Asymptotic Analysis for Schrödinger Hamiltonians via Birkhoff-Gustavson Normal Form

Kaoutar Ghomari[a], **Bekkai Messirdi**[b] and **San Vũ Ngọc**[c]

[a]Department of Mathematics and Computer Sciences, ENP-Oran, BP 1523 El'Mnaouar 31000, Algeria.
E-mail adress: kaoutar.ghomari@gmail.com, ghomari_kaoutar@yahoo.fr
[b]Department of Mathematics, University of Oran Es-Senia, BP 1524 El'Mnaouar 31000, Algeria.
E-mail adress: messirdi.bekkai@univ-oran.dz.
[c]Mathematics Research Institute IRMAR, University of Rennes 1 and Institut Universitaire de France, 263, Avenue du Général Leclerc, 35042 Rennes CEDEX, France.
E-mail adress: san.vu-ngoc@univ-rennes1.fr

Abstract
This article reviews the Birkhoff-Gustavson normal form theorem (BGNF) near an equilibrium point of a quantum Hamiltonian. The BGNF process is thereafter used to investigate the spectrum of Schrödinger operators in the 1:1, 1:2 and 1:3 resonances. A computer program is proposed to compute the coefficients of the BGNF up to any order.

Key words and phrases : Birkhoff Normal Form, Harmonic oscillator, Bargmann representation, Resonances, Fermi resonance.

1 Introduction

The topic under consideration in this paper is the computation of the Birkhoff-Gustavson normal form and its application to the calculation of the quantum mechanical spectra of Schrödinger operators.

An old and important problem in quantum mechanics is the investigation of the discrete spectrum of selfajoint operators. There are several classical methods for the numerical computation of eigenvalues. Many of them amount to writing a finite dimensional approximation of the operator in a suitable basis, and performing numerical diagonalization. It is well known that the choice of basis is delicate and crucial : a bad choice can easily lead to very poor numerical accuracy. With this respect, when quantum Birkhoff-Gustavson normal form can be used, they generally give excellent results.

(0) **2000 MSC** : 58K50, 81S10, 81Q10

The theory of normal forms is one of the theories that allow us to analyse the spectrum of a Hamiltonian near an equilibrium position of a smooth potential. This mathematical theory has a rather long history, dating back to Poincaré, and has received much attention. The first rigorous set-up, in the framework of Hamiltonian classical mechanics, was given in [4] by Birkhoff in the case where the quadratic approximation of the hamiltonian is a sum of harmonic oscillators with non-resonant frequencies; it has been extended then to the resonant case by Gustavson [8].

Several physicists in the 1980's have started to think about a quantum version of the Birkhoff-Gustavson normal form (BGNF). The main idea is based on two steps. The first one is the classical step: find the normal form by canonical transformations of the coordinates and momenta; the second one is to quantize this normal form. The first step is well studied and now considered rather straightforward, but the quantization of the normal form addresses the fundamental question of how to quantize a classical problem in which the coordinates and momenta does not appear in a simple manner. Even in the Birkhoff-Gustavson procedure, it is not clear *a priori* which quantization scheme would be the most natural. One can consult for this the works of M. K. Ali [1] where he makes the comparison between various notions of quantization.

The BGNF played an important role in classical mechanics in permitting, for example, to investigate the stability of elliptic trajectories [6]. It has been applied with remarkable success in molecular physics and became a very powerful tool, attested by the excellent numerical results obtained in [12] and more recently in [9] and [10].

On the mathematics side, the development of sophisticated tools for performing functional analysis in phase space, starting with pseudodifferential operators, microlocal and semiclassical analysis, has been very important for a better understanding and more accurate applications of quantum normal forms. The BGNF for pseudodifferential operators near a non-degenerate minimum of the symbol has been used by several authors, see for example the works of Bambusi [2] about semiclassical normal forms; also the article by Sjöstrand [11] that treats the non-resonant case and the one by Charles and Vu Ngoc [5] for the resonant case.

The goal of this article is to exhibit explicit calculations of the BGNF in some simple resonant situations which can be encountered in physical models, like small molecules. This article is organized as follows :

In section 2, we first start with recalling the procedure that leads Schrödinger operators $P = -\frac{h^2}{2}\Delta + V(x)$, when V is a smooth potential, to their Birkhoff-Gustavson normal form $\tilde{P} = \hat{H}_2 + \hat{K}$, where $\hat{K}$

commutes with the harmonic oscillator $\hat{H}_2$. In this procedure, the quantization and normalization steps are combined at each order, contrary to, for instance, [11], where quantization was applied only after the full classical normal form was obtained.

In section 3, we calculate the BGNF in the 1:1, 1:2 and 1:3 resonances. We introduce the creation and annihilation operators and Bargmann transform and finally we inject everything in Bargmann space. This allows an easy computation of the principal coefficients of the normal form in the three cases.

In section 4, one of the main goals of this work, we calculate the spectrum $\sigma(P)$ of the operator P thanks to the analysis of the spectrum $\sigma(\hat{K})$ of the restriction of $\hat{K}$ to the eigenspaces of $\hat{H}_2$. Since $\hat{H}_2$ and $\hat{K}$ commute, one finally gets the spectrum of P, up to a small error term, simply by adding to $\sigma(\hat{K})$ the corresponding explicit eigenvalue of $\hat{H}_2$.

All the results in sections 3 and 4 were carefully done by hand. However, it is clear that the computation of higher order approximations, involving higher order terms of the Birkhoff-Gustavson normal form, becomes very soon intractable for human abilities. On the other hand, the normal form algorithm is clear enough to be implemented on a computer. We propose in section 5 a program, whose code is available on-line[(1)], which is based on the non-commutative calculus of Weyl algebra and that can easily give the quantum Birkhoff-Gustavson normal form of a given Hamiltonian up to any order.

2 BGNF theorem

We recall the Birkhoff-Gustavson normal form theorem, BGNF, which is fundamental for this work.

Consider on $L^2(\mathbb{R}^n)$ the Schrödinger operator

$$P = -\frac{\hbar^2}{2}\Delta + V(y) \tag{1}$$

where $\hbar > 0$, Δ is the $n-$dimensional Laplacian and V is a smooth real potential on $\mathbb{R}^n$, having a non-degenerate global minimum at 0 which we shall call here the origin. By a linear unitary change of variables in local coordinates near 0, one can assume that the hessian matrix $V''(0)$ is diagonal, let $(\nu_1^2, ..., \nu_n^2)$ be its eigenvalues, with $\nu_j > 0$. The rescaling $x_j = \sqrt{\nu_j} y_j$ transforms P into a perturbation of the harmonic oscillator $\hat{H}_2$:

$$P = \hat{H}_2 + W(x) \tag{2}$$

[(1)] http://blogperso.univ-rennes1.fr/san.vu-ngoc/public/divers/birkhoff_0.4.tgz

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

$$\mathcal{E} = \mathbb{C}[\![x, \xi, \hbar]\!] = \mathbb{C}[\![x_1, ..., x_n, \xi_1, ..., \xi_n, \hbar]\!]$$
$$x = (x_1, ..., x_n) \ , \ \xi = (\xi_1, ..., \xi_n)$$

of formal power series of $(2n+1)$ variables with complex coefficients, where the degree of the monomial $x^\alpha \xi^\beta \hbar^\ell$ is defined to be $|\alpha| + |\beta| + 2\ell$, $\alpha, \beta \in \mathbb{N}^n$, $\ell \in \mathbb{N}$.

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 cofficients of degree $< N$ vanish. Let $A \in \mathcal{E}$, we shall need in this article the Weyl bracket $[.,.]_W$ defined on polynomials by :

$$[f, g]_W = \sigma_W(\widehat{f}\widehat{g} - \widehat{g}\widehat{f}) \text{ , for all } f, g \in \mathcal{E} \tag{3}$$

where $\widehat{f}$ and $\widehat{g}$ are the (formal) Weyl quantizations of symbols f and g, and σ_W is the complete Weyl symbol map. The Weyl quantization of a polynomial in (x, ξ) consists in replacing x_j by the multiplication by x_j operator, and ξ_j by $\frac{\hbar}{i}\frac{\partial}{\partial x_j}$, and averaging all the possible orderings of the variables x an ξ. Thus, for instance, the Weyl quantization of $x_1\xi_1$ is the differential operator $\frac{\hbar}{i}(x_1\frac{\partial}{\partial x_1} + \frac{1}{2})$. Then the bracket defined in (3) can be computed recursively according to the rules $[x_j, x_k]_W = [\xi_j, \xi_k]_W = [\hbar, x_j]_W = [\hbar, \xi_j]_W = 0$ and $[\xi_j, x_k]_W = \frac{\hbar}{i}\delta_{j,k}$, where $\delta_{j,k}$ is the Kronecker index.

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

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

$$e^{i\hbar^{-1}ad_A}(H_2 + L) = H_2 + K \tag{BGNF}$$

where $K = K_3 + K_4 + ...$, with $K_j \in \mathcal{D}_j$ commutes with H_2 :

$$[H_2, K]_W = 0$$

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

Notice that the sum

$$e^{i\hbar^{-1}ad_A}\left(H_2+L\right)=\sum_{l=0}^{\infty}\frac{1}{\ell!}\left(\frac{i}{\hbar}ad_A\right)^{\ell}\left(H_2+L\right) \tag{4}$$

is usually not convergent in the analytic sense, even if L comes from an analytic function, but it is always convergent in the topology of $\mathcal{E}$ because the map $B\mapsto\frac{i}{\hbar}ad_A(B)=\frac{i}{\hbar}[A,B]_W$ sends $\mathcal{O}_N$ into $\mathcal{O}_{N+1}$

The equation (BGNF) is called the Birkhoff-Gustavson normal form of the operator P at the origin.

3 Birkhoff-Gustavson normal form in the 1:1, 1:2 and 1:3 resonances

3.1 Creation and annihilation operators

Let X_j denote the operator of multiplication by x_j and Y_j the operator $\frac{\partial}{\partial x_j}$ in $L^2\left(\mathbb{R}^n\right)$.

$$\begin{aligned} a_j\left(\hbar\right)&=\frac{1}{\sqrt{2\hbar}}\left(X_j+\hbar Y_j\right)=\frac{1}{\sqrt{2\hbar}}(x_j+\hbar\frac{\partial}{\partial x_j}) \\ b_j\left(\hbar\right)&=\frac{1}{\sqrt{2\hbar}}\left(X_j-\hbar Y_j\right)=\frac{1}{\sqrt{2\hbar}}(x_j-\hbar\frac{\partial}{\partial x_j}) \end{aligned} \tag{5}$$

are respectively called the operators of creation and annihilation in $L^2\left(\mathbb{R}^n\right)$.

The operators $a_j\left(\hbar\right)$ and $b_j\left(\hbar\right)$ formally satisfy :

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

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

$$\hat{H}_2=\hbar\sum_{j=1}^{n}\nu_j(a_j\left(\hbar\right)b_j\left(\hbar\right)-\frac{1}{2}) \tag{6}$$

3.2 Bargmann representation

In this paragraph, we recall some standard results concerning the space $\mathcal{B}_{\mathcal{F}}$ of Bargmann-Fock (simply called the Bargmann space) and the Bargmann transform. For more details one can consult [3].

