$\lambda^{app.}(p) = p \cdot \lambda_0 + \mathcal{O}(1/p) \; . \tag{7.5.35}$$

Proof:
This is just a version of the Euler-Mac Laurin Formula on Riemann sums (or a variation of the result on the thermodynamic limit given previously).
Note that, because of the invariance by circular permutation, we shall actually prove the nicer

$$\lambda^{app.}(p) = p \cdot \lambda_0 + \mathcal{O}(\exp -\kappa p) \ , \tag{7.5.36}$$

for some $\kappa > 0$.
We have to compare

$$\frac{\mu(m)}{m} := (2m)^{-1} \sum_{k=0}^{m-1} (1 - \alpha \cos(2\pi k/m))^{\frac{1}{2}} \ , \tag{7.5.37}$$

and the corresponding integral

$$(4\pi)^{-1} \int_0^{2\pi} (1 - \alpha \cos\theta)^{\frac{1}{2}} d\theta \ . \tag{7.5.38}$$

Let $v(\theta) = (1 - \alpha\cos\theta)^{\frac{1}{2}}$. Then the right hand side of (7.5.37) can be written as

$$\frac{1}{2} \int_0^{2\pi} v(\theta) u_m(\theta) d\theta \ , \tag{7.5.39}$$

with

$$u_m(\theta) = \sum_{k \in \mathbb{Z}} \frac{1}{m} \delta(\theta - 2\pi \frac{k}{m}) \ .$$

The Fourier coefficients of u_m are given by

$$\hat{u}_m(j) = \frac{1}{2\pi} \quad \text{if } \exp -ij\frac{2\pi}{m} = 1 \ ,$$

and

$$\hat{u}_m(j) = 0 \ ,$$

otherwise.
Using the Plancherel formula in (7.5.39), we get

$$\begin{array}{ll} \frac{\mu(m)}{m} & = \frac{1}{2} \sum_{\nu \in \mathbb{Z}} \hat{v}(\nu m) \\ & = \int_0^{2\pi} v(\theta) d\theta + \frac{1}{2} \sum_{\nu \neq 0} \hat{v}(\nu m) \ . \end{array} \tag{7.5.40}$$

Here

$$\hat{v}(\nu m) = (2\pi)^{-1} \int_0^{2\pi} v(\theta) \exp -i\nu m\theta \ d\theta \ .$$

and depending on the sign of ν, we shall deform the integration contour into the upper or the lower half plane. v (in our particular case) being holomorphic in a band $\theta \in [0, 2\pi] + i[-\epsilon, +\epsilon]$ for some $\epsilon > 0$, we get easily the exponential decay. Consequently (7.5.36) and a fortiori the weaker statement of the lemma are proved.

We now observe that,

$$\text{the number of intervals } \mathrm{I}_\ell \text{ is majorized by } n_{\mathcal{C}} \; . \tag{7.5.41}$$

We then deduce from (7.5.34) and (7.5.35) that

$$\mathrm{Tr}\ ((\tilde{Q}_{I_\ell})^{\frac{1}{2}}) \geq n_{I_\ell} \cdot \lambda_0 - C \; . \tag{7.5.42}$$

Summing up over all intervals, we get

$$\mathrm{Tr}\ (Q_{\mathcal{C}}^{\frac{1}{2}}) \geq (\sum_\ell n_{I_\ell}) \cdot \lambda_0 - C \cdot n_{\mathcal{C}} \geq (m\lambda_0) - C_1 \cdot (n_{\mathcal{C}} + 1) \; .$$

We then obtain the existence of a constant C_2 such that

$$\mathrm{Tr}\ (Q_{\mathcal{C}}^{\frac{1}{2}}) \geq \lambda^{app.}(m) - C_2 \cdot (n_{\mathcal{C}} + 1) \; .$$

We have also equality for $\mathcal{C} = \emptyset$, and consequently

$$\mathrm{Tr}\ (Q_{\mathcal{C}}^{\frac{1}{2}}) \geq \lambda^{app.}(m) - 2\, C_3 \cdot n_{\mathcal{C}} \; . \tag{7.5.43}$$

It remains only to prove Lemma 7.5.7.

Proof of Lemma 7.5.7:
We change a little the notation in order to come back to the case when $I = \{1, \dots, m\}$. We have now to compare the first eigenvalues $\tilde{\lambda}_{1,m}$ and $\hat{\lambda}_{1,m}$ of the two following operators on $L^2(I\!R^m)$

$$-\Delta + \frac{a}{2} \sum_{k=1}^{m-1} (x_k - x_{k+1})^2 + \frac{v''(s)}{2} \sum_{k=1}^{m} x_k^2 \; ,$$

and

$$-\Delta + \sum_{k=1}^{m} [\frac{a}{2}(x_k - x_{k+1})^2 + \frac{v''(s)}{2} x_k^2] \; .$$

We clearly have the inequality

$$\tilde{\lambda}_{1,m} \leq \hat{\lambda}_{1,m} \ .$$

We have consequently to find an upper bound on $\hat{\lambda}_{1,m}$. Let us consider the first normalized eigenfunction of the first operator $\tilde{\psi}_m$ and we have now to prove the existence of a constant $C_0 > 0$ such that for all m we have

$$\langle (x_1 - x_m)^2 \tilde{\psi}_m \mid \tilde{\psi}_m \rangle \leq C_0 \ . \tag{7.5.44}$$

We deduce (7.5.44) from

$$||x_1 \cdot \tilde{\psi}_m||^2 \leq \ C_1 \ , \tag{7.5.45}$$

and

$$||x_m \cdot \tilde{\psi}_m||^2 \leq \ C_1 \ . \tag{7.5.46}$$

We now diagonalize the quadratic form $\tilde{Q}_m(x)$ in the form

$$\tilde{Q}_m(x) = \sum_k \tilde{\omega}_k(m) y_k^2$$

We have

$$x_1 = \sum_k \tilde{a}_{1,k}(m) \cdot y_k \tag{7.5.47}$$

with the property that

$$\sum_k |\tilde{a}_{1,k}(m)|^2 = 1 \ . \tag{7.5.48}$$

We then deduce immediately

$$||x_1 \tilde{\psi}_m||^2 = \sum \tilde{\omega}_\ell(m)^{-\frac{1}{2}} |a_{1,\ell}|^2 \leq \tilde{\omega}_1(m)^{-\frac{1}{2}} \ . \tag{7.5.49}$$

It remains only to verify that every eigenvalue of the matrix associated to $\tilde{Q}_m$ is estimated from below independently of m. But this follows immediately of the lower bound

$$\frac{a}{2} \sum_{k=1}^{m-1} (x_k - x_{k+1})^2 + \sum_{k=1}^{m} \frac{v''(s)}{2} x_k^2 \geq \frac{v''(s)}{2} \sum_{k=1}^{m} x_k^2 \ . \tag{7.5.50}$$

The proof of (7.5.46) is the same.

A simpler proof [30] of (7.5.29).
A simpler proof can take better in account the algebraic structure of the problem. It is a direct consequence of the following algebraic lemma

Lemma 7.5.9 *:*
Let A and B two real symmetric positive $p \times p$ matrices such that

- *A is definite positive*
- *$A - B$ is positive .*

Then

$$Tr\,[A^{\frac{1}{2}} - B^{\frac{1}{2}}] \leq \frac{1}{\sigma}||A - B||_{Tr}\ , \tag{7.5.51}$$

where σ is the smallest eigenvalue of $A^{\frac{1}{2}} + B^{\frac{1}{2}}$.

Proof:
The proof is based on a tricky commutator argument. We write

$$A^{\frac{1}{2}} - B^{\frac{1}{2}} = \left(A - B + [A^{\frac{1}{2}}\ ,\ B^{\frac{1}{2}}]\right)\left(A^{\frac{1}{2}} + B^{\frac{1}{2}}\right)^{-1}\ ,$$

and similarly

$$A^{\frac{1}{2}} - B^{\frac{1}{2}} = \left(A^{\frac{1}{2}} + B^{\frac{1}{2}}\right)^{-1}\left(A - B - [A^{\frac{1}{2}}\ ,\ B^{\frac{1}{2}}]\right)\ .$$

Let us now take the trace of the sum and use the cyclicity of the trace. We get immediately

$$\mathrm{Tr}\ (A^{\frac{1}{2}} - B^{\frac{1}{2}})\ \ =\ \ \mathrm{Tr}\ \left(\left(A^{\frac{1}{2}} + B^{\frac{1}{2}}\right)^{-1}(A - B)\right)\ .$$

So we obtain the estimate (7.5.51).
We can then apply the Lemma with $A = Q$ and $B = Q_{\mathcal{C}}$. We observe that

$$||A - B||_{Tr} = v''(s)\ n_{\mathcal{C}}$$

and we can choose

$$\sigma = (v''(s))^{\frac{1}{2}}\ .$$

We then get the following improvement of (7.5.29):

$$\mathrm{Tr}\ \ Q^{\frac{1}{2}} \leq\ \mathrm{Tr}\ \ Q_{\mathcal{C}}^{\frac{1}{2}} + n_{\mathcal{C}}(v''(s))^{\frac{1}{2}}\ . \tag{7.5.52}$$

[30] This proof was communicated to us by F. Nier who discussed about the proof with C. Gérard. Many thanks for this improvement.

7.6 Harmonic approximation for the transfer operator

We have already presented the quadratic case. The aim of this subsection is to prove in the same spirit why the harmonic approximation at the bottom is valid in the case of the transfer operator. We consider the operator

$$K_V^h = \exp -\frac{V}{2h} \cdot \exp \frac{h}{a}\Delta \cdot \exp -\frac{V}{2h} \,, \tag{7.6.1}$$

whose distribution kernel is

$$K_V^h(x,y) = h^{-\frac{p}{2}} \exp -\frac{1}{h}\left(\frac{V(x)}{2} + \frac{a}{4}|x-y|^2 + \frac{V(y)}{2}\right) \,. \tag{7.6.2}$$

We shall prove

Proposition 7.6.1 *:*
Let us assume that V is symmetric

$$V(-x) = V(x) \,,$$

has one or two non degenerate minima $\pm x_c$ such that

$$V(x_c) = 0 \,.$$

Let us also assume that V satisfies [31] *for some $C > 0$*

$$V(x) \geq \frac{1}{C}|x|^{\frac{1}{C}} - C$$

and that, for some $\rho > 0$, for suitable constants C_α,

$$|\partial_x^\alpha V(x)| \leq C_\alpha \langle V(x)\rangle^{(1-\rho|\alpha|)_+} \,.$$

Then the largest eigenvalue $\mu_1(h)$ of the operator K_V^h satisfies

$$\lim_{h\to\infty} \mu_1(h) = \mu_1^0 \tag{7.6.3}$$

where μ_1^0 is the largest eigenvalue corresponding to the harmonic Kac operator

$$K_{V_0} = \exp -\frac{V_0}{2} \cdot \exp \Delta \cdot \exp -\frac{V_0}{2} \,. \tag{7.6.4}$$

[31] These assumptions are not optimal!

Here we observe that the last operator is unitary equivalent (use the scaling $x = h^{\frac{1}{2}} y$) to the h-dependent

$$K_{V_0}^h = \exp -\frac{V_0}{2h} \cdot \exp h\Delta \cdot \exp -\frac{V_0}{2h} \, .$$

The lower bound:
We start from the mini-max principle

$$\mu_1(h) = \sup_{\{u \mid ||u||=1\}} \langle K_V^h u, u \rangle \, .$$

The upper bound follows then from a good choice of u. We take the following choice. If u_0 is the first normalized positive eigenfunction of K_{V_0} (this is a gaussian), we introduce $u_0^h(x) := h^{-\frac{p}{2}} u_0(\frac{(x-x_c)}{h^{\frac{1}{2}}})$ and compute $\langle K_V^h u_0^h, u_0^h \rangle$ by the Laplace integral method. The minimum of the phase is obtained for $x = y = x_c$ and it is easy to see that

$$\begin{aligned} \langle K_V^h u_0^h, u_0^h \rangle &= \langle K_{V_0}^h u_0^h, u_0^h \rangle + \mathcal{O}(h) \\ &= \langle K_{V_0} u_0, u_0 \rangle + \mathcal{O}(h) \, . \end{aligned}$$

Here we have used a dilation between the first line and the second line.
So we have obtained

$$\mu_1(h) \geq \mu_1^0 - Ch \tag{7.6.5}$$

for a suitable constant C. This gives the lower bound.

Exercise 7.6.2 *:*
Control [32] *the proof with respect to p in the case when*

$$V(x) = \sum_i v(x_i) + \frac{b}{4} \sum_i |x_i - x_{i+1}|^2$$

One is actually more interested in a control of $-\ln \mu_1(h)/p$.

The upper bound
We will just establish the equivalent of the "IMS" decomposition. The first point is a general formula associated to any partition of unity ϕ_j satisfying

$$\sum_j \phi_j^2 = 1 \, .$$

[32] I have not verified if the exercise is easy!

We have

$$\langle K_V^h u, u\rangle = \sum_j \langle K_V^h \phi_j\, u\,,\, \phi_j\, u\rangle + \frac{1}{2}\sum_j \int [\phi_j(x)-\phi_j(y)]^2 K_V^h(x,y) u(x) u(y)\, dxdy\,. \tag{7.6.6}$$

We now take the same partition of unity as introduced for the Schrödinger operator.

Let us first control the error term.

Starting from

$$\phi_j(x) - \phi_j(y) = (x-y)\cdot \int_0^1 \nabla\phi_j(tx+(1-t)y)dt\,,$$

we get the estimate

$$\begin{array}{ll}(\phi_j(x)-\phi_j(y))^2 & \leq |x-y|^2 \cdot |\int_0^1 \nabla\phi_j(tx+(1-t)y)dt|^2 \\ & \leq |x-y|^2\cdot \int_0^1 |\nabla\phi_j(tx+(1-t)y)|^2 dt\,.\end{array}$$

Summing up over j, we obtain

$$\sum_j (\phi_j(x)-\phi_j(y))^2 \leq |x-y|^2 \cdot \int_0^1 \left[\sum_j |\nabla\phi_j(tx+(1-t)y)|^2\right] dt\,.$$

For our partition of unity, we get

$$\sum_j (\phi_j(x)-\phi_j(y))^2 \leq C\cdot |x-y|^2 \cdot h^{-\frac{4}{5}}\,. \tag{7.6.7}$$

The remainder estimate [33] is then obtained by giving an estimate from above in $\mathcal{L}(L^2)$ of the operator whose distribution kernel is

$$(x,y)\mapsto R_V^h(x,y) = |x-y|^2 K_V^h(x,y).$$

This is analyzed by the Schur lemma saying that for a symmetric kernel

$$||R_V^h||_{\mathcal{L}(L^2)} \leq \sup_x\Big(\int R_V^h(x,y)dy\Big)\,.$$

[33] In all our estimates, we can assume that u is positive (we know that the maximum is obtained for a positive u) and the upper bound on the kernel is justified.

We have consequently just to compute

$$h^{-\frac{p}{2}} \int_y |x-y|^2 \exp -\frac{1}{h}\left(\frac{V(x)}{2} + \frac{a}{4}|x-y|^2 + \frac{V(y)}{2}\right)\, dy\ ,$$

which is majorized by

$$h^{-\frac{p}{2}} \int_y |x-y|^2 \exp -\frac{1}{h}\left(\frac{V(x)}{2} + \frac{a}{4}|x-y|^2\right)\, dy\ .$$

This gives

$$(\int R_V^h(x,y)dy) \leq Ch \exp -\frac{V(x)}{2h}$$

and finally

$$||R_V^h||_{\mathcal{L}(L^2)} \leq Ch\ . \tag{7.6.8}$$

Putting together (7.6.8) and (7.6.7), we finally obtain for the remainder

$$|\frac{1}{2}\sum_j \int [\phi_j(x) - \phi_j(y)]^2 K_V^h(x,y)u(x)u(y)\, dxdy| \leq Ch^{\frac{1}{5}}||u||^2 \tag{7.6.9}$$

Terms corresponding to the harmonic approximation:

We now take $j = \pm 1$ and consider the operator K_V^h restricted to functions with support in say $|x - x_c| \leq h^{\frac{2}{5}}$. We then observe using the harmonic approximation and limiting ourselves to $u \geq 0$ that

$$\begin{aligned} \langle K_V^h \phi_{\pm 1} u, \phi_{\pm 1} u\rangle &\leq \exp Ch^{\frac{1}{5}} \langle K_{V_0}^h \phi_{\pm 1} u, \phi_{\pm 1} u\rangle \\ &\leq \mu_1^0 \cdot \exp Ch^{\frac{1}{5}} ||\phi_{\pm 1} u||^2\ . \end{aligned} \tag{7.6.10}$$

It remains now to estimate from above $\langle K_V^h \phi_0 u, \phi_0 u\rangle$. One easily gets that

$$\langle K_V^h \phi_0 u, \phi_0 u\rangle \leq C \exp -\delta h^{-\frac{1}{5}} ||\phi_0 u||^2\ . \tag{7.6.11}$$

Putting everything together, we have proved the estimate

$$\langle K_V^h u, u\rangle \leq \mu_1^0 (1 + \mathcal{O}(h^{\frac{1}{5}}))||u||^2\ . \tag{7.6.12}$$

This estimate is quite analogous to what was obtained for the Schrödinger operator.

Remark 7.6.3 *:*
It would be interesting to control with respect with the dimension. This is not necessarily easy !

Exercise 7.6.4 *:*
Analyze in the same spirit the operator whose kernel is

$$(x,y) \mapsto h^{-p} \cdot \exp -\frac{V(x)}{2} \exp -\frac{|x-y|^2}{h^2} \exp -\frac{V(y)}{2} \ .$$

For the lower bound, use the Laplace method but use first the change of variables $u = x + y$, $v = x - y$.

