

# Normal forms and semi-classical approximation

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## 1 Introduction

Quantum Mechanics was born at the beginning of the last century with the quantization rules for the harmonic oscillator and for the hydrogen atom. Such rules were almost immediately extended to more general systems by the so called Bohr–Sommerfeld quantization rule: ‘the actions of the classical system can assume only those values which are integer multiples of  $\hbar$ ’. However the actions are defined only in some special situations, and moreover, at present time the Schrödinger equation is the paradigm of quantum mechanics. A question naturally arises: Is there any relation between the eigenvalues of the Schrödinger operator and the numbers obtained by Bohr–Sommerfeld quantization rule (when available)?

According to common wisdom, the ‘Bohr–Sommerfeld numbers’ are a first approximation to the eigenvalues of the Schrödinger operator in the so called semiclassical limit. However precise mathematical results on the subject have been obtained only in the eighties and a good understanding of the problem has been only recently achieved. In particular it is now clear how to compute higher order corrections to the eigenvalues: This is done through suitable normal form procedures.

In the present article we will discuss the above questions for the case of perturbed harmonic oscillators, a case which on the one hand is physically relevant and on the other is well understood. We will only briefly discuss the quantization of perturbations of integrable systems.

## 2 A Statement

On  $L^2(\mathbb{R}^n)$  consider the Schrödinger operator

$$\hat{H} = -\frac{\hbar^2}{2}\Delta + V \tag{2.1}$$

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where  $\Delta$  is the  $n$  dimensional Laplacian and  $V$  is a smooth real potential having an absolute nondegenerate minimum at the origin. We are interested in the eigenvalues of (2.1) close to zero. Introduce coordinates adapted to the normal modes, namely such that

$$V(x) = \sum_{i=1}^n \frac{\omega_i^2 x_i^2}{2} + O(\|x\|^3) .$$

Assume

H1) Nonresonance: There exist  $\gamma > 0$  and  $\tau \in \mathbb{R}$  such that, for any  $k \in \mathbb{Z}^n - \{0\}$  one has

$$|\omega \cdot k| \geq \frac{\gamma}{|k|^\tau} \quad (2.2)$$

H2)  $V(x) > 0$  for  $x \neq 0$ , and

$$\liminf_{|x| \rightarrow \infty} V(x) > 0$$

H3)  $V \in C^\infty(\mathbb{R}^n)$  and for any  $r \geq 0$  there exists  $C_r$  such that

$$\left| \frac{\partial^{|\alpha|} V}{\partial x^\alpha}(x) \right| \leq C_{|\alpha|} \langle x \rangle^m, \quad \forall \alpha \in \mathbb{N}^n,$$

where we used the notation  $\langle x \rangle := (1 + \|x\|^2)^{1/2}$ .

**Theorem 2.1.** *Assume (H1,H2,H3) hold. Then, for any positive  $N, M$  there exist positive constants  $h_{N,M}, \epsilon_{N,M}, C_{N,M}^1, C_{N,M}^2$ , and a smooth function*

$$\mathcal{Z}_{N,M}(I_1, \dots, I_n; \hbar)$$

such that,  $\forall 0 < \epsilon \leq \epsilon_{N,M}$ , and  $0 < \hbar \leq \hbar_{N,M} \epsilon$  the eigenvalues of (2.1) in  $[0, \epsilon)$  have the representation

$$\lambda_k = \left(k + \frac{1}{2}\right) \cdot \omega \hbar + \mathcal{Z}_{N,M} \left( \left(k + \frac{1}{2}\right) \hbar; \hbar \right) + R_{NM}(k, \hbar), \quad k \in \mathbb{N}^n, k_j \geq 1 \quad (2.3)$$

where

$$|R_{NM}(k, \hbar)| \leq C_{N,M}^1 \epsilon^N + C_{N,M}^2 \left(\frac{\hbar}{\epsilon}\right)^M$$

More precisely, for any  $k \in \mathbb{N}^n$  such that

$$\left(k + \frac{1}{2}\right) \cdot \omega \hbar + \mathcal{Z}_{N,M} \left( \left(k + \frac{1}{2}\right) \hbar; \hbar \right) \in [0, \epsilon), \quad (2.4)$$

there exists an eigenvalue  $\lambda_k \in [0, \epsilon)$  for which (2.3) holds, and viceversa, for any eigenvalue in  $[0, \epsilon)$  there exists a  $k$  satisfying (2.3) and (2.4). The function  $\mathcal{Z}_{N,M}(I_1, \dots, I_n; 0)$  coincides with the classical Birkhoff Normal Form of the system computed up to order  $N$ .

The proof of the theorem is constructive, in the sense that it provides an algorithm allowing to construct explicitly, by elementary operations, the function  $\mathcal{Z}_{N,M}$ . One could choose  $\epsilon = \epsilon(\hbar) = \hbar^\delta$  with some positive  $\delta < 1$ , obtaining a simpler statement valid for the eigenvalues in  $[0, \hbar^\delta]$ . It is also possible to weaken the nonresonance condition (H1) to the condition  $\omega \cdot k \neq 0$  for  $k \in \mathbb{Z}^n - \{0\}$ .

