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Quantum Birkhoff normal forms and semiclassical analysis

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Abstract.

The goal of this text is to motivate for an effective version of the quantum Birkhoff normal form, which gives precise spectral asymptotics even in the presence of resonances, in the semiclassical limit. Microlocal analysis, via pseudo-differential operators and Toeplitz operators is used in order to achieve this.

Foreword — The following text is a written version of a talk I delivered at IHES during the conference on *Non commutativity*. It is based on a joint work with Laurent Charles (Paris 6). A more complete article with all details of the proofs appears in [7]. For this reason, the purpose of this text is not to give any precise proof, but instead to convey some important ideas in a simple language.

§1. Introduction

The story starts with quantum mechanics. Consider the linear Schrödinger operator $\hat{H} = -\frac{\hbar^2}{2}\Delta + V(x)$, acting on $\mathbb{R}^n$. Suppose the function V, called the *potential*, is smooth, and confining. By *smooth*, we mean here of class C^∞. However, similar results certainly hold for analytic potentials. By *confining*, we mean that V has a global minimum at some point $x_0 \in \mathbb{R}^n$: $\liminf_{\|x\|\to\infty} V(x) > V(x_0)$.

In (quantum) mechanical terms, we say that one has a *potential well* at x_0. The quantum theory asserts that the *eigenfunctions* of $\hat{H}$ are the stationary states of the system, and the corresponding *eigenvalues* are

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a measure of the energy of these states. The presence of a potential well has the effect to trap the particle inside the well, thus generating a family of stationary states which are bound to it, with a corresponding *discrete spectrum* of energies.

The state with lowest energy is called the *ground state* and is of primary importance since it is the physically most stable state. For instance, a quantum molecule subject to no exterior excitation is expected to live in its ground state. In everyday's life, though, molecules are excited through, for instance, physical or chemical reactions. Thus, they (often momentarily) occupy some states with more energy, called *excited states.*

In this text, our goal is to compute the energies of such *weakly excited states.* It is well known that in general, no precise information is known about these energies. Of course they are just eigenvalues of some self-adjoint operator, but having a grip on their numerical values requires... well, numerical computations. Here, we wish to disprove this statement. It is equally well established that, *in the limit of small values of* $\hbar$ (the so-called semiclassical limit), one can expect more information, because quantities computable from *classical mechanics* become relevant.

And in fact, it is not so uncommon in quantum chemistry that, after reducing all physical parameters, one ends up with a Schrödinger operator like $\hat{H}$, with a parameter $\hbar$ which, if not the original Planck constant, is nevertheless rather small. Since the 1970's, is has been widely recognised that semiclassical approximations can have practical importance in molecular spectroscopy.

Following Sjöstrand's terminology, we will reserve the word *excited state* for a state whose energy is above a *fixed* distance from the ground state energy. By fixed we mean independent of $\hbar$. Thus, in this text, we shall be rather interested in states whose energy *tends to the ground state energy.* These are called *semi-excited states.*

For such low energies, it particularly makes sense to replace the potential V by a Taylor expansion around the minimum of the well, truncated to an arbitrary order. If the minimum of V is non degenerate, then we expect to be able to express the eigenvalues of $\hat{H}$ as perturbations of the case of a positive definite quadratic form, which is exactly solvable. However, from the works of Poincaré and Birkhoff in classical mechanics, we know that, instead of a mere Taylor polynomial, some kind of averaging of the higher order terms known as *Birkhoff's normal form* will provide a much better approximation.

The rest of this text aims at using the Birkhoff normal form in the context of the Schrödinger operator, in order to give precise asymptotics of eigenvalues corresponding to semi-excited states of $\hat{H}$.

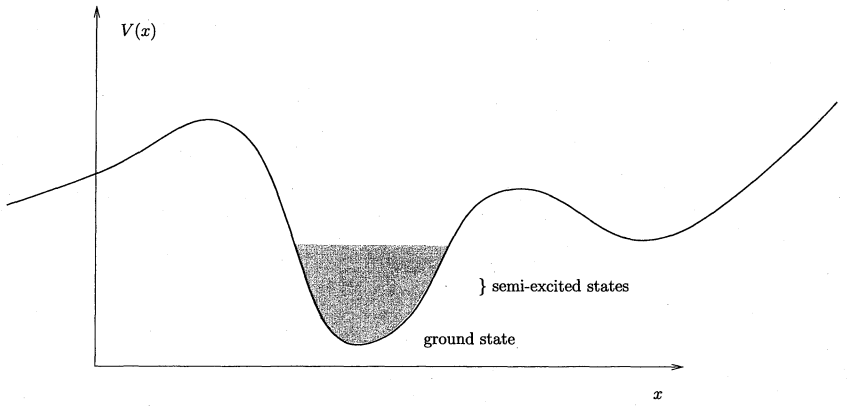

Fig. 1. A confining potential

§2. Hamiltonian mechanics

Using a Birkhoff normal form implies accepting to transfer our system immediately in *phase space*. And in fact, since we shall be using canonical transformations, which mix position and momentum variables, the notion of a potential itself looses its meaning.