Let us consider the space

$$\mathcal{B}_{\mathcal{F}} = \left\{ \varphi(z) \text{ holomorphic function on } \mathbb{C}^n \ ; \ \int_{\mathbb{C}^n} |\varphi(z)|^2 \, d\mu_n(z) < +\infty \right\}$$

where $d\mu_n(z)$ is the Gaussian measure defined by $d\mu_n(z) = \pi^{-n} e^{-\frac{|z|^2}{\hbar}} d^n z = \pi^{-n} e^{-\frac{|z|^2}{\hbar}} d^n x d^n y$. $\mathcal{B}_{\mathcal{F}}$ is a Hilbert space when it is equipped with the natural inner product :

$$< f, g >= \int_{\mathbb{C}^n} f(z) \overline{g(z)} d\mu_n(z)$$

Theorem 2 ([3]) *There exists a unitary mapping $T_{\mathcal{B}}$ from $L^2(\mathbb{R}^n)$ to $\mathcal{B}_{\mathcal{F}}$ defined by*

$$(T_{\mathcal{B}} f)(z) = \frac{2^{n/4}}{(2\pi\hbar)^{3n/4}} \int_{\mathbb{R}^n} f(x) \, e^{-\frac{1}{2}\left(z^2+x^2\right)+\sqrt{2}xz} \pi^{-n} d^n x \qquad (7)$$

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

We recall that $\hat{H}_2$ is essentially self-adjoint with a discrete spectrum $\sigma(\hat{H}_2)$ which consists of the eigenvalues:

$$\lambda_N = \hbar \left(< \nu, \alpha > + \frac{|\nu|}{2} \right) = \hbar \left(N + \frac{|\nu|}{2} \right) \ , \ N =< \nu, \alpha >= \sum_{j=1}^{n} \nu_j \alpha_j$$

$$\nu = (\nu_1, ..., \nu_n), \ \alpha = (\alpha_1, ..., \alpha_n) \in \mathbb{N}^n \text{ and } |\nu| = \sum_{j=1}^{n} \nu_j .$$

The associated eigenspaces are $\mathcal{H}_N = vect \left\{ \psi_\alpha(x) \ ; \ < \nu, \alpha >= N \right\}$ where $\psi_\alpha(x) = e^{-\frac{1}{2}x^2} P_\alpha(x)$ are the standard Hermite functions (here $P_\alpha(x)$ is a polynomial of degree $|\alpha|$) which constitute an orthonormal hilbertian basis $\{\psi_\alpha(x)\}_\alpha$ of $L^2(\mathbb{R}^n)$.

Then we have the following theorem :

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

In the Bargmann representation of quantum mechanics, physical states are mapped into entire functions of a complex variable z, whereas the creation and annihilation operators play the role of differentiation and multiplication with respect to z, respectively.

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

$$T_{\mathcal{B}}\left(a_j\left(\hbar\right)\right)T_{\mathcal{B}}^{-1}=D_j \text{ and } T_{\mathcal{B}}\left(b_j\left(\hbar\right)\right)T_{\mathcal{B}}^{-1}=Z_j \tag{8}$$

The Bargmann transform of the harmonic oscillator is given by

$$\hat{H}_2^{\mathcal{B}}=T_{\mathcal{B}}\left(\hat{H}_2\right)T_{\mathcal{B}}^{-1}=\hbar\sum_{j=1}^{n}\nu_j(z_j\frac{\partial}{\partial z_j}+\frac{1}{2}) \tag{9}$$

and the eigenspace associated to the eigenvalue λ_N is the linear subspace spanned by the functions $\frac{z^{\alpha_1}}{\sqrt{\alpha_1!}}\frac{z^{\alpha_2}}{\sqrt{\alpha_2!}}$ such that $\nu_1\alpha_1+\nu_2\alpha_2=N$:

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

3.3 BGNF in the 1:1 resonance

Consider the following harmonic oscillator

$$\hat{H}_2=\frac{1}{2}\left(-\hbar^2\frac{\partial^2}{\partial x_1^2}+x_1^2\right)+\frac{1}{2}\left(-\hbar^2\frac{\partial^2}{\partial x_2^2}+x_2^2\right)$$

with symbol

$$H_2=\left|z_1\right|^2+\left|z_2\right|^2$$

where $z_j=\frac{1}{\sqrt{2}}\left(x_j+i\xi_j\right)$; $j=1,2$.
The Bargmann transform of $\widehat{H}_2$ is given by

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

Suppose now we are in the situation of the BGNF theorem (cf. equation (2)) : we want to understand the spectrum of an operator of the form $\widehat{H}_2+\widehat{L}$, where L is a perturbation term of order at least 3. From the theorem, it is enough to study the spectrum of the normalized perturbation $\widehat{K}$ (see [5]). The crucial question is therefore to compute the first non-trivial term of the symbol K. Throughout the paper, when K is a formal series in $\mathcal{E}$, we use the notation K_j to denote the homogeneous part of degree j, and $K^{(N)}:=K_0+K_1+\cdots+K_N$.

Since $[H_2,K_3]_W=0$ and thus $\{H_2,K_3\}=0$, we have

$$K_3=\sum_{2\ell+|\beta|+|\gamma|=3}c_{\alpha\beta}^{(3)}\hbar^\ell z^\alpha\overline{z}^\beta \text{ such that } <\nu,\beta-\alpha>=0.$$

In other words, K_3 is a linear combination of order 3 monomials $\hbar^\ell z^\alpha \overline{z}^\beta$ such that $< \nu, \beta - \alpha >= 0$.

The condition of 1:1 resonance, $\nu_1 = \nu_2 = 1$, is expressed by

$$< \nu, \beta - \alpha >= 0 \Leftrightarrow \alpha_1 + \alpha_2 = \beta_1 + \beta_2 \qquad (\textbf{res } 1{:}1)$$

where $\alpha = (\alpha_1, \alpha_2)$, $\beta = (\beta_1, \beta_2) \in \mathbb{N}^2$.

We notice that no monomial exists in $\mathcal{D}_3$ verifying at the same time $|\alpha| + |\beta| = 3$ and the resonance relation (**res** $1:1$). This means $K_3 = 0$. Thus we need to calculate K_4, as a linear combination of monomials $z_1^{\alpha_1} z_2^{\alpha_2} \overline{z}_1^{\beta_1} \overline{z}_2^{\beta_2}$ of order 4. We check that the couples $\alpha = (\alpha_1, \alpha_2)$ and $\beta = (\beta_1, \beta_2)$ which verify at the same time $|\alpha| + |\beta| = 4$ and the resonance relation (**res** $1:1$) are :

$$\alpha = \beta = (1,1)\,,\ \alpha = \beta = (2,0)\,,\ \alpha = \beta = (0,2)\,,$$
$$\alpha = (2,0) \text{ and } \beta = (0,2)\,,\ \alpha = (0,2) \text{ and } \beta = (2,0)$$

Thus K_4 is generated by the monomials :

$$|z_1|^2 |z_2|^2 \ ,\ |z_1|^4 \ ,\ |z_2|^4 \ ,\ z_1^2 \overline{z}_2^2 \ ,\ \overline{z}_1^2 z_2^2 \ ,\ \hbar^2$$

Since K is real, one can write

$$K_4 = \lambda_1 |z_1|^4 + \lambda_2 |z_2|^4 + \lambda_3 |z_1|^2 |z_2|^2 + \lambda_4 \operatorname{Re}\left(z_1^2 \overline{z}_2^2\right) + \lambda_5 \hbar^2 \qquad (10)$$

Evaluation of coefficients λ_j :

By the BGNF, the order 4 perturbation W_4 turns into a new term K_4 which we will obtain as the projection onto the kernel of ad_{H_2} of the term

$$W_4 + \frac{i}{2\hbar}[A_3, W_3]_W, \qquad (11)$$

where A_3 is defined by the relation

$$W_3 = \frac{i}{\hbar} ad_{H_2}(A_3)\,. \qquad (12)$$

Indeed, applying the theorem 1 of Birkhoff-Gustavson to $H_2 + W = H_2 + W_3 + W_4 + \ldots$, we obtain polynomials $A_3 \in \mathcal{D}_3$ and $K_3 \in \mathcal{D}_3$ such as

$$e^{i\hbar^{-1} ad_{A_3}}\left(H_2 + W_3 + \mathcal{O}_4\right) = H_2 + K_3 + \mathcal{O}_4 \qquad (13)$$

where K_3 and H_2 commute. We have

$$(13) \Leftrightarrow H_2 + W_3 + \frac{i}{\hbar}\left[A_3, H_2\right]_W + \mathcal{O}_4 = H_2 + K_3 + \mathcal{O}_4.$$

Since

$$\mathcal{D}_3 = \ker\left(i\hbar^{-1}ad_{H_2}\right) \oplus \mathrm{Im}\left(i\hbar^{-1}ad_{H_2}\right), \tag{14}$$

we may split $W_3 = W_{3,1} + \frac{i}{\hbar}\left[H_2, W_{3,2}\right]_W$ where $W_{3,1} \in \mathcal{D}_3$ commutes with H_2, and $W_{3,2} \in \mathcal{D}_3$. Therefore $K_3 = W_{3,1}$ and we can set $A_3 = W_{3,2}$; however, in the $\mathbf{1}:\mathbf{1}$ resonance, $\ker\left(i\hbar^{-1}ad_{H_2}\right) \cap \mathcal{D}_3 = \{0\}$, hence $K_3 = W_{1,3} = 0$, and therefore A_3 is defined by the relation (12).

Now, let $A_3 = \sum\limits_{|\alpha|+|\beta|=3} a_{\alpha,\beta} z^\alpha \bar{z}^\beta$ and $W_3 = \sum\limits_{|\alpha|+|\beta|=3} c_{\alpha,\beta} z^\alpha \bar{z}^\beta$, then (12) gives:

$$\begin{aligned}\sum_{|\alpha|+|\beta|=3} c_{\alpha,\beta} z^\alpha \bar{z}^\beta &= \frac{i}{\hbar} ad_{H_2}\left(\sum_{|\alpha|+|\beta|=3} a_{\alpha,\beta} z^\alpha \bar{z}^\beta\right) \\ &= \frac{i}{\hbar}\sum_{|\alpha|+|\beta|=3} h < \nu, \beta-\alpha > a_{\alpha,\beta} z^\alpha \bar{z}^\beta\end{aligned}$$

from where

$$a_{\alpha,\beta} = -i\frac{c_{\alpha,\beta}}{< \nu, \beta-\alpha >} \tag{15}$$

and from the $\mathbf{1}:\mathbf{1}$ resonance relation we obtain

$$a_{\alpha,\beta} = -i\frac{c_{\alpha,\beta}}{\beta_1+\beta_2-\alpha_1-\alpha_2},\ \forall \alpha,\beta \in \mathbb{N}^2\ ;\ \ |\alpha|+|\beta| = 3$$

It remains to find K_4; since $K_3 = 0$, the normal form writes

$$e^{i\hbar^{-1}ad_{(A_3+A_4)}}\left(H_2 + W_3 + W_4 + \mathcal{O}_5\right) = H_2 + K_4 + \mathcal{O}_5 \tag{16}$$

with $[K_4, H_2] = 0$. We have

$$\begin{aligned}e^{i\hbar^{-1}ad_{(A_3+A_4)}}\left(H_2 + W_3 + W_4 + \mathcal{O}_5\right) &= H_2 + W_3 + W_4 + \frac{i}{\hbar}\left[A_3, H_2\right]_W + \frac{i}{\hbar}\left[A_4, H_2\right]_W \\ &+ \frac{i}{\hbar}\left[A_3, W_3\right]_W + \frac{1}{2!}\left(\frac{i}{\hbar}\right)^2 \left[A_3, \left[A_3, H_2\right]_W\right]_W + \mathcal{O}_5 \\ &= H_2 + W_4 + \frac{i}{\hbar}\left[A_3, W_3\right] + \frac{i}{2\hbar}\left[A_3, \frac{i}{\hbar}\left[A_3, H_2\right]\right] + \mathcal{O}_5\end{aligned}$$

because from (12), we have, $\frac{i}{\hbar}\left[A_3, H_2\right]_W = -\frac{i}{\hbar}\left[H_2, A_3\right]_W = -W_3$. So

$$\begin{aligned}(16) &\Leftrightarrow W_4 + \frac{i}{\hbar}\left[A_4, H_2\right]_W + \frac{i}{\hbar}\left[A_3, W_3\right]_W + \frac{i}{2\hbar}\left[A_3, \frac{i}{\hbar}\left[A_3, H_2\right]_W\right]_W + \mathcal{O}_5 = R_4 + \mathcal{O}_5 \\ &\Leftrightarrow W_4 + \frac{i}{\hbar}\left[A_4, H_2\right]_W + \frac{i}{\hbar}\left[A_3, W_3\right]_W - \frac{i}{2\hbar}\left[A_3, W_3\right]_W + \mathcal{O}_5 = R_4 + \mathcal{O}_5 \\ &\Leftrightarrow W_4 + \frac{i}{\hbar}\left[A_4, H_2\right]_W + \frac{i}{2\hbar}\left[A_3, W_3\right]_W + \mathcal{O}_5 = K_4 + \mathcal{O}_5\end{aligned}$$