8 Decay of the eigenfunctions and applications

8.1 Introduction

As we have already seen when comparing the spectrum of the harmonic oscillator and of the Schrödinger operator, it could be quite important to know **a priori** how the eigenfunction decays in the classically forbidden region. The Agmon's [Ag] estimates give a very efficient [34] way to control such a decay. This is unfortunately much more difficult with respect to the dimension. We refer to [He88] or to the original papers for details and complements.

8.2 Energy inequalities

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

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

Proposition 8.2.1 :
Let Ω be a bounded open domain in $I\!R^m$ with C^2 boundary. Let $V \in C^0(\bar{\Omega}; I\!R)$ and ϕ a real valued lipschitzian function on $\bar{\Omega}$. Then, for any $u \in C^2(\bar{\Omega}; I\!R)$ with $u_{/\partial\Omega} = 0$, we have

$$\begin{aligned} h^2 \textstyle\int_\Omega |\nabla(\exp\phi/h\ u)|^2\ dx + \int_\Omega (V - |\nabla\phi|^2)\exp 2\phi/h\ u^2\ dx = \\ \textstyle\int_\Omega \exp 2\phi/h\ (S_h u)(x)\cdot u(x)\ dx\ . \end{aligned} \tag{8.2.1}$$

Proof:
In the case when ϕ is a $C^2(\bar{\Omega})$- function, this is an immediate consequence of the Green-Riemann formula

$$\int_\Omega |\nabla v|^2 dx = -\int_\Omega \Delta v\cdot v\, dx\ , \tag{8.2.2}$$

for all $v \in C^2(\bar{\Omega})$ such that $v_{/\partial\Omega} = 0$.
This can actually be extended to $u \in H_0^1(\Omega)$.
To treat the general case, we just write ϕ as a limit as $\epsilon \to 0$ of $\phi_\epsilon = \chi_\epsilon \star \phi$ where $\chi_\epsilon(x) = \chi(\frac{x}{\epsilon})\,\epsilon^{-m}$ is the standard mollifier and we remark that $\nabla\phi$ is almost everywhere the limit of $\nabla\phi_\epsilon = \nabla\chi_\epsilon \star \phi$.

[34] cf the contributions of Helffer-Sjöstrand [HeSj84-87] and Simon [Si84] in the 80's. The reader can also look at the historical notes in Reed-Simon [ReSi78] (p. 355-356) for older results concerning the decay of eigenfunctions.

8.3 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 $I\!R^n$. This metric is degenerated 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 of the length of piecewise C^1 paths connecting x and y:

$$d_{(V-E)_+}(x,y) = \inf_{\left\{\begin{array}{c}\gamma\\ \gamma(0)=x\ ,\ \gamma(1)=y\end{array}\right\}} \int_0^1 [(V(\gamma(t))-E)_+]^{\frac{1}{2}} |\gamma'(t)| dt\ . \tag{8.3.1}$$

When there is no ambiguity, we shall write more simply $d_{(V-E)_+} = d$. Similarly to the Euclidean case, we obtain the following properties

- Triangular inequality
$$|d(x',y)-d(x,y)| \leq d(x',x)\ ,\ \forall x,x',y \in I\!R^m \tag{8.3.2}$$

- $$|\nabla_x d(x,y)|^2 \leq (V-E)_+(x)\ a.e.\ x\ . \tag{8.3.3}$$

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

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

The most useful case will be the case when U is the set $\{x \mid V(x) \leq E\}$. We then measure through $d(x,U)$ the distance to the classical region.

8.4 Decay of eigenfunctions for the Schrödinger operator.

When u_h is a normalized eigenfunction of the Dirichlet realization in Ω satisfying $S_h u_h = \lambda(h) u_h$ then (8.2.1) gives roughly that $\exp\phi/h\ u_h$ is well controlled (in L^2) in a region

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

by $\exp\left(\sup_{\Omega\setminus\Omega_1}\phi(x)/h\right)$. 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

$$\exp(1-\epsilon)d(x)/h\; u_h = \mathcal{O}(\exp\epsilon/h)\;, \tag{8.4.1}$$

for any $\epsilon > 0$.
More precisely we get for example the following theorem

Theorem 8.4.1 *:*
Let us assume that V is C^∞, semibounded and satisfies

$$\lim\inf_{|x|\to\infty} V > \inf V = 0 \tag{8.4.2}$$

and

$$V(x) > 0 \;\; \textit{for } |x| \neq 0\;. \tag{8.4.3}$$

Let u_h be a (family of) normalized eigenfunctions such that

$$S_V(h)u_h = \lambda_h u_h\;, \tag{8.4.4}$$

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

$$||\nabla(\exp d/h \cdot u_h)||_{L^2(K)} + ||\exp d/h \cdot u_h||_{L^2(K)} \leq C_{\epsilon,K}\exp\epsilon/h \tag{8.4.5}$$

where $x \to d(x)$ is the Agmon distance between x and 0 attached to the Agmon metric $V\cdot dx^2$.

Useful improvements in the case when $E = \min V$ and when the minima are non degenerate can be obtained by controlling more carefully with respect to h. It is also possible to control the eigenfunction at ∞. This was actually the initial goal of S. Agmon [Ag]

Proof:
Let us choose some $\epsilon > 0$. We shall use the identity (8.2.1) with

- V replaced by $V - \lambda_h$,
- $\phi = (1-\delta) d(x,U)$, with δ small enough depending on ϵ,
- $u = u_h$, and
- $S_h = -h^2\Delta + V - \lambda_h$.

Let
$$\Omega_\delta^+ = \{x \in \Omega\ ,\ V(x) \geq \delta\}$$
and
$$\Omega_\delta^- = \{x \in \Omega\ ,\ V(x) < \delta\}\ .$$
We deduce from (8.2.1)
$$\begin{array}{l} h^2 \int_\Omega |\nabla(\exp \frac{\phi}{h} u_h)|^2 dx + \int_{\Omega_\delta^+} (V - \lambda_h - |\nabla \phi|^2) \exp \frac{2\phi}{h}\, u_h^2\, dx \\ \qquad \leq \sup_{x\in\Omega_\delta^-} |V(x) - \lambda_h - |\nabla\phi|^2| \left(\int_{\Omega_\delta^-} \exp \frac{2\phi}{h}\, u_h^2\, dx\right)\ . \end{array}$$
Then, for some constant C independent of $h \in]0,h_0]$ and $\delta \in]0,1]$, we get
$$\begin{array}{l} h^2 \int_\Omega |\nabla(\exp \frac{\phi}{h} u_h)|^2 dx + \int_{\Omega_\delta^+} (V - \lambda_h - |\nabla \phi|^2) \exp \frac{2\phi}{h}\, u_h^2\, dx \\ \qquad \leq C \cdot \left(\int_{\Omega_\delta^-} \exp \frac{2\phi}{h}\, u_h^2\, dx\right)\ . \end{array}$$
Let us observe now that on Ω_δ^+ we have (with $\phi = (1-\delta)d(\cdot,U)$)
$$V - \lambda_h - |\nabla\phi|^2 \geq (2-\delta)\delta^2 + o(1)\ .$$
Choosing $h(\delta)$ small enough, we then get for any $h \in]0, h(\delta)]$
$$V - \lambda_h - |\nabla\phi|^2 \geq \delta^2\ .$$
This permits to get the estimate
$$\begin{array}{l} h^2 \int_\Omega |\nabla(\exp \frac{\phi}{h} u_h)|^2 dx + \delta^2 \int_{\Omega_\delta^+} \exp \frac{2\phi}{h}\, u_h^2\, dx \\ \qquad \leq C \cdot \left(\int_{\Omega_\delta^-} \exp \frac{2\phi}{h}\, u_h^2\, dx\right)\ , \end{array}$$
and finally
$$\begin{array}{l} h^2 \int_\Omega |\nabla(\exp \frac{\phi}{h} u_h)|^2 dx + \delta^2 \int_{\Omega} \exp \frac{2\phi}{h}\, u_h^2\, dx \\ \qquad \leq \tilde{C} \cdot \exp \frac{a(\delta)}{h}\ , \end{array}$$

where $a(\delta) = 2 \sup_{x \in \Omega_\delta^-} \phi(x)$. We now observe that $\lim_{\delta \to 0} a(\delta) = 0$ and the end of the proof is then easy.

Applications:
As a first corollary, we can compare different Dirichlet problems corresponding to different open sets Ω_1 and Ω_2 containing a unique well U attached to an energy E. If for example $\Omega_1 \subset \Omega_2$, one can prove the existence of a bijection b between the spectrum of $S_{(h,\Omega_1)}$ in an interval $I(h)$ tending (as $h \to 0$) to E and the corresponding spectrum of $S_{(h,\Omega_2)}$ such that $|b(\lambda) - \lambda| = \mathcal{O}(\exp -S/h)$ (under a weak assumption on the spectrum at $\partial I(h)$). S is here any constant such that

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

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

8.5 Splitting between the two first eigenvalues

The control of the decay of the eigenfunctions has also immediate consequences on the splitting. To understand what is needed, let us recall the following classical formula for the splitting which is nothing else than a version of the minimax principle applied to the orthogonal of $I\!R \cdot u_1$,

$$\lambda_2 - \lambda_1 = \inf_{\left\{ \begin{array}{c} \phi \ ; \ \phi \in C_0^\infty \ , \\ \int \phi(x)\, u_1^{(m)}(x)^2\, dx = 0 \end{array} \right\}} \left[\left(\int |h \nabla \phi|^2 \, u_1^{(m)}(x)^2 \, dx \right) / \left(\int |\phi|^2 \, u_1^{(m)}(x)^2 \, dx \right) \right] \ . \tag{8.5.1}$$

Here $u_1^{(m)}$ denotes the first normalized eigenfunction of the Schrödinger operator. The estimates about the splitting are then deduced from a good choice of ϕ and from a precise information on the decay of $u_1^{(m)}$ in suitable domains.

We first begin by an exercise which is not related to the tunneling effect but gives a universal estimate for the splitting. We take here $h = 1$ and $\phi(x) = x_i$. We assume to simplify that the potential V is symmetric. Then the formula above gives (modulo an argument of regularization [35] because the map $x \mapsto x_i$

[35] Consider the sequence $x \mapsto x_i \theta(\frac{|x|}{n})$ and let $n \to \infty$ in what is obtained.

does not belong to C_0^∞)

$$\lambda_2 - \lambda_1 \leq \frac{1}{\int |x_i|^2 \, u_1^{(m)}(x)^2 \, dx} \ . \tag{8.5.2}$$

Using the uncertainty principle,

$$||tu||_{L^2(I\!R)} \cdot ||u'||_{L^2(I\!R)} \geq 1 \ , \ \forall u \in \mathcal{S}(I\!R) \ ,$$

we get

$$\lambda_2 - \lambda_1 \leq \int |\partial_{x_i} \, u_1^{(m)}(x)|^2 \, dx \ . \tag{8.5.3}$$

Summing over i we get the more symmetric

$$\lambda_2 - \lambda_1 \leq \frac{1}{m} \int (-\Delta u_1^{(m)}(x)) \cdot u_1^{(m)}(x)) \, dx \ , \tag{8.5.4}$$

and if $V^{(m)}$ is positive

$$\lambda_2 - \lambda_1 \leq \frac{\lambda_1(m)}{m} \ . \tag{8.5.5}$$

This is a well known inequality due to Payne-Polya-Weinberger [PPW56].

Let us now consider the double well situation. The potential v is symmetric and has two non degenerate minima. We now choose a function ϕ in C_0^∞ which satisfies

$$\phi(x) = -\phi(-x)$$

and

$$\phi = 1$$

in a neighborhood of the critical point x_c of V. We recall also that the first eigenfunction is even

$$u_1^{(m)}(x) = u_1^{(m)}(-x) \ .$$

We have used here that the first eigenvalue is simple and that the first eigenfunction can be chosen strictly positive (Perron-Frobenius argument).
As a consequence we have effectively

$$\int \phi(x) u_1^{(m)}(x)^2 dx = 0 \ .$$

We observe also using the Agmon estimates that

$$\int \phi(x)^2 u_1^{(m)}(x)^2 \, dx = 1 + \mathcal{O}(\exp -\frac{S}{h}) \, ,$$

and that

$$\int |\nabla \phi(x)|^2 u_1^{(m)}(x)^2 dx = \mathcal{O}(\exp -\frac{S}{h}) \, ,$$

for some $S > 0$. Coming back to the formula giving the splitting we obtain

$$\lambda_2 - \lambda_1 = \mathcal{O}(\exp -\frac{S}{h}) \, . \tag{8.5.6}$$

In the situation of a symmetric double well, we have consequently two eigenvalues whose difference is exponentially small.

Exercise 8.5.1 *:*
According to the result concerning the decay of the first eigenfunction, show that S can be seen as any real number such that

$$S < d_{(V-E)_+}(x_c, -x_c) \, .$$

Remark 8.5.2 *:*
In some generical cases, one can actually give a more precise estimate for the splitting in the form

$$\lambda_2 - \lambda_1 = h^{\frac{1}{2}} A_m(h)(\exp -\frac{S_m}{h}) \, , \tag{8.5.7}$$

where S_m is the Agmon's distance between the two wells and $A_m(h)$ is a non zero function admitting an expansion of the type $A_m(h) \sim \sum_j a_{m,j} h^j$. This was obtained[36] *in this form in [HeSj84-87] and in a weaker form but*

[36] The rigorous study of the splitting (which was present very soon after the beginning of the foundations of the Quantum mechanics, see Landau-Lifschitz [LaLi74]) was motivated, as is for example mentioned in the notes of Reed-Simon [ReSi78] (p. 62-63), by the problems posed by M. Kac [KaTho69]. In the case $m = 1$, the first rigorous proof seems to be given by E. Harrell [Ha80], using the theory of ordinary differential equations, see also Combes-Duclos-Seiler [CDS91].
We just mention the "Instantons" method as for example presented by Coleman [Co77] which did not lead to completely rigorous proofs untill more recently [Hard88].
We emphasize that the "difficult" part in the study of the splitting is to get a lower bound.

sooner by Jona-Lasinio, Martinelli, Scoppola [J.LMS81] and B. Simon [Si84]. Independently a rather sketchy proof was given by V.P. Maslov [Mas84]. This result was already announced at the international conference in Warshaw (1983), (See later more rigorous versions of this proof in [DoKoMa91]) who refers to previous work by himself in 1977 and to Polyakov.
A good control with respect to the dimension is still an open problem. See however the so called instructive example given before where, in a particular case, the explicit dependence with respect to the dimension can be obtained. It is hoped for example the (DK) model that (8.5.7) is true with $S_m = mS_1$ and for $h \leq h_0$ with h_0 independent of m. The Ising model with transverse field presented in Subsection 2.5 suggests that it can be true. S.Y. Dobrokhotov and Kolokoltsov propose formal results in [DoKo93] and [DoKo94]. Helffer-Sjöstrand obtained for the model (K) (and for $\nu > \nu_c$) the weaker

$$\lambda_2 - \lambda_1 \leq \exp -(\frac{\epsilon m}{h}) \,, \tag{8.5.8}$$

for some $\epsilon > 0$ but for $m \leq Ch^{-N_0}$.This does not permit to take the limit $m \to +\infty$. The extension of the result to the (DK) model was presented in [He94e] which gives more precise results on this subject. Let us also observe that this restriction is also not present in the recent contribution of V.S. Barbulyak and Yu. G. Kondrat'ev [BaKo92] on a connected problem.

8.6 Decay for the eigenfunctions of the transfer operator

8.6.1 Preliminary remarks

As already used in the preceding subsection, the first eigenfunction u_1 can be chosen as strictly positive. The potential on $I\!R^p$ V being even, we get also

$$u_1(x) = u_1(-x) \,. \tag{8.6.1}$$

We keep also the assumptions that

$$V \geq 0 \,,$$

$$\frac{1}{C}|x|^2 - C \leq V(x) \leq C(|x|^2 + 1)$$

and V has one or two nondegenerate minima, with $V = 0$.

We now write that u_1 is the first normalized eigenfunction in the form

$$u_1(x;h) = \frac{1}{\mu_1(h)} \int K_V(x,y;h) u_1(y;h) dy \; . \tag{8.6.2}$$

Using Cauchy-Schwarz, we get immediately

$$O < u_1(x;h) \leq \alpha^{-1} (\int K_V(x,y)^2 dy)^{\frac{1}{2}} \tag{8.6.3}$$

We get immediately the following estimate

$$O < u_1(x;h) \leq C \cdot h^{-\frac{p}{4}} \cdot \exp - \frac{V(x)}{2h} \; . \tag{8.6.4}$$

This means that the eigenfunction is strongly localized near the minima of V. This will permit to used cutoff function in order to construct quasimodes attached to each well. We observe here that we are working with operators which are not local, but pseudolocal in a weak sense. The pseudolocality is obtained through the interaction term $\frac{a}{h} \cdot |x-y|^2$. This is a weaker pseudolocality than the pseudolocality observed in the semi-classical study of the Kac operator where the pseudolocality was obtained through an interaction in $\frac{1}{h^2} \cdot |x-y|^2$. This will change the properties and the way of thinking for this problem. The case a large will be more reminiscent of the semiclassical case as we shall see in the next subsubsection.

8.6.2 Improved decay estimates, comparison with the semiclassical results.

We just sketch some improvements and discuss for a large the connexion with the Agmon distance measuring the decay in the semi-classical situation.

Our starting point is (8.6.4). We immediately observe that we can implement this upper bound in (8.6.2) and we get for any compact K the estimate from above

$$0 < u_1(x;h) \leq C_K \cdot h^{-\frac{3p}{4}} \exp - \phi_1(x)/h \; , \; \forall x \in K$$

with

$$\phi_1(x) = \frac{1}{2} V(x) + \inf_y [\frac{a}{4}(x-y)^2 + V(y)] \; .$$

We see that it is strictly better, and we observe the inequalities

$$\frac{1}{2}V(x) \leq \phi_1(x) \leq \frac{1}{2}V(x) + \frac{a}{4} \text{ dist } (x, \{\pm x_c\})^2 .$$

We see that it is strictly better that what was obtained in (8.6.4).