Instead of being a complication, it reveals that everything we will do is much more general than expected. It will allow us to treat as well not only the Schrödinger operator, but any observable in phase space (subject to suitable assumptions). This remark was essentially made by mathematicians in the late 60's (Maslov, Hörmander), leading to microlocal analysis.

Thus, let us now recall the objects we need from classical Hamiltonian mechanics.

Phase space. — Most of the time we shall deal with the phase space $\mathbb{R}^{2n}$, equipped with canonical variables $(x,\xi) = (x_1,\dots,x_n,\xi_1,\dots,\xi_n)$. The *Hamiltonian function*, which physically represents the energy of the system, is denoted by $H(x,\xi)$. For instance, the classical energy corresponding to the Schrödinger operator is

$$H(x,\xi) = \frac{1}{2}\|\xi\|^2 + V(x),$$

where one recognises the sum of the kinetic and the potential energies.

Any function on $\mathbb{R}^{2n}$ gives rise to a *dynamical system*, known as Hamilton's equations :

$$\begin{cases} \dot{x} = \frac{\partial H}{\partial \xi} \\ \dot{\xi} = -\frac{\partial H}{\partial x} \end{cases}$$

A better geometrical understanding of Hamilton's equation is provided by looking more generally at a phase space as a *symplectic manifold* (M, ω). Then H defines a vector field $\mathcal{X}_H$ on M by the equation $\omega(\mathcal{X}_H, \cdot) = -dH$. The corresponding Hamiltonian dynamical system is $\frac{dm}{dt} = \mathcal{X}_H(m)$. In $\mathbb{R}^{2n}$, one takes $\omega = \sum_j d\xi_j \wedge dx_j$.

The most basic fact of Hamiltonian mechanics is that the function H is always *invariant* under the Hamiltonian flow. As we shall see, the purpose of the Birkhoff normal form is to provide us with an *additional invariant function.*

Classical wells. — When a classical particle is inside a potential well, and if its energy is not sufficient to let it jump over the *potential barrier*, then it stays forever in the well. This phenomenon is not limited to the position variable x. It follows directly from the conservation of energy for a general Hamiltonian function H that one can have potential wells in full phase space. The precise definition is given below; although we will consider only global wells, many of the constructions should have some interest for local wells too.

Definition 2.1. *We will say that a Hamiltonian function H has a* ***non-degenerate global well*** *at the point $z_0 \in \mathbb{R}^{2n}$ if z_0 is a non-degenerate global minimum of H :*

$$H(z_0) = 0,\ dH(z_0) = 0,\ H"(z_0) \text{ is positive definite.}$$
$$\text{Moreover } \exists E_\infty > 0 \text{ such that } \{H \leqslant E_\infty\} \text{ is compact.}$$

In this situation, the point z_0 is *fixed point* for the classical dynamics, and for any energy $E \leqslant E_\infty$, trajectories in $H^{-1}(E)$ are complete.

The classical Birkhoff normal form. — The classical Birkhoff normal form has been used in mechanics for quite a long time [2]. It is a refinement of the averaging method. The easiest way to understand it is at the level of formal power series.

Suppose we need precise information about the dynamics of a classical system *near the bottom of a well* z_0. Because trajectories have small energies, they will stay close to z_0, and using Taylor series approximations is a natural idea. The crudest approximation is the quadratic part H_2 :

$$H = H_2 + \mathcal{O}((x, \xi)^3).$$

Of course, H_2 is a positive definite quadratic form. It is pleasant to observe that the dynamics of H_2 is completely explicit and easy to compute. Indeed, as a simple exercise in linear algebra [19, proposition 3.1.1] will show, *up to a canonical linear change of coordinates, H_2 is a sum of harmonic oscillators.* So, there are positive real numbers $\nu_1, \dots, \nu_n$ such that, in some new canonical variables (x, ξ),

$$H_2(x,\xi) = \sum_{j=1}^{n} \nu_j (x_j^2 + \xi_j^2)/2. \tag{1}$$

Such a Hamiltonian is obviously completely integrable. In fact, it follows easily from this formula that the dynamics of H_2 consists of *quasiperiodic* translations of speed $(\nu_1, \dots, \nu_n)$ in the tori $x_j^2 + \xi_j^2 = \text{const}_j$, $\forall j$.

Now, in order to get a good approximation of the dynamics of H, one has to take into account the next term in the Taylor series, H_3. The idea of the averaging method is that the error in doing so can be greatly reduced by replacing H_3 by its average along the flow of H_2. The Birkhoff normalisation procedure pushes this idea to any order. It can be stated as follows.

Theorem 2.2 (Birkhoff). *There exist new formal canonical coordinates (x, ξ), tangent to the identity, and a formal Taylor series*

$$K = K_3 + K_4 + \cdots, \qquad \textit{with } K_j \textit{ homogeneous of degree } j \textit{ in } (x,\xi)$$

such that

$$H(x,\xi) = H_2 + K$$

where K is invariant under the flow of H_2: $\{H_2, K\} = 0$.

The obvious and crucial question for a mathematician is how to make this effective. In other words, what information about the dynamics does this formal statement contains?