A theorem very close to 2.1 was proved by Sjostrand (1992) by a method different from the one that will be presented here (see also Graffi and Paul (1987)). In the analytic or Gevrey case<sup>1</sup> the error can be reduced to be exponentially small with the parameters (Bambusi, Graffi and Paul 1999). Previous results dealing with compact perturbations of the harmonic oscillator were obtained by Bellissard and Vittot (1990). It is possible to deal also with the resonant case in which (H1) is violated. In this case the spectrum of the complete system is qualitatively different from the spectrum of the harmonic one. The normal form allows to compute the main qualitative differences (see sect.6 below).

### 3 Birkhoff Normal Form

In this section we recall the procedure leading to classical Birkhoff Normal Form, whose quantization leads to the proof of theorem 5.3.

#### 3.1 Birkhoff's Theorem

The operator (2.1) is the quantization of the classical Hamiltonian

$$\sum_{i=1}^n \frac{\xi_i^2}{2} + V(x) . \quad (3.1)$$

Denote

$$H_0(\xi, x) := \sum_{j=1}^n \omega_j I_j , \quad I_j := \frac{\xi_j^2 + \omega_j^2 x_j^2}{2\omega_j} \quad (3.2)$$

then we have

**Theorem 3.1.** *For any positive integer  $N \geq 2$  there exist a neighborhood  $\mathcal{U}_N$  of the origin and a canonical transformation  $\mathcal{T}_N : \mathbb{R}^{2n} \supset \mathcal{U}_N \rightarrow \mathbb{R}^{2n}$  which puts the system (3.1) in Birkhoff Normal Form up to order  $N$ , namely such that*

$$H \circ \mathcal{T}_N = H_0 + Z^N + R_N \quad (3.3)$$

where  $Z^N$  Poisson commutes with  $H_0$ , namely  $\{H_0; Z^N\} \equiv 0$  and  $R_N$  is small, i.e.

$$|R_N(\xi, x)| \leq C_N \|(\xi, x)\|^{N+1} \quad (3.4)$$

<sup>1</sup>We recall that a  $C^\infty$  function  $f(x)$  is Gevrey in some domain if there exist constants  $C, \sigma$  such that, for all multiindexes  $\alpha \in \mathbb{N}^n$  one has

$$\left| \frac{\partial^{|\alpha|} f}{\partial x^\alpha} \right| \leq C^{|\alpha|} (\alpha!)^\sigma$$

in the whole domain.

Moreover, if the frequencies are nonresonant namely

$$\omega \cdot k \neq 0, \quad \forall k \in \mathbb{Z}^n \setminus \{0\}, \quad (3.5)$$

the function  $Z^N$  depends on the actions  $I_j$  only.

We recall that the Poisson Bracket of two functions  $f$  and  $g$  is defined by

$$\{f; g\} := \sum_{j=1}^n \left( \frac{\partial f}{\partial \xi_j} \frac{\partial g}{\partial x_j} - \frac{\partial f}{\partial x_j} \frac{\partial g}{\partial \xi_j} \right) = -\{g; f\},$$

and coincides with the Lie derivative of  $g$  with respect to the Hamiltonian vector field of  $f$ .

*Remark 3.2.* In the case where the frequencies fulfill (H1) and the potential  $V$  is analytic (or of Gevrey class) the remainder can be reduced to be exponentially small with  $\|(\xi, x)\|$ .

### 3.2 Scheme of the proof

Make the rescaling  $\xi = \epsilon \xi', x = \epsilon x'$ . In terms of the primed variables the Hamiltonian of the system (3.1) takes the form

$$H_\epsilon(\xi', x') = H_0(\xi', x') + \epsilon W(x'), \quad (3.6)$$

with

$$W(x') := \frac{V(\epsilon x') - \epsilon^2 \sum_{j=1}^n \omega_j^2 (x'_j)^2 / 2}{\epsilon^3} = W_3(x') + \epsilon W_4(x') + \dots \quad (3.7)$$

and  $W_l$  is the Taylor polynomial of order  $l$  of  $V$ . In what follows we will omit primes from the scaled variables.

Given an auxiliary Hamiltonian  $\chi_3$ , denote by  $\Phi_\epsilon^3$  the flow of the corresponding Hamiltonian vector field. We construct  $\chi_3$  so that  $H_\epsilon \circ \Phi_\epsilon^3$  is in normal form up to order  $\epsilon^2$ .

