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Semiclassical Birkhoff-Gustavson normal forms and spectral asymptotics for nearly resonant Schrödinger operators

Abdelkader BOUREBAI* Kaoutar GHOMARI† San VŨ NGỌC ‡

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Abstract

The concept of near resonances for harmonic approximations of semiclassical Schrödinger operators is introduced and explored. Combined with a natural extension of the Birkhoff-Gustavson normal form, we obtain formulas for approaching the discrete spectrum of such operators which are both accurate and easy to implement. We apply the theory to the physically important case of the near Fermi (*i.e.* $1 : 2$) resonance, for which we propose explicit expressions and numerical computations.

1 Introduction and motivation

We are interested in the description of the discrete spectrum of a semiclassical Schrödinger operator \hat{P}_ε

$$\hat{P}_\varepsilon(\hbar) := -\frac{\hbar^2}{2}\Delta + V_\varepsilon(x), \quad (1)$$

where V_ε is a smooth confining potential on \mathbb{R}^n depending smoothly on a small parameter $\varepsilon \in \mathbb{R}$, and $\hbar > 0$ is a small parameter.

More precisely, by “confining potential” we mean that there exist some real value $E_\infty > 0$ and a small $\varepsilon_0 > 0$ such that for all $E < E_\infty$, the

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region $\bigcup_{|\varepsilon| \leq \varepsilon_0} V_\varepsilon^{-1}((-\infty, E))$ is bounded in \mathbb{R}^n . Moreover, we also assume that V_ε grows at most polynomially at infinity, in the sense of the usual pseudo-differential symbol classes, uniformly with respect to ε :

$$\begin{aligned} \exists m, \forall N \in \mathbb{N}, \exists C_N, \forall |\varepsilon| \leq \varepsilon_0, \forall \alpha \in \mathbb{N}^n \text{ s.t. } |\alpha| \leq N, \\ \forall x \in \mathbb{R}^n \quad |\partial^\alpha V_\varepsilon(x)| \leq C_N (1 + \|x\|^2)^{m/2}. \end{aligned}$$

This ensures that \hat{P}_ε has discrete spectrum in $(-\infty, E)$.

Let $E_{0,\varepsilon} = \min V_\varepsilon$. We will assume that this minimum is reached at a unique point and is non-degenerate; hence when studying the spectrum of P_ε near $E_{0,\varepsilon}$, it is natural to consider the harmonic approximation of P_ε . As we will see in Section 2, up to an error of order $\mathcal{O}(\varepsilon^\infty)$, we may assume that this approximation is smooth in ε . Let us first consider $\varepsilon = 0$. In the harmonic approximation of P_0 , which is the quantization of a quadratic Hamiltonian of the form

$$H_2(x, \xi) = \sum_{j=1}^n \frac{\omega_j}{2} (x_j^2 + \xi_j^2),$$

two extreme cases may occur. Either the frequencies $(\omega_1, \dots, \omega_n)$ are independent over \mathbb{Q} (this is the *non-resonant case*), or they are, up to some common multiple, all integers. Of course intermediate cases may happen, see Definition 3.4. In the first case, a well-known result of Birkhoff [2] (following Poincaré) states that the full symbol H of P_0 , which is a perturbation of H_2 , is formally completely integrable: there are canonical coordinates (x, ξ) and a smooth map f such that

$$H(x, \xi) = f(I_1, \dots, I_n) + \mathcal{O}(x, \xi)^\infty, \quad (2)$$

where I_j is the action given by

$$I_j := \frac{1}{2} (x_j^2 + \xi_j^2).$$

Although the Birkhoff idea was soon used by physicists to deal with quantum Hamiltonians, a rigorous proof of the quantum validity of the Birkhoff normal form, in the semiclassical limit, is much more recent, see [19]. This non-resonant case is stable under perturbations of order $\mathcal{O}(\varepsilon)$ if the quadratic term H_2 is invariant, in the sense that one can write a combined Birkhoff normal form in all variables (x, ξ, ε) (and then a semiclassical Birkhoff normal form in $(x, \xi, \varepsilon, \hbar)$ will hold). If one adds diophantine conditions on the frequencies ω_j , so that they become badly approximated by rationals, then it is expected that one can accommodate perturbations of the quadratic

term, and even strengthen the result by using KAM stability, similarly to the case of diophantine tori in [11]. See also [16].

In this paper, we focus on the resonant case, where the situation is quite different. For simplicity, we will always consider the fully resonant case, where all frequencies are integers, up to a common multiple. There is an extension of the Birkhoff normal form for the resonant case, which was worked out by Gustavson [9, 7] (although the general scheme was already known to Poincaré — see also Moser’s paper [17]), where it was shown that, in addition to the completely integrable normal form (2), another formal series of *resonant terms* has to be considered, which makes the resulting series much more difficult to analyze (it will be, generically, non-integrable, see [6]). The full semiclassical analysis of resonant harmonic approximations of general pseudodifferential operators was carried out in [3].