If we try to iterate, we finally are interested in the largest function $\phi_\infty(x)$ which satisfies

$$|\phi_\infty(x) - \phi_\infty(y)| \leq \frac{1}{2}V(x) + \frac{a}{4}|x-y|^2 + \frac{1}{2}V(y) . \tag{8.6.5}$$

This will be indeed the natural candidate for measuring the decay.

One has actually a natural construction in order to get this function. We define $\phi_0 = \frac{V}{2}$ and ϕ_1 as before and introduce by recursion

$$\phi_n(x) = \frac{V(x)}{2} + \inf_y [\frac{V(y)}{2} + \frac{a}{4}|x-y|^2 + \phi_{n-1}(y)] .$$

It is easy to see that this sequence is increasing with respect to n and that

$$\frac{1}{2}V(x) \leq \phi_n(x) \leq \frac{1}{2}V(x) + \frac{a}{4} \text{ dist } (x, \{\pm x_c\})^2 .$$

We can then define the limit $\phi_\infty(x)$ which satisfies

$$\phi_\infty(x) = \frac{V(x)}{2} + \inf_y [\frac{V(y)}{2} + \frac{a}{4}|x-y|^2 + \phi_\infty(y)] .$$

This limit can be seen as locally Lipschitzian. For the proof we observe that $x \mapsto |x-y|^2$ has this property and that for any compact F in $I\!R^p$ then there exists another compact F' such that, for all n and for all $x \in F$ the minimum $\inf_y(\frac{V(y)}{2} + \frac{a}{4}|x-y|^2 + \phi_n(y))$ is attained at a point y_n in F'. This function can play the role of the distance to the minima of V and gives a good measure of the decay of the first eigenfunction.

The case a large, or the come back of the Agmon distance:

The other case of interest is the case when a is large. We now consider a function $d_\infty(x)$ such that

$$|\nabla d_\infty(x)|^2 \leq V(x) \quad a.e \ , \ d_\infty(\pm x_c) = 0 \ , \ d_\infty \geq 0.$$

We recognize here that the Agmon distance to the minimas satisfies these conditions and we observe in this case that, for any $\epsilon > 0$, $(1-\epsilon)a^{\frac{1}{2}}d_\infty(x)$ satisfies (8.6.5) for a large enough.
We have indeed (assuming Hess V bounded)

$$\begin{aligned} |d_\infty(x) - d_\infty(y)| & \leq \tfrac{1}{2}|x-y|[|\nabla d_\infty(x)| + |\nabla d_\infty(y)|]) + \mathcal{O}(|x-y|^2) \\ & \leq \tfrac{V(x)}{2\sqrt{a}} + \tfrac{V(y)}{2\sqrt{a}} + \tfrac{\sqrt{a}}{4}|x-y|^2 + \mathcal{O}(|x-y|^2) \end{aligned}$$

Multipling by $(1-\epsilon)a^{\frac{1}{2}}$ it is easy to conclude.

8.6.3 The quadratic case

The explicit computation when V is quadratic and $p = 1$ ($v(x) = \frac{c}{2} \cdot x^2$) is also enlightning. We are looking for a solution of:

$$\phi_\infty(x) = \inf_y \frac{1}{4}(x^2 + a|x-y|^2 + y^2) + \phi_\infty(y) \ .$$

It is rather clear from our construction that $\phi_\infty(x)$ is quadratic and we are consequently looking for b such that

$$\frac{1}{2} b\, x^2 = \inf_y \frac{1}{4}(c\, x^2 + a|x-y|^2 + c\, y^2) + \frac{1}{2} b\, y^2 \ .$$

An immediate computation gives that the minimum is obtained for $y = ax/(a+c+2b)$.

$$2b(a+c+2b) = c(a+c+2b) + a(c+2b) \ .$$

This is fortunately a second order equation whose unique positive solution is

$$b = \frac{1}{2}\sqrt{c(2a+c)} \ .$$

These computations are of course immediately related to the explicit computations we have done concerning the harmonic Kac operator which can be seen as $\exp S$ where S is an explicit harmonic oscillator.

9 WKB Constructions

9.1 Introduction

The WKB constructions are first constructed in order to find approximations for the lowest eigenvalues. We shall concentrate on the construction corresponding to the lowest level. The other important point in these WKB constructions is that they also permit to get a good approximation of the one-well eigenfunction and not only in a small neighborhood of the minimum. Although, this will not be analyzed in these notes[37]

We shall try to work in parallel with three different problems :

- the Schrödinger operator
- the Laplace integral
- the transfer operator

9.2 WKB for the Schrödinger operator, formal approach

9.2.1 WKB, first approach

We are looking for a WKB solution of the form

$$u^{wkb}(x;h) = h^{-\frac{p}{4}} a(x,h) \exp -\phi_0(x)/h \ ,$$

for the Schrödinger equation

$$S_V = -h^2\Delta + V(x) \ ,$$

in the neighborhood of a non degenerate minimum of the potential V defined on $I\!R^p$. The potential V is C^∞ , defined in an interval around the minimum which is assumed to be at 0. We precize that we are looking for a real positive phase ϕ_0 and for an amplitude admitting an expansion

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

[37]See the book [He88] and the original paper [HeSj84-87].

The research of a formal WKB solution corresponds to the simultaneous research of $a(x;h)$ and of $E(h) \sim \sum_{j=0}^{\infty} E_j\, h^j$ such that

$$(-h^2\Delta + V(x) - E(h))\,(a(\cdot,h)\exp -\phi_0(\cdot)/h) \sim 0$$

that is

$$(V - |\nabla\phi_0|^2)a + 2h\,\nabla\phi_0\cdot\nabla a - h\,\Delta a + h\,\Delta\phi_0\,a - E(h)a \sim 0\ . \qquad (9.2.1)$$

This leads first to

$$V(x) - |\nabla\phi_0(x)|^2 - E_0 = 0\ . \qquad (9.2.2)$$

This equation is called the eiconal equation. Assuming that a solution of this equation has been found, we then obtain a system of equations which we shall call transport equations

$$\begin{array}{lll}
(\mathrm{T}_1) & 2\nabla\phi_0(x)\cdot\nabla a_0 + (\Delta\phi_0 - E_1)a_0 & = 0\ ,\\
(\mathrm{T}_2) & 2\nabla\phi_0(x)\cdot\nabla a_1 + (\Delta\phi_0 - E_1)a_1 & = \Delta a_0 + E_2 a_0,\\
\cdot & & \\
\cdot & & \\
(\mathrm{T}_{\mathrm{k+1}}) & 2\nabla\phi_0(x)\cdot\nabla a_k + (\Delta\phi_0 - E_1)a_k & = \sum_{j=2}^{k} E_j\, a_{k+1-j}\\
 & \qquad + \Delta a_{k-1}\ +\ E_{k+1}\, a_0\ . &
\end{array} \qquad (9.2.3)$$

These equations have all the same structure. There is a real vector field X defined as

$$X = 2\nabla\phi_0\cdot\nabla$$

which will vanish at 0 (and this determine $E_0 = 0 = \min V$), a function $g = (\Delta\phi_0 - E_1)$ which has to vanish at 0 (and this will determine E_1, assuming that $a_0(0) = 1$) and a function f which will be either identically 0 (in the case of (T_1)) or which will be given by

$$f = \sum_{j=2}^{k} E_j a_{k+1-j} + \Delta a_{k-1} + E_{k+1} a_0\ ,$$

and will vanish at 0 and this will determine E_{k+1}.
We have then to solve

$$Xu + gu = f$$

with $u(0) = 1$ in the case of (T_1) and with $u(0) = 0$ in the other cases.
We shall see later how to solve these equations in the general case. In order to meet the difficulties in successive steps, let us first consider the one dimensional case.

9.2.2 The case of dimension $p = 1$

Let us first rewrite the eiconal equation. We get in dimension 1

$$\phi_0'(t)^2 = V(t)\ .$$

This gives explicitely

$$\phi_0(t) = \int_0^t \frac{s}{|s|} V^{\frac{1}{2}}(s)ds\ ,$$

which is clearly well defined and C^∞ in a neighborhood of 0. We recall that we take $E_0 = \min V = 0$. Let us now look at the transport equation

$$2\phi_0'(t)a_0'(t) + (E_1 - \phi_0''(t))a_0(t) = 0\ ,$$

with the initial condition

$$a_0(0) = 1\ .$$

E_1 is determined by

$$E_1 = \phi_0''(0)\ .$$

We can solve explicitely this ordinary differential equation by observing that

$$(\ln a_0)' = -\frac{1}{2}\frac{(E_1 - \phi_0''(t))}{\phi_0'(t)}\ .$$

All the other equations have the same structure and can be solved using the variation of constants.

9.2.3 The case of dimension $p \geq 1$

We consider a variant of the formal WKB method essentially adapted to the first eigenvalue. We are looking for a WKB solution of the form

$$u^{wkb}(x;h) = h^{-\frac{p}{4}} \exp -\phi(x,h)/h\ ,$$

for the Schrödinger equation

$$S_{(h,V)} = -h^2\Delta + V(x)\ ,$$

in the neighborhood of a non degenerate minimum of the potential V. The potential V is C^∞ , defined in some ball in $I\!\!R^p$. We precize that we are looking for a real phase ϕ admitting an expansion

$$\phi(x,h) \sim \sum_{j=0}^{\infty} h^j \ \phi_j(x)$$

and we observe that the form of the WKB solution is not exactly the standard one which was in the form

$$\hat{u}^{wkb}(x,h) = h^{-\frac{p}{4}} a(x,h) \exp -\phi_0(x)/h \ .$$

The choice of u^{wkb} is adapted to an approximation of the first eigenfunction and will permit a better control with respect to the dimension p. The construction will work well under the following assumptions

- $V(0) = \nabla V(0) = 0$,
- $V \in C^\infty(B(0,1); I\!\!R)$
- Hess $V(0) \geq \sigma > 0$

The research of a formal WKB solution corresponds to the simultaneous research of $\phi(x;h)$ and of $E(h) \sim \sum_{j=0}^{\infty} E_j \ h^j$ such that

$$(-h^2\Delta + V(x) - E(h)) \exp -\phi(x;h)/h \sim 0$$

that is

$$V - |\nabla\phi|^2 + h^2\Delta\phi - E(h) \sim 0 \ . \tag{9.2.4}$$

This leads to the following system of equations which we shall call "eiconal" equation for the first one and transport equations for the other.

$$\begin{array}{lll}
(\mathrm{E}) & V(x) - |\nabla\phi_0(x)|^2 & = 0 \ , \\
(\mathrm{T_1}) & 2\nabla\phi_0(x)\cdot\nabla\phi_1 & = \Delta\phi_0(x) - E_1 \ , \\
(\mathrm{T_2}) & 2\nabla\phi_0(x)\cdot\nabla\phi_2 & = \Delta\phi_1(x) - E_2 - |\nabla\phi_1|^2 \ , \\
\cdot & & \\
\cdot & & \\
(\mathrm{T_k}) & 2\nabla\phi_0(x)\cdot\nabla\phi_k & = \Delta\phi_{k-1}(x) - (\nabla\phi_1\cdot\nabla\phi_{k-1} \\
& & \qquad +\nabla\phi_2\cdot\nabla\phi_{k-2} + \cdots + \nabla\phi_{k-1}\cdot\nabla\phi_1) - E_k \ .
\end{array}$$

Again the equations take the form

$$Xu = f$$

but this time, we take the initial condition $u(0) = 0$. At each step, the necessary condition that the left hand side vanishes determines E_k.

9.3 WKB for the Laplace integral, formal approach

Let us assume that we are in the conditions to apply the Laplace method in the neighborhood of the point 0. We want to analyze a new proof for the existence of a complete expansion for which the control with respect to the dimension will be easier. We remain in this subsection to a very formal level.

Theorem 9.3.1 *:*
Let us assume that Φ is a C^∞ potential defined in a neighborhood of O in $I\!R^p$ such that

$$\Phi(0) = O\ ;\ \Phi \geq 0\ ;\quad \textit{Hess}\ \Phi(0) > 0\ .$$

Then there exists a formal series

$$f(x,h) \sim \sum_j f_j(x) \cdot h^j \tag{9.3.1}$$

and a series

$$E(h) \sim \sum_{j \geq 0} E_j \cdot h^j \tag{9.3.2}$$

s.t in the sense of the formal series in h but in a fixed sufficiently small neighborhood of 0 B , the following equation is satisfied

$$|\nabla f|^2 - \Phi - h \ln \det(\ \textit{Hess}\ f) \sim E(h)\ . \tag{9.3.3}$$

Of course this statement and the origin of the equation could appear mysterious and it is probably better to give the following " formal" corollary:

Corollary 9.3.2 *:*
If

$$J(h) := (1/h\pi)^{\frac{p}{2}} \cdot (\int \exp(-\frac{1}{h}\Phi(x))\ dx)\ ,$$

then, at the level of the formal expansions [38] *,*

$$(\ln J(h)) \sim h^{-1} \sum_j E_j \, h^j \ , \quad \text{as } h \to 0 \ . \tag{9.3.4}$$

Proof of the corollary:
This is just an application of the formal Laplace's method. The integral becomes

$$(1/h\pi)^{\frac{p}{2}} \cdot \left(\int \exp \left[-\frac{1}{h} \Phi(x) - \ln \det \ \text{Hess } f(x,h) \right] dy \right)$$

where we perform the change of variable

$$y = \nabla f(x,h) \ .$$

At least formally, it is then clear that Theorem 9.3.1, gives that

$$(1/\pi h)^{\frac{p}{2}} \cdot \left(\int \exp(-\frac{1}{h} \sum y_j^2 + \frac{1}{h} E(h)) \ dy \right)$$

So finally, using $\int \exp -y^2 dy = \sqrt{\pi}$,

$$\ln J^f(h) \sim h^{-1} E(h) \ .$$

Of course everything is for the moment formal but the control of the coefficients is what is basic for the future. Let us study the first terms of the expansion in powers of h. We take $E_0 = 0$ and the first equation is simply

$$|\nabla f_0|^2 = \Phi - E_0 = \Phi \ ,$$

which is the standard eiconal equation. The solution of the first eiconal equation corresponds actually to a proof of a special case of the Morse Lemma where the change of variable can be taken with the specific form $y = \nabla f(x)$. The second equation is

$$2 \nabla f_0 \cdot \nabla f_1 = \ln \det \ \text{Hess } f_0 - E_1$$

which is quite analogous to the transport equation (T_1) in the Schrödinger case. We get actually as in the Schrödinger case a complete expansion observing (in order to obtain the complete expansion) the following standard lemma

[38] This means that for the moment we have not controlled any remainder term. $J(h)$ is defined only at the level of the formal expansions given by the formal stationary phase theorem. We shall return later on to a control of the remainder terms. We prefer to write $J^f(h)$ or $J^{form}(h)$ when we speak of the formal expansion.

Lemma 9.3.3 *:*
Let $]-a,+a[\ni t\mapsto A(t)$ *a* C^1*-family of positive definite* $q\times q$ *symmetric matrices. Then we have*

$$\frac{d}{dt}\ln\det A(t) = \;Tr\;(A(t)^{-1}A'(t))\;. \tag{9.3.5}$$

9.4 WKB for the transfer operator, formal approach

9.4.1 Eiconal and transport equation

We want to produce WKB solution when we are near the minimum of the potential.
We have the following identities assuming that everything is differentiable. We start from

$$\phi(x)=\inf_y[\Theta(x,y)+\phi(y)]\;,$$

with

$$\Theta(x,y)=w(x,y)+\frac{v(x)}{2}+\frac{v(y)}{2}\;.$$

If we assume that the minimum is obtained for a unique regular $y(x)$ we get

$$\phi(x)=\Theta(x,y(x))+\phi(y(x))\;,$$

and

$$\partial_y\Theta(x,y(x))+\nabla\phi(y(x))=0\;.$$

Differentiating with respect to x, we first obtain

$$\nabla\phi(x)=\partial_x\Theta(x,y(x))\;.$$

We are looking for a Lagrangian manifold [39] $\Lambda_\phi=\{(x,\xi)\in I\!R^{2p}|\xi=\nabla\phi(x)\}$ which is invariant by the canonical relation attached to Θ:

$$C_\Theta=\{(x,\xi,y,\eta)\in I\!R^{4p}|\xi=\partial_x\Theta(x,y)\;,\;\eta=-\partial_y\Theta(x,y)\}$$

We recall that in the case of Schrödinger we found a Lagrangian manifold inside $p(x,\xi)=:\xi^2-V(x)=0$ by looking for an invariant outgoing lagrangian

[39] This will be defined later. If the projection $(x,\xi)\mapsto x$ on the space $\xi=0$ restricted to Λ_ϕ is a diffeomorphism, what follows could be taken as a definition of a Lagrangian submanifold.

manifold invariant by the flow H_p. Here we have the same phenomenon in a discrete version. Let us express the diffeomorphism κ whose graph is C_Θ in the case when $w(x,y) = \frac{a}{4}|x-y|^2$.
We find the equations :

$$\begin{aligned} \xi &= (\nabla v)(x) + \tfrac{a}{2}(x-y) \\ \eta &= -(\nabla v)(y) + \tfrac{a}{2}(x-y)\ . \end{aligned}$$

and this gives the expression for κ

$$\begin{aligned} y &= x + \tfrac{2}{a}(\nabla v)(x) - \tfrac{2}{a}\xi && := y(x,\xi)\ , \\ \eta &= -(\nabla v)(y(x,\xi)) + \xi - (\nabla v)(x) && := \eta(x,\xi)\ . \end{aligned}$$

One get also a similar expression for κ^{-1}.
Let us look at the fixed points of the diffeomorphisms. We look for the points such that $y(x,\xi) = x$, $\eta(x,\xi) = \xi$ and get $\xi = 0$, $\nabla v(x) = 0$.
We find consequently as fixed points the points $(x,0)$ where x is a critical value of v. In particular, if we assume that 0 is a non degenerate minimum of v, $(0,0)$ is a fixed point and we have just to verify, in order to apply the general theory of Smale [Sm1], if we have an hyperbolic point for the diffeomorphism attached to C_Θ:

$$(x,\xi) \mapsto (y,\eta)$$

with $(x,\xi,y,\eta) \in C_\Theta$. This means that the derivative of the diffeomorphism at the fixed point has no eigenvalues of modulus 1. In our case, we shall see (look at the quadratic case) that there are exactly [40] p eigenvalues of modulus < 1 and p eigenvalues of modulus > 1 . The regularity of the stable manifold is an old result due to Smale [Sm1] (See also [Sm2] (p. 751) or [Ir]). The property that these stable manifolds are Lagrangian is obtained as in the continuous case.
Once we have solved this problem, we arrive naturally to the study of the WKB problem. Find $\phi(x;h)$ and $E(h)$ such that

$$K_v \exp -\phi(\cdot;h)/h \sim E(h) \exp -\phi(\cdot;h)/h\ .$$

Another approach could be:
Find $a(x;h)$ and $E(h)$ such that

$$(K_v a \exp -\phi(\cdot)/h)(x) \sim E(h) a(\cdot;h) \exp -\phi(\cdot)/h\ .$$

[40] We find actually that the eigenvalues are real positive.