*Remark 3.3.* Given a  $C^\infty$  function  $g$  one has<sup>2</sup>  $g \circ \Phi_\epsilon^3 \sim \sum_{l=0}^{\infty} \epsilon^l g_l$ , with

$$g_0 := g, \quad g_l = \frac{1}{l} \{\chi_3; g_{l-1}\}, \quad l \geq 1. \quad (3.8)$$

If both  $g$  and  $\chi_3$  are analytic then the series of  $g \circ \Phi_\epsilon^3$  can be shown to converge in a neighbourhood of the origin. Using (3.8) to compute  $H_\epsilon \circ \Phi_\epsilon^3$  we get

$$H_\epsilon \circ \Phi_\epsilon^3 = H_0 + \epsilon[W_3 + \{\chi_3; H_0\}] + O(\epsilon^2).$$

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<sup>2</sup>where  $\sim$  denotes the fact that the l.h.s. is asymptotic to the r.h.s. For a precise definition see sect. 4 below.

So  $H_\epsilon \circ \Phi_\epsilon^3$  is in normal form up to  $O(\epsilon^2)$  provided  $\chi_3$  fulfills the so called *Homological Equation*:

$$W_3 + \{\chi_3; H_0\} = Z_3 \quad (3.9)$$

where the unknown function  $Z_3$  has to be in normal form. Remark that, since the operator

$$\chi \mapsto \{\chi; H_0\}$$

maps linearly polynomials of degree  $l$  into polynomials of degree  $l$ , equation (3.9) can be interpreted as a linear equation in the finite dimensional space of polynomials of degree three in the phase space variables.

**Lemma 3.4.** *The Homological Equation (3.9) admits a solution  $(\chi_3, Z_3)$ .*

*Proof.* Introduce the canonical coordinates  $(\zeta, \eta)$  by

$$\zeta_j := \frac{1}{\sqrt{2}} \left( \frac{\xi_j}{\sqrt{\omega_j}} + ix_j \sqrt{\omega_j} \right) ; \quad \eta_j := \frac{1}{i\sqrt{2}} \left( \frac{\xi_j}{\sqrt{\omega_j}} - ix_j \sqrt{\omega_j} \right) . \quad (3.10)$$

In these variables the unperturbed Hamiltonian  $H_0$  reads  $H_0 = \sum_{j \geq 1} i\omega_j \zeta_j \eta_j$  and  $W_3$  is transformed in a different polynomial, again of third order. The important fact is that in these coordinates the eigenvectors of the linear operator  $\{H_0; \cdot\}$  are the monomials

$$\zeta^k \eta^l \equiv \zeta_1^{k_1} \dots \zeta_n^{k_n} \eta_1^{l_1} \dots \eta_n^{l_n}$$

Indeed one has  $\{H_0; \zeta^k \eta^l\} = i\omega \cdot (k - l) \zeta^k \eta^l$ . As a consequence, writing

$$W_3(\zeta, \eta) = \sum_{k, l} C_{k, l} \zeta^k \eta^l$$

one can define the resonant set

$$\mathcal{R} := \{(k, l) : \omega \cdot (k - l) = 0\}$$

and

$$Z_3(\zeta, \eta) := \sum_{k, l \in \mathcal{R}} C_{k, l} \zeta^k \eta^l , \quad \chi_3(\zeta, \eta) := \sum_{k, l \notin \mathcal{R}} \frac{C_{k, l}}{i\omega \cdot (k - l)} \zeta^k \eta^l \quad (3.11)$$

Going back to the original variables one has the solution of the Homological Equation.  $\square$

**Definition 3.5.** The function  $Z_3$  solving (3.9) will be called the *resonant part* of  $W_3$  and will be denoted by  $\langle W_3 \rangle$ .

Using the function  $\chi_3$  one can transform the Hamiltonian to the form

$$H_0 + \epsilon Z_3 + \epsilon^2 R_3$$

*Remark 3.6.* Equation (3.8) allows to construct directly the Taylor expansion of  $R_3$  in terms of the Taylor expansion of  $W$  and of its Poisson Brackets with  $\chi_3$ .

Iterating the construction (which however slightly changes due to the presence of  $Z_3$ ) one gets the proof of theorem 3.1.

*Remark 3.7.* In the nonresonant case  $\omega \cdot (k - l) = 0$  implies  $k = l$ , therefore the resonant part of a polynomial is the sum of monomials of the form

$$\zeta^k \eta^k = I_1^{k_1} \dots I_n^{k_n} ,$$

i.e. it is a function of the actions only. Moreover in this case one has  $Z_3 = 0$ , while in general  $Z_4 \neq 0$ .

## 4 Some symbolic calculus

To understand how to quantize the procedure of Birkhoff Normal Form we have to study the classical–quantum correspondence. It is well known that there are some different procedures in order to associate an operator to a classical observable. Here we concentrate on Weyl quantization rule.

