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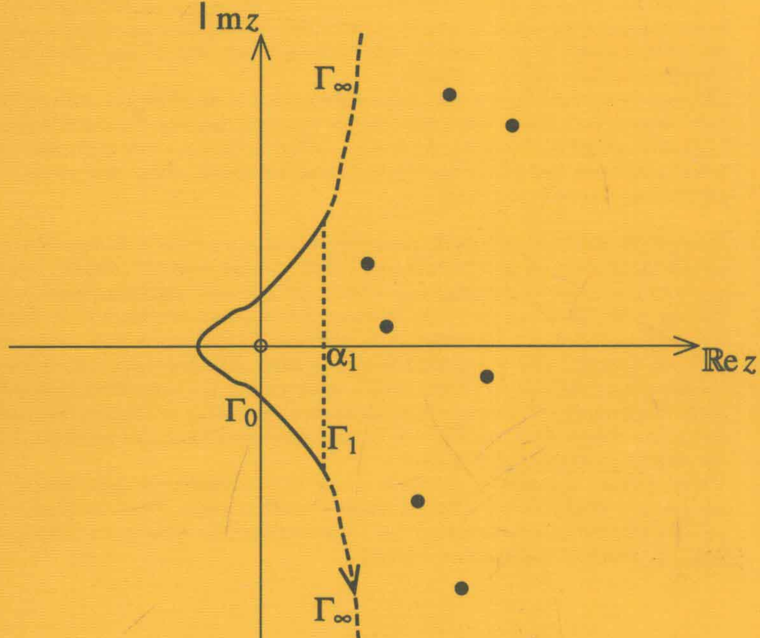
Bernard Helffer
Francis Nier

Hypoelliptic Estimates and Spectral Theory for Fokker-Planck Operators and Witten Laplacians



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Authors

Bernard Helffer

Laboratoire de Mathématiques
UMR CNRS 8628
Université Paris-Sud
Bâtiment 425
91404 Orsay
France

e-mail: bernard.helffer@math.u-psud.fr

Francis Nier

IRMAR UMR CNRS 6625
Université de Rennes 1
Campus de Beaulieu
35042 Rennes Cedex
France

e-mail: francis.nier@univ-rennes1.fr

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Foreword

This text is an expanded version of informal notes prepared by the first author for a minicourse of eight hours, reviewing the links between hypoelliptic techniques and the spectral theory of Schrödinger type operators. These lectures were given at Rennes for the workshop "Equations cinétiques, hypoellipticité et Laplacien de Witten" organized in February 2003 by the second author. Their content has been substantially completed after the workshop by the two authors with the aim of showing applications to the Fokker-Planck operator in continuation of the work by Hérau-Nier. Among other things it will be shown how the Witten Laplacian occurs as the natural elliptic model for the hypoelliptic drift diffusion operator involved in the kinetic Fokker-Planck equation. While presenting the analysis of these two operators and improving recent results, this book presents a review of known techniques in the following topics : hypoellipticity of polynomial of vector fields and its global counterpart, global Weyl-Hörmander pseudo-differential calculus, spectral theory of non self-adjoint operators, semi-classical analysis of Schrödinger type operators, Witten complexes and Morse inequalities.

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Introduction

This text presents applications and new issues for hypoelliptic techniques initially developed for the regularity analysis of partial differential operators. The main motivation comes from the theory of kinetic equation and statistical physics. We will focus on the Fokker-Planck (Kramers) operator:

$$K = v \cdot \partial_x - (\partial_x V(x)) \cdot \partial_v - \Delta_v + \frac{v^2}{4} - \frac{n}{2} = X_0 - \Delta_v + \frac{v^2}{4} - \frac{n}{2}\,, \tag{1.1}$$

and the Witten Laplacian

$$\Delta^{(0)}_{\Phi/2,h} := -h^2\Delta + \frac{1}{4}|\nabla\Phi|^2 - \frac{h}{2}\Delta\Phi\,, \tag{1.2}$$

where

$$\Phi(x,v) = \frac{v^2}{2} + V(x)$$

is a classical hamiltonian on $\mathbb{R}^{2n}_{x,v}$ and

$$X_0 = v \cdot \partial_x - (\partial_x V(x)) \cdot \partial_v$$

is the corresponding hamiltonian vector field.
The aim of this text is threefold:

1. exhibit the strong relationship between these two operators,
2. review the known techniques initially devoted to the analysis of hypoelliptic differential operators and show how they can become extremely efficient in this new framework,
3. present, complete or simplify the existing recent results concerned with the two operators (1.1) and (1.2).