and therefore K_4 must be the projection onto $\mathcal{D}_4 \cap \ker\left(i\hbar^{-1} ad_{H_2}\right)$, in the splitting (14), of the term

$$W_4 + \frac{i}{2\hbar}\left[A_3, W_3\right]_W. \tag{17}$$

In order to compute this projection, we express W_3 in terms of the more convenient complex variables : $z_j = \frac{1}{\sqrt{2}}\left(x_j + i\xi_j\right)$, so $x_j = \frac{1}{\sqrt{2}}\left(z_j + \bar{z}_j\right)$, and we get, by Taylor expansion:

$$\begin{aligned}
W_3 = & \frac{1}{2\sqrt{2}.3!}\left[\frac{\partial^3 W(0)}{\partial x_1^3}\left(z_1+\bar{z}_1\right)^3 + \frac{\partial^3 W(0)}{\partial x_2^3}\left(z_2+\bar{z}_2\right)^3\right.\\
&\left. + 3\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2}\left(z_1+\bar{z}_1\right)^2\left(z_2+\bar{z}_2\right) + 3\frac{\partial^3 W(0)}{\partial x_1 \partial x_2^2}\left(z_1+\bar{z}_1\right)\left(z_2+\bar{z}_2\right)^2\right]\\
= & \frac{1}{2\sqrt{2}.3!}\left[\frac{\partial^3 W(0)}{\partial x_1^3}\left(z_1^3 + 3z_1^2\bar{z}_1 + 3z_1\bar{z}_1^2 + \bar{z}_1^3\right)\right.\\
& + \frac{\partial^3 W(0)}{\partial x_2^3}\left(z_2^3 + 3z_2^2\bar{z}_2 + 3z_2\bar{z}_2^2 + \bar{z}_2^3\right)\\
& + 3\frac{\partial^3 V(0)}{\partial x_1^2 \partial x_2}\left(z_1^2 z_2 + z_1^2\bar{z}_2 + \bar{z}_1^2 z_2 + \bar{z}_1^2\bar{z}_2 + 2z_1 z_2\bar{z}_1 + 2z_1\bar{z}_1\bar{z}_2\right)\\
& \left. + 3\frac{\partial^3 V(0)}{\partial x_1 \partial x_2^2}\left(z_2^2 z_1 + z_2^2\bar{z}_1 + \bar{z}_2^2 z_1 + \bar{z}_2^2\bar{z}_1 + 2z_2 z_1\bar{z}_2 + 2z_2\bar{z}_2\bar{z}_1\right)\right].
\end{aligned}$$

By the relation (15) we get

$$\begin{aligned}
A_3 = & -i\frac{1}{2\sqrt{2}.3!}\left[\frac{\partial^3 W(0)}{\partial x_1^3}\left(-\frac{1}{3}z_1^3 - 3z_1^2\bar{z}_1 + 3z_1\bar{z}_1^2 + \frac{1}{3}\bar{z}_1^3\right)\right]\\
& + \frac{\partial^3 W(0)}{\partial x_2^3}\left(-\frac{1}{3}z_2^3 - 3z_2^2\bar{z}_2 + 3z_2\bar{z}_2^2 + \frac{1}{3}\bar{z}_2^3\right)\Bigg]\\
& + 3\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2}\left(-\frac{1}{3}z_1^2 z_2 - z_1^2\bar{z}_2 + \bar{z}_1^2 z_2 + \frac{1}{3}\bar{z}_1^2\bar{z}_2 - 2z_1 z_2\bar{z}_1 + 2z_1\bar{z}_1\bar{z}_2\right)\\
& + 3\frac{\partial^3 W(0)}{\partial x_1 \partial x_2^2}\left(-\frac{1}{3}z_2^2 z_1 - z_2^2\bar{z}_1 + \bar{z}_2^2 z_1 + \frac{1}{3}\bar{z}_2^2\bar{z}_1 - 2z_2 z_1\bar{z}_2 + 2z_2\bar{z}_2\bar{z}_1\right)\Bigg]
\end{aligned}$$

Now, we must calculate $\frac{i}{2\hbar}\left[A_3, W_3\right]_W$. By the Moyal Formula:

$$\frac{i}{2\hbar}\left[A_3, W_3\right]_W = \frac{1}{2}\left\{A_3, W_3\right\} - \frac{\hbar^2}{2^3 3!}\Pi^3\left(A_3, W_3\right) + \mathcal{O}_5 \tag{18}$$

where we use the bidifferential operator $\Pi(f,g) := f\Pi g$ given by

$$\{f,g\} = f\Pi g = \sum_{j=1}^{n}\frac{\partial f}{\partial \xi_j}\frac{\partial g}{\partial x_j} - \frac{\partial f}{\partial x_j}\frac{\partial g}{\partial \xi_j} = -if\left(\frac{\overleftarrow{\partial}}{\partial \bar{z}}\frac{\overrightarrow{\partial}}{\partial z} - \frac{\overleftarrow{\partial}}{\partial z}\frac{\overrightarrow{\partial}}{\partial \bar{z}}\right)g \tag{19}$$

and

$$\Pi^3 = i\left[\frac{\overleftarrow{\partial^3}}{\partial\bar{z}^3}\frac{\overrightarrow{\partial^3}}{\partial z^3} - 3\frac{\overleftarrow{\partial^2}}{\partial\bar{z}^2}\frac{\overrightarrow{\partial^2}}{\partial z^2}\frac{\overleftarrow{\partial}}{\partial z}\frac{\overrightarrow{\partial}}{\partial\bar{z}} + 3\frac{\overleftarrow{\partial}}{\partial\bar{z}}\frac{\overrightarrow{\partial}}{\partial z}\frac{\overleftarrow{\partial^2}}{\partial z^2}\frac{\overrightarrow{\partial^2}}{\partial\bar{z}^2} - \frac{\overleftarrow{\partial^3}}{\partial z^3}\frac{\overrightarrow{\partial^3}}{\partial\bar{z}^3}\right] \quad (20)$$

$$= i\sum_{j=1}^{n}\frac{\overleftarrow{\partial^3}}{\partial\bar{z}_j^3}\frac{\overrightarrow{\partial^3}}{\partial z_j^3} - 3\frac{\overleftarrow{\partial^3}}{\partial\bar{z}_j^2\partial z_j}\frac{\overrightarrow{\partial^3}}{\partial z_j^2\partial\bar{z}_j} + 3\frac{\overleftarrow{\partial^3}}{\partial\bar{z}_j\partial z_j^2}\frac{\overrightarrow{\partial^3}}{\partial z_j\partial\bar{z}_j^2} - \frac{\overleftarrow{\partial^3}}{\partial z_j^3}\frac{\overrightarrow{\partial^3}}{\partial\bar{z}_j^3}$$

Since A_3 and W_3 are in function of $z^\alpha\bar{z}^\beta$, we can compute the Poisson brackets using the following nice formula :

Lemma 5 $\forall\alpha,\beta,\alpha',\beta'\in\mathbb{N}^n$*:*

$$\left\{z^\alpha\bar{z}^\beta, z^{\alpha'}\bar{z}^{\beta'}\right\} = -iz^{\alpha+\alpha'}\bar{z}^{\beta+\beta'}\sum_{j=1}^{n}\begin{vmatrix}\alpha_j & \beta_j\\ \alpha'_j & \beta'_j\end{vmatrix}\frac{1}{z_j\bar{z}_j} \quad (21)$$

Particular cases:
$\left\{z^\alpha, z^\beta\right\} = 0$; $\left\{\bar{z}^\alpha, \bar{z}^\beta\right\} = 0$; $\left\{z^\alpha, \bar{z}^\beta\right\} = -iz^\alpha\bar{z}^\beta\sum_{j=1}^{n}\alpha_j\beta_j\frac{1}{z_j\bar{z}_j}$.

Proof.

$$\left\{z^\alpha\bar{z}^\beta, z^{\alpha'}\bar{z}^{\beta'}\right\} = -i\sum_{j=1}^{n}\frac{\partial z_1^{\alpha_1}...z_n^{\alpha_n}\ \bar{z}_1^{\beta_1}...\bar{z}_1^{\beta_1}}{\partial\bar{z}_j}\frac{\partial z_1^{\alpha'_1}...z_n^{\alpha'_n}\ \bar{z}_1^{\beta'_1}...\bar{z}_1^{\beta'_1}}{\partial z_j}$$
$$-\frac{\partial z_1^{\alpha_1}...z_n^{\alpha_n}\ \bar{z}_1^{\beta_1}...\bar{z}_1^{\beta_1}}{\partial z_j}\frac{\partial z_1^{\alpha'_1}...z_n^{\alpha'_n}\ \bar{z}_1^{\beta'_1}...\bar{z}_1^{\beta'_1}}{\partial\bar{z}_j}$$
$$= -i\sum_{j=1}^{n}\beta_j\alpha'_j z^{\alpha+\alpha'-e_j}\ \bar{z}^{\beta+\beta'-e_j} - \alpha_j\beta'_j z^{\alpha+\alpha'-e_j}\ \bar{z}^{\beta+\beta'-e_j}$$
$$= -i\sum_{j=1}^{n}\left(\beta_j\alpha'_j - \alpha_j\beta'_j\right)z^{\alpha+\alpha'-e_j}\ \bar{z}^{\beta+\beta'-e_j}$$

which gives the result. ■

After a long but straightforward calculation by hand and via this last lemma, we arrive to gather all monomials of $\frac{1}{2}\{A_3, W_3\}$, that are in K_4, and we obtain:

$$-\frac{1}{2}\left(\frac{1}{3!2\sqrt{2}}\right)^2\left[60\left\{\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)^2+\left(\frac{\partial^3 W(0)}{\partial x_1^2\partial x_2}\right)^2\right\}|z_1|^4\right.$$
$$+60\left\{\left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)^2+\left(\frac{\partial^3 W(0)}{\partial x_2^2\partial x_1}\right)^2\right\}|z_2|^4$$
$$+\left\{72\left[\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_1^2\partial x_2}\right)+\left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_2^2\partial x_1}\right)+\right.\right.$$
$$\left.\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_2^2\partial x_1}\right)+\left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_1^2\partial x_2}\right)\right]$$
$$\left.+96\left[\left(\frac{\partial^3 W(0)}{\partial x_1^2\partial x_2}\right)^2+\left(\frac{\partial^3 W(0)}{\partial x_2^2\partial x_1}\right)^2\right]\right\}|z_1|^2|z_2|^2$$
$$-3\left\{\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_1^2\partial x_2}\right)+\left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_2^2\partial x_1}\right)\right.$$
$$\left.\left.+\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_2^2\partial x_1}\right)+\left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_1^2\partial x_2}\right)\right\}\operatorname{Re}\left(z_1^2\overline{z}_2^2\right)\right]$$

and the second term of (18) is simply

$$-\frac{\hbar^2}{2^3 3!}\Pi^3\left(A_3,W_3\right)=\frac{1}{2^3 3!}.192\left(\frac{1}{2\sqrt{2}.3!}\right)^2\left[\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)^2+\left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)^2\right]\hbar^2$$
$$=\frac{1}{72}\left[\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)^2+\left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)^2\right]\hbar^2$$

Let's now, look for all monomials of W_4 that should belong to K_4.

We have

$$W_4\left(x_1,x_2\right)=\frac{1}{4!}\left(\frac{\partial^4 W(0)}{\partial x_1^4}x_1^4+\frac{\partial^4 W(0)}{\partial x_2^4}x_2^4+4\frac{\partial^4 W(0)}{\partial x_1^3\partial x_2}x_1^3x_2\right.$$
$$\left.+4\frac{\partial^4 W(0)}{\partial x_2^3\partial x_1}x_2^3x_1+6\frac{\partial^4 W(0)}{\partial x_1^2\partial x_2^2}x_1^2x_2^2\right)$$

We know from (10) that only the monomials x_1^4, x_2^4 and $x_1^2x_2^2$ in $W_4\left(x_1,x_2\right)$ may contribute to K_4.