To a function  $f \in \mathcal{S}(\mathbb{R}^{2n})$  (Schwartz class), we associate an operator  $\hat{f}$  acting on functions  $\psi \in \mathcal{S}(\mathbb{R}^n)$ , which is defined by

$$[\hat{f}\psi](x) := \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n \times \mathbb{R}^n} f\left(\frac{x+y}{2}, \xi\right) e^{\frac{i(x-y)\cdot\xi}{\hbar}} \psi(y) dy d\xi \quad (4.1)$$

**Definition 4.1.** The operator (4.1) is called the *Weyl quantization of  $f$*  and in turn  $f$  is called the *symbol* of  $\hat{f}$ .

Using the method of oscillatory integrals Weyl quantization rule can be extended to much more general observables  $f$ . We recall that roughly speaking the method of oscillatory integrals consists in giving meaning to a formal expression of the form (4.1) by using successive integration by parts (see e.g. Martinez 2001).

**Definition 4.2.** A function  $f \in C^\infty(\mathbb{R}^{2n})$  will be called a *smooth symbol of class  $S(\langle z \rangle^m)$*  if, for any  $r \geq 0$  there exists  $C_r$  such that

$$\left| \frac{\partial^{|\alpha|} f}{\partial z^\alpha}(z) \right| \leq C_{|\alpha|} \langle z \rangle^m , \quad \forall \alpha \in \mathbb{N}^{2n} ,$$

where  $\langle z \rangle$  is defined as in sect. 2.

It is useful to extend such a definition to functions explicitly depending also on  $\hbar$ . This can be done in a straightforward way by asking the constants  $C_r$  to be independent of  $\hbar$  in a neighbourhood of the origin. Different classes of symbols can also be defined, but for our purpose this class is enough.

**Theorem 4.3.** Let  $f \in S(\langle z \rangle^m)$ ,  $m \in \mathbb{R}$ , and  $\psi \in \mathcal{S}(\mathbb{R}^n)$ , then the formal expression (4.1) is a well defined oscillatory integral.

*Example 4.4.* Under Weyl quantization rule one has

$$\begin{aligned}\hat{\xi}_j &= i\hbar\partial_{x_j}, \quad \hat{x}_j = x_j \text{ (multiplication operator)} \\ \widehat{\xi_j x_j} &= \frac{1}{2}(\hat{\xi}_j \hat{x}_j + \hat{x}_j \hat{\xi}_j)\end{aligned}$$

**Definition 4.5.** A sequence  $(f_j)_{j \geq 0}$  with  $f_j \in S(\langle z \rangle^m)$  will be called the asymptotic expansion of  $f \in S(\langle z \rangle^m)$ , if for any integer  $N$  there exist two positive constants  $C_N, \hbar_N$  such that

$$f = \sum_{j=0}^N \hbar^j f_j + R_N$$

with  $|R_N(z, \hbar)| \leq C_N \hbar^{N+1} \langle z \rangle^m$ , and  $\hbar \in (0, \hbar_N)$ .

The key point for the quantization of the normal form procedure is the following

**Theorem 4.6.** Let  $f \in S(\langle z \rangle^{m_1})$ , and  $g \in S(\langle z \rangle^{m_2})$ , then there exists a unique  $F \in S(\langle z \rangle^{m_1+m_2})$  such that

$$\hat{F} = \hat{f} \hat{g} \quad (\text{Operator product!})$$

moreover one has

$$F = e^{\frac{i\hbar}{2}(\partial_x \cdot \partial_\eta - \partial_y \cdot \partial_\xi)}(f(x, \xi)g(y, \eta))\Big|_{y=x, \eta=\xi}. \quad (4.2)$$

Finally  $F$  admits an asymptotic expansion in  $\hbar$  which coincides with the formal expansion of (4.2).

The proof is obtained by using eq. (4.1) to write down an expression for  $\hat{f} \hat{g} \psi$  and obtain a formula for  $F$ . Then one shows that the formula is well defined and therefore the result is not formal.

**Definition 4.7.** In the above context, the symbol  $G$  of

$$\frac{i}{\hbar} [\hat{f}; \hat{g}] =: \hat{G}$$

will be called the *Moyal Bracket of  $f$  and  $g$*  and will be denoted by  $\{f; g\}_M$ .

By formula (4.2) one has in particular

$$\{f; g\}_M = \{f; g\} + \hbar^2 \Delta_1(f, g) + O(\hbar^4), \quad (4.3)$$

where

$$\Delta_1(f, g) = -\frac{1}{24} \left( \frac{\partial^3 f}{\partial \xi^3} \frac{\partial^3 g}{\partial x^3} - 3 \frac{\partial^3 f}{\partial \xi^2 \partial x} \frac{\partial^3 g}{\partial x^2 \partial \xi} + 3 \frac{\partial^3 f}{\partial \xi \partial x^2} \frac{\partial^3 g}{\partial x \partial \xi^2} - \frac{\partial^3 f}{\partial x^3} \frac{\partial^3 g}{\partial \xi^3} \right)$$

where we used a vector notation for the derivatives. If either  $f$  or  $g$  are polynomials of degree less or equal than 2 then

$$\{f; g\}_M = \{f; g\} . \quad (4.4)$$

Given a selfadjoint operator  $A$  and a smooth function  $G : \mathbb{R} \rightarrow \mathbb{R}$  it is well known how to define by spectral theorem the operator  $G(A)$ . Suppose now that  $A = \hat{f}$  for some symbol  $f$ . In general one has  $G(\hat{f}) \neq \widehat{G \circ f}$ . However, by symbolic calculus (i.e. using eq. (4.2)) one has