At this point, an easy answer can be given. Simply truncate at some order N the canonical change of coordinates. Then consider the polynomial K^N obtained by truncating the series K at the order N. Then in the new variables, $\{H, K^N\}$ vanishes up to order N, which means that K^N is an approximate integral of motion for H. Notice that, in general, by just truncating the change of coordinates we loose the symplectic structure. However, several tricks are known, which make the change of coordinates a true canonical diffeomorphism; one is to consider *generating functions* [1]; another, more natural, is to construct the canonical transformation as a flow at time one of some auxiliary Hamiltonian.

Let us recall that having an additional integral of motion for a Hamiltonian system is interesting because it "reduces the number of degrees of freedom". Precisely, it implies that the motion takes place in a submanifold of dimension $2n-2$. But this is not the only asset of the method, and the power of the Birkhoff normal form also comes from the fact that, in general, one can do much better, just looking at the quadratic part H_2 :

- if the "frequencies" ν_j are independent over $\mathbb{Q}$ (one usually talks about "non-resonant" frequencies), then $K = f(I_1, \ldots, I_n)$ with $I_j = (x_j^2+\xi_j^2)/2$. So we have actually n independent, Poisson commuting integrals of motion ! Therefore, the dynamics is (formally) completely integrable and the flow of H winds densely on a Lagrangian n-torus.
- if the frequencies are completely resonant: $\nu_j = \nu_c \kappa_j$ with coprime integers $\kappa_j \in \mathbb{N}$ and $\nu_c \in \mathbb{R}^+$, then there is no (obvious) integral for H, apart from K. But, on the other hand, a nice feature appears : the flow of H_2 is periodic.
- Of course, intermediate cases can occur. But we won't deal with them here.

An outstanding question about Birkhoff's normal form is the convergence of the series. Already raised by Poincaré this problem is still not completely understood. Although we shall in fact not use any convergence properties, let us mention briefly two recent results that shed some light on this issue. The first one is due to Perez–Marco [14] and Gong [10] who say that, given a fixed, non-resonant, quadratic part H_2, then the Birkhoff normal form K is generically divergent, in a space of analytic Hamiltonians. The second result, obtained by Zung [21], shows that the canonical transformation (and hence the normal form itself) is convergent as soon as the analytic Hamiltonian H is *analytically completely integrable.*

From a physicist's viewpoint, the interesting question is probably elsewhere. For instance, how about a version of Birkhoff's normal form suitable for *quantum mechanics*? The main incentive of our work is to give a precise answer to this. Of course, many authors have already considered this problem. To begin with, physicists in the 1970's have started to notice that using Birkhoff's normal form at a formal level, for polynomial observables on phase space give very accurate numerics. They made the crucial observation that *resonances* should be taken into account. Due to small divisors, treating an almost resonant system as a perturbation of a resonant one is much wiser, numerically speaking, than considering it as a non-resonant system. It is possible to give a

mathematical version of this in terms of asymptotic expansions. That's the reason why we will use semiclassical analysis.

§3. Quantum mechanics

Let us recall now our initial motivation from quantum mechanics. The Schrödinger operator is

$$P = -\frac{h^2}{2}\Delta + V(x). \tag{2}$$

Assume that the potential V is smooth on $\mathbb{R}^n$ and has a global, non-degenerate minimum at $x_0 = 0$ with $V(0) = 0$. Then the quadratic form $V''(0)$ is positive definite; hence there exists a unitary linear change of coordinates on $\mathbb{R}^n$ which makes $V''(0)$ diagonal. Let us denote by $(\nu_1^2, \ldots, \nu_n^2)$ its eigenvalues, with $\nu_j > 0$.

Now, the simple rescaling $x_j \mapsto \sqrt{\nu_j} x_j$ transforms P into a perturbation of the harmonic oscillator $\hat{H}_2$:

$$P = \hat{H}_2 + W(x), \qquad \text{with } \hat{H}_2 = \sum_{i=1}^{n} \frac{\nu_j}{2}\left(-\hbar^2 \frac{\partial^2}{\partial x_j^2} + x_j^2\right),$$

where $W(x)$ is a smooth potential of order $\mathcal{O}(|x|^3)$ at the origin.

Our results will apply not only to such an operator, but also to any *pseudo-differential operator* P in some standard symbol class, that is self-adjoint and that possesses a non-degenerate global well in the sense of definition 2.1. In is not the purpose of this paper to explain in details the pseudo-differential calculus that will be used. (In fact, one can even argue that it is not so crucial.) However, we do need good properties such as a pseudo-differential functional calculus, and for this we will use the classes defined by the metric $(\|x\|^2 + \|\xi\|^2)^{\frac{m}{2}}$, $m \in \mathbb{Z}$, and assume that P is elliptic at infinity. Then P is essentially self-adjoint and has a discrete spectrum below E_∞. These classes are easy to work with but the ellipticity condition is too restrictive for Schrödinger operators. This is not too bad since, for the study of the discrete spectrum near the origin, one can always replace the initial Schrödinger operator by a good pseudo-differential operator in these simple classes (see for instance [12]).

