

# Hamiltonians Spectrum in Fermi Resonance via The Birkhoff-Gustavson Normal Form

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## Abstract

We investigate in this paper the theorem of Birkhoff normal form near an equilibrium point in infinite dimension and discuss the dynamical consequences for Schrödinger Hamiltonians. We calculate also the spectrum in Fermi resonance by using the Bargmann transform.

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## 1 Introduction

One of the theories that allows us to calculate the spectrum of some non-resonant hamiltonian near an equilibrium position of a regular potential is the theory of the normal forms used by Birkhoff [3] to treat some dynamic systems, it has been extended then to the resonant case by Gustavson [5].

The Birkhoff-Gustavson normal form (BGNF) received, in some decades ago, a lot of attention in the description of the dynamic systems. A quantum description via the BGNF implies two steps, the first one is to search for the normal form by canonical transformations of the coordinates and second one is to quantify the normal form. But notice that the coordinates don't often appear in a simple way and therefore that the quantification won't be obvious in the majority of the cases (see e.g.[1]). The quantification that would appear the better adapted to have good enough results is the one of Weyl and it is

what one uses in this work.

Let's add on this the excellent numeric calculations that show that the BGNF became a very powerful tool in the molecular physics (see e.g.[6, 7]).

The BGNF for pseudodifferential operators near non degenerate minimum of the symbol has been used by several authors; in particular the article of Sjöstrand [8] treats the non resonant case and the one of Charles and Vu Ngoc [4] treats the resonant case, from where this work is inspired.

Now, we recall the theorem of Birkhoff-Gustavson normal form (BGNF) which is fundamental for this work.

Let's suppose that  $P = -\frac{\hbar^2}{2}\Delta + V(x)$  is a Schrödinger hamiltonian with a smooth potential  $V$  on  $\mathbb{R}^n$  and 0 is a non-degenerate global minimum for  $V$  which we shall call here the origin. By a linear, unitary change of variable in local coordinates near 0, one can assume that the hessian matrix  $V''(0)$  is diagonal, let  $(\nu_1^2, \dots, \nu_n^2)$  be its eigenvalues, with  $\nu_j > 0$ . The rescaling  $x_j \rightarrow \sqrt{\nu_j}x_j$  transforms  $P$  into a perturbation of the harmonic oscillator  $\hat{H}_2$  :

$$P = \hat{H}_2 + W(x)$$

with  $\hat{H}_2 = \sum_{j=1}^n \frac{\nu_j}{2} \left( -\hbar^2 \frac{\partial^2}{\partial^2 x_j^2} + x_j^2 \right)$ , where  $W(x)$  is a smooth potential of order  $\mathcal{O}(|x|^3)$  near the origin.

We work with the space  $\mathcal{E} = \mathbb{C}[x, \xi, \hbar] = \mathbb{C}[x_1, \dots, x_n, \xi_1, \dots, \xi_n, \hbar]$  of polynomials of  $(2n + 1)$  variables with complex coefficients, where the degree of the monomial  $x^\alpha \xi^\beta \hbar^\ell$  is defined by  $|\alpha| + |\beta| + 2\ell$ ,  $\alpha, \beta \in \mathbb{N}^n$ ,  $\ell \in \mathbb{N}$ . Let  $\mathcal{D}_N$  be the finite dimensional vector space spanned by monomials of degree  $N$  and  $\mathcal{O}_N$  the subspace of  $\mathcal{E}$  consisting of formal series whose coefficients of degree  $< N$  vanish. Let  $A \in \mathcal{E}$ , We shall need in this article the Weyl bracket  $[\cdot, \cdot]_W$  defined on  $\mathcal{E}$  by:

$$ad_A(B) = [A, B]_W = \widehat{A}\widehat{B} - \widehat{B}\widehat{A} \quad \text{for all } B \in \mathcal{E}$$

where  $\widehat{A}$  and  $\widehat{B}$  are the Weyl quantizations of symbols  $A$  and  $B$ .

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

**Theorem 1** *Let  $H_2 \in \mathcal{D}_2$  be admissible and  $L \in \mathcal{O}_3$ , then there exists  $A \in \mathcal{O}_3$  and  $K \in \mathcal{O}_3$  such that:*

$$\begin{aligned} e^{i\hbar^{-1}ad_A}(H_2 + L) &= H_2 + KBGNF & (1) \\ [H_2, K]_W &= 0 \end{aligned}$$

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

**BGNF** is the Birkhoff-Gustavson normal form of the operator  $P$  near the origin.

In the section 2, one first starts with calculating the BGNF in the 1:2 resonance, we introduce the creation and annihilation operators and Bergmann transform and finally we inject the all in Bargmann space.