**Lemma 4.8.** *Denote  $I_j(x, \xi) = (\omega_j^2 x_j^2 + \xi_j^2)/2\omega_j$ . Then, for any positive integer  $k$  there exists a function  $F_k(I_j, \hbar)$  such that*

$$\widehat{(I_j)^k} = F_k(\hat{I}_j, \hbar)$$

where the right hand side is defined by spectral calculus. Moreover  $F_k$  can be computed explicitly by the recursion formula  $F_{k+1} = I_j F_k + F_{k-1} \hbar^2 (k^2 - k + 1)/4$ .

As a consequence of this fact and of the fact that  $[\hat{I}_j, \hat{I}_l] = 0$  one has that the Weyl quantization of a polynomial function of the actions is a function of the action operators.

## 5 Semiclassical normal form

Let  $\chi$  be a smooth symbol such that  $\hat{\chi}$  is selfadjoint, and consider the group of unitary operators  $X_\epsilon := \exp\left(\frac{i\epsilon}{\hbar} \hat{\chi}\right)$ . Let  $g$  be a smooth symbol; apply the unitary transformation  $X_\epsilon$  to  $\hat{g}$ , namely compute  $X_\epsilon \hat{g} X_\epsilon^{-1}$ . By the remark that (on a suitable domain)

$$\frac{d}{d\epsilon}(X_\epsilon \hat{g} X_\epsilon^{-1}) = X_\epsilon \frac{i}{\hbar} [\hat{\chi}; \hat{g}] X_\epsilon^{-1} ,$$

one has (formally!)<sup>3</sup> the expansion of  $X_\epsilon \hat{g} X_\epsilon^{-1}$  in  $\epsilon$ :

$$X_\epsilon \hat{g} X_\epsilon^{-1} = \sum_{l \geq 0} \epsilon^l \widehat{g_{q,l}}$$

where

$$\widehat{g_{q,0}} := \hat{g}, \quad \widehat{g_{q,l}} = \frac{1}{l} \frac{i}{\hbar} [\hat{\chi}; \widehat{g_{q,l-1}}] , \quad l \geq 1 . \quad (5.1)$$

Equivalently the symbol of  $X_\epsilon \hat{g} X_\epsilon^{-1}$  is formally given by  $\sum_l \epsilon_l g_{q,l}$  with

$$g_{q,0} := g, \quad g_{q,l} := \frac{1}{l} \{\chi; g_{q,l-1}\}_M , \quad l \geq 1 . \quad (5.2)$$

from which one sees a remarkable similitude with the classical equation. Moreover (5.2) converges to (3.8) when  $\hbar \rightarrow 0$ .

<sup>3</sup>such a series can be interpreted as an asymptotic expansion provided one restricts the domain at each step of the approximation

Applying the unitary transformation generated by  $\hat{\chi}$  to the Hamiltonian operator  $\hat{H}_\epsilon$  (cf. eq. (3.6)) one has  $X_\epsilon \hat{H}_\epsilon X_\epsilon^{-1} = \widehat{H}_q^1$  with

$$H_q^1 = H_0 + \epsilon[W_3 + \{\chi; H_0\}_M] + O(\epsilon^2) \quad (5.3)$$

$$\equiv H_0 + \epsilon[W_3 + \{\chi; H_0\}] + O(\epsilon^2) \quad (5.4)$$

where we used the fact that  $H_0$  is a quadratic polynomial so that (4.4) holds. It is thus clear that lemma 3.4 allows to solve also the *Quantum Homological Equation* appearing in this context and to determine the symbol of the operator generating the unitary transformation putting the Hamiltonian operator in normal form up to corrections of order  $\epsilon^2$ . Moreover, one can compute in terms of Moyal brackets (of polynomials!) the expansion of the symbol of the new remainder and of the normal form. Iterating the construction one generates a well defined *Semiclassical Normal Form* of the quantum system.