Denote by $\lambda_1(\hbar) \leqslant \lambda_2(\hbar) \leqslant \cdots$ these eigenvalues, repeated with their multiplicities. In 1983, almost independently, Simon [15, 16] and Helffer–Sjöstrand [12] proved that for any fixed j, $\lambda_j(\hbar)$ admits an asymptotic expansion in *half-integer* powers of $\hbar$. The presence of non-integers powers of $\hbar$ was a bit surprising at that time, maybe because

they never appear in one degree of freedom and, more generally, in integrable cases. However, in two degrees of freedom with — for instance — a $1:2$ resonance (which means that $\nu_2/\nu_1 = 2$) then such half-integer powers of $\hbar$ are generic.

Thus, these "low-lying eigenvalues" are well understood. However, they describe the system only at very low energies, of order $\mathcal{O}(\hbar)$. We wish now to say something about semi-excited states, that is to say energies much larger that $C\hbar$ but, still, that tend to zero as $\hbar$ tends to zero.

The first answer was given in 1992 by Sjöstrand [17], and concerns the case where the frequencies are non-resonant. In this situation, we expect the spectrum to behave as the spectrum of a completely integrable system, which it does indeed :

Theorem 3.1 (Sjöstrand). *If the ν_i's are independent over $\mathbb{Q}$, then for any $\delta \in (0,1)$,*

$$\mathrm{Spec}(P) \cap [0, C\hbar^\delta] = \{f(\hbar(k_1 + \tfrac{1}{2}), \dots, \hbar(k_n + \tfrac{1}{2}); \hbar), \quad k_i \in \mathbb{Z}\} + O(\hbar^\infty)$$

where $f = f(I_1, \dots, I_n; \hbar)$ admits an asymptotic expansion in integral powers of $\hbar$, in the C^∞ topology.

Let us give some heuristics in order to understand this result and to see what one could do in the general case.

- *The non-resonant case.* This is actually the easiest case. Formally, the Hamiltonian function H is completely integrable; hence, under some canonical transformation, it can be written as
$$H = f(I_1, \dots, I_n)$$
for some formal function $f : \mathbb{R}^n \to \mathbb{R}$, where the functions I_j are *action integrals* $I_j(x,\xi) = \frac{1}{2}(x_j^2 + \xi_j^2)$. Then, one can quantise the canonical transformation, in which case the quantum Hamiltonian $\hat{H}$ now becomes microlocally unitarily equivalent to $f(\hat{I}_1, \dots, \hat{I}_n)$, with $\hat{I}_j = \frac{1}{2}(-\hbar^2 \frac{\partial^2}{\partial x_j^2} + x_j^2)$. Of course, these operators $\hat{I}_j$ are just 1D harmonic oscillators, whose spectrum is the set $\{\hbar(k + 1/2); k \in \mathbb{N}\}$. Since H is confining, this "normal form" really gives a good approximation to the spectrum of $\hat{H}$. This is what Sjöstrand's theorem says.
- *The resonant case.* We assume here that, up to a common multiple, all frequencies ν_j are integers. Then the Hamiltonian flow of H_2 is periodic, and the Birkhoff normal form says that, up to some canonical transformation, one is reduced to the case

where H *commutes* with the S^1-action generated by H_2. So, naturally, one would like to *reduce* the system with respect to this action. However, this is not easy, for at least two reasons. The first difficulty is that this S^1 action is in general not free. The orbit space cannot be expected to be a manifold; it will have orbifold singularities in general. The simplest example is the 1 : 2 resonance for which the orbit space has the "tear"-like shape displayed in figure 2. The second technical difficulty

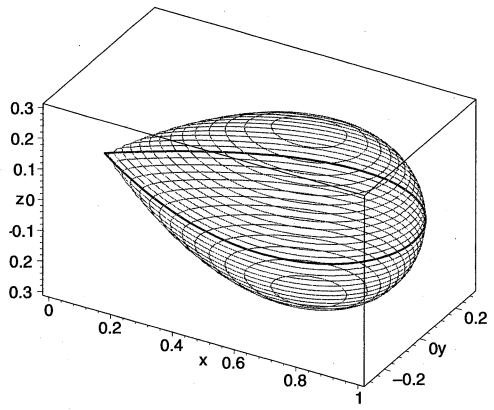

Fig. 2. The orbit space of the 1 : 2 resonance Hamiltonian $H = \frac{1}{2}(x_1^2 + \xi_1^2) + x_2^2 + \xi_2^2$

concerns quantisation. Because of their power and flexibility, we have chosen to work with pseudo-differential operators. However, they still have some intrinsic rigidity as they serve to quantise very particular phases spaces : cotangent spaces. And in general, the cotangent structure is lost after reduction. So we need a more geometric quantisation that would work on orbifolds...

In the middle of the 1970's, several people started to consider the question of quantising a system with symmetry with microlocal tools. It has led to many very interesting results concerning eigenvalues *clusters*, and more general statements about the commutation of quantisation and reduction. This area of research combines in a remarkable way analysis, geometry and algebra, in the spirit of Atiyah–Singer's index theorem.

Concerning eigenvalues clusters, the pioneers were Chazarain [8], Weinstein [20], Colin de Verdière [9], and Guillemin [11]. The result they were interested in was roughly the following.