Now, if we let $x_j = \frac{1}{\sqrt{2}} (z_j + \bar{z}_j)$, then:

$$x_1^4 = \frac{1}{4} (z_1 + \overline{z}_1)^4 = \frac{1}{4}(z_1^4 + 4z_1^2 |z_1|^2 + \underbrace{6 |z_1|^4}_{\text{in } K_4} + 4\overline{z}_1^2 |z_1|^2 + \overline{z}_1^4)$$

$$x_2^4 = \frac{1}{4} (z_2 + \overline{z}_2)^4 = \frac{1}{4}(z_2^4 + 4z_2^2 |z_2|^2 + \underbrace{6 |z_2|^4}_{\text{in } K_4} + 4\overline{z}_2^2 |z_2|^2 + \overline{z}_2^4)$$

$$\begin{aligned} x_1^2 x_2^2 &= \frac{1}{4} (z_1 + \overline{z}_1)^2 (z_2 + \overline{z}_2)^2 \\ &= \frac{1}{4} \Big[z_1^2 z_2^2 + \underbrace{z_1^2 \overline{z}_2^2}_{\text{in } K_4} + 2\overline{z}_1^2 |z_2|^2 + \underbrace{\overline{z}_1^2 z_2^2}_{\text{in } K_4} + \overline{z}_1^2 \overline{z}_2^2 \\ &\quad + 2\overline{z}_1^2 |z_2|^2 + 2z_2^2 |z_1|^2 + 2 |z_1|^2 \overline{z}_2^2 + 4\underbrace{|z_1|^2 |z_2|^2}_{\text{in } K_4} \Big] \end{aligned}$$

from where, we get the other part of the terms of K_4, that is:

$$\frac{1}{16} \frac{\partial^4 W(0)}{\partial x_1^4} |z_1|^4 + \frac{1}{16} \frac{\partial^4 W(0)}{\partial x_2^4} |z_2|^4 + \frac{1}{4} \frac{\partial^4 W(0)}{\partial x_1^2 \partial x_2^2} |z_1|^2 |z_2|^2 + \frac{1}{8} \frac{\partial^4 W(0)}{\partial x_1^2 \partial x_2^2} \operatorname{Re}\left(z_1^2 \overline{z}_2^2\right)$$

finally we gather all terms that are in K_4, and we obtain the coefficients we were looking for:

Theorem 6 *The quantum Birkhoff-Gustavson normal form of the Schrödinger hamiltonian in* $1:1$ *resonance* $H_2 + W$ *is equal to* $H_2 + K_4 + \mathcal{O}_5$ *with*

$$K_4 = \lambda_1 |z_1|^4 + \lambda_2 |z_2|^4 + \lambda_3 |z_1|^2 |z_2|^2 + \lambda_4 \operatorname{Re}\left(z_1^2 \overline{z}_2^2\right) + \lambda_5 \hbar^2,$$

where

$$\lambda_1 = \frac{1}{16}\frac{\partial^4 W(0)}{\partial x_1^4} - \frac{1}{2}\left(\frac{1}{3!2\sqrt{2}}\right)^2 60 \left\{ \left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)^2 + \left(\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2}\right)^2 \right\}$$

$$\lambda_2 = \frac{1}{16}\frac{\partial^4 W(0)}{\partial x_2^4} - \frac{1}{2}\left(\frac{1}{3!2\sqrt{2}}\right)^2 60 \left\{ \left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)^2 + \left(\frac{\partial^3 W(0)}{\partial x_2^2 \partial x_1}\right)^2 \right\}$$

$$\begin{aligned}\lambda_3 = {} & \frac{1}{4}\frac{\partial^4 W(0)}{\partial x_1^2 \partial x_2^2} + 72 \left[\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2}\right) + \left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_2^2 \partial x_1}\right) \right. \\ & + \left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_2^2 \partial x_1}\right) + \left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2}\right) \\ & \left. +96 \left(\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2}\right)^2 + \left(\frac{\partial^3 W(0)}{\partial x_2^2 \partial x_1}\right)^2 \right]\end{aligned}$$

$$\begin{aligned}\lambda_4 = {} & \frac{1}{8}\frac{\partial^4 W(0)}{\partial x_1^2 \partial x_2^2} - 3 \left[\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2}\right) + \left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_2^2 \partial x_1}\right) \right. \\ & \left. + \left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_2^2 \partial x_1}\right) + \left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2}\right) \right]\end{aligned}$$

$$\lambda_5 = \frac{1}{72}\left[\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)^2 + \left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)^2 \right]$$

The Weyl quantization of K_4 gives a concrete representation of this normal form as a polynomial differential operator :

$$\begin{aligned}\hat{K}_4 = {} & \lambda_1 \left(x_1^4 + \hbar^4 \frac{\partial^4}{\partial x_1^4} - 2\hbar^2 x_1^2 \frac{\partial^2}{\partial x_1^2} - 4\hbar^2 x_1 \frac{\partial}{\partial x_1} - \hbar^2 \right) \\ & +\lambda_2 \left(x_2^4 + \hbar^4 \frac{\partial^4}{\partial x_2^4} - 2\hbar^2 x_2^2 \frac{\partial^2}{\partial x_2^2} - 4\hbar^2 x_2 \frac{\partial}{\partial x_2} - \hbar^2 \right) \\ & +\lambda_3 \left(x_1^2 x_2^2 - \hbar^2 x_1^2 \frac{\partial^2}{\partial x_1^2} - \hbar^2 x_2^2 \frac{\partial^2}{\partial x_2^2} + \hbar^4 \frac{\partial^2}{\partial x_1^2}\frac{\partial^2}{\partial x_2^2} \right) \\ & +\lambda_4 \left[x_1^2 x_2^2 + \hbar^2 x_1^2 \frac{\partial^2}{\partial x_2^2} + \hbar^2 x_2^2 \frac{\partial^2}{\partial x_1^2} + \hbar^4 \frac{\partial^2}{\partial x_1^2}\frac{\partial^2}{\partial x_2^2} \right. \\ & \left. - 4\hbar^2 x_1 x_2 \frac{\partial}{\partial x_1}\frac{\partial}{\partial x_2} + 2\hbar^2 x_1 \frac{\partial}{\partial x_1} + 2\hbar^2 x_2 \frac{\partial}{\partial x_2} + \hbar^2 \right] \\ & +\lambda_5 \hbar^2\end{aligned} \quad (22)$$

Using the creation and annihilation operators we get:

$$\begin{aligned}\hat{K}_4 = & 2\hbar^2\lambda_1\left[a_1^2(\hbar)\, b_1^2(\hbar) + b_1^2(\hbar)\, a_1^2(\hbar) - 1\right] \\ & +2\hbar^2\lambda_2\left[a_2^2(\hbar)\, b_2^2(\hbar)\, b_2^2(\hbar)\, a_2^2(\hbar) - 1\right] \\ & +2\hbar^2\lambda\left({}_3 a_1(\hbar)\, b_1(\hbar)\, a_2(\hbar)\, b_2(\hbar)\right. \\ & \left. + b_1(\hbar)\, a_1(\hbar)\, b_2(\hbar)\, a_2(\hbar) - \frac{1}{2}\right) \\ & +2\hbar^2\lambda_4[a_1^2(\hbar)\, b_2^2(\hbar) + a_2^2(\hbar)\, b_1^2(\hbar)]) \\ & +\lambda_5\hbar^2\end{aligned} \tag{23}$$

and by using Bargmann representation, we get

$$\begin{aligned}\hat{K}_4^{\mathcal{B}} = & T_{\mathcal{B}}\left(\widehat{K}_4\right)T_{\mathcal{B}}^{-1} = 2\hbar^2\left[\lambda_1\left(1 + 4z_1\frac{\partial}{\partial z_1} + 2z_1^2\frac{\partial^2}{\partial z_1^2}\right)\right. \\ & +\lambda_2\left(1 + 4z_2\frac{\partial}{\partial z_2} + 2z_2^2\frac{\partial^2}{\partial z_2^2}\right) \\ & +\lambda_3\left(1 + z_1\frac{\partial}{\partial z_1} + z_2\frac{\partial}{\partial z_2} + 2z_1z_2\frac{\partial^2}{\partial z_1\partial z_2}\right) \\ & \left.+\lambda_4\left(z_1^2\frac{\partial^2}{\partial z_2^2} + z_2^2\frac{\partial^2}{\partial z_1^2}\right)\right] \\ & +\lambda_5\hbar^2 \\ = & 2\hbar^2\left(2\lambda_1 z_1^2\frac{\partial^2}{\partial z_1^2} + 2\lambda_2 z_2^2\frac{\partial^2}{\partial z_2^2} + 2\lambda_3 z_1z_2\frac{\partial^2}{\partial z_1\partial z_2} + \lambda_4\left(z_1^2\frac{\partial^2}{\partial z_2^2} + z_2^2\frac{\partial^2}{\partial z_1^2}\right)\right. \\ & \left. + (4\lambda_1 + \lambda_3)\, z_1\frac{\partial}{\partial z_1} + (4\lambda_2 + \lambda_3)\, z_2\frac{\partial}{\partial z_2} + \left(\lambda_1 + \lambda_2 + \lambda_3 + \frac{\lambda_5}{2}\right)\right)\end{aligned} \tag{24}$$

3.4 BGNF in the 1:2 resonance (Fermi resonance)

Let

$$\widehat{H}_2 = \frac{1}{2}\left(-\hbar^2\frac{\partial^2}{\partial x_1^2} + x_1^2\right) + \left(-\hbar^2\frac{\partial^2}{\partial x_2^2} + x_2^2\right)$$

with symbol

$$H_2 = |z_1|^2 + 2\,|z_2|^2$$

where $z_j = \frac{1}{\sqrt{2}}\left(x_j + i\xi_j\right)$; $j = 1, 2$.

The Bargmann transform of $\widehat{H}_2$ is given by

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

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

$$K_3 = \sum_{2\ell+|\beta|+|\gamma|=3} c_{\alpha\beta}^{(3)}\hbar^\ell z^\alpha \overline{z}^\beta$$

such that $< \nu, \beta - \alpha >= 0$.

The condition of 1:2 resonance, $\nu_1 = 1, \nu_2 = 2$, is expressed by

$$< \nu, \beta - \alpha >= 0 \Leftrightarrow \alpha_1 + 2\alpha_2 = \beta_1 + 2\beta_2 \qquad (\textbf{res } 1{:}2)$$

where $\alpha = (\alpha_1, \alpha_2)$,$\beta = (\beta_1, \beta_2) \in \mathbb{N}^2$.
To obtain 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 $\beta = (\beta_1, \beta_2)$ which verify at the same time $|\alpha| + |\beta| = 3$ and the resonance relation (**res** $1:2$) are :

$$\alpha = (0,1) \text{ and } \beta = (2,0)$$
$$\alpha = (2,0) \text{ and } \beta = (0,1)$$

Thus, K_3 is generated by the monomials

$$z_2\overline{z}_1^2 \ , \ z_1^2\overline{z}_2$$

Since K is real, we can write

$$K_3 = \mu \operatorname{Re}(z_1^2\overline{z}_2) = \frac{\mu}{2}(z_2\overline{z}_1^2 + z_1^2\overline{z}_2), \ \mu \in \mathbb{R} \qquad (25)$$

Evaluation of coefficient μ :

The term of third degree in Taylor series of W near the origine is

$$W_3(x_1, x_2) = \frac{1}{3!}\left[\frac{\partial^3 W(0)}{\partial x_1^3}x_1^3 + \frac{\partial^3 W(0)}{\partial x_2^3}x_2^3 + 3\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2}x_1^2 x_2 + 3\frac{\partial^3 W(0)}{\partial x_2^2 \partial x_1}x_2^2 x_1\right]$$

where $W(x_1, x_2) = \sum\limits_{j \geqslant 3} W_j(x_1, x_2)$ given in formula (2).
If we put $x_j = \frac{1}{\sqrt{2}}(z_j + \overline{z}_j)$, We remark that, only the coefficient of $x_1^2 x_2$ in $W_3(x_1, x_2)$ corresponds to the coefficient of K_3, because:

$$x_1^2 x_2 = \frac{1}{2\sqrt{2}}\left(z_1^2 z_2 + \underbrace{z_1^2\overline{z}_2 + \overline{z}_1^2 z_2}_{\text{in } K_3} + \overline{z}_1^2\overline{z}_2 + 2|z_1|^2 z_2 + 2|z_1|^2\overline{z}_2\right)$$

we obtain, the term in K_3 :

$$\frac{1}{2}.\frac{1}{2\sqrt{2}}\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2}(z_1^2\overline{z}_2 + \overline{z}_1^2 z_2) = \frac{1}{2\sqrt{2}}\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2}\operatorname{Re}(z_1^2\overline{z}_2)$$