*Example 5.1.* Denote by  $Z_{q,l}$ ,  $l = 1, 2, \dots$  the term added to the Semiclassical Normal Form at the  $l^{\text{th}}$  step of the iterative construction. Explicitly the first terms are given by

$$Z_{q,1} = \langle W_3 \rangle = Z_3 \quad (5.5)$$

$$Z_{q,2} = \langle W_4 \rangle + \frac{1}{2} \langle \{\chi_3; W_3\}_M \rangle + \frac{1}{2} \langle \{\chi_3; Z_3\}_M \rangle \quad (5.6)$$

$$\begin{aligned} Z_{q,3} &= \langle W_5 \rangle + \langle \{\chi_4; Z_3\}_M \rangle + \frac{1}{3} \langle \{\chi_3; H_2\}_M \rangle \\ &+ \frac{1}{2} \langle \{\chi_3; W_{3,1}\}_M \rangle + \langle \{\chi_3; W_4\}_M \rangle \end{aligned} \quad (5.7)$$

where, according to definition 3.5  $\langle \cdot \rangle$  is the resonant part of its argument,  $\chi_j$  is (formally) the symbol of the operator generating the  $j^{\text{th}}$  unitary transformation, and

$$H_2 := \frac{1}{2} \langle \{\chi_3; Z_3 - W_3\}_M \rangle, \quad W_{3,1} := \{\chi_3; W_3\}_M.$$

Remark that all the Moyal brackets involved contain polynomials of degree at most 4, so that they can be computed exactly using formula (4.3) which in this case does not contain corrections of order  $\hbar^4$ .

The problem in order to make rigorous the previous construction is that all the series involved are in general divergent. Moreover it is not possible to show that the remainders appearing when truncating such series are small in a reasonable sense. Nevertheless it is possible, using the tools of microlocal analysis, to show that the Semiclassical Normal Form contains essentially all the informations on the part of the spectrum close to zero.

The precise relation between the spectrum of the original Hamiltonian and the spectrum of the Semiclassical Normal Form is captured by the following definition

Let  $H_1(\epsilon, \hbar)$ ,  $H_2(\epsilon, \hbar)$  be two families of selfadjoint operators, set  $\text{Spec}_\epsilon(H_{1,2}) := \text{Spec}(H_{1,2}) \cap [0, \epsilon)$ .

**Definition 5.2.** We say that

$$\text{Spec}_\epsilon(H_1) = \text{Spec}_\epsilon(H_2) \pmod{\epsilon^\infty + (\hbar/\epsilon)^\infty}$$

if for any  $N, M > 0$  there exist  $C_{N,M}^1$  and  $C_{N,M}^2$  such that for any  $\lambda_1 \in \text{Spec}_\epsilon(H_1)$  there exists  $\lambda_2 \in \text{Spec}_\epsilon(H_2)$  such that  $\lambda_1 = \lambda_2 + R_{N,M}$  with

$$|R_N| \leq C_{N,M}^1 \epsilon^N + C_{N,M}^2 (\hbar/\epsilon)^M \quad (5.8)$$

and conversely. Eq. (5.8) has to hold for any couple  $(\hbar, \epsilon)$  with  $\epsilon$  and  $(\hbar/\epsilon)$  small enough.

**Theorem 5.3.** Assume (H2, H3), assume also

(H1') There exist  $\gamma > 0$  and  $\tau \in \mathbb{R}$  such that, for any  $k \in \mathbb{Z}^n$  one has

$$\text{either } \omega \cdot k = 0 \quad \text{or} \quad |\omega \cdot k| \geq \frac{\gamma}{|k|^\tau} \quad (5.9)$$

Then there exists a polynomial function  $\mathcal{Z}_q$  such that one has

$$\text{Spec}_\epsilon(\hat{H}) = \text{Spec}_\epsilon(\hat{H}_0 + \widehat{\mathcal{Z}}_q) \pmod{\left(\epsilon^\infty + \left(\frac{\hbar}{\epsilon}\right)^\infty\right)} \quad (5.10)$$

The polynomial  $\mathcal{Z}_q$  coincides with the Semiclassical Normal Form defined at the beginning of the section.

*Scheme of the proof.* It consists of six steps. (1) make the unitary transformation  $(U\psi)(x) := \epsilon^{n/4} \psi(\epsilon^{1/2}x)$  which transforms the Hamiltonian operator (2.1) into the Weyl quantized of  $\epsilon H_\epsilon := \epsilon(H_0 + \epsilon^{1/2}W)$ , but a Weyl quantization where  $\hbar$  is substituted by  $\hbar' := \hbar/\epsilon$ . (2) make a cutoff of  $H_\epsilon$ , namely, fix  $R$  and consider a smooth function  $t$  such that  $t(s) \equiv 1$  for  $|s| \leq R$ ,  $t(s) \equiv 0$  for  $|s| \geq 2R$ , define  $a(x, \xi) := W(x)t(\|(\xi, x)\|)$  and (3) compare the spectrum of the Hamiltonian  $\hat{H}_\epsilon$  with the spectrum of  $H^t := H_0 + \epsilon a$ . By microlocal analysis one has that, in any fixed bounded interval such spectra coincide modulo  $\hbar^\infty$  (see e.g. Martinez 2001). (4) Rescale back the variables, namely apply the transformation  $U_\epsilon^{-1}$  to  $H^t$ . (5) Apply the normal form algorithm to the so obtained Hamiltonian showing that all the series involved are convergent in suitable norms. (6) Use again microlocal analysis to show that the spectrum of the Semiclassical Normal Form coincides with the spectrum of the normalized operator with compactly supported symbol.  $\square$

*Remark 5.4.* Fix an arbitrary  $1 > \delta > 0$  and link  $\epsilon$  to  $\hbar$  by  $\epsilon := \hbar^\delta$ . Then one obtains a simplified statement according to which the spectrum of (2.1) in  $[0, \hbar^\delta)$  coincides modulo  $\hbar^\infty$  with the spectrum of  $\hat{H}_0 + \widehat{\mathcal{Z}}_q$  in the same interval.