At the mathematical level the analysis of these two operators leads to explore or revisit various topics, namely: hypoellipticity of polynomials of vector fields and its global counterpart, global Weyl-Hörmander pseudo-differential calculus, spectral theory of non self-adjoint operators, semi-classical analysis of Schrödinger type operators, Witten complexes and Morse inequalities. The point of view chosen in this text is, instead of considering more complex physical models, to focus on these two operators and to push as far as possible the analysis. In doing so, new results are obtained and some new questions arise about the existing mathematical tools.

We will prove that $(e^{-tK})_{t\geq 0}$ and $(e^{-t\Delta^{(0)}_{\Phi/2}})_{t\geq 0}$ are well defined contraction semigroups on $L^2(\mathbb{R}^{2n}, dx\, dv)$ for any $V \in \mathcal{C}^\infty(\mathbb{R}^n_x)$. Meanwhile the Maxwellian

$$M(x,v) = \begin{cases} e^{-\frac{\Phi(x,v)}{2}} & \text{if} \quad e^{-\frac{\Phi(x,v)}{2}} \in L^2(\mathbb{R}^{2n}) \\ 0 & \text{else} \,, \end{cases}$$

is the (unique up to normalization) equilibrium for K and $\Delta^{(0)}_{\Phi/2}$:

$$KM = \Delta^{(0)}_{\Phi/2} M = 0 \,.$$

Two questions arise from statistical physics or the theory of kinetic equations:
Question 1:
Is there an exponential return to the equilibrium ? By this, we mean the existence of $\tau > 0$ such that:

$$\left\| e^{-tP} u - c_u M \right\| \leq e^{-\tau t} \left\| u \right\| \,, \; \forall u \in L^2(\mathbb{R}^{2n}) \,,$$

where $P = K$ or $P = \Delta^{(0)}_{\Phi/2}$ and c_u (in the case $M \neq 0$) is the scalar product in $L^2(\mathbb{R}^{2n})$ of u and $M/||M||$.
Question 2:
Is it possible to get quantitative estimates of the rate τ ?

For $P = \Delta^{(0)}_{\Phi/2}$ which is essentially self-adjoint it is reduced to the estimate of its first nonzero eigenvalue. Several recent articles, like [DesVi], [EckPiRe-Be], [EckHai1], [EckHai2], [HerNi], [Re-BeTh1], [Re-BeTh2], [Re-BeTh3], [Ta1], [Ta2] and [Vi1], analyzed this problem for operators similar to K, with various approaches going from pure probabilistic analysis to pure partial differential equation (PDE) techniques and to spectral theory. The point of view developed here is PDE oriented and will strongly use hypoelliptic techniques together with the the spectral theory for non self-adjoint operators.

Note that a related and preliminary result in this "spectral gap" approach concerns the compactness of the resolvent. One of the results which establish the strong relationship between K and $\Delta^{(0)}_{\Phi/2}$ says:

Theorem 1.1.
The implication

$$\left((1+K)^{-1} \text{ compact}\right) \Rightarrow \left((1+\Delta^{(0)}_{\Phi})^{-1} \text{ compact}\right) \tag{1.3}$$

holds under the only assumption $V \in \mathcal{C}^\infty(\mathbb{R}^n)$[1].

[1] Indeed the $\mathcal{C}^\infty$ regularity is not the crucial point here and the most important fact is that nothing is assumed about the behaviour at infinity.

In [HerNi] the reverse implication was proved for quite general elliptic potentials, satisfying for some $\mu \geq 1$,

$$|\partial_x^\alpha V(x)| \leq C_\alpha \langle x\rangle^{2\mu-|\alpha|} \text{ and } C^{-1}\langle x\rangle^{2\mu} \leq 1 + |V(x)| \leq C^\alpha \langle x\rangle^{2\mu} .$$

Among other things in the present text, we will explore as deeply as possible the validity of the following conjecture:

Conjecture 1.2.
The Fokker-Planck operator (1.1) has a compact resolvent if and only if the Witten Laplacian on 0-forms (1.2) has a compact resolvent.