Theorem 7 *The quantum Birkhoff-Gustavson normal form of the Schrödinger hamiltonian in $1:2$ resonance $H_2 + W$ is equal to $H_2 + K_3 + \mathcal{O}_4$ with*

$$K_3 = \mu \operatorname{Re}(z_1^2\overline{z}_2)$$

where

$$\mu = \frac{1}{2\sqrt{2}}\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2}$$

The calculation of $\hat{K}_3$ Weyl quantization of K_3 give us:

$$\hat{K}_3 = \mu \widehat{\mathrm{Re}\left(z_1^2\overline{z}_2\right)} = x_1^2 x_2 - 2\hbar^2 x_1 \frac{\partial}{\partial x_1}\frac{\partial}{\partial x_2} + \hbar^2 x_2 \frac{\partial^2}{\partial x_1^2} - \hbar^2 \frac{\partial}{\partial x_2}$$

Using the creation and annihilation operators we get,

$$\hat{K}_3 = \sqrt{2}\mu\hbar^{3/2}\left(a_2\left(\hbar\right)b_1^2\left(\hbar\right) + a_1^2\left(\hbar\right)b_2\left(\hbar\right)\right) \tag{26}$$

and by using Bargmann representation, we get

$$\widehat{K}_3^{\mathcal{B}} = T_{\mathcal{B}}\left(\widehat{K}_3\right)T_{\mathcal{B}}^{-1} = \sqrt{2}\mu\hbar^{3/2}\left(z_2\frac{\partial^2}{\partial z_1^2} + z_1^2\frac{\partial}{\partial z_2}\right) \tag{27}$$

3.5 BGNF in the 1:3 resonance

Now, we consider

$$\widehat{H}_2 = \frac{1}{2}\left(-\hbar^2\frac{\partial^2}{\partial x_1^2} + x_1^2\right) + \frac{3}{2}\left(-\hbar^2\frac{\partial^2}{\partial x_2^2} + x_2^2\right)$$

with symbol

$$H_2 = \left|z_1\right|^2 + 3\left|z_2\right|^2$$

where $z_j = \frac{1}{\sqrt{2}}\left(x_j + i\xi_j\right)$; $j = 1, 2$.

The Bargmann transform of $\widehat{H}_2$ is given by

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

The condition of 1:3 resonance, $\nu_1 = 1, \nu_2 = 3$ is expressed by the resonance relation :

$$< \nu, \beta - \alpha >= 0 \Leftrightarrow \alpha_1 + 3\alpha_2 = \beta_1 + 3\beta_2 \tag{\textbf{res} 1:3}$$

where $\alpha = (\alpha_1, \alpha_2)$, $\beta = (\beta_1, \beta_2) \in \mathbb{N}^2$

We see that no monomial exists in $\mathcal{D}_3$ verifying at the same time $|\alpha| + |\beta| = 3$ and the resonance relation (**res** $1:3$) .This means $K_3 = 0$. Thus, we need to calculate $K_4 \in \mathcal{D}_4$ satisfying the relation (**res** $1:3$) . We check that the couples $\alpha = (\alpha_1, \alpha_2)$ and $\beta = (\beta_1, \beta_2)$ which verify at the same time $|\alpha| + |\beta| = 4$ and the resonance relation (**res** $1:3$) are :

$$\begin{aligned}&\alpha = \beta = (1,1)\,,\ \alpha = \beta = (2,0)\,,\ \alpha = \beta = (0,2)\,,\\ &\alpha = (3,0)\ \text{ and } \beta = (0,1)\,,\ \alpha = (0,1)\ \text{ and } \beta = (3,0)\end{aligned}$$

Thus, K_4 is generated by the monomials :

$$|z_1|^4 \ , \ |z_2|^4 \ , \ |z_1|^2 |z_2|^2 \ , \ z_1^3\bar{z}_2 \ , \ \bar{z}_1^3 z_2 \ , \ \hbar^2$$

since K is real, on can write

$$K_4 = \gamma_1 |z_1|^4 + \gamma_2 |z_2|^4 + \gamma_3 |z_1|^2 |z_2|^2 + \gamma_4 \operatorname{Re}\left(z_1^3\bar{z}_2\right) + \gamma_5\hbar^2 \qquad (28)$$

Evaluation of the coefficients γ_j : We have to calculate

$$A_3 = \sum_{|\alpha|+|\beta|=3} a_{\alpha,\beta} z^\alpha \bar{z}^\beta$$

where the coefficients $a_{\alpha,\beta}$ are given by the formula (15) , we get:

$$\begin{aligned} A_3 = & -i\frac{1}{2\sqrt{2}.3!}\left[\frac{\partial^3 W(0)}{\partial x_1^3}\left(-\frac{1}{3}z_1^3 - 3z_1^2\bar{z}_1 + 3z_1\bar{z}_1^2 + \frac{1}{3}\bar{z}_1^3\right)\right] \\ & + \frac{\partial^3 W(0)}{\partial x_2^3}\left(-\frac{1}{9}z_2^3 - z_2^2\bar{z}_2 + z_2\bar{z}_2^2 + \frac{1}{9}\bar{z}_2^3\right)\Big] \\ & +3\frac{\partial^3 W(0)}{\partial x_1^2\partial x_2}\left(-\frac{1}{5}z_1^2 z_2 + z_1^2\bar{z}_2 - \bar{z}_1^2 z_2 + \frac{1}{5}\bar{z}_1^2\bar{z}_2 - \frac{2}{3}z_1 z_2\bar{z}_1 + \frac{2}{3}z_1\bar{z}_1\bar{z}_2\right) \\ & + 3\frac{\partial^3 W(0)}{\partial x_1\partial x_2^2}\left(-\frac{1}{7}z_2^2 z_1 - \frac{1}{5}z_2^2\bar{z}_1 + \frac{1}{5}\bar{z}_2^2 z_1 + \frac{1}{7}\bar{z}_2^2\bar{z}_1 - 2z_2 z_1\bar{z}_2 + 2z_2\bar{z}_2\bar{z}_1\right)\Big] \end{aligned}$$

By the same way as in the 1 : 1 resonance, a long straightforward calculation by hand and via **Lemma 5**, we arrive to gather all terms of $\frac{i}{2\hbar}[A_3, W_3]_W$, that are in K_4, and we obtain:

$$\begin{aligned} & -\frac{1}{2}\left(\frac{1}{3!2\sqrt{2}}\right)^2 \left[\left\{60\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)^2 + \frac{684}{15}\left(\frac{\partial^3 W(0)}{\partial x_1^2\partial x_2}\right)^2\right\}|z_1|^4\right. \\ & + \left\{20\left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)^2 + \frac{2484}{35}\left(\frac{\partial^3 W(0)}{\partial x_2^2\partial x_1}\right)^2\right\}|z_2|^4 \\ & + \left\{72\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)\left(\left(\frac{\partial^3 W(0)}{\partial x_1^2\partial x_2}\right) + \left(\frac{\partial^3 W(0)}{\partial x_2^2\partial x_1}\right)\right)\right. \\ & +24\left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)\left(\left(\frac{\partial^3 W(0)}{\partial x_1^2\partial x_2}\right) + \left(\frac{\partial^3 W(0)}{\partial x_2^2\partial x_1}\right)\right) \\ & \left. +\frac{864}{35}\left(\frac{\partial^3 W(0)}{\partial x_2^2\partial x_1}\right)^2 - \frac{288}{5}\left(\frac{\partial^3 W(0)}{\partial x_1^2\partial x_2}\right)^2\right\}|z_1|^2|z_2|^2 \\ & \left. + \left\{\frac{432}{5}\left(\frac{\partial^3 W(0)}{\partial x_1^2\partial x_2}\right)\left(\frac{\partial^3 W(0)}{\partial x_1\partial x_2^2}\right) - 24\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_1^2\partial x_2}\right)\right\}\operatorname{Re}\left(z_1^2\bar{z}_2^2\right)\right] \\ & + \left[\frac{1}{72}\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)^2 + \frac{1}{216}\left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)^2\right]\hbar^2 \end{aligned}$$

Now, for the calculation of all monomials of W_4 that should belong in K_4, we remark from (28) that only the monomials x_1^4, x_2^4, $x_1^2 x_2^2$ and $x_1^3 x_2$ in $W_4(x_1, x_2)$ may contribute to K_4.
The calculation of coefficients of $|z_1|^4$, $|z_2|^4$ and $|z_1|^2|z_2|^2$ is already do in the $1:1$ resonance.
What remains us to calculate, that is the one of $\mathrm{Re}(z_1^3\overline{z}_2)$.
If we let $x_j = \frac{1}{\sqrt{2}}(z_j + \bar{z}_j)$, then:

$$x_1^3 x_2 = \frac{1}{4}(z_1^3 z_2 + \underbrace{z_1^3\overline{z}_2}_{\text{in } K_4} + 3z_1^2\overline{z}_1 z_2 + 3z_1^2\overline{z}_1\overline{z}_2 + 3z_1\overline{z}_1^2 z_2 + 3z_1\overline{z}_1^2\overline{z}_2 + \underbrace{\overline{z}_1^3 z_2}_{\text{in } K_4} + \overline{z}_1^3\overline{z}_2)$$

therefore, the coefficient of $\mathrm{Re}(z_1^3\overline{z}_2)$ is exactly:

$$\frac{1}{24}\frac{\partial^4 W(0)}{\partial x_1^3 \partial x_2}$$

finally we gather all terms that are in K_4, and we obtain the coefficients we were looking for:

Theorem 8 *The quantum Birkhoff-Gustavson normal form of the Schrödinger hamiltonian in* $1:3$ *resonance* $H_2 + W$ *is equal to* $H_2 + K_4 + \mathcal{O}_5$ *with*

$$K_4 = \gamma_1 |z_1|^4 + \gamma_2 |z_2|^4 + \gamma_3 |z_1|^2 |z_2|^2 + \gamma_4 \mathrm{Re}\left(z_1^3\overline{z}_2\right) + \gamma_5 \hbar^2$$

where

$$\gamma_1 = \frac{1}{16}\frac{\partial^4 W(0)}{\partial x_1^4} - \frac{1}{2}\left(\frac{1}{3!2\sqrt{2}}\right)^2 \left\{60\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)^2 + \frac{684}{15}\left(\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2}\right)^2\right\}$$

$$\gamma_2 = \frac{1}{16}\frac{\partial^4 W(0)}{\partial x_2^4} - \frac{1}{2}\left(\frac{1}{3!2\sqrt{2}}\right)^2 \left\{20\left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)^2 + \frac{2484}{35}\left(\frac{\partial^3 W(0)}{\partial x_2^2 \partial x_1}\right)^2\right\}$$

$$\begin{aligned}\gamma_3 = {} & \frac{1}{12}\frac{\partial^4 W(0)}{\partial x_1^2 \partial x_2^2} - \frac{1}{2}\left(\frac{1}{3!2\sqrt{2}}\right)^2 \left\{72\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2} + \frac{\partial^3 W(0)}{\partial x_2^2 \partial x_1}\right)\right. \\ & +24\left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)\left(\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2} + \frac{\partial^3 W(0)}{\partial x_2^2 \partial x_1}\right) \\ & \left. + \frac{864}{35}\left(\frac{\partial^3 W(0)}{\partial x_2^2 \partial x_1}\right)^2 - \frac{288}{5}\left(\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2}\right)^2\right\}\end{aligned}$$

$$\gamma_4 = \frac{1}{24}\frac{\partial^4 W(0)}{\partial x_1^3 \partial x_2} - \frac{1}{2}\left(\frac{1}{3!2\sqrt{2}}\right)^2 \left(\frac{\partial^3 W(0)}{\partial x_1^2 \partial x_2}\right)\left\{\frac{432}{5}\left(\frac{\partial^3 W(0)}{\partial x_1 \partial x_2^2}\right) - 24\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)\right\}$$

$$\gamma_5 = \frac{1}{72}\left(\frac{\partial^3 W(0)}{\partial x_1^3}\right)^2 + \frac{1}{216}\left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)^2$$