Let us take the second approach. We want the formal following identity

$$E(h)a(x;h) = h^{-\frac{p}{2}} \int a(y;h) \cdot \exp -\frac{1}{h}[\Theta(x,y) + \phi(y) - \phi(x)] \, dy$$

Applying the Laplace integral method, we get

$$E_0 \, a_0(x) = c \cdot a_0(y(x))(\det[\nabla^2_{yy}\Theta + \nabla^2\phi])^{-\frac{1}{2}}(y(x))$$

A necessary condition, in order to solve, is

$$E_0 = c \cdot (\det[\nabla^2_{yy}\Theta + \nabla^2\phi])^{-\frac{1}{2}}(0) \; .$$

Then we have for a_0 the formula

$$a_0(x) = \prod_{n=1}^{\infty} \theta(y^{(n)}(x)) \; ,$$

with by definition

$$y^{(n)}(x) = y(y^{(n-1)}(x)) \; ,$$

and

$$\theta(y) = \left(\frac{\det[\nabla^2_{yy}\Theta + \nabla^2\phi](0)}{\det[\nabla^2_{yy}\Theta + \nabla^2\phi](y)} \right)^{\frac{1}{2}} \; .$$

We observe here that, for any x sufficiently near the bottom 0 of V, we have

$$y^{(n)}(x) \to 0$$

and the convergence is exponentially rapid as it appears in the proof. Let us observe also that for our particular Θ $\nabla^2_{yy}\Theta$ is independent of x:

$$(\nabla^2_{yy}\Theta)(y,x) = \frac{a}{2} \, I + \frac{1}{2} \, \text{Hess} \, V(y) \; .$$

In order to see what is going on, let us come back to the one dimensional quadratic case. We recall that we have

$$\phi(y) = \frac{b}{2} y^2$$

with

$$b = \frac{1}{2}\sqrt{c(2a+c)}$$

and

$$y(x) = \frac{a}{c+a+2b}x \ .$$

Of course we do not need the discussion in this case, but what will be relevant for our discussion is the property that

$$||y(x)|| \leq k||x||$$

for $0 < k < 1$ for a suitable norm (as can be seen in the proof of the stable manifold theorem). This is what will make the procedure convergent.

By continuing to apply the Laplace transform in order to cancel the different powers of h we obtain as next equation

$$E_1 a_0(x) + E_0 a_1(x) = c \cdot a_1(y(x))(\det[\nabla^2_{yy}\Theta + \nabla^2\phi])^{-\frac{1}{2}}(y(x)) + c_1(x)$$

where c_1 depends on a_0 and its derivatives of order less or equal to 2. It seems better to look for a_1 in the form

$$a_1(x) = a_0(x) \cdot b_1(x) \ ,$$

and c_1 in the form

$$c_1(x) = E_0 \, a_0(x) \cdot d_1(x) \ .$$

We then obtain

$$E_1 \, a_0(x) + E_0 \, a_0(x) \cdot b_1(x) =$$
$$c \cdot a_0(y(x)) \cdot b_1(y(x))(\det[\nabla^2_{yy}\Theta + \nabla^2\phi])^{-\frac{1}{2}}(y(x)) \ + \ E_0 \, a_0(x) \cdot d_1(x) \ ,$$

or, using the equation satisfied by a_0,

$$b_1(x) = b_1(y(x)) + (d_1(x) - \frac{E_1}{E_0}) \ .$$

We meet the necessary condition which determines actually E_1

$$d_1(0) - \frac{E_1}{E_0} = 0 \ ,$$

and the equation takes the structure

$$b_1(x) = b_1(y(x)) + \theta_1(x) \ ,$$

with $\theta_1(0) = 0$. We then obtain a formula for b_1 by iterating the functional equation

$$b_1(x) = \sum_{n=0}^{\infty} \theta_1(y^{(n)}(x)) \ .$$

9.4.2 The analysis of the diffeomorphism in the quadratic case

In order to verify this property of hyperbolicity, let us explicite the computation of the diffeomorphism κ:

$$(y, \eta) = \kappa(x, \xi)$$

in the quadratic case. After diagonalization of the potential v we can reduce our consideration to the two-dimensional case. The map κ is in this case linear and given by the 2×2 matrix

$$M_\kappa = \begin{pmatrix} \frac{(a+c)}{a} & -\frac{2}{a} \\ -\frac{1}{2a}c(c+2a) & \frac{(a+c)}{a} \end{pmatrix}$$

The two eigenvalues are given by

$$\lambda_\pm = \frac{(a+c)}{a} \pm \frac{1}{a}\sqrt{c(c+2a)}$$

and one verifies that

$$0 < \lambda_- < 1$$

and

$$\lambda_+ > 1 \ .$$

We have consequently an hyperbolic point (saddle point situation) and a one dimensional subspace Λ_- on which κ is contracting, that is the eigenspace attached to λ_-. One finds the equation

$$\xi = \frac{1}{2}\sqrt{c(c+2a)}x$$

and as in the case of the Schrödinger operator one has

$$\xi = \phi'(x)$$

that is ϕ is the generating function of Λ_-.

9.5 Around the stable manifold theorem

9.5.1 Two theorems for solving eiconal and transport equations

We now will sketch the proof of the main theorems permitting to solve the eiconal equation and the transport equations.

Theorem 9.5.1 *:*
If V is a C^∞ potential on a neighborhood of 0 in $I\!R^p$ such that

$$V(0) = 0\ ,\ V(x) \geq 0\ ,\quad \textit{Hess}\ V(0) > 0\ .$$

Then there exists a C^∞ function ϕ_0 with the same properties such that

$$|\nabla\phi|^2 = V$$

in a suitable neighborhood of 0.

Remark 9.5.2 *:*
If we are just interested in getting the first eigenvalue modulo $\mathcal{O}(h^\infty)$ it is sufficient to solve a formal eiconal equation in the sense of the formal series in powers of x at 0. We only need to solve

$$|\nabla\phi_0|^2 = V + \mathcal{O}(|x|^\infty)\ .$$

This appears to be much more easy.

The second statement is

Theorem 9.5.3 *:*
Let X be a C^∞ real vector field defined in a neighborhood of 0. Let us assume that the linear part at 0 of the vector fields is given by

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

Let b be a C^∞ function such that $b(0) = 0$. Then for each C^∞ function g defined in a neighborhood of 0 such that $g(0) = 0$ and for each $\gamma \in I\!R$, there exists a unique C^∞ function f defined in a neighborhood U of 0 such that

$$\begin{array}{ll} (X+b)f & = g \\ f(0) & = \gamma \end{array}$$

in U.

9.5.2 Around the proof

Let us first prove the second theorem. We shall do as if it was all the time possible [41] to linearize the vectorfield X on X_0. This is actually not always true but gives a good intuition. The actual proof uses direct estimates on the flow and comparison with the linearized vector at the origin. So we have to solve in the new coordinates the equation

$$\begin{aligned} (X_0 + b)f &= g \\ f(0) &= \gamma \end{aligned}$$

One easily reduces the problem to the case $\gamma = 0$.
We have now two complementary approaches.

The first one is the formal approach. We expand everything in powers of x and solve easily using the condition that for $|\alpha| \neq 0$ the condition $\sum_j \nu_j \alpha_j \neq 0$ is satisfied. The linearization procedure is not necessary for this part. In the same way, we can solve the eiconal equation formally in powers of x. (See the remark above).

The second one is to use the flow ϕ_t of the vector field.
We recall that the flow ϕ_t is the map $\rho \mapsto \phi_t(\rho)$ associating to ρ the solution $x(t;\rho)$ of the equation

$$dx/dt = X(x(t))\ ,\ x(0) = \rho\ .$$

In the linear case the flow is explicitely given by

$$\phi_t = (\exp At)\ ,$$

if A is the matrix such that $X_0 = \sum_{ij} A_{ij} x_i \partial_{x_j}$.
Here we have actually assumed that A is diagonal which makes the next estimates easier to verify.
From this we get immediately the property that

$$\| \phi_t(y) \| \leq C \exp(-\min_j \nu_j |t|) \cdot \| y \|\ ,$$

[41] This is actually not possible when the eigenvalues of the eigenvalues of the linearized vector field at the 0 are not independent over $\mathbb{Z}$. We refer to [HeSj84-87] for a detailed proof or to what will be done in the next section.

for $t < 0$, where the ν_j are the eigenvalues of A. What is decisive here is of course that $\mathrm{Re}\ \nu_j > 0$. Then if $g(0) = 0$ and $b(0) = 0$, the solution will be given by

$$f(y) = \int_{-\infty}^0 g(\phi_t(y)) \exp(-\int_t^0 b(\phi_s(y))ds)\, dt\ .$$

Let us just verify that the integral has a meaning. If $|g(y)| \leq C_N \cdot |y|^N$ for some N then we have

$$\begin{array}{rl} |g(\phi_t(y))| & \leq C_N \cdot C^N\ (\exp - (N \min_j \nu_j |t|)\,) \cdot\ |y|^N \\ |\int_t^0 b(\phi_s(y))ds| & \leq C_0 |t| \cdot |y|\ . \end{array}$$

So we get for $|y| \leq \varepsilon_0$

$$|g(\phi_t(y))\ \int_t^0 b(\phi_s(y))ds| \leq \tilde{C}_N \cdot C^N\ \exp - \Big((N \min_j \nu_j - \varepsilon_0)|t| \Big)\ |y|^N\ .$$

For $N \in I\!N^*$ and ε_0 small enough, this gives the exponential decay and permits to define the integral. Let us also observe that if g is flat then f is flat (and in this case we do not need to assume that $b(0) = 0$. We can also verify that the argument works for the derivatives.

Sketch of the proof for the eiconal equation.

The idea of the proof is to determine the phase ϕ as the generating function of a Lagrangian manifold $\Lambda^+ = \{(x, \nabla\phi(x))\ ,\ x \in W\}$ where W is a neighborhood of 0 and lying in $q^{-1}(0)$ where

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

A minicourse in symplectic geometry.
Let us recall some minimal definitions in symplectic geometry. Our space $I\!R^{2p}$ is a symplectic manifold, that is a C^∞ manifold M where, at each point m, a non degenerate $2-$form[42] ω_m is given (that is a bilinear non degenerate antisymmetric map on T_mM). Here the $2-$ form is constant and given by

$$\omega = \sum_j d\xi_j \wedge dx_j\ .$$

[42]The map $m \mapsto \omega_m$ is also assumed to be C^∞.

A C^∞ submanifold of M Λ is called Lagrangian if, at each point λ, the tangent space $T_\lambda\Lambda$ is a lagrangian plane in $T_\lambda M$. This means that $\dim T_\lambda\Lambda = p = \frac{\dim M}{2}$ and that, for all $u, v \in T_\lambda\Lambda \times T_\lambda\Lambda$, we have

$$\omega_\lambda(u, v) = 0 \; .$$

If the projection of Λ (in $I\!R^{2p}$) on $I\!R^p_x$ $(x, \xi) \mapsto x$ is a local diffeomorphism, then we can define locally Λ by

$$\xi = \theta(x) \; .$$

The expression that Λ is lagrangian then gives the equations

$$\partial\theta_i/\partial x_j = \partial\theta_j/\partial x_i \; .$$

Then we get by standard differential geometry the local existence of ϕ such that

$$\theta_j(x) = (\partial\phi/\partial x_j)(x) \; .$$

ϕ is called the generating function.
In a symplectic manifold, the hamiltonian vector field H_q associated to a function q is well defined by the isomorphism between the tangent space $T_m M$ and the cotangent space $T^*_m M$ associating to a vector $u \in T_m M$ the linear form

$$v \mapsto \omega_m(u, v) \; .$$

In this isomorphism, H_q is associated to the 1-form dq.
The hamiltonian flow is then the flow associated to the Hamiltonian vector field and the basic property is the so-called conservation of the energy

$$q(\phi_t(x, \xi)) = q(x, \xi) \; .$$

Analysis of the hamiltonian vector field:

Let us now consider in a neighborhhod of 0 in $I\!R^{2p}$ the hamiltonian q whose taylor expansion satisfies

$$q(x, \xi) = |\xi|^2 - \sum_j \mu_j x_j^2 + \mathcal{O}(|x, \xi|^3).$$

Then the hamiltonian flow H_q has the following structure

$$H_q = 2\left(\sum_j \xi_j \frac{\partial}{\partial x_j} + \sum_j \mu_j x_j \frac{\partial}{\partial \xi_j}\right) \ + \ \mathcal{O}(|x,\xi|^2) \ ,$$

whose linear part is

$$Y_0 = 2\left(\sum_j \xi_j \frac{\partial}{\partial x_j} + \sum_j \mu_j x_j \frac{\partial}{\partial \xi_j}\right) \ .$$

The analysis of the structure of the flow near $(0,0)$ is then related to the study of the socalled "fundamental" matrix defined by

$$F = 2\begin{pmatrix} 0 & I \\ \frac{1}{2}\text{ Hess } V(0) & 0 \end{pmatrix}$$

whose eigenvalues are given by $\pm 2\sqrt{\mu_j}$ for $j = 1, \ldots, p$. Let us denote by $\Lambda_0^{\pm}$ the positive (resp. negative) eigenspace. It is clear in this very simple situation that $\Lambda_0^{\pm}$ is the set of the (x,ξ) such that $\exp(-tF)(x,\xi)$ tends to 0 as $\pm t$ tends to $+\infty$. Λ_0^+ is called the outgoing stable manifold and Λ_0^- is called the ingoing stable manifold.
Moreover, we observe by direct computation that $\Lambda_0^{\pm}$ is a Lagrangian plane in $I\!R^{2p}$ determined by the equations

$$\xi_j = \pm\sqrt{\mu_j} x_j \ .$$

We observe that these $p-$dimensional subspaces are well parametrized by the projection in the x variables and the generating function is explicitely given by

$$\phi_0(x) = \frac{1}{2}\sum_j \sqrt{\mu_j} x_j^2$$

or in the more invariant way by

$$\phi_0(x) = \frac{1}{2}\langle x | (\text{ Hess } V(0))^{\frac{1}{2}} x\rangle \ .$$

What we need to show now is that everything which was done for this linearized vector field Y_0 is also true locally in the neighborhood of $(0,0)$ for the vector H_q. This is just the object of the locally stable manifold theorem.
The theorem is the following

Theorem 9.5.4 *(The local stable manifold theorem for flows) :*
Under suitable assumptions (Hyperbolic singular point), there exists in a neighborhood of this point two C^∞ *submanifolds* Λ^+ *and* Λ^- *tangent to* Λ_0^+ *and* Λ_0^- *at* $(0,0)$ *and invariant by the flow of* H_q ϕ_t *and characterized in a suitable neighborhoofd* U *of* 0 *as*

$$\Lambda_\pm = \{(x,\xi) \in U \mid \phi_t(x,\xi) \to 0 \quad as \quad \mp t \to \infty\}$$

Moreover we have the following properties:

- *These local submanifolds* $\Lambda^\pm$ *are Lagrangian.*
- *For some* $\epsilon_0 > 0$ *and some constant* C

$$||\phi_t(x,\xi)|| \leq C \cdot \exp \pm\epsilon_0 t ||(x,\xi)|| \;\; for \; (x,\xi) \in \Lambda_\pm, \;\; as \;\; \mp t \to \infty \, .$$

- *Similar properties hold for the derivatives.*

All the properties are general for hyperbolic point of general vector field. We mean by that that the eigenvalues of the matrix associated to the linearized vector field at the critical point are all with non-zero real part.
What is particular to our situation is the fact that there is an equal number of eigenvalues with real part > 0 and with real part < 0 which gives two $p-$ dimensional stable manifolds (exchanged by the map $(x,\xi) \mapsto (x,-\xi)$) and the Hamiltonian character which implies that these two manifolds are lagrangian.
For the general proof of the local stable manifold theorem, let us refer for example to the excellent book of Irwin [Ir] (p.151-152). In this book, this is just explained as a kind of corollary of the corresponding theorem for diffeomorphisms which we already mentioned and whose proof is detailed from p. 144 to 148 (see also our next subsection). We emphasize for the student (or the reader) that we need only the local version of the stable manifold theorem. The global version is much more involved.