Hypoelliptic techniques enter at this level twice:

1. in the proof of the equivalence when it is possible;
2. in order to get effective criteria for the compactness of $(1 + \Delta_{\Phi/2}^{(0)})^{-1}$.

In this direction, the present text provides a (non complete) review of various techniques due to Hörmander [Hor1], Kohn [Ko], Helffer-Mohamed [HelMo], Helffer-Nourrigat [HelNo1, HelNo2, HelNo3, HelNo4], while emphasizing new applications of rather old results devoted to subellipticity of systems by Maire [Mai1, Mai2], Trèves [Tr2] and Nourrigat [No1]. Among those works, one can distinguish at least two methods for the treatment of the hypoellipticity, one referred to as Kohn's method which is not optimal but flexible enough to permit several variants and another one which is based on the idea initiated by Rothschild-Stein [RoSt] and developed by Helffer-Nourrigat to approximate the operators by left invariant operators on nilpotent Lie groups.
By writing

$$\Delta_{\Phi/2}^{(0)} = \Delta_{V/2}^{(0)} \otimes \mathrm{Id}_v + \mathrm{Id}_x \otimes (-\Delta_v + \frac{v^2}{4} - \frac{n}{2})$$

and

$$\Delta_{V/2}^{(0)} = -\Delta_x + \frac{1}{4}|\nabla V|^2 - \frac{1}{2}\Delta V(x) ,$$

which can also be expressed in the form

$$\Delta_{V/2}^{(0)} = \sum_{j=1}^{n} L_j^* L_j = \sum_{j=1}^{n} X_j^2 + Y_j^2 + i\,[X_j, Y_j] ,$$

with $L_j = X_j + Y_j$, $X_j = \partial_{x_j}$, $Y_j = \frac{1}{2i}\partial_{x_j} V(x)$, the conditions on $V(x)$ which ensure the compactness of $(1 + \Delta_{\Phi/2}^{(0)})^{-1}$ can be analyzed very accurately with nilpotent techniques.
Although it is possible to write K as a non commutative polynomial of ∂_{x_j}, $\partial_{x_j} V(x)$, ∂_{v_j}, v_j, the relationship between K and $\Delta_{\Phi/2}^{(0)}$ is more clearly exhibited after writing

$$K = X_0 + b^* b = X_0 + \sum_{j=1}^{n} b_j^* b_j$$

which looks like a "type 2 Hörmander's operators", $X_0 + \sum_{j=1}^n Y_j^2$ if one replaces the vector field Y_j by the annihilation operators

$$b_j = \partial_{v_j} + \frac{v_j}{2}\ , \text{ for } j = 1, \ldots, n\ ,$$

associated with the harmonic oscillator hamiltonian

$$b^* b = -\Delta_v + \frac{v^2}{4} - \frac{n}{2}\ .$$

We will follow and improve the variant of the Kohn's method used by Hérau-Nier in [HerNi] which was partly inspired by former works of Eckmann-Pillet-Rey-Bellet [EckPiRe-Be], Eckmann-Hairer [EckHai1]. Precisely our results will require one of the two following assumptions after setting

$$h(x) = \sqrt{1 + |\nabla V(x)|^2}\ .$$

Assumption 1.3.
The potential $V(x)$ belongs to $\mathcal{C}^\infty(\mathbb{R}^n)$ and satisfies:

$$\forall \alpha \in \mathbb{N}^n,\ |\alpha| \geq 1, \exists C_\alpha \ s.t.\ \forall x \in \mathbb{R}^n\ ,\ |\partial_x^\alpha V(x)| \leq C_\alpha h(x)\ , \tag{1.4}$$

$$\exists M\ ,\ C \geq 1\ ,\ s.t\ \forall x \in \mathbb{R}^n\ ,\ h(x) \leq C\ \langle x \rangle^M\ , \tag{1.5}$$

and the coercivity condition

$$\exists M\ ,\ C \geq 1\ ,\ s.t.\ \forall x \in \mathbb{R}^n\ ,\ C^{-1}\ \langle x \rangle^{1/M} \leq h(x)\ . \tag{1.6}$$