Theorem 3.2 (Weinstein, Guillemin, Colin de Verdière). *Let P be an elliptic, self-adjoint pseudo-differential operator on a compact manifold. If the Hamiltonian flow of the principal symbol p is* simply periodic *(in particular without fixed points), and the subprincipal symbol vanishes, then the spectrum is clustered on an arithmetic progression $\alpha + \beta(N\hbar + \gamma)$, $N \in \mathbb{Z}$.*

The proof of this theorem follows from the idea that on can always perturb P by a subprincipal term, in such a way that $\exp(-iP/\beta\hbar) =$

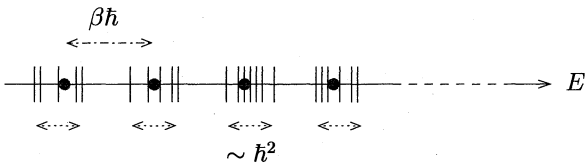

Fig. 3. The spectrum is separated into clusters.

$C.Id$, for some non-vanishing constants β, C. Actually, the assumption on the subprincipal symbol can be somewhat relaxed (its average along the flow should be constant), see [5]; see also [4] for the computation of the shift α.

The original statement was not actually in terms of a small parameter $\hbar$. In fact, the extension of this result to $\mathbb{R}^n$, including a full-fledged semiclassical version was worked out later by Helffer and Robert. Many other interesting development occurred too, like the discovery by Boutet de Monvel and Guillemin [5] that the number of eigenvalues in each cluster could be computed as a Hilbert–Samuel polynomial, a kind of Atiyah–Singer, Riemann–Roch formula. Please consult these references, or [7], for a more accurate version of the (hi)story.

Such a result naturally raises two questions : first, the conditions on the flow is quite restrictive. A general S^1 action has isotropy. Thus, to begin with, is there a version of this theorem that would include fixed points? The second question is deeper : the existence of clusters if a first step; what can we say about the internal structure of each cluster? These two points are at the heart of our concerns here.

Thus, our main result can be split into two theorems, formulated as follows.

Theorem 3.3 ([7]). *Let P be the Schrödinger operator as in (2). Assume that the frequencies ν_j are coprime integers.*

(1) *There exists $\hbar_0 > 0$ and $C > 0$ such that for every $\hbar \in (0, \hbar_0]$*

$$\mathrm{Spec}(P) \cap (-\infty, C\hbar^{\frac{2}{3}}) \subset \bigcup_{E_N \in \mathrm{Spec}(\hat{H}_2)} \left[E_N - \frac{\hbar}{3}, E_N + \frac{\hbar}{3}\right].$$

(2) *When $E_N \leqslant C\hbar^{\frac{2}{3}}$, let $m(E_N, \hbar) = \#\mathrm{Spec}(P) \cap \left[E_N - \frac{\hbar}{3}, E_N + \frac{\hbar}{3}\right]$. Then $m(E_N, \hbar)$ is precisely the dimension of $\ker(\hat{H}_2 - E_N)$.*

The first point asserts the existence of clusters, centred on the eigenvalues E_N of $\hat{H}_2$, which are in an arithmetic progression of reason $\hbar$:

$$E_N = \hbar\left(\frac{|\nu|}{2} + N\right), \quad N \in \mathbb{N}.$$

The factor of $1/3$ in $\frac{\hbar}{3}$ is just here to show that, when h_0 is small enough, the clusters are indeed separated from each other.

The second point ensures that each cluster contains the expected number of eigenvalues, that is, the multiplicity of E_N.

The first two points essentially say that, in this asymptotic region of energy less that $C\hbar^{\frac{2}{3}}$, the spectrum of P behaves like a regular perturbation of the spectrum of $\hat{H}_2$.

Theorem 3.4 ([7]). *In the situation of the preceding theorem, one can describe the internal structure of the N-eth cluster of eigenvalues as follows.*

Let $k = k(x, \xi)$ be the average of W along the flow of H_2. Let $S_N \subset \mathbb{R}^{2n}$ be the ellipsoid :

$$S_N = \{(x, \xi) \in \mathbb{R}^{2n}, \quad H_2(x, \xi) = E_N\}.$$

Let

$$E_N + \lambda_1(E_N, \hbar), \ldots, E_N + \lambda_{m(E_N,\hbar)}(E_N, \hbar)$$

be the eigenvalues of P in this N-eth band $\left[E_N - \frac{\hbar}{3}, E_N + \frac{\hbar}{3}\right]$.

Then, uniformly for $\hbar < \hbar_0$ and N such that $E_N \leqslant C\hbar^{\frac{2}{3}}$,

$$\lambda_1(E_N, \hbar) = \inf_{(x,\xi) \in S_N} k(x, \xi) + (E_N)^{\frac{3}{2}} \mathcal{O}(N^{-1}), \tag{3}$$

$$\lambda_{m(E_N,\hbar)}(E_N, \hbar) = \sup_{(x,\xi) \in S_N} k(x, \xi) + (E_N)^{\frac{3}{2}} \mathcal{O}(N^{-1}) \tag{4}$$

and for any function $g \in C^\infty(\mathbb{R})$,

$$\sum_{i=1}^{m(E_N,\hbar)} g\Big(\frac{\lambda_i(E_N,\hbar)}{(E_N)^{\frac{3}{2}}}\Big) = \Big(\frac{1}{2\pi\hbar}\Big)^{n-1} \int_{S_N} g\Big(\frac{k(x,\xi)}{(E_N)^{\frac{3}{2}}}\Big) \mu_{E_N}(x,\xi) + \mathcal{O}(N^{2-n})$$

where μ_{E_N} *is the Liouville measure of* S_N.