The Weyl quantization of $\mathrm{Re}\left(z_1^3\overline{z}_2\right)$ is

$$\widehat{\mathrm{Re}\left(z_1^3\overline{z}_2\right)} = x_1^3 x_2 - \hbar^4 \frac{\partial^3}{\partial x_1^3}\frac{\partial}{\partial x_2} - 3\hbar^2 x_1 \frac{\partial}{\partial x_1}\frac{\partial}{\partial x_2} - 3\hbar^2 x_1 \frac{\partial}{\partial x_2} \\ -3\hbar^2 x_1 x_2 \frac{\partial^2}{\partial x_1^2} - 3\hbar^2 x_2 \frac{\partial}{\partial x_1}$$

The Weyl quantization of the rest of K_4 is already calculated in 1:1 resonance.
Using the creation and annihilation operators we get,

$$\widehat{\mathrm{Re}\left(z_1^3\overline{z}_2\right)} = 2\hbar^2 \left(a_1^3(\hbar)\, b_2(\hbar) + b_1^3(\hbar)\, a_2(\hbar)\right)$$

So,

$$\begin{aligned}\hat{K}_4 = & \, 2\hbar^2\gamma_1 \left(a_1^2(\hbar)\, b_1^2(\hbar) + b_1^2(\hbar)\, a_1^2(\hbar) - 1\right) \\ & +2\hbar^2\gamma_2 \left(a_2^2(\hbar)\, b_2^2(\hbar)\, b_2^2(\hbar)\, a_2^2(\hbar) - 1\right) \\ & +2\hbar^2\gamma_3 \left(a_1(\hbar)\, b_1(\hbar)\, a_2(\hbar)\, b_2(\hbar)\right. \\ & \left. + b_1(\hbar)\, a_1(\hbar)\, b_2(\hbar)\, a_2(\hbar) - \frac{1}{2}\right) \\ & +2\hbar^2\gamma_4 \left(a_1^3(\hbar)\, b_2(\hbar) + b_1^3(\hbar)\, a_2(\hbar)\right) \\ & +\gamma_5\hbar^2 \end{aligned} \tag{29}$$

The Bargmann representation give us:

$$\begin{aligned}\widehat{K}_4^{\mathcal{B}} = & \, T_{\mathcal{B}}\left(\widehat{K}_4\right) T_{\mathcal{B}}^{-1} \\ = & \, 2\hbar^2\gamma_1 \left[\left(1 + 4z_1\frac{\partial}{\partial z_1} + 2z_1^2\frac{\partial^2}{\partial z_1^2}\right) + \gamma_2\left[1 + 4z_2\frac{\partial}{\partial z_2} + 2z_2^2\frac{\partial^2}{\partial z_2^2}\right]\right. \\ & \left. + \gamma_3\left(1 + z_1\frac{\partial}{\partial z_1} + z_2\frac{\partial}{\partial z_2} + 2z_1 z_2\frac{\partial^2}{\partial z_1\partial z_2}\right) + \gamma_4\left(z_2\frac{\partial^3}{\partial z_1^3} + z_1^3\frac{\partial}{\partial z_2}\right) + \frac{\gamma_5}{2}\right] \\ = & \, 2\hbar^2\left[2\gamma_1 z_1^2\frac{\partial^2}{\partial z_1^2} + 2\gamma_2 z_2^2\frac{\partial^2}{\partial z_2^2} + 2\gamma_3 z_1 z_2\frac{\partial^2}{\partial z_1\partial z_2} + \gamma_4\left(z_2\frac{\partial^3}{\partial z_1^3} + z_1^3\frac{\partial}{\partial z_2}\right)\right. \\ & \left. + (4\gamma_1 + \gamma_3)\, z_1\frac{\partial}{\partial z_1} + (4\gamma_2 + \gamma_3)\, z_2\frac{\partial}{\partial z_2} + \left(\gamma_1 + \gamma_2 + \gamma_3 + \frac{\gamma_5}{2}\right)\right] \end{aligned} \tag{30}$$

4 Spectrum in the 1:1, 1:2 and 1:3 resonances

4.1 Spectrum in the 1:1 resonance

In this section we analyse the spectrum of the restriction of $\hat{K}_4$ to the eigenspace of $\widehat{H}_2$ by computing the matrix elements $\hat{K}_4^{\mathcal{B}}(\varphi_\alpha)$.

First we have,

$$\begin{aligned}
\frac{\partial\varphi_{(\alpha_1,\alpha_2)}}{\partial z_1} &= \frac{\partial}{\partial z_1}\left(\frac{z_1^{\alpha_1}}{\sqrt{\alpha_1!}}\frac{z_2^{\alpha_2}}{\sqrt{\alpha_2!}}\right) = \alpha_1\frac{z_1^{\alpha_1-1}}{\sqrt{\alpha_1!}}\frac{z_2^{\alpha_2}}{\sqrt{\alpha_2!}}\\
&= \sqrt{\alpha_1}\frac{z_1^{\alpha_1-1}}{\sqrt{(\alpha_1-1)!}}\frac{z_2^{\alpha_2}}{\sqrt{\alpha_2!}} = \sqrt{\alpha_1}\varphi_{(\alpha_1-1,\alpha_2)}\\
\frac{\partial^2\varphi_{(\alpha_1,\alpha_2)}}{\partial z_1^2} &= \sqrt{\alpha_1}\sqrt{\alpha_1-1}\varphi_{(\alpha_1-2,\alpha_2)}\\
\frac{\partial\varphi_{(\alpha_1,\alpha_2)}}{\partial z_2} &= \sqrt{\alpha_2}\varphi_{(\alpha_1,\alpha_2-1)}\\
\frac{\partial^2\varphi_{(\alpha_1,\alpha_2)}}{\partial z_2^2} &= \sqrt{\alpha_2}\sqrt{\alpha_2-1}\varphi_{(\alpha_1,\alpha_2-2)}\\
\frac{\partial^2\varphi_{(\alpha_1,\alpha_2)}}{\partial z_1\partial z_2} &= \sqrt{\alpha_1}\sqrt{\alpha_2}\varphi_{(\alpha_1-1,\alpha_2-1)}
\end{aligned}$$

and

$$\begin{aligned}
z_1\varphi_{(\alpha_1,\alpha_2)} &= z_1\left(\frac{z_1^{\alpha_1}}{\sqrt{\alpha_1!}}\frac{z_2^{\alpha_2}}{\sqrt{\alpha_2!}}\right) = \frac{z_1^{\alpha_1+1}}{\sqrt{\alpha_1!}}\frac{z_2^{\alpha_2}}{\sqrt{\alpha_2!}}\\
&= \sqrt{\alpha_1+1}\frac{z_1^{\alpha_1+1}}{\sqrt{(\alpha_1+1)!}}\frac{z_2^{\alpha_2}}{\sqrt{\alpha_2!}} = \sqrt{\alpha_1+1}\varphi_{(\alpha_1+1,\alpha_2)}\\
z_1^2\varphi_{(\alpha_1,\alpha_2)} &= \sqrt{\alpha_1+2}\sqrt{\alpha_1+1}\varphi_{(\alpha_1+2,\alpha_2)}\\
z_2\varphi_{(\alpha_1,\alpha_2)} &= \sqrt{\alpha_2+1}\varphi_{(\alpha_1,\alpha_2+1)}\\
z_2^2\varphi_{(\alpha_1,\alpha_2)} &= \sqrt{\alpha_2+2}\sqrt{\alpha_2+1}\varphi_{(\alpha_1,\alpha_2+2)}\\
z_1z_2\varphi_{(\alpha_1,\alpha_2)} &= \sqrt{\alpha_1+1}\sqrt{\alpha_2+1}\varphi_{(\alpha_1+1,\alpha_2+1)}
\end{aligned}$$

Thus,

$$\begin{aligned}
\hat{K}_4^{\mathcal{B}}\varphi_{(\alpha_1,\alpha_2)} &= 2\hbar^2(2\lambda_1 z_1^2\frac{\partial^2\varphi_{(\alpha_1,\alpha_2)}}{\partial z_1^2} + 2\lambda_2 z_2^2\frac{\partial^2\varphi_{(\alpha_1,\alpha_2)}}{\partial z_2^2} + 2\lambda_3 z_1 z_2\frac{\partial^2\varphi_{(\alpha_1,\alpha_2)}}{\partial z_1\partial z_2}\\
&\quad +\lambda_4[z_2^2\frac{\partial^2\varphi_{(\alpha_1,\alpha_2)}}{\partial z_1^2} + z_1^2\frac{\partial^2\varphi_{(\alpha_1,\alpha_2)}}{\partial z_2^2}] + (4\lambda_1+\lambda_3)\, z_1\frac{\partial\varphi_{(\alpha_1,\alpha_2)}}{\partial z_1}\\
&\quad + (4\lambda_2+\lambda_3)\, z_2\frac{\partial\varphi_{(\alpha_1,\alpha_2)}}{\partial z_2} + \left(\lambda_1+\lambda_2+\lambda_3+\frac{\lambda_5}{2}\right)\varphi_{(\alpha_1,\alpha_2)})\\
&= 2\hbar^2(2\lambda_1 z_1^2\sqrt{\alpha_1(\alpha_1-1)}\varphi_{(\alpha_1-2,\alpha_2)} + 2\lambda_2 z_2^2\sqrt{\alpha_2(\alpha_2-1)}\varphi_{(\alpha_1,\alpha_2-2)}\\
&\quad +2\lambda_3 z_1 z_2\sqrt{\alpha_1\alpha_2}\varphi_{(\alpha_1-1,\alpha_2-1)} + \lambda_4(z_2^2\sqrt{\alpha_1(\alpha_1-1)}\varphi_{(\alpha_1-2,\alpha_2)}\\
&\quad +z_1^2\sqrt{\alpha_2(\alpha_2-1)}\varphi_{(\alpha_1,\alpha_2-2)}) + (4\lambda_1+\lambda_3)\, z_1\sqrt{\alpha_1}\varphi_{(\alpha_1-1,\alpha_2)}\\
&\quad + (4\lambda_2+\lambda_3)\, z_2\sqrt{\alpha_2}\varphi_{(\alpha_1,\alpha_2-1)} + \left(\lambda_1+\lambda_2+\lambda_3+\frac{\lambda_5}{2}\right)\varphi_{(\alpha_1,\alpha_2)})
\end{aligned}$$

$$
\begin{aligned}
&= 2\hbar^2 \left[2\lambda_1\alpha_1 (\alpha_1 - 1) \varphi_{(\alpha_1,\alpha_2)} + 2\lambda_2\alpha_2 (\alpha_2 - 1) \varphi_{(\alpha_1,\alpha_2)} + 2\lambda_3\alpha_1\alpha_2\varphi_{(\alpha_1,\alpha_2)} \right. \\
&\quad +\lambda_4 \left(\sqrt{\alpha_1(\alpha_1-1)(\alpha_2+1)(\alpha_2+2)}\varphi_{(\alpha_1-2,\alpha_2+2)} \right. \\
&\quad \left.\left. + \sqrt{(\alpha_1+1)(\alpha_1+2)\alpha_2(\alpha_2-1)}\varphi_{(\alpha_1+2,\alpha_2-2)}) \right) \right] \\
&\quad + (4\lambda_1 + \lambda_3)\, \alpha_1\varphi_{(\alpha_1,\alpha_2)} + (4\lambda_2 + \lambda_3)\, \alpha_2\varphi_{(\alpha_1,\alpha_2)} + \left(\lambda_1 + \lambda_2 + \lambda_3 + \frac{\lambda_5}{2} \right) \varphi_{(\alpha_1,\alpha_2)} \\
&= 2\hbar^2 \left\{ \lambda_4 \sqrt{\alpha_1(\alpha_1-1)(\alpha_2+1)(\alpha_2+2)}\varphi_{(\alpha_1-2,\alpha_2+2)} \right. \\
&\quad + [2\lambda_1\alpha_1 (\alpha_1 - 1) + 2\lambda_2\alpha_2 (\alpha_2 - 1) + 2\lambda_3\alpha_1\alpha_2 + (4\lambda_1 + \lambda_3)\, \alpha_1 \\
&\quad + (4\lambda_2 + \lambda_3)\, \alpha_2 + \left(\lambda_1 + \lambda_2 + \lambda_3 + \frac{\lambda_5}{2} \right) \Big] \varphi_{(\alpha_1,\alpha_2)} \\
&\quad \left. + \lambda_4 \sqrt{(\alpha_1+1)(\alpha_1+2)\alpha_2(\alpha_2-1)}\varphi_{(\alpha_1+2,\alpha_2-2)} \right\}
\end{aligned}
$$