Let us just say a few words on the Lagrangian character of these stable manifolds which is usually not mentioned in the standard literature. Let us do this for the outgoing manifold. The argument is easily transfered to the other manifold. We just start from the following property satisfied for any point m of a symplectic manifold, for any vectors u and v in $T_m M$ and any canonical map [43]

κ:

$$\omega_m(u,v) = \omega_{\kappa(m)}((D\kappa)_m\, u\ ,\ (D\kappa)_m\, v).$$

We know take $m=(x,\xi)\in\Lambda^+$, u and v in $T_{(x,\xi)}\Lambda^+$ and $\kappa=\phi_t$.
Taking the limit as $t\rightarrow-\infty$, we see, according to the stable manifold theorem that $||(D\phi_t)_m u||_{\mathbb{R}^{2p}}$ and $||(D\phi_t)_m v||_{\mathbb{R}^{2p}}$ tend to 0 as $t\rightarrow-\infty$, and noting that ω_m is independent of m, we get immediately

$$\lim_{t\rightarrow-\infty}\omega_{\phi_t(x,\xi)}((D\phi_t)_{(x,\xi)}u\ ,\ (D\phi_t)_{(x,\xi)}v) = 0\ .$$

We observe also that in a sufficiently small neighborhood of $(0,0)$ the Lagrangian manifold can be parametrized in x and due to the Lagrangian character, this gives the existence of a generating function $\phi(x)$ such that

$$\Lambda_+ = \{(x,\xi)\mid \xi=\nabla\phi(x)\}\ .$$

We can fix the function ϕ by the condition

$$\phi(0)=0\ .$$

Let us also note that the condition that

$$T_{(0,0)}\Lambda^+ = \Lambda_0^+$$

gives in particular that

$$\phi(x)=\phi_0(x)+\mathcal{O}(|x|^3)\ .$$

In particular it is clear that $\phi(x)\geq 0$ near 0.

Let us also observe that

$$q_{/\Lambda^+}=0$$

This is an immediate consequence of the conservation of the energy by the flow, of the definition of the outgoing manifold and of the fact that $q(0,0)=0$.

[43]that is preserving the symplectic two form,

Other links are important to mention in order to understand the complete hamiltonian picture.
If $(x(t), \xi(t))$ is a "bicharacteristic" solution of the hamiltonian system living on Λ^+ then we have

$$\xi(t) = \nabla\phi(x(t)) \ ,$$

and consequently

$$dx/dt = 2\nabla\phi(x(t)) \ .$$

Consequently the projection of the bicharacteristic is an integral curve of the vector field $2\nabla\phi$.
Conversely if $x(t)$ is an integral curve of $2\nabla\phi$ such that $\lim_{t\to-\infty} x(t) = 0$ (which is true if $x(0)$ is in a suitable neighborhood of 0) then $(x(t), \xi(t) = \nabla\phi(x(t))$ is a bicharacteristic curve for H_q.

9.5.3 The stable manifold for diffeomorphisms:

We shall follow here the nice exposition of Irwin [Ir]. Let us start from a diffeomorphism $f\colon\ X \mapsto X$, and let p be a fixed point of f. The stable set of f at p is the set

$$\{x \in X \ : \ f^n(x) \to p \ \text{ as } \ n \to \infty\}.$$

We notice that this set is always non-empty, since it contains p. The unstable set of f at p is the stable set of f^{-1} at p.
Given any open neighborhood U of p, we define the local stable set of $f_{/U}$ at p to be the set of all $x \in U$ such that $(f^n(x) : n \geq 0)$ is a sequence in U converging to p. We shall say that the point p is hyperbolic if the tangent map of f at p T is a hyperbolic linear automorphism, that is if it has no eigenvalue of module 1. We can then decompose the tangent space T_pX as the sum

$$E := T_pX = E_s \oplus E_u$$

where E_s is the stable subspace corresponding to the subspace attached to the eigenvalues of module < 1 (the complex space attached to these eigenvalues being stable by complex conjugation, it is the complexified of a real space that we call E_s) and E_u is the unstable space. Because we shall apply a fixed point theorem it is better to introduce the following suitable norm

$$||\cdot||_E = \max(|\cdot|_s\ ,\ |\cdot|_u)$$

where $|\cdot|_s$ (resp. $|\cdot|_u$) is chosen such that $||T_s||_{\mathcal{L}(E_s)} < a < 1$ and $||T_u^{-1}||_{\mathcal{L}(E_u)} < a < 1$. Here we have denoted by T_s the restriction of T to E_s and similarly for T_u.

Exercise 9.5.5 *:*
Prove that it is possible.

The basic theorem we need is the following:

Theorem 9.5.6 *(Local stable manifold theorem):*
Let B a closed ball in E with center 0 and radius b. Let $\eta : B \mapsto E$ be Lipschitz with constant κ, where $\kappa < 1 - a$. Suppose $\eta(0) = 0$. Then there is a unique map $h : B_s \mapsto B_u$ such that graph h is the stable set of $(T + \eta)_{/B}$ at 0. Moreover the map h is Lipschitz, and C^r when η is C^r.

Proof:

We denote by $\mathcal{S}_0(B)$ the set of the sequences in B converging to 0 as $n \to \infty$. This is complete for the natural norm.
We are looking for elements in $\mathcal{S}_0(B)$ of the form $((T + \eta)^n(x)\ :\ n \geq 0)$ for some $x = (x_s, x_u) \in B$. These sequences can be easily identified to the sequences whose first term belong to the points of the local stable manifold.
We now observe that $\gamma \in \mathcal{S}_0(B)$ is such a sequence iff

$$\gamma(n) = \chi(x_s, \gamma)(n) \tag{9.5.1}$$

for some x_s in B_s, where[44]

$$\chi(x_s, \gamma)(n) = \begin{cases} ((T + \eta)_s\gamma(n - 1)\ , T_u^{-1}(\gamma_u(n + 1) - \eta_u\gamma(n))) & \text{for } n > 0 \\ (x_s, T_u^{-1}(\gamma_u(1) - \eta_u\gamma(0))) & \text{for } n = 0\ , \end{cases} \tag{9.5.2}$$

and $\eta = (\eta_s, \eta_u) : B \mapsto E_s \times E_u$.
The useful feature of (9.5.1) is that the sequence γ appears as the fixed point

[44]We observe that $(T+\eta)_s\gamma(n-1) = T_s\gamma_s(n-1)+\eta_s\gamma(n-1)$. There is a small ambiguity in the notation which does not lead to any confusion if we observe that $(Tu)_s = T_s u_s$ for all $u \in E$.

of a contraction of $\mathcal{S}_0(B)$ (depending on a parameter x_s). According to our choice of norms, we get easily the following estimate

$$|\chi(x_s, \gamma) - \chi(x_s, \gamma')| \leq (a + \kappa)|\gamma - \gamma'| \, . \tag{9.5.3}$$

We have consequently defined a map $\chi \; : \; B_s \times \mathcal{S}_0(B) \mapsto \mathcal{S}_0(B)$ which is contracting with respect to γ and Lipschitz on the first factor, since

$$|\chi(x'_s, \gamma) - \chi(x_s, \gamma)| = |x'_s - x_s| \, .$$

Then the contracting map theorem gives the existence of a unique map $g : B_s \mapsto \mathcal{S}_0$ such that, for all $x_s \in B_s$, (9.5.1) holds with γ replaced by $g(x_s)$. Correspondingly there is for each $x_s \in B_s$ a unique point $g(x_s)(0)$ of the local stable set with stable component x_s. Thus the map of the theorem is given by $h(x_s) = (g(x_s)(0))_u$. The contracting map theorem gives the Lipschitz character of g. It is then easy to get the same property for h. One can also prove the inequality for the fixed point

$$|\gamma(n)| \leq (a + \kappa)^n b \, .$$

Remark 9.5.7 *:*
One could have worked similarly with $\mathcal{S}_0(B)$ replaced by $\mathcal{B}(B)$ the subspace of all bounded sequences in B. One obtains similarly a fixed point which will be by uniqueness the same map g. Thus we have also proved that the local stable manifold may be characterized as the set of all points x whose iterates $(T + \eta)^n(x)$ for $n \geq 0$ form a bounded sequence.

From the stable manifold theorem for the diffeomorphisms to the stable manifold theorem for the flows:

If ϕ_t is the flow attached to a C^∞-vector with an hyperbolic singular point p, the theorem for flow is a direct consequence of the theorem for the diffeomorphisms applied to $f = \phi_{t=1}$ by observing the following

Exercise 9.5.8 *:*
Show that if p is a fixed point of a flow ϕ_t then for any neighborhood U of p then there exists a neighborhood V of p such that $\phi_t(x) \in U$ for all $x \in V$ and all $t \in [0, 1]$.

This permits to prove that $\phi_t(x) \to p$ as $t \to +\infty$ iff $\phi_n(x) \to p$ as $n \to +\infty$ for $n \in I\!N$.
One can also get easily the invariance by the flow ϕ_t of the stable set for ϕ_1.

10 WKB constructions in large dimension

10.1 Introduction

We shall just analyze the eiconal equation and the transport equations for the Schrödinger equation in the situation with large dimension. Most of the techniques have been initiated by J.Sjöstrand [Sj93a], [Sj93b] and [Sj92b]. We shall limit our study in a small neighborhood of some minimum of the potential which is now assumed to be at 0. We first recall the following definition of the 0-standard functions [45] with weights:

Definition 10.1.1 *:*
A (family of) scalar function $a^{(m)}(x)$ defined on an open set $W^{(m)}$ in $I\!R^m$ *is called* 0*-standard if, for any $k \in I\!N^*$, there exists a constant C_k independent of m such that, for any x in $W^{(m)}$, we have*

$$|\langle \nabla^{(k)} a^{(m)}(x), t_1 \otimes \cdots \otimes t_k \rangle| \leq C_k \; |t_1|_{p_1,\rho_1} \cdots |t_k|_{p_k,\rho_k} \tag{10.1.1}$$

for all $t_1, \ldots\ldots, t_k$ in $I\!R^m$, all p_j in $[1,\infty]$ with

$$1 = \frac{1}{p_1} + \ldots + \frac{1}{p_k}\;,\; 1 = \rho_1 \ldots\ldots \rho_k$$

where $|.|_{p,\rho}$ is the norm[46] in ℓ^p_ρ .

In this course we shall limit ourself essentially to the case when all the weights ρ_j are equal to 1 but other weights are important for treating the exponential convergence of the thermodynamic limit of the coefficients of the semiclassical expansion of the first eigenvalue.

As mentioned above our family of open sets $W^{(m)}$ will be a ℓ^∞ ball

$$B_\infty(0,\epsilon) = \{x \in I\!R^m \mid |x_j| \leq \epsilon\}\;.$$

Let us observe that all our models are 0-standard.

[45] Although we say "functions", it is quite important to understand that we are actually dealing with a sequence of functions parametrized by the dimension m.

[46] For $u \in I\!R^m$, the ℓ^p_ρ norm of u is defined by $|u|_{p,\rho} = \left(\sum_j \rho(j)|u_j|^p\right)^{\frac{1}{p}}$

We have already seen how the formal WKB method works. We are looking for a WKB solution of the form

$$u^{wkb}(x;h) = \exp -\phi(x,h)/h \ ,$$

for the Schrödinger equation

$$S_V = -h^2\Delta + V(x) \ ,$$

in the neighborhood of a non degenerate minimum of the potential V. The potential V is C^∞ , defined in a ℓ^∞-ball centered at the minimum and with fixed radius in $I\!R^m$ and we shall sometimes assume that this radius is normalized as equal to 1.
We state that we are looking for a real phase ϕ admitting an expansion

$$\phi(x,h) \sim \sum_{j=0}^{\infty} h^j \ \phi_j(x) \ .$$

The choice of u^{wkb} is adapted to an approximation of the first eigenfunction and will permit a better control with respect to the dimension m. The construction works well under the following assumptions

- $V(0) = \nabla V(0) = 0$,
- $V \in C^\infty(B(0,1); I\!R)$
- Hess $V(0) \geq \rho > 0$

The research of a formal WKB solution corresponds to the simultaneous research of $\phi(x;h)$ and of $E(h) \sim \sum_{j=0}^{\infty} E_j \ h^j$ such that

$$(-h^2\Delta + V(x) - hE(h)) \exp -\phi(x;h)/h \sim 0$$

that is

$$V - |\nabla\phi|^2 + h\Delta\phi - hE(h) \sim 0 \ . \tag{10.1.2}$$

This leads to the following system of equations which we have called "eiconal" equation

$$
\begin{array}{lll}
(\mathrm{E}) & V(x) - |\nabla \phi_0(x)|^2 & = 0 \ , \\
(\mathrm{T}_1) & 2\nabla \phi_0(x) \cdot \nabla \phi_1 & = \Delta \phi_0(x) - E_0 \ , \\
(\mathrm{T}_2) & 2\nabla \phi_0(x) \cdot \nabla \phi_2 & = \Delta \phi_1(x) - E_1 - |\nabla \phi_1|^2 \ , \\
\cdot & & \\
\cdot & & \\
(\mathrm{T}_\mathrm{k}) & 2\nabla \phi_0(x) \cdot \nabla \phi_k & = \Delta \phi_{k-1}(x) - (\nabla \phi_1 \cdot \nabla \phi_{k-1} \\
& & \qquad + \nabla \phi_2 \cdot \nabla \phi_{k-2} + \cdots + \nabla \phi_{k-1} \cdot \nabla \phi_1) - E_{k-1} \ .
\end{array}
$$

The rigorous treatment with control with respect to the dimension was introduced by J.Sjöstrand. We give here one of the simplest theorems in this direction.

Theorem 10.1.2 *:*
Let $d > 0$. Let $V^{(m)}$ be a (family of) C^∞ potentials defined in a ball $B_\infty(0, d)$ admitting a unique minimum at 0 and satisfying

- *Strict convexity:*

$$
\textit{Hess}\ V^{(m)}(x) \geq \sigma > 0 \ , \quad \textit{for } x \in B_\infty(0, d) \textit{ for } \sigma > 0 \ , \tag{10.1.3}
$$

- $$
V^{(m)} \text{ is } 0 - \text{standard in } B_\infty(0, d) \ , \tag{10.1.4}
$$

- $$
\textit{Hess}\ V^{(m)}(0) = D^{(m)} + A^{(m)} \ , \tag{10.1.5}
$$

  where $D^{(m)}$ is diagonal (positive definite) and

$$
||A^{(m)}||_{\mathcal{L}(\ell^p, \ell^p)} \leq r_1 \ < \ r_0 \leq \lambda_{min}(D) \ ,
$$

  for all p s.t. $1 \leq p \leq \infty$.

Then, if r_1 is small enough [47]*, there exists, in a possibly smaller $B_\infty(0, d')$, a unique formal solution* [48] *$(E(h), \phi(x, h))$ of the "eiconal" system such that the ϕ_j are 0-standard and the E_j are $\mathcal{O}_j(m)$.*

---

[47] Much better results have been obtained by J. Sjöstrand.
[48] everything is m-dependent but r_1, r_0 and σ are m-independent.

10.2 The eiconal equation

10.2.1 Sketch of the construction

We sketch the construction of ϕ_0 and explain why this solution is 0-standard. This is done by a careful analysis of the construction of the outgoing manifold Λ starting in $T^*I\!R^m$ of the point $(0,0)$ and associated with the hamiltonian flow H_q where $q(x,\xi) = \xi^2 - V(x)$. This was already presented in the preceding section without to pay attention to the dimension. The phase ϕ_0 is then the generating function of this manifold, that is locally

$$\Lambda = \{(x,\xi)\ |\xi = \nabla \phi_0(x)\}\ .$$

10.2.2 A trace Lemma

We shall use at many places the following lemma [49],

Lemma 10.2.1 *:*

$$|\ \ Tr\ \ A| \leq ||A||_{\mathcal{L}(\ell^\infty,\ell^1)}\ . \tag{10.2.1}$$

Proof of the lemma:
Put $t_j = \omega^j$, where ω is a m :th root of unity. We observe that $|t|_\infty = 1$ and so we get

$$|\langle At|\bar{t}\rangle| \leq ||A||_{\mathcal{L}(\ell^\infty,\ell^1)}\ . \tag{10.2.2}$$

On the other hand,

$$\langle At|\bar{t}\rangle = \sum_0^{m-1}\sum_0^{m-1} a_{j,k}\omega^{j-k} = \sum_0^{m-1} b_\nu \omega^{-\nu}\ , \tag{10.2.3}$$

with

$$b_\nu = \sum_{j-k\equiv -\nu \bmod (m)} a_{j,k}\ . \tag{10.2.4}$$

We now notice that

$$b_0 = \text{ Tr }\ A\ .$$

[49]We follow the proof given by J. Sjöstrand [Sj93a].

Choosing $\omega = \omega_0^k$, where ω_0 is a primitive root of unity, we get from (10.2.2)-(10.2.4)

$$|\sum_{\nu=0}^{m-1} b_\nu {\omega_0^{-k\nu}}| \leq ||A||_{\mathcal{L}(\ell^\infty,\ell^1)} \ , \ \text{for } k = 0, 1, \cdots, m-1 \ , \tag{10.2.5}$$

so

$$|\sum_{k=0}^{m-1}\sum_{\nu=0}^{m-1} b_\nu {\omega_0^{-k\nu}}| \leq m||A||_{\mathcal{L}(\ell^\infty,\ell^1)} \ . \tag{10.2.6}$$

Here we notice that the double sum in (10.2.5) is equal to mb_0, since $\sum_{k=0}^{m-1} {\omega_0^{-k\nu}}$ is equal to zero when $1 \leq \nu \leq m-1$ and is equal to m when $\nu = 0$. Hence (10.2.4) reduces to

$$|b_0| \leq ||A||_{\mathcal{L}(\ell^\infty,\ell^1)}$$

which is precisely the statement of the lemma.