This theorem explains, in a weak sense, the repartition of eigenvalues in each cluster. This repartition is shaped by the symbol k, which plays the role of an *effective principal symbol* for the reduced system. The results are what one would expect when viewing each separate cluster as a semiclassical system on its own.

Of course, the result holds as well for any elliptic pseudo-differential operator with a non-degenerate global well, and with completely resonant frequencies. The adjustments needed in the statement are the following : the formula for k in terms of the symbol of p is less straightforward, and the spectrum has to be shifted by the $\hbar$ times the value at the origin of the subprincipal symbol of P. (In the theorems above we have used the fact that the Schrödinger operator has a vanishing subprincipal symbol.)

The proof of the theorem is not given here; instead, we will try to emphasise the main ingredients needed.

§4. The methods

4.1. The quantum Birkhoff normal form

A crucial observation, which enables us to merely think about a quantum version of Birkhoff's normal form, is that the essential ingredient of the normalisation procedure lies in *Lie algebra* properties of the Poisson bracket. Thus, in the quantum setting, even if the algebra of observables is not commutative, one can implement a Birkhoff normal form thanks to the Lie algebra structure given by commutators. Of course, the fact that commutators, in the semiclassical limit, gives Poisson brackets, is a strong incentive for believing that this is indeed the right observation.

As in the classical setting, the first step is to understand the *formal* structure of the quantum Birkhoff normal form.

We work with the space

$$\mathscr{E} = \mathbb{C}\,[\![x_1, \ldots, x_n, \xi_1, \ldots, \xi_n, \hbar]\!],$$

and define the *weight* of the monomial $x^\alpha \xi^\beta \hbar^\ell$ to be $|\alpha|+|\beta|+2\ell$. Indeed, it turns out that this grading, modelled after scaling properties of the harmonic oscillator, is particularly well adapted to our problem.

The finite dimensional vector space spanned by monomials of weight N is denoted by $\mathscr{D}_N$. Let $\mathscr{O}_N$ be the subspace consisting of formal series whose coefficients of weight strictly less than N vanish. $(\mathscr{O}_N)_{N\in\mathbb{N}}$ is a filtration

$$\mathscr{E} = \mathscr{O}_0 \supset \mathscr{O}_1 \supset \cdots, \qquad \bigcap_N \mathscr{O}_N = \{0\}.$$

The formal quantum Birkhoff normal form can be expressed as follows.

Theorem 4.1. *Let $H_2 \in \mathscr{D}_2$ be the harmonic oscillator (as in equation (1)) and $L \in \mathscr{O}_3$. Then there exists $A \in \mathscr{O}_3$ and $K \in \mathscr{O}_3$ such that*

- $e^{i\hbar^{-1}\mathrm{ad}_A}(H_2 + L) = H_2 + K$;
- $[K, H_2] = 0$.

Moreover if H_2 and L have real coefficients then A and K can be chosen to have real coefficients as well.

Because we will use Weyl's quantization to transform these power series into operators, polynomials with real coefficients will give symmetric operators.

Thus, formally, a suitable conjugation by a unitary formal operator reduces $P = H_2 + L$ to a new operator, $H_2 + K$, admitting a quantum integral, K. Since such a conjugation should leave the spectrum invariant, one expects to be able to calculate the spectrum of P from the study of the normal form $H_2 + K$.

From this formal statement, and similarly to the classical case, one has to understand two aspects : The first is, how to describe formal series that commute with H_2; as before, this depends on arithmetic properties of the frequencies ν_j. The second aspect is to find a way to replace the formal series by asymptotic expansions. This is the role of semiclassical and microlocal analysis, for which we don't give any detail here (they can be found in [7]. The net result is the following statement :

Theorem 4.2 (Quantum Birkhoff normal form [7])**.** *Let P be a semiclassical self-adjoint pseudo-differential operator of order zero such that the principal symbol p admits a non-degenerate global well.*

Then for any compact domain $D \subset \mathbb{R}^{2n}$ containing the origin in its interior there exists a pseudo-differential operator K of order zero such that

- $[K, \hat{H}_2] = 0$;
- *K vanishes microlocally outside of D;*

- *the total Weyl symbol $\sigma_W(K)$ is in $\mathscr{O}_3$, and can be formally obtained algorithmically by the formal quantum Birkhoff normalisation procedure;*

and for each $\eta > 0$ there exists $E_0 > 0$, $\hbar_0 > 0$ and for each N a constant $C_N > 0$ such that for all $(\hbar, E) \in [0, \hbar_0] \times [0, E_0]$,

$$\left(\lambda_j^P \leqslant E \text{ or } \lambda_j^Q \leqslant E\right) \Rightarrow \left|\lambda_j^P - \lambda_j^Q\right| \leqslant C_N(E^N + \hbar^N),$$

where $Q = Q((1+\eta)E) := (\hat{H}_2 + K)_{\restriction \Pi^{\hat{H}_2}_{(-\infty,(1+\eta)E]}(L^2(\mathbb{R}^n))}$.