We see that the basis $\mathcal{H}_N^{\mathcal{B}}$ is stable by $\hat{K}_4^{\mathcal{B}}$ because,

$$
\alpha_1 - 2 + (\alpha_2 + 2) = \alpha_1 + \alpha_2 = N \quad \text{and} \quad \alpha_1 + 2 + (\alpha_2 - 2) = \alpha_1 + \alpha_2 = N
$$

where $\mathcal{H}_N^{\mathcal{B}} = \left\{ \varphi_{(N-\ell,\ell)}\ ;\ \ell = 0, 1, ..., E\left[\frac{N}{2}\right] \right\}$.
One can verify easily that the matrix $\widehat{K}_4^{\mathcal{B}}$ in $\mathcal{H}_N^{\mathcal{B}}$ is symetric. Indeed,

$$
\begin{aligned}
\widehat{K}_4^{\mathcal{B}}\varphi_{(\alpha_1+2,\alpha_2-2)} = 4\hbar^2 [&\lambda_4 \sqrt{(\alpha_1+2)(\alpha_1+1)(\alpha_2-1)\alpha_2}\varphi_{(\alpha_1,\alpha_2)} + \\
&(2\lambda_1 (\alpha_1+2)(\alpha_1+1) + 2\lambda_2 (\alpha_2-2)(\alpha_2-3) \\
&+2\lambda_3 (\alpha_1+2)(\alpha_2-2) + (4\lambda_1+\lambda_3)(\alpha_1+2) \\
&+ (4\lambda_2+\lambda_3)(\alpha_2-2) + \left(\lambda_1 + \lambda_2 + \lambda_3 + \frac{\lambda_5}{2} \right))\varphi_{(\alpha_1+2,\alpha_2-2)} \\
&+\lambda_4 \sqrt{(\alpha_1+4)(\alpha_1+3)(\alpha_2-2)(\alpha_2-3)}\varphi_{(\alpha_1+4,\alpha_2-4)}]
\end{aligned}
$$

One gets,

$$
\begin{aligned}
\widehat{K}_4^{\mathcal{B}}\varphi_{(N-\ell,\ell)} = 4\hbar^2 \Big(&\lambda_4 \sqrt{(\ell+1)(\ell+2)(N-\ell)(N-\ell-1)}\varphi_{(N-\ell-2,\ell+2)} \\
&+(2\lambda_1 (N-\ell)(N-\ell-1) + 2\lambda_2\ell(\ell-1) + \lambda_3 (N-\ell)\,\ell \\
&+ (4\lambda_1+\lambda_3)(N-\ell) + (4\lambda_2+\lambda_3)\,\ell + \left(\lambda_1 + \lambda_2 + \lambda_3 + \frac{\lambda_5}{2} \right))\varphi_{(N-\ell,\ell)} \\
&+ \lambda_4 \sqrt{\ell(\ell-1)(N-\ell+1)(N-\ell+2)}\varphi_{(N-\ell+2,\ell-2)} \Big)
\end{aligned}
\tag{31}
$$

Thus,

Proposition 9 *The matrix of $\widehat{K}_4^{\mathcal{B}}$, in the basis $\mathcal{H}_N^{\mathcal{B}}$ is :*

$$2\hbar^2 \begin{pmatrix} d_{N,0} & A_{N,0} & & & \vdots & & \\ A_{N,0} & d_{N,1} & \ddots & & \vdots & \mathbf{0} & \\ \cdots & \ddots & \ddots & \ddots & \vdots & \cdots & \cdots \\ & & A_{N,\ell-1} & d_{N,\ell} & A_{N,\ell} & \ddots & \\ & \mathbf{0} & & A_{N,\ell} & d_{N,\ell+1} & \ddots & \ddots \\ & & & & \vdots & \ddots & \ddots \end{pmatrix} \tag{32}$$

where, for $\ell = 0, 1, ..., E\left[\frac{N}{2}\right]$:

$$\begin{cases} A_{N,\ell} = \lambda_4 \sqrt{(\ell+1)(\ell+2)(N-\ell)(N-\ell-1)} \\ d_{N,\ell} = 2\lambda_1 (N-\ell)(N-\ell-1) + 2\lambda_2 \ell (\ell-1) + 2\lambda_3 (N-\ell)\ell \\ + (4\lambda_1+\lambda_3)(N-\ell) + (4\lambda_2+\lambda_3)\ell + \left(\lambda_1+\lambda_2+\lambda_3+\frac{\lambda_5}{2}\right) \end{cases}$$

4.2 Spectrum in the 1:2 resonance

By computing $\hat{K}_3^{\mathcal{B}}(\varphi_\alpha)$, we get

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

we see that the basis $\mathcal{H}_N^{\mathcal{B}}$ is stable by $\widehat{K}_3^{\mathcal{B}}$ because,

$\alpha_1 - 2 + 2(\alpha_2+1) = \alpha_1 + 2\alpha_2 = N$ and $\alpha_1 + 2 + 2(\alpha_2 - 1) = \alpha_1 + 2\alpha_2 = N$

where $\mathcal{H}_N^{\mathcal{B}} = \left\{ \varphi_{(N-2\ell,\ell)} \; ; \; \ell = 0, 1, ..., E\left[\frac{N}{2}\right] \right\}$.
The matrix of $\widehat{K}_3^{\mathcal{B}}$ in $\mathcal{H}_N^{\mathcal{B}}$ is symetric, since

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

Thus,

$$\begin{aligned} \widehat{K}_3^{\mathcal{B}} \varphi_{(N-2\ell,\ell)} &= \sqrt{2}\mu\hbar^{\frac{3}{2}} \left(\sqrt{(\ell+1)(N-2\ell)(N-2\ell-1)}\varphi_{(N-2\ell-2,\ell+1)} \right. \\ &\quad \left. + \sqrt{(N-2\ell+2)(N-2\ell+1)\ell}\varphi_{(N-2\ell+2,\ell-1)} \right) \end{aligned} \tag{33}$$

Proposition 10 *The matrix of $\widehat{K}_3^{\mathcal{B}}$ in the basis $\mathcal{H}_N^{\mathcal{B}}$ is:*

$$\sqrt{2}\mu\hbar^{\frac{3}{2}}\begin{pmatrix} 0 & m_0 & & \vdots & & \\ m_0 & 0 & \ddots & \vdots & \mathbf{0} & \\ \cdots & \ddots & 0 & m_\ell \cdots & \cdots & \\ & & m_\ell & 0 & \ddots & \\ & \mathbf{0} & & \ddots & 0 & \ddots \\ & & & \vdots & \ddots & 0 \end{pmatrix} \tag{34}$$

where for $\ell = 0, 1, ..., E\left[\frac{N}{2}\right]$:

$$m_\ell = \sqrt{(\ell+1)(N-2\ell)(N-2\ell-1)}$$

In the case of Fermi resonance, the half integer powers of $\hbar$ are present, the coefficient of $\hbar^{3/2}$ is then the average along the flow of $\widehat{H}_2$ of the term of order 3 in the Taylor expansion of the symbol.

4.3 Spectrum in the 1:3 resonance

We have,

$$\frac{\partial^3\varphi_{(\alpha_1,\alpha_2)}}{\partial z_1^3} = \sqrt{\alpha_1}\sqrt{\alpha_1-1}\sqrt{\alpha_1-2}\varphi_{(\alpha_1-3,\alpha_2)}$$
$$z_1^3\varphi_{(\alpha_1,\alpha_2)} = \sqrt{\alpha_1+3}\sqrt{\alpha_1+2}\sqrt{\alpha_1+1}\varphi_{(\alpha_1+3,\alpha_2)}$$

then,

$$z_1^3\frac{\partial\varphi_{(\alpha_1,\alpha_2)}}{\partial z_2} + z_2\frac{\partial^3\varphi_{(\alpha_1,\alpha_2)}}{\partial z_1^3} = \sqrt{(\alpha_1+3)(\alpha_1+2)(\alpha_1+1)\alpha_2}\varphi_{(\alpha_1+3,\alpha_2-1)} + \sqrt{\alpha_1(\alpha_1-1)(\alpha_1-2)(\alpha_2+1)}\varphi_{(\alpha_1-3,\alpha_2+1)}$$

Therefore,

$$\begin{aligned}\widehat{K}_4^{\mathcal{B}}\varphi_{(\alpha_1,\alpha_2)} = 2\hbar^2 \Big(&\gamma_4\sqrt{\alpha_1(\alpha_1-1)(\alpha_1-2)(\alpha_2+1)}\varphi_{(\alpha_1-3,\alpha_2+1)} \\ &+(2\gamma_1\alpha_1(\alpha_1-1)+2\gamma_2\alpha_2(\alpha_2-1)+2\gamma_3\alpha_1\alpha_2+(4\gamma_1+\gamma_3)\alpha_1 \\ &+(4\gamma_2+\gamma_3)\alpha_2+\left(\gamma_1+\gamma_2+\gamma_3+\frac{\gamma_5}{2}\right))\varphi_{(\alpha_1,\alpha_2)} \\ &+\gamma_4\sqrt{(\alpha_1+3)(\alpha_1+2)(\alpha_1+1)\alpha_2}\varphi_{(\alpha_1+3,\alpha_2-1)}\Big)\end{aligned}$$

The basis $\mathcal{H}_N^{\mathcal{B}} = \left\{\varphi_{(N-3\ell,\ell)}\ ;\ \ell = 0, 1, ..., E\left[\frac{N}{2}\right]\right\}$ is stable by $\widehat{K}_4^{\mathcal{B}}$ because,

$\alpha_1+3+3(\alpha_2-1) = \alpha_1+3\alpha_2 = N$ and $\alpha_1-3+3(\alpha_2+1) = \alpha_1+3\alpha_2 = N$

and the matrix of $\widehat{K}_4^{\mathcal{B}}$ in $\mathcal{H}_N^{\mathcal{B}}$ is symetric since

$$\begin{aligned}
\widehat{K}_4^{\mathcal{B}}\varphi_{(\alpha_1+3,\alpha_2-1)} = 2\hbar^2 \Big[& \gamma_4\sqrt{(\alpha_1+3)(\alpha_1+2)(\alpha_1+1)\alpha_2}\varphi_{(\alpha_1,\alpha_2)} \\
& + (2\gamma_1(\alpha_1+3)(\alpha_1+2) + 2\gamma_2(\alpha_2-1)(\alpha_2-2) + 2\gamma_3(\alpha_1+3)(\alpha_2-1) \\
& + (4\gamma_1+\gamma_3)(\alpha_1+3) + (4\gamma_2+\gamma_3)(\alpha_2-1) \\
& + \left(\gamma_1+\gamma_2+\gamma_3+\frac{\gamma_5}{2}\right)\Big]\varphi_{(\alpha_1+3,\alpha_2-1)} \\
& + \gamma_4\sqrt{(\alpha_1+6)(\alpha_1+5)(\alpha_1+4)(\alpha_2-1)}\varphi_{(\alpha_1+6,\alpha_2-2)}\Big]
\end{aligned}$$