10.2.3 Construction of solutions of the eiconal equation

We recall that we are working in a ℓ^∞-neighborhood of the minimum of the potential supposed to be at 0 in $I\!R^m$. Put $A_0 = \text{ Hess } V(0)$ and we assume that

$$A_0 = D_0 + B \ , \tag{10.2.7}$$

where D_0 is a positive diagonal matrix with diagonal elements in $[r_0, d_0]$, with $r_0 > 0$ and d_0 independent of m, and where

$$||B||_{\mathcal{L}(\ell^p)} \leq \delta \quad \text{ for } \quad 1 \leq p \leq \infty \ . \tag{10.2.8}$$

δ is of course assumed to be strictly less than r_0 but, because we are not looking for the optimal result, we shall perhaps take δ "small enough" later but independently of the dimension m. Let us write

$$A_0^{\pm\frac{1}{2}} = (2\pi i)^{-1} \int_\Gamma z^{\pm\frac{1}{2}} (z - A_0)^{-1} dz \ , \tag{10.2.9}$$

where Γ is a suitable contour around the spectrum of A_0 that we can choose independent of m. Then, if δ is small enough, we can expand $(z - A_0)^{-1}$ and obtain (uniformly with respect to $z \in \Gamma$)

$$(z - A_0)^{-1} = (z - D_0)^{-1} + \mathcal{O}(\delta) \quad \text{ in } \mathcal{L}(\ell^p) \quad , \forall p \in [1, \infty] \ .$$

Hence, integrating over Γ,

$$A_0^{\pm\frac{1}{2}} = D_0^{\pm\frac{1}{2}} + C_\pm \ , \quad \text{where} \quad ||C_\pm||_{\mathcal{L}(\ell^p)} \leq C_3 \delta \ . \tag{10.2.10}$$

Using the assumption of 0-standardness, we get

$$\begin{aligned} \langle \nabla V(x) - \text{ Hess } V(0) x, t\rangle &= \textstyle\int_0^1 (1-s)\langle (\nabla^3 V)(sx), t \otimes x \otimes x\rangle \; ds \\ &= \mathcal{O}(1) |t|_1 \, |x|_\infty^2 \ , \end{aligned} \tag{10.2.11}$$

and hence by duality

$$|\nabla V(x) - \text{ Hess } V(0) x|_\infty \leq C |x|_\infty^2 \ . \tag{10.2.12}$$

Let[50] $q(x,\xi) = \frac{1}{2}\xi^2 - V(x)$ the hamiltonian in the classically forbidden region and $q_0 = \frac{1}{2}\xi^2 - \frac{1}{2}$ Hess $Vx \cdot x$, its quadratic approximation. Then if we consider, the corresponding hamiltonian vector fields, we deduce from (10.2.12)

$$|H_q - H_{q_0}|_\infty \leq C |x|_\infty^2 \ . \tag{10.2.13}$$

We have now to compare the two corresponding flows.
Let us first look at the H_{q_0} flow. It is convenient to look for coordinates adapted to the two stable Lagrangian planes for the flow. This is indeed what we have done when explaining the standard proof of the stable manifold theorem. So we introduce

$$x_\pm = \frac{1}{2}\left(x \pm \text{ Hess } V(0)^{-\frac{1}{2}} \xi\right) \ , \ \xi_\pm = \frac{1}{2}\left(\pm \text{ Hess } V(0)^{\frac{1}{2}} x + \xi\right) \ , \tag{10.2.14}$$

and we notice that

$$x = x_+ + x_- \ , \ \xi = \xi_+ + \xi_- \ , \tag{10.2.15}$$

$$\xi_\pm = \pm \text{ Hess } V(0)^{\frac{1}{2}} x_\pm \ . \tag{10.2.16}$$

The stable Lagrangian planes $\Lambda_\pm^0$ are given by $x_\pm = 0$ or equivalently by $\xi_\pm = 0$.
Since Hess $V(0)^{\pm\frac{1}{2}}$ are uniformly bounded in $\mathcal{L}(\ell^\infty)$, we also have

$$|x_\pm|_\infty + |\xi_\pm|_\infty \leq C |(x,\xi)|_\infty \ . \tag{10.2.17}$$

[50]It is easier to have $\frac{1}{2}\xi^2$ for the computations.

Let us remark that we have two natural symplectic systems of coordinates given by $(2^{\frac{1}{2}}x_+, 2^{\frac{1}{2}}\xi_-)$ and $(2^{\frac{1}{2}}x_-, 2^{\frac{1}{2}}\xi_+)$. The equations for the H_{q_0} flow take the simpler form

$$\partial_t x_\pm(t) = \pm \text{ Hess } V(0)^{\frac{1}{2}} x_\pm(t) \ , \ \partial_t \xi_\pm(t) = \pm \text{ Hess } V(0)^{\frac{1}{2}} \xi_\pm(t) \ . \quad (10.2.18)$$

Combining (10.2.12) and (10.2.13) with the fact that Hess $V(0)^{\pm\frac{1}{2}}$ are uniformly bounded in $\mathcal{L}(\ell^\infty)$, we get the following estimates for the H_q-flow

$$\begin{array}{ll} |\partial_t x_\pm(t) \mp \text{ Hess } V(0)^{\frac{1}{2}} x_\pm(t)|_\infty & \leq C|x(t)|_\infty^2 \\ |\partial_t \xi_\pm(t) \mp \text{ Hess } V(0)^{\frac{1}{2}} \xi_\pm(t)|_\infty & \leq C|x(t)|_\infty^2 \ . \end{array} \quad (10.2.19)$$

We are now looking for nice neighborhoods of the invariant manifolds. For this, let us introduce the region

$$\Omega_{\epsilon_1,\epsilon_2} = \{(x,\xi) \in I\!\!R^{2m} \ ; \ |\xi_-|_\infty \leq \epsilon_1 |x|_\infty \ , \ |x|_\infty < \epsilon_2\} \ .$$

The boundary $\partial\Omega_{\epsilon_1,\epsilon_2}$ is a disjoint union of two pieces

$$\begin{array}{ll} \partial^-\Omega_{\epsilon_1,\epsilon_2} & = \{(x,\xi) \in \partial\Omega_{\epsilon_1,\epsilon_2} \ ; \ |x|_\infty < \epsilon_2\}, \\ \partial^+\Omega_{\epsilon_1,\epsilon_2} & = \{(x,\xi) \in \partial\Omega_{\epsilon_1,\epsilon_2} \ ; \ |x|_\infty = \epsilon_2\} \ . \end{array}$$

We then have the

Lemma 10.2.2 *:*
If ϵ_1 and ϵ_2 satisfy $\epsilon_j > 0$, ϵ_1 and ϵ_2/ϵ_1 sufficiently small, then the following holds for any trajectory $t \mapsto (x(t), \xi(t))$ of H_q.
If $(x(t_0), \xi(t_0)) \in \partial^+\Omega_{\epsilon_1,\epsilon_2}$ for some t_0 then $(x(t), \xi(t)) \notin \bar{\Omega}_{\epsilon_1,\epsilon_2}$ for $t - t_0 > 0$ small enough.
If $(x(t_0), \xi(t_0)) \in \partial^-\Omega_{\epsilon_1,\epsilon_2}$ for some t_0 then $(x(t), \xi(t)) \in \Omega_{\epsilon_1,\epsilon_2}$ for $t - t_0 > 0$ small enough.

In other words, the lemma says that the flow enters through $\partial^-\Omega_{\epsilon_1,\epsilon_2}$ and leaves through $\partial^+\Omega_{\epsilon_1,\epsilon_2}$.

Proof of the lemma:

We shall study the derivatives of the Lipschitz continuous function: $t \mapsto |\xi_-(t)|_\infty$ and $t \mapsto |x(t)|_\infty$.

If $f(t)$ is locally Lipschitz on some interval, then [51] $f'(t)$ exists almost everywhere and defines an element in L^∞_{loc} with the property that

$$f(t_2) - f(t_1) = \int_{t_1}^{t_2} f'(t)dt \; .$$

In our case it is easier to compute observing that the map $u \mapsto |u|$ is differentiable outside of O and that it has a left derivative at 0 equal to -1 and a right derivative equal to $+1$. We recall also that $\max(f,0) = \frac{1}{2}(f + |f|)$ so $\max(|f|,|g|) = \frac{1}{2}(|f| + |g|) + \frac{1}{2}||f| - |g||$. This gives effectively the easy way to compute the derivative of the different norms.
Now using (10.2.19) and the fact that $\text{Hess}\, V(0)^{\frac{1}{2}}$ is a small perturbation in $\mathcal{L}(\ell^\infty)$ of a diagonal matrix with strictly positive diagonal elements [52], we get

$$\partial_t |\xi_-(t)|_\infty \leq -C^{-1} |\xi_-(t)|_\infty + \mathcal{O}(|x(t)|_\infty^2) \text{ a.e .} \tag{10.2.20}$$

Similarly, we have also almost evrywhere

$$\partial_t |x(t)|_\infty \geq C^{-1} |x_+(t)|_\infty - C|x_-(t)|_\infty + \mathcal{O}(|x(t)|_\infty^2) \text{ a.e .} \tag{10.2.21}$$

In $\bar{\Omega}_{\epsilon_1,\epsilon_2}$, we get using (10.2.21), (10.2.16), the assumption on $\text{Hess}\, V(0)$ and the definition of $\Omega_{\epsilon_1,\epsilon_2}$,

$$\partial_t |x(t)|_\infty \geq C^{-1} |x_+(t)|_\infty - C\epsilon_1 |(x,\xi)|_\infty \; . \tag{10.2.22}$$

[51] Confer for example the book by Rudin [Rud].

[52] In order to detail the argument, let us first look at the one dimensional situation.
If $y(t)$ is a solution of $y'(t) = -ay(t)$ for some $a > 0$ then we observe that $|y(t)|' = -a|y(t)|$ a.e..
If $y(t)$ is a solution of $y'(t) \leq -ay(t) + Dy(t)^2$ for some $a > 0$ then we observe that $|y(t)|' \leq -a|y(t)| + Dy(t)^2$ a.e..
We now look at the two dimensional situation.
If $y_j(t)$ $(j = 1,2)$ is a solution of $y_j'(t) = -a_j y_j(t)$ for some $a_j > 0$ then let us consider $y(t) := \max(|y_1|,|y_2|)$. Using the above formula, we have almost everywhere $y'(t) = |x_1(t)|'$ if $|x_1| \geq |x_2|$ (and we have in this case $y(t) = |x_1(t)|$),
and
$y'(t) = |x_2(t)|'$ if $|x_1| \leq |x_2|$ (and we have in this case $y(t) = |x_2(t)|$).
We consequently obtain in this case
$|y(t)|' \leq -\inf(a_1,a_2)|y(t)|$.

Here C has been changed. We have used also that $\epsilon_2/\epsilon_1 \leq \delta_0$ with δ_0 small enough and that ϵ_1 is small enough.
Changing again the constants we obtain

$$\partial_t |x(t)|_\infty \geq [C^{-1} - C\epsilon_1] |(x,\xi)|_\infty \,. \tag{10.2.23}$$

In particular we get that, for ϵ_1 small enough, (and with ϵ_2/ϵ_1 small enough,) $\partial_t |x(t)|_\infty > 0$ almost everywhere for $(x(t),\xi(t))$ near $\partial^+\Omega_{\epsilon_1,\epsilon_2}$, which proves the first statement in the lemma.

If now $(x(t_0),\xi(t_0)) \in \partial^-\Omega_{\epsilon_1,\epsilon_2} \setminus \{(0,0)\}$, then $|\xi_-(t_0)|_\infty = \epsilon_1 \, |x(t_0)|_\infty$ and (10.2.20) implies that for t sufficiently near t_0

$$\partial_t |\xi_-(t)|_\infty \leq -C^{-1} |\xi_-(t)|_\infty + \mathcal{O}\left((\epsilon_1^{-1} |\xi_-(t)|_\infty)^2 \right) \text{ a.e .} \tag{10.2.24}$$

which is strictly negative provided that $\epsilon_1^{-2} |\xi_-|_\infty$ is sufficiently small, i.e. if $\epsilon_1^{-1} |x(t)|_\infty \leq \epsilon_2/\epsilon_1$ is sufficiently small. In view of (10.2.23), we have also $\partial_t |x(t)| > 0$ near $t = t_0$, and hence

$$\partial_t [|\xi_-(t)|_\infty / |x(t)|_\infty] = (\partial_t |\xi_-(t)|_\infty) / |x(t)|_\infty \; - \; |\xi_-(t)|_\infty ||\partial_t x(t)| / |x(t)|_\infty^2 < 0$$

almost everywhere for t sufficiently near t_0. The second statement follows easily.

The lemma is proved.

Evolution of the tangent vectors:

The control of the properties of the stable manifold goes through the study of its tangent space. Because its stability through the Hamiltonian flow, it is natural to follow the evolution of a tangent vector through the flow. We first recall the identity

$$\langle \text{ Hess } V(x) - \text{ Hess } V(0), t_1 \otimes t_2 \rangle = \int_0^1 \langle \nabla^3 V(sx), x \otimes t_1 \otimes t_2 \rangle ds \,. \tag{10.2.25}$$

Using our assumption of 0-standardness of V, we then obtain

$$|| \text{ Hess } V(x) - \text{ Hess } V(0) ||_{\mathcal{L}(\ell^p)} \leq C |x|_\infty \,,\; 1 \leq p \leq \infty \tag{10.2.26}$$

The evolution of a tangent vector $t = (t_x, t_\xi)$ under the H_q-flow is given by the system

$$\partial_s \begin{pmatrix} t_x \\ t_\xi \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ \text{Hess } V(x(s)) & 0 \end{pmatrix} \begin{pmatrix} t_x \\ t_\xi \end{pmatrix} \tag{10.2.27}$$

As before, we decompose t along the tangent spaces to the two stable manifolds at 0, and write $t = t^+ + t^-$, $t^\pm = (t_x^\pm, t_\xi^\pm)$ with

$$\left.\begin{array}{ll} t_x^\pm & = \frac{1}{2}(t_x \pm \text{ Hess } V(0)^{-\frac{1}{2}} t_\xi) \\ t_\xi^\pm & = \frac{1}{2}(\pm \text{ Hess } V(0)^{\frac{1}{2}} t_x + t_\xi) \end{array}\right\} \tag{10.2.28}$$

We restrict now to integral curves living in $|x|_\infty \leq \epsilon_2$ and we get from (10.2.27)-(10.2.28)

$$\partial_s t_x^+ = \frac{1}{2}(t_\xi + \text{ Hess } V(0)^{-\frac{1}{2}} \cdot \text{ Hess } V(x(s)) t_x) \; ,$$

and consequently, by combining with (10.2.26)

$$\begin{array}{rcll} \partial_s t_x^+ & = & \text{Hess } V(0)^{\frac{1}{2}} t_x^+ + \mathcal{O}(1)|x(s)|_\infty |t|_p & \\ & = & \text{Hess } V(0)^{\frac{1}{2}} t_x^+ + \mathcal{O}(1)\epsilon_2 |t|_p & \text{in } \ell^p \; . \end{array} \tag{10.2.29}$$

Similarly, we obtain also

$$\begin{array}{rll} \partial_s t_x^- & = - \text{ Hess } V(0) t_\xi^- + \mathcal{O}(1)|x(s)|_\infty |t|_p & \\ & = - \text{ Hess } V(0) t_\xi^- + \mathcal{O}(1)\epsilon_2 |t|_p & \text{in } \ell^p \; , \end{array} \tag{10.2.30}$$

and

$$\begin{array}{rll} \partial_s t_\xi^\pm & = \pm \text{ Hess } V(0)^{\frac{1}{2}} t_\xi^\pm + \mathcal{O}(1)|x(s)|_\infty |t|_p & \\ & = \pm \text{ Hess } V(0)^{\frac{1}{2}} t_\xi^\pm + \mathcal{O}(1)\epsilon_2 |t|_p & \text{in } \ell^p \; . \end{array} \tag{10.2.31}$$

Everything is here uniform with respect to p.
As in the case of the hamiltonian equation, we get from (10.2.31), the following inequations

$$\begin{array}{rl} \partial_s |t_\xi^+|_\infty & \geq C^{-1}|t_\xi^+|_\infty - C|x(s)|_\infty |t_\xi^-|_\infty \\ & \geq C^{-1}|t_\xi^+|_\infty - C\epsilon_2 |t_\xi^-|_\infty \; , \end{array} \tag{10.2.32}$$

and

$$\begin{array}{rl} \partial_s |t_\xi^-|_\infty & \geq -C^{-1}|t_\xi^-|_\infty + C|x(s)|_\infty |t_\xi^+|_\infty \\ & \geq -C^{-1}|t_\xi^-|_\infty - C\epsilon_2 |t_\xi^+|_\infty \; . \end{array} \tag{10.2.33}$$

This is true under the condition that ϵ_2 is small enough and we have used that $|t|_\infty \sim |t_\xi^+|_\infty + |t_\xi^-|_\infty$ where $\sim$ means that the constants appearing in the equivalence are independent of the dimension.
But looking at the variation of $|t_\xi^-| - c\,|t_\xi^+|$, we find that

$$V_c := \{t \in I\!R^{2m}\ ;\ |t_\xi^-|_\infty \leq c\,|t_\xi^+|\}$$

is stable under the differentiated flow under the condition that c satisfies the conditions

$$C^2\epsilon_2 < c < C^{-2}\epsilon_2^{-1}\ . \tag{10.2.34}$$

We now consider a Lagrangian plane $\Lambda(0)$ of the form $t_\xi = (\text{ Hess } V(0)^{\frac{1}{2}} + R(0))t_x$ with $R(0)$ symmetric and $||R(0)||_{\mathcal{L}(\ell^\infty)} \leq \alpha$.
We now observe that for α small enough, this can also be written as $t_\xi^- = S(0)t_\xi^+$.
Let us compute the link between S and R. We first observe that we have

$$t_\xi^+ + t_\xi^- = (\text{ Hess } V(0)^{\frac{1}{2}} + R(0)) \text{ Hess } V(0)^{-\frac{1}{2}}(t_\xi^+ - t_\xi^-)\ .$$

$$2(I - \frac{1}{2}R(0) \text{ Hess } V(0)^{-\frac{1}{2}})t_\xi^- = R(0) \text{ Hess } V(0)^{-\frac{1}{2}}t_\xi^+$$

This gives

$$S(0) = \frac{1}{2}(I + R(0) \text{ Hess } V(0)^{-\frac{1}{2}})(I - \frac{1}{2}R(0) \text{ Hess } V(0)^{-\frac{1}{2}})^{-1}$$

and it is easy to see that if $\alpha < \alpha_0$ then there exists C such that if $||R|| \leq \alpha$ then $||S|| \leq C||R|| \leq C\alpha$. The converse is also true.
It is better to follow the evolution of S. If we take c of the order of ϵ_2, we see that, as long as the trajectory remains in $\Omega_{\epsilon_1,\epsilon_2}$, then the inequality $||S(0)|| \leq c$ will imply $||S(s)|| \leq c$.
Coming back to the R representation, we get that if $\Lambda(0)$ has the form $t_\xi = (\text{ Hess } V(0)^{\frac{1}{2}} + R(0))t_x$ with $\alpha = \epsilon_2$, then there exists a constant C such that the image $\Lambda(s) \in T_{(x(s),\xi(s))}(I\!R^{2m})$ under the differential of the flow, is of the form

$$t_\xi = (\text{ Hess } V(0)^{\frac{1}{2}} + R(s))t_x$$

with

$$||R(s)||_{\mathcal{L}(\ell^\infty)} \leq C\epsilon_2\ .$$

The reconstruction of the stable manifold:

We have already a construction of the local stable manifold in some neighborhood of the origin 0. We want to control this neighborhood independently of the dimension. We shall use however the initial local manifold as starting point of the construction with control with respect to the dimension.