The section 3 is the goal of this work, we calculate the spectrum  $\sigma(P)$  of operator  $P$  while passing by the calculation of the spectrum  $\sigma(\hat{K}_3)$  of the restriction of  $\hat{K}_3$  to the eigenspace of  $\hat{H}_2$ . Since  $\hat{H}_2$  et  $\hat{K}_3$  commute one finally gets  $\sigma(P) = \sigma(\hat{H}_2) + \sigma(\hat{K}_3)$ .

## 2 BGNF in the 1:2 resonance

### 2.1 Creation and annihilation operators

We denote by  $X_j$  the operator of multiplication by  $x_j$  and  $Y_j$  the operator of derivation  $\frac{\partial}{\partial x_j}$  in  $L^2(\mathbb{R}^n)$ .  $a_j(\hbar) = \frac{1}{\sqrt{2\hbar}}(X_j + \hbar Y_j) = \frac{1}{\sqrt{2\hbar}}\left(x_j + \hbar \frac{\partial}{\partial x_j}\right)$  and  $b_j(\hbar) = \frac{1}{\sqrt{2\hbar}}(X_j - \hbar Y_j) = \frac{1}{\sqrt{2\hbar}}\left(x_j - \hbar \frac{\partial}{\partial x_j}\right)$  are respectively called the operators of creation and annihilation in  $L^2(\mathbb{R}^n)$ .

The operators  $a_j(\hbar)$  and  $b_j(\hbar)$  verify:

$$\begin{aligned} a_j^*(\hbar) &= b_j(\hbar) \quad , \quad b_j^*(\hbar) = a_j(\hbar) \\ [a_j(\hbar), b_k(\hbar)] &= \delta_{jk} \quad , \quad [a_j(\hbar), a_k(\hbar)] = 0 \quad , \quad [b_j(\hbar), b_k(\hbar)] = 0 \end{aligned}$$

While rewriting  $\hat{H}_2$  according to  $a_j(\hbar)$  and  $b_j(\hbar)$ , one gets

$$\hat{H}_2 = \hbar \sum_{j=1}^n \nu_j \left( a_j(\hbar) b_j(\hbar) - \frac{1}{2} \right)$$

### 2.2 Bargmann representation

In this paragraph, we recall some standards results concerning the classic space  $\mathcal{B}_{\mathcal{F}}$  of Bargmann-Fock or simply the Bargmann space, for more details one can consult [2].  $\mathcal{B}_{\mathcal{F}} = \{\varphi(z)$  holomorphic function on  $\mathbb{C}^n$  ;  $\int_{\mathbb{C}^n} |\varphi(z)|^2 d\mu_n(z) < +\infty\}$  where  $d\mu_n(z)$  is the Gaussian measure defined by  $d\mu_n(z) = \pi^{-n} e^{-\frac{|z|^2}{\hbar}} d^n z$ .  $\mathcal{B}_{\mathcal{F}}$  is a Hilbert space when it is equipped with the natural inner product  $\langle f, g \rangle = \int_{\mathbb{C}^n} f(z) \overline{g(z)} d\mu_n(z)$ .

**Theorem 2** *There exists a unitary mapping  $T_{\mathcal{B}}$  of  $L^2(\mathbb{R}^n)$  onto  $\mathcal{B}_{\mathcal{F}}$  defined by*

$$T_{\mathcal{B}}f(x) = \varphi(z) = 2^{n/4} (2\pi\hbar)^{-3n/4} \int_{\mathbb{R}^n} f(x) e^{-\frac{1}{2}(z^2+x^2)+\sqrt{2}xz} \pi^{-n} d^n x$$

$T_{\mathcal{B}}$  is called the Bargmann transform.

We recall that the spectrum  $\sigma(\hat{H}_2)$  of  $\hat{H}_2$  is constituted of eigenvalues  $\lambda_N = \hbar \left( \langle \nu, \alpha \rangle + \frac{|\nu|}{2} \right) = \hbar \left( N + \frac{|\nu|}{2} \right)$ , where  $\nu = (\nu_1, \dots, \nu_n)$  and  $N = \langle \nu, \alpha \rangle$ . The eigenspace  $\mathcal{H}_N = \{ \psi_{\alpha}(x) \text{ such that } \langle \nu, \alpha \rangle = N \}$  is constituted of Hermite functions  $\psi_{\alpha}(x) = e^{-x^2/2} P_{\alpha}(x)$  which form an orthonormal hilbertian basis  $\{ \psi_{\alpha}(x) \}_{\alpha}$  of  $L^2(\mathbb{R}^n)$ , where  $P_{\alpha}(x)$  is a polynomial of degree  $\alpha$ . Then we have the following theorem:

**Theorem 3** *The isometry  $T_{\mathcal{B}}$  makes correspond the functions  $\{ \psi_{\alpha}(x) \}_{\alpha}$  to the functions  $\left\{ \frac{z^{\alpha}}{\sqrt{\alpha!}} \right\}_{\alpha}$  that constitute an orthonormal hilbertian basis of  $\mathcal{B}_{\mathcal{F}}$ .*

**Proposition 4** *If we note by  $Z_j$  the operator of multiplication by  $z_j$  and by  $D_j$  the operator of derivation  $\frac{\partial}{\partial z_j}$  on  $\mathcal{B}_{\mathcal{F}}$ , then :*

$$T_{\mathcal{B}}(a_j(\hbar)) T_{\mathcal{B}}^{-1} = D_j \text{ and } T_{\mathcal{B}}(b_j(\hbar)) T_{\mathcal{B}}^{-1} = Z_j$$

The Bargmann transform of the harmonic oscillator is given by

$$\hat{H}_2^{\mathcal{B}} = T_{\mathcal{B}}(\hat{H}_2) T_{\mathcal{B}}^{-1} = \hbar \sum_{j=1}^n \nu_j \left( z_j \frac{\partial}{\partial z_j} + \frac{1}{2} \right)$$

The eigenspace associated to the eigenvalues  $\lambda_N$  is  $\mathcal{H}_N^{\mathcal{B}} = T_{\mathcal{B}}(\mathcal{H}_N) T_{\mathcal{B}}^{-1} :$

$$\mathcal{H}_N^{\mathcal{B}} = \text{vect} \left\{ \varphi_{\alpha} = \varphi_{(\alpha_1, \alpha_2)} = \frac{z^{\alpha_1}}{\sqrt{\alpha_1!}} \frac{z^{\alpha_2}}{\sqrt{\alpha_2!}} \text{ such that } \nu_1 \alpha_1 + \nu_2 \alpha_2 = N \right\}$$

### 2.3 The 1:2 resonance (Fermi resonance)

We consider  $\hat{H}_2 = \frac{1}{2} \left( -\hbar^2 \frac{\partial^2}{\partial x_1^2} + x_1^2 \right) + \left( -\hbar^2 \frac{\partial^2}{\partial x_2^2} + x_2^2 \right)$  with symbol  $H_2 = \frac{1}{2} |z_1|^2 + |z_2|^2$  where  $z_j = x_j + i\xi_j$ . The Bargman transform of  $\hat{H}_2$  is

$$\hat{H}_2^{\mathcal{B}} = T_{\mathcal{B}}(\hat{H}_2) T_{\mathcal{B}}^{-1} = \hbar \left( z_1 \frac{\partial}{\partial z_1} + 2z_2 \frac{\partial}{\partial z_2} + \frac{3}{2} \right)$$

Since  $[H_2, K_3]_W = 0$  and  $\{H_2, K_3\} = 0$ , it is sufficient to calculate the Weyl symbol

$$K_3 = \sum_{2\ell+|\alpha|+|\beta|=3} \hbar^\ell z^\alpha \bar{z}^\beta \quad \text{such that } \alpha_1 + 2\alpha_2 = \beta_1 + 2\beta_2 \quad (\mathbf{res1} : 2)$$

where  $\alpha = (\alpha_1, \alpha_2)$  and  $\beta = (\beta_1, \beta_2)$ . To calculate  $K_3$ , it is necessary to look for

all monomials of order 3 that satisfy the Fermi resonance relation (**res 1 : 2**). The couples  $\alpha = (\alpha_1, \alpha_2)$  and  $\beta = (\beta_1, \beta_2)$  that verify at a time  $|\alpha| + |\beta| = 3$  and the relation (**res 1 : 2**) are:

1)  $\alpha = (0, 1)$  and  $\beta = (2, 0)$ . Thus,  $K_3 = z_2 \bar{z}_1^2$ .

2)  $\alpha = (2, 0)$  and  $\beta = (0, 1)$ . Thus,  $K_3 = z_1^2 \bar{z}_2$ .