When it comes to ε perturbations, possibly affecting the harmonic term H_2 , one may argue that resonant case is not generic: for most perturbations of a resonant Hamiltonian H_0 , the perturbed Hamiltonian H_ε will be non-resonant. Thus, it is tempting to claim that, in most physical situations, one can restrict oneself to the set of non-resonant ε and thus stick to the completely integrable normal form (2). However, this normal form is in general not convergent [15], and, as $\varepsilon \rightarrow 0$, it is expected that the famous appearance of *small denominators* will make it more and more divergent, hindering the effectiveness of the approximation (unless the full Hamiltonian is known to be integrable and analytic, see [21]).

This phenomenon of near resonances has been recognized as crucial in molecular spectroscopy. Thus, for the study of the dynamics of highly excited vibrational states, Joyeux shows in his article [13] that the resonant Birkhoff-Gustavson procedure can yield more accurate results than the standard Birkhoff procedure, even when the Hamiltonian is *not* resonant. He considers the HCP molecule, called phosphatine, where the calculation of the fundamental frequencies leads to $\omega_1 \approx 1256$ (C-P stretch), $\omega_2 \approx 650$ (bend), and $\omega_3 \approx 3479\text{cm}^{-1}$ (C-H stretch). The Hamiltonian obtained by the non-resonant Birkhoff normal form (also called the Dunham expansion) is the formal series

$$H_D = \sum_i \omega_i I_i + \sum_{i \leq j} x_{ij} I_i J_j + \sum_{i \leq j \leq k} y_{ijk} I_i J_j I_k + \dots$$

Joyeux computed levels of HCP up to 22000cm^{-1} above the bottom of the well by truncating the series at various orders, and compared the results to the exact quantum levels of HCP relative to the ground state. Using ℓ^1 , ℓ^2 and ℓ^∞ norms to estimate the discrepancy with respect to the exact quantum

computation, he observed a rapid divergence, see [13, Table 1], which limits the interest of this Hamiltonian to at most 4th or 5th order, which is not satisfactory. The article therefore concludes that the Dunham expansion is very far from being sufficient for whatever quantitative purpose.

Given that the relation between both fundamental frequencies ω_1 and ω_2 , namely $\omega_1 - 2\omega_2 \approx -44\text{cm}^{-1}$ is a *near resonance* relation, Joyeux proposed, as a next step, to take this resonance into account in the formal expansion, and to compare once again the results of the calculations of the energy levels of the HCP molecule. For this, he considered the following Hamiltonian:

$$H = H_D + \sum_{m \geq 1} H_F^{(m)},$$

$$H_F^{(m)} = 2I_1^{\frac{m}{2}} I_2^m \cos(m\varphi_1 - 2m\varphi_2) \times \left(k^{(m)} + \sum_i k_i^{(m)} I_i + \sum_{i \leq j} k_{ij}^{(m)} I_i I_j + \dots \right),$$

which he calls the Fermi resonance Hamiltonian (in Physics or Chemistry literature, the 2 : 1 resonance is traditionally called the Fermi resonance, see Section 3.2). The terms in H_F are precisely those given by the Birkhoff-Gustavson procedure in case of an exact 2 : 1 resonance. It is then noticed that the results of the computations of energy levels are much more accurate with this modified Hamiltonian.

From this study comes the motivation and main goal of our work, which is a description of the spectrum of semiclassical Schrödinger operators $\hat{P}_\varepsilon(\hbar)$ given in (1), for which the harmonic frequencies are close to resonance. For this purpose, we build on the paper [3] which gives precise semiclassical asymptotics for an exact, full resonance, by restricting the Hamiltonian to the eigenspaces of the resonant harmonic oscillator (whose dimensions tend to infinity in the semiclassical limit). Our main results are organized as follows:

In Section 2, we consider the first step of this work, which consists in transforming the initial Schrödinger Hamiltonian \hat{P}_ε into a perturbation of the harmonic oscillator (Proposition 3.1). For this, we need a diagonalization result of symmetric real matrices depending smoothly on small parameter ε (Theorem 2.1).

Section 3 has a double goal. On the one hand, we prove in Theorem 3.3 that the Birkhoff-Gustavson normal form (BGNF) theorem can be extended to handle Schrödinger operators \hat{P}_ε depending on the parameter ε (where the harmonic frequencies also depend on the parameter ε); on the other hand,

we give an explicit construction of the BGNF in the near Fermi resonance, in Theorems 3.5 and 3.6.

In Section 4, we give the exact matrix representation of the “polyads” generated by the first non-trivial Birkhoff correction of the Fermi resonance, *i.e.* the restriction of the quantum BGNF to the various eigenspaces of the resonant harmonic oscillator (Theorem 4.2).