We next consider the evolution of certain lagrangian manifolds in $\Omega_{\epsilon_1,\epsilon_2}$ of the form $\xi = \nabla\phi(x)$ satisfying

$$|| \text{ Hess } \phi(x) - \text{ Hess } V(0)^{\frac{1}{2}} ||_{\mathcal{L}(\ell^\infty)} \leq \epsilon_2$$

for all x in the projection of $\Omega_{\epsilon_1,\epsilon_2}$.
Let us define

$$\Lambda(s) = \{\exp(sH_q)(\rho) \ ; \ \rho \in \Lambda(0), \exp(\sigma H_q)(\rho) \in \Omega_{\epsilon_1,\epsilon_2} \text{ for } 0 \leq \sigma \leq s\} \ .$$

Since the points of $\Lambda(s)$ with $|x| \neq 0$ move outwards and cross $\partial^+\Omega_{\epsilon_1,\epsilon_2}$, we see that for small $s \geq 0$,$\Lambda(s)$ is closed in $\Omega_{\epsilon_1,\epsilon_2}$, Lagrangian (as the image of a closed subset of $\Lambda(0) \cup \Omega_{\epsilon_1,\epsilon_2}$ by a symplectic map) and of the form $\xi = \nabla\phi_s(x)$. The stability remark we gave before about the evolution of tangent Lagrangian subspaces implies that

$$|| \text{ Hess } \phi_s(x) - \text{ Hess } V(0)^{\frac{1}{2}} ||_{\mathcal{L}(\ell^\infty)} \leq C\epsilon_2 \ . \tag{10.2.35}$$

The argument can be iterated (without additional factors C in the last estimate [53]) and we conclude that for all $s \geq 0$, $\Lambda(s)$ is of the form $\xi = \nabla\phi_s(x)$ with (10.2.35) satisfied.
We now choose $\Lambda(0)$ with the additional property that $\Lambda(0)$ coincides with the stable manifold for the H_q-flow near $(0,0)$. This coincidence is easily obtained in a small but m-dependent small neighborhood of 0. Since all points in $\Omega_{\epsilon_1,\epsilon_2} \setminus \mathcal{V}(0,0)$, where $\mathcal{V}(0,0)$ is a neighborhood of $(0,0)$, are evacuated within some fixed time by the flow, we see that, for s sufficiently large, $\lambda(s) \cup \mathcal{V}(0,0)$ becomes independent of s and equal to the stable outgoing manifold,

$$\begin{aligned} \lambda_+ &= \{\rho \in \Omega_{\epsilon_1,\epsilon_2} \ ; \ \exp(-sH_q(\rho)) \in \Omega_{\epsilon_1,\epsilon_2} \text{ for all } s \geq 0\} \\ &= \{\rho \in \Omega_{\epsilon_1,\epsilon_2} \ ; \ \exp(-sH_q(\rho)) \in \Omega_{\epsilon_1,\epsilon_2} \text{ for all } s \geq 0 \\ &\qquad \text{and } \exp(-sH_q(\rho)) \to (0,0) \text{ when } s \to +\infty\} \ . \end{aligned}$$

[53] Think of our proof coming from R to S

The corresponding phase $\phi(x)$ then satisfies the eiconal equation

$$|\nabla\phi(x)|^2 = V(x) \quad \text{ for } \quad |x|_\infty < \epsilon_2 \, . \tag{10.2.36}$$

By construction, we also have

$$|\nabla\phi(x) - \text{ Hess } V(0)^{\frac{1}{2}} x|_\infty \leq \epsilon_1 |x|_\infty \, , \tag{10.2.37}$$

$$|| \text{ Hess } \phi(x) - \text{ Hess } V(0)^{\frac{1}{2}} ||_{\mathcal{L}(\ell^\infty)} \leq C \, \epsilon_2 \, . \tag{10.2.38}$$

Actually by playing with $\alpha \leq \epsilon_2$, one can get in $|x|_\infty \leq \alpha$ the estimate with ϵ_2 replaced by α, we can finally prove the better

$$|| \text{ Hess } \phi(x) - \text{ Hess } V(0)^{\frac{1}{2}} ||_{\mathcal{L}(\ell^\infty)} \leq C \, |x|_\infty \, . \tag{10.2.39}$$

These estimates give also information about the flow $t \mapsto \exp(-t\nabla\phi(x) \cdot \partial_x)$ because as already observed in the preceding section, this flow is the x-projection of the flow $t \mapsto \exp(-tH_q)$ restricted to Λ_+. Let $]-\infty, 0] \ni s \mapsto (x(s), \xi(s)) \in \Lambda_+$ be an H_q integral curve. According to (10.2.23), there is a constant $C > 0$ such that $\partial_s |x(s)| \geq C^{-1}|x(s)|$ and hence by the Gronwall's lemma

$$|\exp(-t\nabla\phi(x) \cdot \partial_x)(x)|_\infty \leq \exp(-\frac{t}{C}) \; |x|_\infty \, , \; \text{ for } \; t \geq 0 \, . \tag{10.2.40}$$

If c satisfies (10.2.34), then $T_{x(s),\xi(s)}\Lambda_+ \subset V_c$ for $s \leq 0$ and (10.2.32) shows that there exists a constant $C > 0$ such that $\partial_s |t_\xi^+| \geq C^{-1}|t_\xi^+|$, if $s \mapsto (t_x(s), t_\xi(s)) \in T\Lambda_+$ is an integral curve of the differentiated flow. We now take $c \leq \frac{1}{2}$. Since $|t_\xi^-| \leq c|t_\xi^+|$, we have $|t_x| \sim |t_\xi^+|$ and we conclude, again by Gronwall's Lemma, that

$$|t_x(s)| \geq \frac{1}{C} \exp(\frac{s - \tilde{s}}{C}) \; |t_x(\tilde{s})|$$

for $\tilde{s} < s$. This can actually be interpreted as an estimate on the differential of the flow $\exp(-t\nabla\phi(x) \cdot \partial_x)$ and for some new constant C we have

$$||d\left(\exp(-t\nabla\phi(x) \cdot \partial_x)\right)||_{\mathcal{L}(\ell^\infty)} \leq \exp(-\frac{t}{C}) \, |x|_\infty \, , \; \text{ for } \; t \geq 0 \, . \tag{10.2.41}$$

Summing up, we have proved

Proposition 10.2.3 *:*
If δ is small enough, then there exists $\epsilon > 0$ independent of m such that the eiconal equation $|\nabla\phi|^2 = V$ has a positive solution ϕ_0 in $\{x \in I\!R^m \ |x|_\infty \leq \epsilon\}$. Moreover this solution satisfies (10.2.37), (10.2.39), (10.2.40) and (10.2.41) for some constant C. The constants ϵ_1 and ϵ_2 can be chosen arbitrarily small if δ and ϵ are strictly positive and small enough. Moreover the phase ϕ_0 is 0-standard.

Here we emphasize that all the constants are chosen independently of the dimension m.

10.3 Transport equation

The lemma permits to show that $\Delta\phi_0$ is 0-standard and the necessary and sufficient condition to solve (T_1) is then

$$E_0 = (\Delta\phi_0)(0) \ .$$

This condition determines E_0, gives an estimate of E_0 as a consequence of the 0-standard character of ϕ_0 and $\Delta\phi_0$.

$$\phi_1(x) = \int_{-\infty}^{0} (\Delta\phi_0 - E_0) \exp(t\nabla\phi_0 \cdot \partial_x)(x) dt$$

which can be studied modulo a good knowledge of the flow attached to $\nabla\phi_0 \cdot \partial_x$.

10.4 About the origin of the 0-standard functions

In the first papers devoted to the subject by J. Sjöstrand, an assumption of holomorphy was done on the potential near the minima. This makes the proof a little easier because the Cauchy inequalities permit to control all the derivatives once the first one were controlled. We shall briefly see here how it leads naturally to the notion of standard function. This notion of 0-standard function is also related to the notion of a C^∞ map defined in a ball of a possibly infinite dimensional Banach space. Although we are working in finite dimension, it is really basic to think in terms of a normed space in order to control everything with respect to the dimension. Let us nethertheless

observe that the estimates for the definition of 0-standard function concern the derivatives of order greater than one.
The following proposition is at the origin of the notion of 0-standard function:

Proposition 10.4.1 *:*
Let $0 < r_1 < r_0$. *Then there is a constant* $C_0 > 0$ *independent of the dimension* m *such that, for every holomorphic function on*

$$\mathbf{B}(\ell^\infty, \mathbb{C}^m; 0, r_0) = \{x \in \mathbb{C}^m \; ; \; |x|_\infty < r_0\}$$

satisfying

$$|\nabla u(x)|_\infty \leq 1 \,,$$

for $|x|_\infty < r_0$, *we have, for* $|x|_\infty < r_1$*:*

$$|\langle \nabla^2 u(x), t_1 \otimes t_2 \rangle| \leq C_0 |t_1|_{p_1} \, |t_2|_{p_2} \tag{10.4.1}$$

when

$$t_j \in \mathbb{C}^m \,,\; 1 = p_1^{-1} + p_2^{-1} \,,\; 1 \leq p_j \leq \infty$$

and

$$|\langle \nabla^3 u(x), t_1 \otimes t_2 \otimes t_3 \rangle| \leq C_0 |t_1|_{p_1} \, |t_2|_{p_2} \, |t_3|_{p_3} \tag{10.4.2}$$

when

$$t_j \in \mathbb{C}^m \,,\; 1 = p_1^{-1} + p_2^{-1} + p_3^{-1} \,,\; 1 \leq p_j \leq \infty \,.$$

In other words and extending the statements of the proposition, u is then 0-standard. What J.Sjöstrand had in mind in introducing this notion was related to the following proposition

Proposition 10.4.2 *:*
If u *is* 0*-standard then*

$$|\nabla(\nabla u \cdot \nabla u)|_\infty \leq C_0 \,, \tag{10.4.3}$$

and

$$|\nabla(\Delta u)|_\infty \leq C_0 \,. \tag{10.4.4}$$

More generally, Δu *and* $\nabla u \cdot \nabla u$ *are* 0*- standard.*

Let us sketch the proof of these propositions. The first one is based on the Cauchy inequalities. Our assumption implies that

$$|\langle \nabla u(x), t_2 \rangle| \leq |t_2|_1 \ ,$$

for $x \in B(0, r_0)$. Let $x \in B(0, r_1)$ and $t_1 \in \ell^\infty$ with $|t_1|_\infty \leq r_0 - r_1$. Let us consider the holomorphic function F of one variable:

$$D(0,1) \ni z \mapsto F(z) := \langle \nabla u(x + z t_1), t_2 \rangle \ ,$$

which is of in module less than $|t_2|_1$ at each point. Applying the Cauchy inequality, we get

$$|F'(0)| \leq \sup_{z \in D(0,1)} |F(z)| \ ,$$

or in other words

$$|\langle \nabla^2 u(x), t_1 \otimes t_2 \rangle| \leq |t_2|_1 \ .$$

For general t_1, we then get

$$|\langle \nabla^2 u(x), t_1 \otimes t_2 \rangle| \leq (r_0 - r_1)^{-1} \, |t_1|_\infty \, |t_2|_1 \ .$$

Since $\nabla^2 u$ is symmetric, we also have

$$|\langle \nabla^2 u(x), t_1 \otimes t_2 \rangle| \leq (r_0 - r_1)^{-1} \, |t_2|_\infty \, |t_1|_1 \ ,$$

and, using the complex interpolation, we get (10.4.1) with $C_0 = (r_0 - r_1)^{-1}$. The inequality (10.4.2) is obtained by similar techniques.
Let us now consider (10.4.3). This is obtained by a simple computation. We have

$$\nabla(\nabla u \cdot \nabla u) = 2(\text{ Hess } u)(\nabla u) \ .$$

It is then easy to conclude (with $C_0 = 2(r_0 - r_1)^{-1}$) using the estimate on ∇u and the estimate on Hess u.
The proof of (10.4.4) is more sophisticated. In order to estimate $\nabla \Delta u = \Delta \nabla u$ in ℓ^∞, we shall consider $\Delta \langle \nabla u, t \rangle$ for $t \in \ell^1$ and we write it as Tr (Hess $\langle \nabla u, t \rangle$). Since u is 0-standard (or since we have (10.4.2)), we obtain

$$|\langle \nabla^2 (\langle \nabla u \ , \ t \rangle), r \otimes s \rangle| \leq C_0 |t|_1 \, |r|_\infty \, |s|_\infty \ .$$

In other words

$$|| \text{ Hess } (\langle \nabla u, t \rangle) ||_{\mathcal{L}(\ell^\infty, \ell^1)} \leq C_0 |t|_1 \ .$$

We then use the trace Lemma 10.2.1 and get (10.4.4).

10.5 About the interversion between the thermodynamic limit and the semiclassical limit

This last subsection is only a presentation of some statements. We refer to [HeSj92a] for details.

We now implement additional assumptions in order to control the convergence of each $E_j(m)/m$ and the assumptions are then analogous to what appear in our study of the thermodynamic limit and first introduced in the semiclassical context in [HeSj92a].

Theorem 10.5.1 *:*
We keep the conditions given in Theorem 10.1.2 and we add the following additional conditions:

- *$V^{(m)}$ is 0-standard in $B_\infty(0,d)$ relatively to the weights ρ_ℓ satisfying:*

$$(*) \qquad \exp(-\kappa) \leq \rho_\ell(j+1)/\rho_\ell(j) \leq \exp(\kappa)\ . \tag{10.5.1}$$

- $$\textit{Hess}\ V^{(m)}(0) = D^{(m)} + A^{(m)}, \tag{10.5.2}$$

  where $D^{(m)}$ is diagonal (positive definite) and

$$||A^{(m)}||_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)} \leq r_1 \ < \ r_0 \leq \lambda_{min}(D)$$

  for all p s.t. $1 \leq p \leq \infty$ and for all ρ satisfying (10.5.1).

- *Invariance by circular permutation:*
  For every m, $V^{(m)}$ satisfies

$$V^{(m)}\left(x_m, x_1, \ldots.., x_{m-1}\right) = V^{(m)}\left(x_1, \ldots., x_m\right)\ . \tag{10.5.3}$$

- *Short range interaction:*
  For all m, n, for all ρ defined on $\{1, \ldots., m+n\}$ verifying $(*)$ and

$$(**) \qquad \rho(j) = 1 \ \textit{ for } j \geq m+1\ , \quad \textit{and } \rho(1) = 1\ ,$$

  the interaction $W^{(m,n)} = V^{(m+n)} - (V^{(m)}\tilde{\oplus}V^{(n)})$, satisfies (10.1.1) and is uniformly 0-standard but for $1 = \rho\rho_1 \ldots.. \rho_k$, instead of $1 = \rho_1 \ldots\ldots \rho_k$.

- *Uniform 0-standardness:*
  The family $(1-t)(V^{(m)}\tilde{\oplus}V^{(n)}) + tV^{(m+n)}$ *is, for* $0 \leq t \leq 1$, *uniformly* 0- *standard for the* ρ*'s satisfying* $(*)$ *and*

$$(***) \qquad \begin{array}{l} \exp -\kappa \leq \rho(n+m)/\rho(1) \leq \exp \kappa \ , \\ \exp -\kappa \leq \rho(m)/\rho(1) \leq \exp \kappa \ . \end{array} \tag{10.5.4}$$

Then the $E_j(m)/m$ *are convergent as* $m \to \infty$ *to some* α_j *and we have, for some* $\kappa_0 > 0$,

$$|E_j(m)/m - \alpha_j| \leq C_j \cdot \exp -(\kappa_0 \cdot m) \tag{10.5.5}$$

Verification of the assumptions for the (DK) model

The verification of (10.1.4) is easy. We first observe (always with the convention that $x_{m+1} = x_1$) that a function of one variable is 0-standard. In particular $x \mapsto v(x_\ell)$ and $x \mapsto x_l^2$ are 0-standard. We observe also that $x \mapsto x_\ell . x_{\ell+1}$ is 0-standard. Finally this property remains for a sum of terms depending of different variables and this gives the property for $V^{(m)}$.

For (10.1.5) we get immediately

$$D^{(m)} = (v''(s) + 2a)I_m \tag{10.5.6}$$

where I_m is the identity in $I\!R^m$, so we have :

$$r_0 = \lambda_{min}(D^{(m)}) = (v''(s) + 2a) \ . \tag{10.5.7}$$

If we denote by τ the operator on $I\!R^m$ defined by:

$$(\tau x)_i = x_{i-1} \ ,$$

we can write

$$A^{(m)} = -(2a)(\tau + \tau^{-1})$$

The eigenvalues of A have been already computed as $-2a \cdot \cos(2\pi\frac{k}{m})$ for $k = 0, 1, \ldots.., m-1$.