So one gets,

$$\begin{aligned}
\widehat{K}_4^{\mathcal{B}}\varphi_{(N-3\ell,\ell)} = 2\hbar^2 \Big(& \gamma_4\sqrt{(\ell+1)(N-3\ell)(N-3\ell-1)(N-3\ell-2)}\varphi_{(N-3\ell-3,\ell+1)} \\
& + [2\gamma_1(N-3\ell)(N-3\ell-1) + 2\gamma_2\ell(\ell-1) + 2\gamma_3\ell(N-3\ell) \\
& + (4\gamma_1+\gamma_3)(N-3\ell) + (4\gamma_2+\gamma_3)\ell + \left(\gamma_1+\gamma_2+\gamma_3+\frac{\gamma_5}{2}\right)]\varphi_{(N-3\ell,\ell)} \\
& + \gamma_4\sqrt{\ell(N-3\ell+1)(N-3\ell+2)(N-3\ell+3)}\varphi_{(N-3\ell+3,\ell-1)}\Big)
\end{aligned} \tag{35}$$

and therefore,

Proposition 11 *The matrix of $\widehat{K}_4^{\mathcal{B}}$ in the basis $\mathcal{H}_N^{\mathcal{B}}$ is :*

$$2\hbar^2 \begin{pmatrix}
d'_{N,0} & B_{N,0} & & & \vdots & & \\
B_{N,0} & d'_{N,1} & \ddots & \ddots & \vdots & \mathbf{0} & \\
\cdots & \ddots & \ddots & B_{N,\ell-1} & & \cdots & \cdots \\
& & \ddots & d'_{N,\ell} & B_{N,\ell} & \ddots & \\
& \mathbf{0} & & B_{N,\ell} & d'_{N,\ell+1} & \ddots & \ddots \\
& & & & \vdots & \ddots & \ddots
\end{pmatrix} \tag{36}$$

where for $\ell = 0, 1, ..., E\left[\frac{N}{2}\right]$:

$$\begin{cases}
B_{N,\ell} = \gamma_4\sqrt{(\ell+1)(N-3\ell)(N-3\ell-1)(N-3\ell-2)} \\
d'_{N,\ell} = (2\gamma_1(N-3\ell)^2 + 2\gamma_2\ell^2 + 2\gamma_3\ell(N-3\ell) \\
+ (3\gamma_1+\gamma_3)(N-3\ell) + (3\gamma_2+\gamma_3)\ell + \left(\gamma_1+\gamma_2+\gamma_3+\frac{\gamma_5}{2}\right))
\end{cases}$$

5 An effective Quantum BGNF program

We have implemented the Quantum Birkhoff-Gustavson normal form in the computer language `ocaml`(2), which is a fast and very expressive functional language, particularly well adapted to mathematical constructions.

(2)`http://caml.inria.fr/index.en.html`

5.1 Overview of the code

The code consists of three modules : Math, Weyl and Birkhoff. The Math module is a functorial interface that defines the axioms of general (non-commutative) associative algebras over an abelian field. This permits the use of the same code for different coefficient rings: real numbers, complex numbers, rationals, or even formal series. For instance, we may declare that we use complex coefficients using the simple line :

```
open Math.ComplexNumbers;;
```

The Weyl module implements the Weyl algebra for formal series $\mathcal{E}$ — defined in Section 2, endowed with the non-commutative Moyal product. Internally, series are stored in hash tables, and the module provides a way to convert them to/from a text representation. The number of variables is arbitrary, it need not be specified. For instance the 1 : 2-oscillator

$$\mathtt{h2} = \frac{1}{2}(x_1^2 + \xi_1^2) + (x_2^2 + \xi_2^2)$$

will be printed as follows:

```
Weyl.print_poly h2;;
1 h^0 x^() ξ^(0,2)
1 h^0 x^(0,2) ξ^()
0.5 h^0 x^() ξ^(2)
0.5 h^0 x^(2) ξ^()
```

For convenience, we also wrote a Maple module that can use copy-pasted text directly to/from Maple notation :

```
Maple.of_poly h2;;
- : string = "0.5*x[1]^2+0.5*xi[1]^2+1*x[2]^2+1*xi[2]^2"
```

As a simple example, the code below computes the Moyal bracket of x^3 and ξ^3 — which is the Weyl symbol of the operator bracket $\frac{i}{\hbar}[x^3, (\frac{\hbar}{i}\frac{\partial}{\partial x})^3]$.

```
let x3 = Maple.to_poly "x[1]^3" in
let xi3 = Maple.to_poly "xi[1]^3" in
let c = Weyl.crochet x3 xi3 in
Maple.of_poly c;;
- : string = "1.5*h^2+-9*x[1]^2*xi[1]^2"
```

Thus we find $\frac{i}{\hbar}[x^3, \xi^3]_W = \frac{3}{2}\hbar^2 - 9x^2\xi^2$.

The Birkhoff module is the core of the normal form algorithm. It implements the proof of Theorem 1 that appears in [5]. It involves an induction where each step consists in solving a cohomological equation. Only Moyal brackets, additions, and multiplication by scalar are used. Here is the code for the induction step :

```
let birkhoff_step order freq k r =
  let n = ordre r in
  let (rn, _) = get_homog r n in
  let (kn, an) = split freq rn in
  let newh = exp_ad an (add k r) order
  and k' = add k kn
  in let r' = add newh (coeff_mult C.mone k') in
    proj_order ~check:true r' (n+1);
    (k', r')
```

If h=k+r, where h is the initial quantum Hamiltonian (or Weyl symbol), k is the normalisation at order n-1 and r is the remainder (of order n, then the function birkhoff_step computes the next-order normalization : h=k'+r', where r' is of order n+1.

For simplicity, we have assumed in this code that the quadratic hamiltonian is of the form $H_2 = \nu_1 x'_1\xi'_1 + \cdots + \nu_n x'_n\xi'_n$: this amounts to writing H_2 in terms of creation and annihilation operators as in (6). In order to deal with harmonic oscillators in real variables (x_j, ξ_j) as in (2), we need to use the change of variables $x'_j = \frac{1}{\sqrt{2}}(x_j + i\xi_j)$, $\xi'_j = \frac{1}{\sqrt{2}}(x_j - i\xi_j)$. We have implemented this change of variables in the code.

5.2 Numerical results for the $1:3$ resonance

We may define H_2 using Maple notation as follows :

```
let h2 = Maple.to_poly "0.5*x[1]^2+0.5*xi[1]^2+1.5*x[2]^2+1.5*xi[2]^2";;
```

Then we convert it to complex coordinates :

```
let h2z = coordz h2;;
Maple.of_poly h2z;;
- : string = "1*x[1]^1*xi[1]^1+3*x[2]^1*xi[2]^1"
```

It has now the required form $H_2 = x'_1\xi'_1 + 3x'_2\xi'_2$. We add now a simple perturbation $W = (x_2)^3$, which we convert to complex coordinates :

```
let w = Maple.to_poly "x[2]^3";;
let wz = coordz w;;
Maple.of_poly vz;;
```

```
- : string =
"1.06066*x[2]^1*xi[2]^2+0.353553*x[2]^3+
1.06066*x[2]^2*xi[2]^1+0.353553*xi[2]^3"
```

Thus we have, in complex coordinates (x'_j, ξ'_j) :

$$W = \frac{17}{16} x'_2 {\xi'_2}^2 + \frac{6}{17} {x'_2}^3 + \frac{17}{16} {x'_2}^2 \xi'_2 + \frac{6}{17} {\xi'_2}^3.$$

and finally we may consider the hamiltonian $H = H_2 + W$:

```
let hz = Weyl.add h2z vz;;
```

Now we define the frequency vector $[1; 3]$, and we may apply the Birkhoff procedure at order 4 :

```
let freq = [| one; of_int 3 |];;
let kz = birkhoff freq hz 4;;
```

We have obtained the normalized Hamiltonian `kz`. We convert it back to real coordinates (x_j, ξ_j) and print it :

```
let k = coordx kz;;
Maple.of_poly k;;
- : string =
"0.5*x[1]^2+0.5*xi[1]^2+0.166667*h^2+-0.625*x[2]^2*xi[2]^2+-0.3125*x[2]^4+
-0.3125*xi[2]^4+1.5*x[2]^2+1.5*xi[2]^2"
```

Reordering terms, we get

$$K = \frac{1}{2}x_1^2 + \frac{1}{2}\xi_1^2 + \frac{3}{2}x_2^2 + \frac{3}{2}\xi_2^2 + \frac{1}{6}\hbar^2 - \frac{5}{8}x_2^2\xi_2^2 - \frac{5}{16}x_2^4 - \frac{5}{16}\xi_2^4 + \mathcal{O}_6 = H_2 + K_4 + \mathcal{O}_6$$

where $K_4 = \frac{1}{6}\hbar^2 - \frac{5}{8}x_2^2\xi_2^2 - \frac{5}{16}x_2^4 - \frac{5}{16}\xi_2^4 = \frac{1}{6}\hbar^2 - \frac{5}{16}(x_2^2 + \xi_2^2)^2$.

It remains to compare to the theoretical results of section 3.5 (Theorem 8), which predicts:

$$K_4 = \gamma_1 |z_1|^4 + \gamma_2 |z_2|^4 + \gamma_3 |z_1|^2 |z_2|^2 + \gamma_4 \operatorname{Re}\left(z_1^3 \overline{z}_2\right) + \gamma_5 \hbar^2$$

Using that $W(x_1, x_2) = x_2^3$, we see from the formulas in Theorem 8 that only the coefficients γ_2 and γ_5 don't vanish; we obtain:

$$\begin{aligned}
K_4 &= \gamma_2 \left|z_2\right|^4 + \gamma_5 \hbar^2 \\
&= -\frac{1}{2}\left(\frac{1}{3!2\sqrt{2}}\right)^2 20\left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)^2 \frac{1}{4}\left(x_2^4+\xi_2^4+2x_2^2\xi_2^2\right) \\
&\quad +\frac{1}{216}\left(\frac{\partial^3 W(0)}{\partial x_2^3}\right)^2 \hbar^2 \\
&= -\frac{1}{2}\left(\frac{1}{3!2\sqrt{2}}\right)^2 20.36.\frac{1}{4}\left(x_2^4+\xi_2^4+2x_2^2\xi_2^2\right)+\frac{1}{216}.36.\hbar^2 \\
&= -\frac{5}{16}\left(x_2^4+\xi_2^4+2x_2^2\xi_2^2\right)+\frac{1}{6}\hbar^2
\end{aligned}$$

hence,

$$H_2+K_4=\frac{1}{2}x_1^2+\frac{1}{2}\xi_1^2+\frac{3}{2}x_2^2+\frac{3}{2}\xi_2^2-\frac{5}{16}x_2^4-\frac{5}{16}\xi_2^4-\frac{5}{8}x_2^2\xi_2^2+\frac{1}{6}\hbar^2,$$

which confirms the computer output.

Of course, we can ask the program to give the normalization at any given order. For instance here is what we get at order 8 :

$$\begin{gathered}
K=\frac{1}{2}\xi_1^2+\frac{3}{2}\xi_2^2+\frac{1}{2}x_1^2+\frac{3}{2}x_2^2 \\
-\frac{5}{16}\xi_2^4+\frac{1}{6}\hbar^2-\frac{5}{8}x_2^2\xi_2^2-\frac{5}{16}x_2^4 \\
-\frac{235}{1152}\xi_2^6+\frac{395}{576}\hbar^2\xi_2^2-\frac{235}{384}x_2^2\xi_2^4-\frac{235}{384}x_2^4\xi_2^2-\frac{235}{1152}x_2^6+\frac{395}{576}\hbar^2x_2^2 \\
-\frac{38585}{165888}\xi_2^8+\frac{100205}{41472}\hbar^2\xi_2^4-\frac{128}{243}\hbar^4-\frac{38585}{41472}x_2^2\xi_2^6-\frac{38585}{27648}x_2^4\xi_2^4-\frac{38585}{41472}x_2^6\xi_2^2 \\
-\frac{38585}{165888}x_2^8+\frac{100205}{20736}\hbar^2x_2^2\xi_2^2+\frac{100205}{41472}\hbar^2x_2^4+\mathcal{O}_{10}
\end{gathered}$$

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