*Remark 5.5.* In the case where the frequencies are nonresonant one has that the symbol of the normal form depends on the actions only. By lemma 4.8 one has that also the quantization of the normal form is a function of the action operators only (explicitly computable), and therefore the spectrum of the normal form is given by a quantization formula as claimed in theorem 2.1.

## 6 The resonant case.

In the case where the frequencies are nonresonant, due to the particular structure of the normal form, one obtains a very precise information on the spectrum. In the case where there are some resonances the situation is more difficult. In order to illustrate what happens we concentrate on the completely resonant case, i.e. the case where all the frequencies are integer multiples of a single fundamental frequency  $\nu$ .

In this case the eigenvalues of  $\hat{H}_0$  form a subset of  $\mathbb{N}\hbar\nu + \frac{1}{2}|\omega|\hbar$  and are degenerate. One expects the nonlinear part to break such a degeneracy and to transform each eigenvalue in a small band. One can use the normal form to study the structure of the so obtained band. To this end the most relevant contribution is due to the first non vanishing term of the normal form. For the sake of definiteness we assume that this is the term of order four, namely  $\mathcal{Z}_4$ . Denote

$$N := \mathcal{Z}_4|_{H_0^{-1}(1)}, \quad B(E) \equiv [E - \frac{1}{3}\nu\hbar, E + \frac{1}{3}\nu\hbar]$$

**Theorem 6.1.** *Fix  $1 > \gamma_1 > \frac{1}{2}$ , then, provided  $\hbar$  is small enough one has*

$$\text{Spec}(\hat{H}) \cap (\hbar, \hbar^{\gamma_1}) \subset \bigcup_{E \in \text{Spec}(\hat{H}_0)} B(E) \quad (6.1)$$

Moreover, denote by

$$E + \lambda_1(E, \hbar) \leq \dots \leq E + \lambda_m(E, \hbar) \quad (6.2)$$

the eigenvalues of  $\hat{H}$  in  $B(E)$  counted with multiplicity, then

$$\lambda_1(E, \hbar) = E^2 \text{Min} N + E^2(O(\hbar/E) + O(E^{\frac{1}{2}})) \quad (6.3)$$

and similarly

$$E^2 \lambda_m(E, \hbar) = E^2 \text{Max} N + E^2(O(\hbar/E) + O(E^{\frac{1}{2}})). \quad (6.4)$$

This statement is due to Bambusi, Charles and Tagliaferro (2003) for previous results see Vũ Ngọc (1998).

Eq. (6.1) shows that the spectrum has a band structure, while eqs.(6.3) and (6.4) allow to compute the minimum and the maximum of each band.

The idea of the proof is as follows. First forget high order terms of the normal form whose effect is included in the error terms. Then due to the commutation property of the normal form with  $\hat{H}_0$  one has that  $\hat{\mathcal{Z}}_4$  restricts to an operator acting on the eigenspaces of  $\hat{H}_0$ . On the classical side one has that by Marsden–Weinstein procedure  $\mathcal{Z}_4$  defines a classical Hamiltonian system on the manifold obtained by symplectic reduction of the original phase space. By the methods of geometric quantization it turns out that the quantum operator acting on an eigenspace of  $\hat{H}_0$  is a Toeplitz operator whose principal symbol is exactly the above reduced classical Hamiltonian. Then the proof follows by classical properties of Toeplitz operators.

We point out that results of this kind are useful in the computation of the molecular spectra (Michel and Zhilinski 2001, Zhilinski 2001).

## 7 Quantization of KAM tori

In this section we present a result on the quantization of KAM tori. It allows to construct part of the spectrum of a close to integrable system.

We recall that a classical Hamiltonian system with  $n$  degrees of freedom is said to be integrable if it has  $n$  integrals of motion independent and in involution. If the energy surface is compact then, by Arnold–Liouville theorem there exists a canonical transformation  $\mathcal{T}_0 : \mathbb{R}^n \times \mathbb{T}^n \supset D \times \mathbb{T}^n \rightarrow \mathbb{R}^{2n}$  introducing action angle variables, namely such that, denoting by  $K_0$  the original integrable Hamiltonian,  $K_0 \circ \mathcal{T}_0$  is independent of the angles  $\phi \in \mathbb{T}^n$ . Here  $D$  is an open bounded domain.