Assumption 1.4.
The potential $V(x)$ belongs to $\mathcal{C}^\infty(\mathbb{R}^n)$ and satisfies (1.4) (1.5) with the coercivity condition (1.6) replaced by the existence of $\rho_0 > 0$ and $C > 0$ such that:

$$\forall x \in \mathbb{R}^n,\ |\nabla h(x)| \leq C\, h(x)\, \langle x \rangle^{-\rho_0}\ . \tag{1.7}$$

Theorem 1.5.
If the potential $V \in \mathcal{C}^\infty(\mathbb{R}^n)$ verifies Assumption 1.3 or Assumption 1.4, then there exists a constant $C > 0$ such that

$$\forall u \in \mathcal{S}(\mathbb{R}^{2n}),\ \left\|\Lambda^{1/4} u\right\|^2 \leq C\left(\|Ku\|^2 + \|u\|^2\right)\ , \tag{1.8}$$

with $\Lambda^2 = (1 + \Delta_{\Phi/2}^{(0)})$

Corollary 1.6.
If the potential $V \in \mathcal{C}^\infty(\mathbb{R}^n)$ satisfies Assumption 1.3 then the operator K has a compact resolvent.
If the potential $V \in \mathcal{C}^\infty(\mathbb{R}^n)$ satisfies Assumption 1.4, then K has a compact resolvent if (and only if) the Witten Laplacian $\Delta_{V/2}^{(0)}$ has a compact resolvent.

After the proof of these results, we show by analyzing the example of a quadratic potential V that the exponent $1/4$ is not optimal. We also address the question whether nilpotent algebra method can be applied directly to the operator K and explain why a naive application of Helffer-Nourrigat results in [HelNo3] does not work. We emphasize that the hypoelliptic estimate (1.8) is not only used for the question of the compactness of $(1+K)^{-1}$. Indeed a variant of it permits to give a meaning to the contour integral

$$e^{-tK} = \frac{1}{2i\pi}\int_{\partial S_K} e^{-tz}(z-K)^{-1}\,dz\;,$$

for $t>0$, although we cannot say more on the numerical range of K, than

$$\{\langle u, Ku\rangle,\; u\in D(K)\}\subset\{z\in\mathbb{C},\,\mathrm{Re}\,z\geq 0\}\;.$$

This last point is crucial in the quantitative analysis of the rate of return to the equilibrium.

We will not reproduce the complete quantitative analysis of [HerNi] which provides upper and lower bounds of the rate of return to the equilibrium for

$$K_{\gamma_0,m,\beta} = v\cdot\partial_x - \frac{1}{m}(\partial_x V(x))\cdot\partial_v - \frac{\gamma_0}{m\beta}\left(\partial_v - \frac{m\beta}{2}v\right)\cdot\left(\partial_v + \frac{m\beta}{2}v\right)$$

in terms of the friction coefficient γ_0, the particle mass m and the inverse temperature β. These bounds are expressed, up to some explicit algebraic factor in (γ_0, m, β), in terms of the first non zero eigenvalue of the semiclassical Witten Laplacian

$$\Delta^{(0)}_{V/2,h} = -h^2\Delta_x + \frac{1}{4}\left|\nabla V(x)\right|^2 - \frac{h}{2}\Delta V(x) \quad \text{with } h=\beta^{-1}\;.$$

The latter part of this text gives an account of the semiclassical analysis of this Witten Laplacian. We will recall the relationship with Morse inequalities according to Witten [Wi], after introducing the whole Witten complex and the corresponding deformed Hodge Laplacians $\Delta^{(p)}_{f,h}$ on all p-forms. After recalling some basic tools in semiclassical analysis, we recall the more accurate results of Helffer-Sjöstrand [HelSj1, HelSj4] stating that the $\mathcal{O}(h^{3/2})$ eigenvalues of these Witten Laplacians are actually $\mathcal{O}(e^{-\frac{C}{h}})$ and that the restriction of the Witten complex, to suitable finite dimensional spectral spaces, leads by a limiting procedure to the orientation complex which was introduced in topology. Finally, we will discuss and propose some improvements about the accurate asymptotics of those exponentially small eigenvalues given, by Bovier-Eckhoff-Gayrard-Klein in [BovGayKl], [BovEckGayKl1] and [BovEckGayKl2]. This last result will at the end be combined with the comparison inequalities of [HerNi] for the rates of trend to the equilibrium between $K_{\gamma_0,m,\beta}$ and $\Delta^{(0)}_{V/2,h}$, $(h=\beta^{-1})$.
Here is an example of quantitative results which can be obtained.