Here $\Pi_J^{\hat{H}_2}$ is the spectral projector of $\hat{H}_2$ on the interval J.

Notice that one of the key points is that we could realise the operator K as a pseudo-differential operator commuting exactly with $\hat{H}_2$, and not only modulo $O(\hbar^\infty)$. The initial spectral problem is thus reduced to the study of the *joint spectrum* of $\hat{H}_2$ and K. Of course, this will play a crucial role when it will come to reducing the system by the S^1 action. One may notice also that, from a technical, but also conceptual viewpoint, the separation between the parameters E and $\hbar$ is important and useful for understanding the limits of the validity of the method.

4.2. Some applications

This quantum Birkhoff normal form will not only be the instrument of the proof of theorems 3.3 and 3.4, but also allows one to quickly recover many related results. Let us mention some of them here.

Polynomial differential operators. — One of the motivations for this work was to justify the many computations done in molecular physics and chemistry which use a truncation of the Birkhoff normal form for obtaining numerically the spectrum of some molecules [13]. And indeed, the theorem, together with an estimate which enters the proof, gives this justification. This estimate concerns the norm of differential operators with polynomial coefficients acting on an eigenspace of $\hat{H}_2$, when the full symbol has a given order. It can be stated as follows :

Lemma 4.3. *Let $K = K(\hbar)$ be a pseudo-differential operator such that*

- *its Weyl symbol k is of order $\mathscr{O}(\hbar^m)$ in a neighbourhood of the origin;*
- *the Taylor expansion of k at the origin is in $\mathscr{O}_\ell$;*
- *K commutes with $\hat{H}_2$.*

Then there exists $C > 0$, $E_0 > 0$, such that

$$\left\| K_{\restriction \ker(\hat{H}_2 - E_N)} \right\| \leqslant C(E_N)^{\ell/2}(\hbar/E_N)^m, \qquad \forall E_N \in (0, E_0] \cap \operatorname{spec}(\hat{H}_2).$$

In view of this lemma, an application of theorem 4.2 yields the following result :

Theorem 4.4. *In the statement of theorem 4.2, one may truncate the formal series of K at the order $\mathcal{O}(\ell+1)$ (in the $\mathcal{E}$-grading). Then, the truncation still commutes with $\hat{H}_2$ and the error on the eigenvalues is $CE^{\frac{\ell+1}{2}} + O(\hbar^\infty)$.*

Semi-excited states. — Sjöstrand's result in the non-resonant case can be recovered by applying the quantum Birkhoff normal form theorem with $E = Ch^\gamma$, for some $\gamma \in (0,1)$. In this regime the theorem precisely says that, up to an error of order $O(\hbar^\infty)$, the eigenvalues of P in this spectral range are the same as the eigenvalues of a completely integrable approximation.

Low-lying eigenvalues. — It is quite remarkable that theorem 4.2 also applies to the study of low-lying eigenvalues by Helffer–Sjöstrand and Simon. Even though we are now at a limiting case of the allowed asymptotic region in the parameter space $(E,\hbar)$, we may just use the theorem with $E = C\hbar$. For such low energies, Q becomes a finite dimensional matrix ! (of size independent of $\hbar$). Then, when $E = E_N$ is an eigenvalue of $\hat{H}_2$, one can scale E out of the principal term $\hat{H}_2$ using the unitary operator $(U_E\Psi)(x) = E^{\frac{n}{4}}\Psi(\sqrt{E}x)$, which identifies $\ker(\hat{H}_2(\hbar) - E_N)$ with $\ker(\hat{H}_2(\hbar/E)-1)$. Conjugating with U_E in the statement of theorem 4.4, a straightforward computation shows that we are left with a polynomial perturbation of $\hat{H}_2$ in the variable $\sqrt{\hbar}$. Standard perturbation theory for matrices then gives us the result, namely, that each eigenvalue admits an asymptotic expansion in half-integer powers of $\hbar$.

4.3. The Bargmann side

The quantum Birkhoff normal form is the first step in the proof of theorems 3.3 and 3.4. It reduces the initial spectral problem to the study of the restriction of some operator K to eigenspaces of the harmonic oscillator. In case of completely resonant frequencies (*ie.* the frequencies ν_j are coprime integers), the spectrum of $\hat{H}_2$ is the set of eigenvalues $E_N = \hbar(\frac{|\nu|}{2} + N)$, $N \in \mathbb{N}$. The "cluster" associated to N is just the spectrum of K restricted to the eigenspace $\ker(\hat{H}_2 - E_N)$. The estimate of lemma 4.3 gives the width of these clusters, as stated in theorem 3.3.