Thus,  $K_3$  belongs to the linear space spanned by  $\{z_2 \bar{z}_1^2, z_1^2 \bar{z}_2\}$ . However we know that  $\widehat{K}_3$  is real, then

$$K_3 = \frac{\mu}{2} ((x_2 + i\xi_2)(x_1 - i\xi_1)^2(x_1 + i\xi_1)^2((x_2 - i\xi_2))) \quad , \mu \in \mathbb{C}$$

$$\begin{aligned} \widehat{K}_3 &= \sqrt{2\mu\hbar^{\frac{3}{2}}} \left( \frac{1}{\sqrt{2\hbar}} \left( x_2 + \hbar \frac{\partial}{\partial x_2} \right) \frac{1}{2\hbar} \left( x_1 - \hbar \frac{\partial}{\partial x_1} \right)^2 \right. \\ &\quad \left. + \frac{1}{2\hbar} \left( x_1 + \hbar \frac{\partial}{\partial x_1} \right)^2 \frac{1}{\sqrt{2\hbar}} \left( x_2 - \hbar \frac{\partial}{\partial x_2} \right) \right) \\ &= \sqrt{2\mu\hbar^{\frac{3}{2}}} (a_2(\hbar) b_1^2(\hbar) + a_1^2(\hbar) b_2(\hbar)) \end{aligned}$$

and using Bargmann representation, we get  $\widehat{K}_3^B = T_B \left( \widehat{K}_3 \right) T_B^{-1} = \sqrt{2\mu\hbar^{\frac{3}{2}}} \left( z_2 \frac{\partial^2}{\partial z_1^2} + z_1^2 \frac{\partial}{\partial z_2} \right)$ .

### 3 Spectrum of $\widehat{K}_3$

While calculating  $\widehat{K}_3^B(\varphi_\alpha)$ , we get

$$\begin{aligned} \widehat{K}_3^B \varphi(\alpha_1, \alpha_2) &= \sqrt{2\mu\hbar^{\frac{3}{2}}} \left( z_2 \frac{\partial^2 \varphi(\alpha_1, \alpha_2)}{\partial z_1^2} + z_1^2 \frac{\partial \varphi(\alpha_1, \alpha_2)}{\partial z_2} \right) \\ &= \sqrt{2\mu\hbar^{\frac{3}{2}}} \left( \sqrt{(\alpha_2 + 1)\alpha_1(\alpha_1 - 1)} \varphi(\alpha_1 - 2, \alpha_2 + 1) \right. \\ &\quad \left. + \sqrt{(\alpha_1 + 2)(\alpha_1 + 1)\alpha_2} \varphi(\alpha_1 + 2, \alpha_2 - 1) \right) \end{aligned}$$

we see well that  $\mathcal{H}_N^B$  is steady by  $\widehat{K}_3^B$  because  $\alpha_1 - 2 + 2(\alpha_2 + 1) = \alpha_1 + 2\alpha_2 = N$  and  $\alpha_1 + 2 + 2(\alpha_2 - 1) = \alpha_1 + 2\alpha_2 = N$  one can verify easily that the matrix  $\widehat{K}_3^B$  in  $\mathcal{H}_N^B$  is symmetric, indeed:

$$\begin{aligned} \widehat{K}_3^B \varphi(\alpha_1 + 2, \alpha_2 - 1) &= \sqrt{2\mu\hbar^{\frac{3}{2}}} \left( \sqrt{(\alpha_1 + 2)(\alpha_1 + 1)\alpha_2} \varphi(\alpha_1, \alpha_2) \right. \\ &\quad \left. + \sqrt{(\alpha_1 + 4)(\alpha_1 + 3)(\alpha_2 - 1)} \varphi(\alpha_1 + 4, \alpha_2 - 2) \right) \end{aligned}$$

so in the basis of  $\mathcal{H}_N^B = \{ \varphi(N - 2l, l) \text{ such that } l = 1, 2, \dots, E[\frac{N}{2}] \}$  one gets,

$$\begin{aligned} \widehat{K}_3^B \varphi_{(\alpha_1, \alpha_2)} &= \sqrt{2\mu\hbar^{\frac{3}{2}}} \left( \sqrt{(l + 1)(N - 2l)(N - 2l - 1)} \varphi(\alpha_1 - 2, \alpha_2 + 1) \right. \\ &\quad \left. + \sqrt{(N - 2l + 2)(N - 2l + 1)l} \varphi(N - 2l + 2, l - 1) \right) \end{aligned}$$

and therefore, the matrix of  $\widehat{K}_3^B$  in the basis of  $\mathcal{H}_N^B$  will be given by:

$$\sqrt{2\mu\hbar^{\frac{3}{2}}} \begin{pmatrix} 0 & m_0 & & \vdots & & \\ m_0 & 0 & \ddots & \vdots & \mathbf{0} & \\ \cdots & \ddots & 0 & m_l & \cdots & \cdots \\ & & & m_l & 0 & \ddots \\ & \mathbf{0} & & \ddots & 0 & \ddots \\ & & & \vdots & \ddots & 0 \end{pmatrix}$$

where,  $m_l = \sqrt{(l + 1)(N - 2l)(N - 2l - 1)}$ ,  $l = 1, 2, \dots, E[\frac{N}{2}]$ .

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