Proposition 1.7.
Assume that the potential V is a C^∞ Morse function with

- *two local minima $U_1^{(0)}$ and $U_2^{(0)}$, such that $V(U_1^{(0)}) < V(U_2^{(0)})$,*
- *one critical point with index 1 $U^{(1)}$,*
- *$V(x) = |x|^2$ for $|x| \geq C$.*

Then for fixed any fixed $\gamma_0 > 0$ and $m > 0$, the rate $\tau(\gamma_0, m, \beta)$ satisfies

$$\liminf_{\beta\to\infty} e^{\beta\left(V(U^{(1)})-V(U_2^{(0)})\right)}\tau(\gamma_0, m, \beta) > 0 \,,$$

$$\text{and} \ \limsup_{\beta\to\infty} \frac{e^{\frac{\beta}{2}\left(V(U^{(1)})-V(U_2^{(0)})\right)}\tau(\gamma_0, m, \beta)}{\beta\log\beta} < +\infty \,.$$

At the level of the methods, there is no strict separation between the qualitative and the quantitative analysis. This is especially true for the maximal estimates obtained for operators on nilpotent Lie algebra: the existence of uniform estimates can indeed lead by a kind of addition of variable procedure standard in physics to semi-classical estimates.

In order to help the reader who is not necessarily specialist in all the techniques, we now give a rather precise description of the contents of the book, chapter by chapter. We mention in particular the possibilities for the reader to omit some part at the first reading.

- In Chapter 2, we present the Hörmander condition for a family of vector fields and the proof given by J. Kohn of the subellipticity of the Hörmander's operators $\sum X_j^2$ and $X_0 + \sum X_j^2$. Although it is a rather standard material, we thought that it was useful to give the details because many other proofs will be modelled on this first one. The use of the pseudo-differential theory is minimal in this chapter, and appears essentially only for operators of the form $\Lambda^s := \phi(x)(1-\Delta)^s\chi(x)$, composed with partial differential operators. We give all the details for the brackets arguments but do not recall how the hypoellipticity can be derived from these subelliptic estimates.
- In Chapter 3, we recall some basic criteria for the compactness of the resolvent of the Schrödinger operator following a paper of Helffer-Mohamed. Again, this is rather standard material but we show how to use the Kohn's argument in the context of global problems. The bracket's technique is used here in order to prove that the form domain of the Schrödinger operator is compactly embedded in L^2. This is simply obtained by showing the continuous imbedding of the form domain in a weighted L^2 space. We have not resisted to the pleasure to present the connected problem of the magnetic bottles.

- In Chapter 4, we recall some elements of the Weyl-Hörmander calculus. The main aim is to construct the analog of the Λ^s appearing in Kohn's proof in a very large context. Because we wanted here to extend as much as possible the previous work of Hérau-Nier in [HerNi], we were naturally led to introduce a rather general class of pseudo-differential operators adapted to this problem. The reader can at the first reading omit this chapter and just take the main result as a fact. The existence of this family $(\Lambda^s)_{s\in\mathbb{R}}$ of pseudo-differential operators when Λ is a globally elliptic or globally quasi-elliptic operator (whose simplest example is the square root of the harmonic oscillator) is rather old (See for example the work by D. Robert in the seventies). Here the Beals criterion in the framework of Weyl-Hörmander calculus allows to consider once and for all possibly degenerate cases. We close the discussion by presenting new results of J.-M. Bony about the geodesic temperance.
- Chapter 5 is the first key chapter. We first show that our Fokker-Planck operators are maximally accretive by extending a self-adjointness criterion of Simader. This result seems to be new. We then analyze various properties of the Fokker-Planck operator. The main point is the analysis of the compactness of the resolvent. Developing an approach initiated by Hérau-Nier and implementing the family Λ^s analyzed in the previous chapter, the proof is a tricky mixture between Kohn's proof of subellipticity, Helffer-Mohamed's proof for the compactness of the resolvent of the Schrödinger operator and of the algebraic structure of the Fokker-Planck operator. The link with a Witten Laplacian is emphasized and this leads to propose a natural necessary and sufficient condition for the compactness of the resolvent of the Fokker-Planck operator which is partially left open. This disproves also that only an Hörmander's type global condition is sufficient. We also analyze carefully the so called quadratic model, recalling on one hand the explicit computations presented in the book by Risken and showing on the other hand how "microlocal analysis" can be used for improving Kohn's type estimates.
- Chapter 6 shows how the previous hypoelliptic estimates permit to control the decay of the semi-group attached to the Fokker-Planck operator. The reader will find here the main motivation coming from the Kinetic theory. Again, we meet, when trying to be more quantitative, the question of estimating carefully the behavior of the lowest non zero eigenvalue of a canonical Witten Laplacian.
- Chapter 7 is devoted to a short description (without proofs) of the characterization of the hypoellipticity for homogeneous operators on nilpotent groups. The main result is a conjecture of Rockland which was proved in the late 70's by Helffer-Nourrigat. The reason for including this presentation in the book is two fold. First the hypoellipticity plays an important role in the analysis of the Fokker-Planck operator and the Witten Laplacian with degenerate ellipticity. Secondly, we consider maximal estimates and the proof of Helffer-Nourrigat was actually establishing as a technical tool a lot of spectral estimates for operators with polynomial coefficients.