It is then easy to verify that, for ρ satisfying $(*)$,

$$||A||_{\mathcal{L}(\ell^p_\rho)} \leq 2a \cdot \exp(\kappa)$$

We observe that one can choose κ such that

$$r_1 = 2a . \exp(\kappa) \ < \ (v''(s) + 2a) \tag{10.5.8}$$

and we shall make this choice now.
Let us now verify the condition on $W^{(m,n)}$ which was given by

$$W^{(m,n)}(x) = \frac{a}{2}\left((x_{m+n} - x_1)^2 + (x_m - x_{m+1})^2 - (x_m - x_1)^2 - (x_{m+n} - x_{m+1})^2\right) .$$

Here it is sufficient to observe that the only j for which $\partial_{x_j} W^{(m,n)}$ are not 0 are $j = 1, m, m+1, m+n$.
Let us verify (10.1.5). We first observe that

$$D_t^{(m+n)} = (1-t)(D^{(m)} \oplus D^{(n)}) + tD^{(m+n)}$$

and

$$A_t^{(m+n)} = (1-t)(A^{(m)} \oplus A^{(n)}) + tA^{(m+n)}.$$

All the properties we need are stable by arithmetical means, so it is sufficient to treat the case $(V^{(m)} \tilde{\oplus} V^{(n)})$ for ρ satisfying $(*)$ and $(***)$ which can be reduced by separation of variables to the study of $V = V^{(m)}$ for ρ satisfying $(*)$.

Conclusion
If we take d small enough in Theorem 10.1.2, we can, using the WKB solution centered at one of the critical points x_c and multiplying by a suitable cut-off function, get a complete expansion of the first eigenvalue of the Dirichlet problem modulo $m\mathcal{O}(h^\infty)$. Actually, we first obtain only an upperbound for this first eigenvalue and it is a little more tricky to obtain the equality which is obtained under the technical condition

$$m \leq C \cdot h^{-N_0} . \tag{10.5.9}$$

Under the condition (10.5.9), one can finally obtain (modulo a uniform $\mathcal{O}(h^\infty)$) the expansion

$$\frac{\lambda_1(m,h)}{m} \sim \sum_j \frac{E_j}{m}\, h^j . \tag{10.5.10}$$

We just sketch how one can get from this some semiclassical expansion without any restriction on m. In order to eliminate the restrictive condition (10.5.9), we come back to the universal control of the thermodynamic limit given in Section 6.4 (more precisely (6.4.2))

$$|(\lim_{m\to+\infty} \frac{\lambda_1(m,h)}{m}) - \frac{\lambda_1(m,h)}{m}| \leq \frac{C}{m} . \tag{10.5.11}$$

Combining (10.5.11), (10.5.10) (under condition (10.5.9) and (10.5.5), one obtains finally pass to the limit $m \to +\infty$ (10.5.10) and we get

$$(\lim_{m\to+\infty} \frac{\lambda_1(m,h)}{m}) \sim \sum_j \alpha_j \; h^j \; . \tag{10.5.12}$$

References

[AbRo] R.Abraham, J.Robbin: Transversal mappings and flows. and inside Appendix by Al Kelley : The stable, center-stable, center, center-unstable, and unstable manifolds. W.A. Benjamin, Inc. New York 1967.

[Ag] S.Agmon: Lecture on exponential decay of solutions of second order elliptic equations. Math. Notes, t.29, *Princeton University Press.*

[BGM] M.Berger, P.Gauduchon, E.Mazet: Spectre d'une variété riemannienne, Springer Lecture Notes in Mathematics 194 (1971).

[CDV93] Y.Colin de Verdière: Cours de DEA, Université de Grenoble, 1993-1994.

[CFKS87] H.L. Cycon, R. Froese, W.Kirsch, B.Simon: Schrödinger operators. *Springer* (1987).

[Die] J. Dieudonné: Calcul infinitésimal. *Hermann.*

[El85] R.S.Ellis: Entropy, large deviations, and statistical mechanics. *Grundlehren der mathematischen Wissenschaften* $n^0$271, *Springer, New York*, (1985).

[Ga83] G.Gallavotti: The elements of mechanics. *Texts and monographs in Physics*, Springer, (1983).

[GlJa87] J.Glimm and A.Jaffe: Quantum physics (a functional integral point of view). *Springer Verlag*, Second edition (1987).

[He84] B.Helffer: Théorie spectrale pour des opérateurs globalement elliptiques. *Astérisque* n^0 112 (1984).

[He88] B.Helffer: Introduction to the semiclassical analysis for the Schrödinger operator and applications. *Springer lecture Notes in Math.*, n^0 1336 (1988).

[Ho] L. Hörmander: The analysis of linear partial differential operators, *Springer Verlag.*

[Hu] D. Huet: Décomposition spectrale et opérateurs, Presses universitaires de France (1976)

[Ir] M.C. Irwin: Smooth dynamical systems, Academic Press (1970).

[ItzDr89] C.Itzykson and J.M.Drouffe: Théorie statistique des champs I. *Savoirs actuels,Interedition/ Editions du CNRS*, (1989).

[LaLi74] L.D. Landau, E.M. Lifschitz: Mécanique quantique, théorie non-relativiste, Editions Mir (1974).

[Pa84] G.Parisi: Statistical field theory. Frontiers in Physics, Addison-Wesley Publishing Company, (1984).

[ReSi72] M.Reed, B.Simon: Methods of modern mathematical Physics. I. Functional analysis. *Academic Press*, (1972).

[ReSi75] M.Reed, B.Simon: Methods of modern mathematical Physics. II. Fourier analysis, selfadjointness. *Academic Press*, (1975).

[ReSi] M.Reed, B.Simon: Methods of modern mathematical Physics. III. *Academic Press*, (1976).

[ReSi78] M.Reed, B.Simon: Methods of modern mathematical Physics. IV. Analysis of operators. *Academic Press*, (1978).

[Ro87] D.Robert: Autour de l'approximation semi-classique. *Birkhäuser*, Vol.68, *Progress in Mathematics*, (1987)

[Roe94] G.Roepstorff: Path integral approach to quantum Physics. *Texts and monographs in Physics*, Springer (1994).

[Rud] W. Rudin: Real and Complex analysis. Mc Graw Hill, New York (1974).

[Ru69] D.Ruelle: Statistical mechanics. *Math. Physics monograph series, W.A.Benjamin, Inc.* (1969).

[Schw] L. Schwartz : Analyse hilbertienne, Collection Méthodes, Hermann 1979, Paris.

[Si74] B.Simon: The $P(\phi)_2$ Euclidean quantum field theory. *Princeton Series in Physics* (1974).

[Si79] B.Simon: Functional integration and quantum physics. *Pure and Applied mathematics* $n^0 86$, Academic press, New york, (1979).

[Si93] B.Simon: The statistical mechanics of lattice gases. Volume 1, *Princeton Series in Physics* (1993).

[Sj82] J.Sjöstrand: Singularités analytiques microlocales. *Astérisque* $\mathrm{n}^0 95$, (1982).

[Thi83] W.Thirring: Volume 4, Quantum Mechanics of large systems. (translated by E.M.Harrell), *Springer Verlag*, (1983).

[Tho72] C. J. Thompson: Mathematical statistical mechanics. *The Macmillan company New York*, (1972).

[Yos] K.Yosida: Functional Analysis, Grundlehren der mathematischen Wissenschaften 123, *Springer Verlag*, (1980).

References

[Alb] C. Albanese: On the spectrum of the Heisenberg Hamiltonian. Journal of statistical Physics 55 (1-2), p. 297-309, (1989).

[BaKo92] V.S. Barbulyak, Y. Kondratév: The quasiclassical limit for the Schrödinger operator and phase transitions in Quantum statistical physics. Functional Analysis and apllications, Vol. 26, n^0 2, p. 61-64, April-June, (1992).

[BeBru90] G.Ben Arous and M.Brunaud: Méthode de Laplace: Etude variationnelle des fluctuations de diffusions de type "champ moyen". *Stochastics and stochastics reports*, Vol.31, p. 79-144, (1990).

[BoHe93] C.Bolley, B.Helffer: An application of semiclassical analysis to the asymptotic study of the supercooling field of a superconducting material Annales de l'institut Henri-Poincaré (Section Physique Théorique), (1993), Vol 58, $\mathrm{n}^0 2$, p.189-233.

[BreHi79] E.Brézin, S.Hikami: Large order behavior of $\frac{1}{N}$ expansion in zero and one dimensions. *J.Phys.A* 12 (6) 1979, pp 759-770.

[BruHe91] M.Brunaud and B.Helffer: Un problème de double puits provenant de la théorie statistico-mécanique des changements de phase (ou relecture d'un cours de M.Kac). *Preprint LMENS*, March 1991.

[Co77] S. Coleman: The use of instantons, Proc. Internat. School of Physics, Erice, (1977).

[CDS91] J.M. Combes, P. Duclos, R. Seiler: Krein's formula and one dimensional multiple well, *Journal of Functional Analysis* 52 (1983), p. 257-301.

[DoKo93] S.Yu.Dobrokhotov, V.N.Kolokoltsov: On amplitude of low energy levels splitting value for Schrödinger operator with double-well potential. *Theoretical and mathematical physics* (Tome 94, $n^0 3$), (March 1993).

[DoKo94] S.Yu.Dobrokhotov, V.N.Kolokoltsov: The double-well splitting of the low energy levels for the Schrödinger operator of discrete Φ^4-models on tori. *Preprint* (1994).

[DoKoMa91] S.Yu.Dobrokhotov, V.N.Kolokoltsov, V.P.Maslov: The splitting of the low lying energy levels of the Schrödinger operator and the asymptotics of the fundamental solution of the equation $hu_t = (h^2\Delta/2 - V(x))\, u$. *Teor. Mat. Fizika* 87:3 (1991), p.323-375. English translation in Theor. Math. Phys.

[DoKoMa92] S.Yu.Dobrokhotov, V.N.Kolokoltsov, V.P.Maslov: Quantization of the Bellman equation, exponential asymptotics and tunneling. *Advances in Soviet Math.* AMS (1992), V.13,p.1-47.

[Hard88] A. Hardarson: Doublewell tunneling via the Feynman-Kac formula, PHD Caltech 1988.

[Ha80] E.M.Harrell: On the rate of asymptotic eigenvalue degeneracy. *Comm.in Math.Phys.*, t.75, 1980, p.239-261.

[He92a] B.Helffer: Problèmes de double puits provenant de la théorie statistico-mécanique des changements de phase, II Modèles de Kac avec champ magnétique. étude de modèles près de la température critique. *Preprint LMENS*, March 1992.

[He92b] B.Helffer: Décroissance exponentielle des fonctions propres pour l'opérateur de Kac: le cas de la dimension > 1. in Operator calculus and spectral theory, *Symposium on operator calculus and spectral theory*, Lambrecht (Germany), December 1991, edited by M.Demuth, B.Gramsch and B.-W.Schulze, *Operator Theory: Advances and Applications*, Vol.57; *Birkhäuser Verlag Basel*, (1992).

[He93a] B.Helffer: Estimations sur les fonctions de corrélation pour des modèles du type de Kac. Exposé au séminaire EDP de l'Ecole Polytechnique, April 1993.

[He93b] B.Helffer: Spectral properties of the Kac operator in large dimension. Proceedings on Mathematical Quantum Theory II: Schrödinger Operators, (August 1993), edited by J.Feldman, R.Froese, and L.M.Rosen. CRM Proceedings and Lecture Notes.

[He94a] B.Helffer: Around a stationary phase theorem in large dimension. *Journal of Functional Analysis*, Vol.119, n^{o}1, January 1994.

[He94b] B.Helffer: Universal estimate of the gap for the Kac operator in the convex case. *Comm. in Math. Physics*, Vol.161, n^o 3, (1994), p.631-642.

[He94c] B.Helffer: Correlation decay and gap of the transfer operator. *Proceedings of the conference in the Euler Institut in St Petersbourg*, (to appear).

[He94d] B.Helffer: Around the transfer operator and the Trotter-Kato formula. *Proceedings of the conference in Holzhau.* (to appear).

[He94e] B.Helffer: Recent results and open problems on Schrödinger operators, Laplace integrals and transfer operators in large dimension. Survey to appear in Advances in Partial Differential equations, Akademie Verlag.

[HeSj84-87] B.Helffer and J.Sjöstrand: Multiple wells in the semiclassical limit.
I *Comm. in PDE* 9(4), p.337-408, (1984),
II *Annales de l'IHP (section Physique théorique)*,
Vol.42, $n^0 2$, (1985), p.127-212.
III *Math.Nachrichten* 124, (1985), p.263-313.

[HeSj92a] B.Helffer, J.Sjöstrand: Semiclassical expansions of the thermodynamic limit for a Schrödinger equation. *Astérisque* 210 (1992), p.135-181.

[HeSj92b] B.Helffer and J.Sjöstrand: Semiclassical expansions of the thermodynamic limit for a Schrödinger equation II. *Helvetica Physica Acta*, Vol.65, (1992), p.748-765 and Erratum, Vol.67, (1994), p.1-3.

[HeSj94] B.Helffer, J.Sjöstrand: On the correlation for Kac like models in the convex case. *Journal of Statistical Physics*, Vol. 74, $\mathrm{n}^0$1-2, p. 349-369, (1994).

[J.LMS81] G. Jona-Lasinio, F. Martinelli, E. Scoppola: New approach to semiclassical limit of quantum mechanics I. Multiple tunneling in one dimension, *Comm. in Math. Phys.* 80, pp. 125-174, (1981).

[Ka62] M.Kac: Statistical mechanics of some one-dimensional systems. Studies in mathematical analysis and related topics: essays in honor of Georges Polya, *Stanford University Press*, Stanford, California (1962), p.165-169.

[Ka66] M. Kac: Mathematical mechanisms of phase transitions. Brandeis lectures (1966), *Gordon and Breach.*

[HelKa63] M.Kac and E.Helfand: *J. Math. Phys.* 4, 1078 (1963).

[KaTho66] M.Kac, C.Thompson: On the mathematical mechanism of phase transition. *Proc.N.A.S.*, Vol.55, 1966 and Erratum Vol 56, (1966) p.1625.

[KaTho69] M.Kac, C.Thompson: Phase transition and eigenvalue degeneracy of a one dimensional anharmonic oscillator. *Studies in Applied Mathematics*, 48 (1969), p.257-264.

[Ken] T. Kennedy: Rayleigh Schrödinger perturbation à la Kirkwood-Thomas, Personal communication (September 1995).

[KiTho] J. Kirkwood, L. Thomas: Expansions and phase transitions for the groundstate in quantum spin systems. Comm. Math. Phys. 91, p.405 (1983).

[Mas84] V.P.Maslov: Global exponential asymptotics of the solutions of the tunnel equations and the large deviation problems. *Tr. Mosk. Inst. Akad. Nauk* 163, (1984), p.150-180. Engl. transl. in *Proc. Stecklov Inst. Math.*4 (1985).

[PPW56] L.E.Payne, G.Polya, H.F.Weinberger: On the ratio of consecutive eigenvalues. *Journal of Math. and Physics* 35, (3), (Oct.1956).

[Si83] B.Simon: Instantons, double wells and large deviations. *Bull.AMS.*,t.8, (1983), p.323-326.

[Si84] B.Simon: Semi-classical Analysis of low lying eigenvalues.
I *Ann.Inst.H.Poincaré* 38,(1983) , p.295-307.
II *Annals of Mathematics*,120, (1984), p.89-118.

[SWYY85] I.M.Singer, B.Wong, S.T.Yau and S.S.T. Yau: An estimate of the gap of the first two eigenvalues of the Schrödinger operator. *Ann. Scuola Norm. Sup. Pisa* (4), 12 (1985), P.319-333.

[Sj91] J.Sjöstrand: Schrödinger in high dimensions. asymptotic constructions and estimates. Proceeding of the french-japanese symposium on algebraic analysis and singular perturbations, CIRM, Luminy, France, (October 1991).

[Sj92a] J.Sjöstrand: Exponential convergence of the first eigenvalue divided by the dimension. for certain sequences of Schrödinger operator. *Astérisque* 210, (1992), p.303-326.

[Sj92b] J.Sjöstrand: Evolution equations in a large number of variables. *Mathematische Nachrichten* 166 (1994) p. 17-53.

[Sj93a] J.Sjöstrand: Potential wells in high dimensions I. *Ann. Inst. Poincaré*, Section Physique théorique, 58 (1), (1993).

[Sj93b] J.Sjöstrand: Potential wells in high dimensions II, more about the one well case. *Ann. Inst. Poincaré*, Section Physique théorique, 58 (1), (1993).

[Sj93c] J.Sjöstrand: On ferromagnetic Laplace integrals and maximum principles. *Preprint de l'université d'Orsay*, June 1993. To appear *Ann.Inst. Fourier.*

[Sj93d] J.Sjöstrand: Estimations sur les corrélations et principes du maximum. *Séminaire Equations aux dérivées partielles de l'Ecole Polytechnique*, October 1993.

[Sj94] J.Sjöstrand: Correlation asymptotics and Witten Laplacians. Preprint, June 1994.

[Sm1] S.Smale: Stable manifolds for differential equations and diffeomorphisms. Ann. Scuola Normale Superiore Pisa 18(1963), p. 97-116.

[Sm2] S.Smale: Differentiable dynamical systems, Bull. Amer. Math. Soc. 73 (1967) p. 747-817.

[Sor93a] V.Sordoni: Schrödinger operators in high dimensions: convex potentials. *Preprint Université Paris-Nord* 94-03, December 1993.

[Sor93b] V.Sordoni: Anharmonic oscillators in high dimension, *Preprint Université Paris-Nord* 94-07, December 1993.

[Sor94] V.Sordoni: Around the method of instantons. in preparation, (1994).

[Tr59] H.Trotter: On the product of semigroups of operators. *Proc.Amer. Math.Soc.* 10 (1959) p.549-551.

[Z-J84] J.Zinn-Justin: The principles of instanton calculus: a few applications. Les Houches, Session XXXIX, (1982), Recent advances in field theory and statistical mechanics, *Elsevier Science Publishers*.

Index