Consider now a close to integrable analytic Hamiltonian system, namely a Hamiltonian system with Hamiltonian

$$K = K_0 + \epsilon K_1$$

where  $\epsilon$  is a small parameter. We assume that, denoting again by  $\mathcal{T}_0$  the canonical transformation introducing action angle variables for the system  $K_0$ , one has that both  $K_0 \circ \mathcal{T}_0$  and  $K_1 \circ \mathcal{T}_0$  are real analytic on  $D \times \mathbb{T}^n$ . Then KAM theory applies. To state the corresponding result denote by  $D_0 \subset D$  a domain whose closure is contained in  $D$ .

**Theorem 7.1.** *Assume that  $\forall I \in D$  one has*

$$\det \left( \frac{\partial^2 (K_0 \circ \mathcal{T}_0)}{\partial I^2} \right) \neq 0 \quad (7.1)$$

*then there exists a positive constant  $\epsilon_*$  and, for any  $\epsilon$  with  $|\epsilon| < \epsilon_*$  there exists a Gevrey canonical transformation  $\mathcal{T}_\epsilon : D_0 \times \mathbb{T}^n \rightarrow \mathbb{R}^{2n}$  and a Cantor set  $D_\epsilon \subset D_0$  with the following properties:*

$$K \circ \mathcal{T}_\epsilon = Z(I) + R(I, \phi, \epsilon), \quad (7.2)$$

*where  $R(I, \phi, \epsilon)$  vanishes at infinite order on  $D_\epsilon$ , i.e., for any multiindex  $\alpha$  there exists  $C_{|\alpha|}$  such that one has*

$$\left| \frac{\partial^{|\alpha|} R}{\partial (I, \phi)^\alpha} (I, \phi, \epsilon) \right| \leq C_{|\alpha|} \exp \left( - \frac{c}{|I - D_\epsilon|^\rho} \right) \quad (7.3)$$

*with a suitable  $\rho > 0$  and  $|I - D_\epsilon|$  denoting the distance from  $D_\epsilon$ . Moreover as  $\epsilon$  tends to zero the measure of  $D_\epsilon$  tends to the measure of  $D_0$ .*

A particular consequence is that the set  $D_\epsilon$  is foliated in invariant tori. From the proof it also turns out that the motion on each torus is quasiperiodic with frequencies fulfilling (H1) of sect. 2. Moreover the tori are linearly stable and even more: they are stable in an exponential sense<sup>4</sup>.

<sup>4</sup>namely, a solution starting  $O(\mu)$  close to a torus takes at least a time  $O(\exp(c/\mu^\rho))$  to double its distance from the torus

Quantizing the normalizing transformation  $\mathcal{T}_\epsilon$  by using the theory of Fourier Integral Operators one can put also the quantum Hamiltonian in a suitable normal form which allows to deduce some spectral informations on the system.

To fix ideas we restrict to the case where  $K$  is a natural system, namely it has the form (3.1), and is close to integrable in the above sense. Fix two parameters  $E_1 < E_2$ , assume (i) that  $K^{-1}([-\infty, E_2 + \delta])$  is compact for some positive  $\delta$ , (ii) that the domain  $D_0$  can be constructed in such a way that  $\mathcal{T}_0 : D_0 \times \mathbb{T}^n \rightarrow K_0^{-1}([E_0, E_1])$  is a bijection and moreover the KAM condition (7.1) holds. Denote by  $\theta \in \mathbb{Z}^n$  the Maslov class of the tori of  $K_0$  (see e.g. Lazutkin 1993) and, having fixed some  $0 < \sigma < 1$ , define the set of indexes

$$\mathcal{I} := \{k \in \mathbb{Z}^n : |D_\epsilon - \hbar(k + \theta/4)| \leq \hbar^\sigma\} \quad (7.4)$$

**Theorem 7.2.** *There exist positive constants  $\hbar_*$ ,  $c$ ,  $C$ , and  $\sigma < 1$ , and a function  $K_q : D_0 \times (0, \hbar_*) \rightarrow \mathbb{R}$  with the following property: For any  $k \in \mathcal{I}$  there exists at least one eigenvalue of  $\hat{K}$  in the interval*

$$\left[ Z_q(\hbar(k + \theta/4), \hbar) - Ce^{-c/\hbar^p}, Z_q(\hbar(k + \theta/4), \hbar) + Ce^{-c/\hbar^p} \right] \quad (7.5)$$

One can also show that a large part of the spectrum is constructed in this way. This is obtained by comparing the semiclassical estimate of the number of eigenvalues in  $[E_1, E_2]$  to the number of eigenvalues thus constructed.

Theorem 7.2 is due to Popov (Popov 2000); The quantization of KAM tori were initiated by Lazutkin and widely developed by Colin de Verdière who obtained a result similar to theorem 7.2 for the case where  $K$  is  $C^\infty$  and describes the geodesic flow on a compact Riemannian manifold (Colin de Verdière 1977).

## 8 Further Readings

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