- Chapter 8 develops the relationship between the nilpotent analysis and the more general analysis of maximal hypoellipticity of polynomial of vector fields. The breakthrough was the paper by Rothschild-Stein which opened the possibility to establish and prove good criteria of maximal hypoellipticity. We very briefly present some ideas of the results obtained in this spirit by Helffer-Nourrigat and Nourrigat during the eightie's.
- Chapter 9 is a first try to apply nilpotent techniques directly to the Fokker-Planck operator. We present the main difficulties and discuss various possible approaches. As an application of these ideas we obtain a first result containing the quadratic Fokker-Planck model, which is far from proving the general conjecture, but leads to optimal estimates.
- Chapter 10 presents how the nilpotent techniques work for particular systems. Instead of looking at the Witten Laplacian, it is better to look at the system corresponding to the first distorted differential of the Witten complex. The analysis of the microlocal maximal hypoellipticity or of the microlocal subellipticity of these systems of complex vector fields, which was done in the eighties mainly motivated by the $\bar{\partial}_b$-problem in complex analysis, gives as byproducts new results for the compactness of the resolvent and for the semi-classical regime. Following a former lecture note of Nourrigat, our presentation (without proof) of the basic results in microlocal analysis can be understood independently of the nilpotent language.
- Chapter 11 is continuing the investigation of the Witten Laplacian on $\mathbb{R}^n$. After recalling its general properties and its relationship with statistical mechanics (this point is detailed in Chapter 12), we present recent criteria for the compactness of its resolvent obtained by the authors and discuss many examples. New results are presented in connection with the subellipticity of some tangential system of vector fields.
- With Chapter 12, we start the presentation of the semi-classical analysis. The chapter is mainly devoted to the analysis of the so called harmonic approximation and we give a flavour of what is going on for large dimension systems which appear naturally in statistical physics.
- Chapter 13 enters more deeply in the analysis of the tunneling effect. Because there are already pedagogical books on the subject, we choose to select some of the important ideas and limit ourselves to the treatment of the first model of the theory: the double well problem.
- Chapter 14 starts the analysis of the Witten Laplacian in the semi-classical regime. We recall how E. Witten uses the harmonic approximation technique for suitable Laplacians on p-forms attached to a distorted complex of the de Rham complex in order to give an analytic proof of the Morse inequalities.
- Chapter 15 is again a key chapter. We now would like to analyze exponentially small effects. We recall (in a sometimes sketchy way) the main steps of the so called Witten-Helffer-Sjöstrand's proof that the Betti numbers are also the cohomology numbers of the orientation complex.

- Chapter 16 explores how this approach permits to understand and partially recover some recent results by Bovier-Gayrard-Klein. We also present the recent results obtained in collaboration with M. Klein. We close the chapter by an application to the splitting for the Witten Laplacian on functions.
- Chapter 17 is devoted to the presentation of the result obtained by Hérau-Nier for the rate of decay for the semi-group associated to the Fokker-Planck operators which was one of the main motivations of the whole study.
- The last chapter gives additional information on quite recent results obtained or announced in the last year.