In order to gain more insight into the internal structure of each cluster, we need to understand the nature of the operator

$$K_{\restriction \ker(\hat{H}_2 - E_N)}.$$

It is not a pseudo-differential operator, simply because it acts on a finite dimensional Hilbert space. However, it does appear as the "symplectic reduction" of a pseudo-differential operator on $\mathbb{R}^n$. Indeed, the operation of restriction of K to the E_N-eigenspace of $\hat{H}_2$ is the quantum analogue to the symplectic reduction of the principal symbol k by the S^1-action generated by the Hamiltonian flow of H_2, at the energy E_N. Enforcing this *quantisation commutes with reduction* philosophy, we have to consider the E_N-eigenspace of $\hat{H}_2$ as the quantisation of the symplectic reduced space $M_{E_N} = H_2^{-1}(E_N)/S^1$. Except in the case where all frequencies are equal to 1 (the co-called $1:1\cdots:1$ resonance), the action has a non-trivial, finite degree isotropy, and M_{E_N} is an *orbifold.* More precisely, it is a *weighted projective space.* In [5], Boutet de Monvel and Guillemin showed how to quantise smooth projective varieties (and more generally contact manifols), and how to endow them with an algebra of microlocal operators, called Toeplitz operators. This book was really a pioneer in building such a deep bridge between algebraic geometry and microlocal analysis. It is expected that nowadays more and more algebraic problems will reveal their microlocal nature through a similar process. Charles showed that Toeplitz operators can be defined also for symplectic orbifolds [6], and here we will use this analytico-geometric machinery to extract some finer spectral results.

The first observation which is needed to pass smoothly from pseudo-differential operators to Toeplitz operators is that, in $\mathbb{R}^n$, they coincide (formally and microlocally), via the *Bargmann transform.*

The second observation, which we already alluded to earlier, it that it is now natural to use the scaling operator U_E, which allows us to fix the energy of $\hat{H}_2$, provided we work with a rescaled semiclassical parameter $h = \hbar/E$.

Thus, we will work now in the *Bargmann space* $\mathscr{B}_h$: the Hilbert space of entire holomorphic functions on $\mathbb{C}^n$ with finite norm, where the norm comes from the scalar product

$$\langle \psi, \psi' \rangle_{\mathbb{C}^n} = \int_{\mathbb{C}^n} (\psi, \psi')(z)\mu(z), \qquad \text{with } (\psi, \psi')(z) = \psi(z)\overline{\psi'(z)}e^{-|z|^2/h}$$

where $|z|^2 = \sum z_i \bar{z}_i$ and μ is the Lebesgue measure on $\mathbb{C}^n = \mathbb{R}^{2n}$.

Operators on $L^2(\mathbb{R}^n)$ can be transported on $\mathscr{B}_h$ via the *Bargmann transform* which is the unitary map $U_{\mathscr{B}} : L^2(\mathbb{R}^n) \to \mathscr{B}_h$ given by

$$U_{\mathscr{B}}(\varphi)(z) = \frac{2^{n/4}}{(2\pi h)^{3n/4}} \int_{\mathbb{R}^n} e^{h^{-1}\left(z\cdot x\sqrt{2} - (z^2+x^2)/2\right)} \varphi(x)dx, \tag{5}$$

where $z \cdot x = \sum z_i x_i$, $z^2 = z \cdot z$, $x^2 = x \cdot x$.

The harmonic oscillator becomes

$$\hat{H}_2^{\mathscr{B}}(h) := U_{\mathscr{B}} \tilde{H}_2(h) U_{\mathscr{B}}^* = h \sum_{j=1}^{n} \nu_j \left(z_j \frac{\partial}{\partial z_j} + \tfrac{1}{2} \right).$$

and $H_2 = \sum_j \nu_j |z_j|^2$.

Using the Bargmann transform, *h-pseudo-differential operators* P are transformed into *semiclassical Toeplitz operators*, that is to say, operators of the form

$$T_g : \mathscr{B}_h \to \mathscr{B}_h, \qquad \psi \mapsto \mathbf{\Pi}^{\mathscr{B}}(g\psi),$$

where $\mathbf{\Pi}^{\mathscr{B}}$ is the orthogonal projector of $L^2(\mathbb{C}^n, e^{-|z|^2/h})$ onto $\mathscr{B}_h$, and $g = g(h)$ is a function on $\mathbb{C}^n$ with an asymptotic expansion in powers of h.

We are now in position to throw K in the Bargmann machinery, in the spirit of [3]. Denote by $\mathbf{H}^N$ the N-th eigenspace of $\hat{H}_2$, and let $K_N : \mathbf{H}^N \to \mathbf{H}^N$ be the restriction of K to $\mathbf{H}^N$.

Recall that M_{E_N} is the symplectic reduced space at energy E_N.

Theorem 4.5 ([7]). *K_N can be identified with a $\frac{1}{N}$-semiclassical* Toeplitz operator on M_1*:*

$$K_N = \mathbf{\Pi}_N g$$

where g is a smooth function on M_1 admitting an asymptotic expansion in powers of N^{-1}.

Once we have this result, theorem 3.4 is essentially an application of known spectral asymptotics for Toeplitz operators, as presented by [5] in the smooth case, and by [6] in the orbifold case. Notice again that the new semiclassical parameter is not $\hbar$ anymore, but N^{-1}. The appearance of a different semiclassical parameter is not surprising when considering that our reduction is a kind of second quantisation, in the sense of physicists, and of second microlocalisation, in the sense of Sjöstrand [18].

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