Finally, in Section 5, we show how the theoretical study can lead to numerical schemes, and we propose, in the case of the Fermi resonance, a detailed numerical illustration of our results, by comparing the “exact” quantum spectrum of \hat{P}_ε with the eigenvalues obtained via the ε -Birkhoff-Gustavson procedure, at order 3.

2 Preparation: smooth diagonalization

In order to obtain the harmonic approximation of the Schrödinger operator (1), we need to diagonalize the Hessian of V_ε at the critical point, in a smooth way. Because our aim is to deal with resonant eigenvalues, we cannot assume that eigenvalues are simple, and we will use the following general result, which is elementary but apparently not often found in the literature (we could not locate a reference).

Theorem 2.1 *Let $A(\varepsilon)$ be a family of $n \times n$ real symmetric, respectively hermitian, matrices depending in a smooth (ie. C^∞) way on a small parameter ε . Then there exists a smooth family of orthogonal, respectively unitary, matrices $U(\varepsilon)$ and smooth functions $\varepsilon \mapsto \lambda_{j,\varepsilon} \in \mathbb{R}$, $j = 1, \dots, n$ such that*

$$U^{-1}(\varepsilon)A(\varepsilon)U(\varepsilon) = \text{diag}(\lambda_{1,\varepsilon}, \dots, \lambda_{n,\varepsilon}) + \mathcal{O}(\varepsilon^\infty).$$

Remark 2.2 This result means that, if we accept to replace the true eigenvalues by approximate eigenvalues which are close to the exact one to any order in ε , then we may smoothly diagonalize the family $A(\varepsilon)$. What may come as a surprise when one first encounters this kind of result is that, in general, it is *not* possible to smoothly diagonalize a smooth family of symmetric matrices in an exact way (unless all eigenvalues are simple). See for instance Example 5.3, section II-5 of the Kato book [14]. On the other hand, positive results are available when the family is analytic, or if one only requires C^1 regularity for the eigenvalues, a result due to Rellich [18], see also [14, Theorem 6.8 Section II-6]. \triangle

Proof. Let us treat the real symmetric case; the Hermitian case will be completely analogous. We reason by induction on the size of the matrix.

The result obviously holds when $n = 1$ (without the $\mathcal{O}(\varepsilon^\infty)$ error term). We may assume that $A(0)$ is diagonal; let $\mu_1 < \dots < \mu_\ell$ be its eigenvalues, with multiplicities d_1, \dots, d_ℓ . By the min-max formula, the eigenvalues of $A(\varepsilon)$ are continuous in ε . Thus, there exists $\rho > 0$ such that the spectrum of $A(\varepsilon)$ is contained in $\bigcup_{j=1}^\ell B(\mu_j, \rho)$, and each ball $B_j := B(\mu_j, \rho)$ contains d_j eigenvalues (counted with multiplicity). This shows that the spectral projector on the generalized eigenspaces,

$$P_{B_j}(\varepsilon) := -\frac{1}{2\pi i} \int_{\partial B_j} (A(\varepsilon) - z)^{-1} dz,$$

is C^∞ in ε . It is now easy to find an orthonormal basis of the generalized eigenspace $E_j(\varepsilon) := P_{B_j}(\mathbb{R}^n)$ that depends smoothly on ε . For instance, one can take a basis $\mathcal{B}(0)$ of $E_j(0)$; for ε small enough, the projection $P_{B_j}(\varepsilon)(\mathcal{B}(0))$ is a basis of $E_j(\varepsilon)$, which we may smoothly orthonormalize by the Gram-Schmidt algorithm. In this way we obtain a smooth bloc-diagonal decomposition: there exists a smooth unitary matrix $V(\varepsilon)$ such that

$$V^{-1}(\varepsilon)A(\varepsilon)V(\varepsilon) = \begin{pmatrix} A_1(\varepsilon) & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & A_\ell(\varepsilon) \end{pmatrix}.$$

where $A_j(\varepsilon) = \mu_j I + \mathcal{O}(\varepsilon)$ is a real symmetric matrix. If $\ell > 1$ we obtain the result by induction. Hence it only remains to consider the case of a unique generalized eigenspace of dimension n : we have

$$A(\varepsilon) = \mu_1 I + \mathcal{O}(\varepsilon).$$

Because the remainder $\mathcal{O}(\varepsilon)$ is smooth, we can write it as $\varepsilon B_1(\varepsilon)$, where $B_1(\varepsilon)$ is smooth (and real symmetric). Therefore the question is reduced to diagonalizing $B_1(\varepsilon)$, and we may repeat the procedure. There are finally only two possibilities:

1. Either there exists $N > 0$ such that, after the N -th iteration, the remainder $B_N(0)$ possesses more than one generalized eigenspace. Then we may split them and obtain the result as above;
2. or for all $N > 0$, $B_N(0)$ has only one generalized eigenspace.

In the second case, we have real constants $c_0 = \mu_1, c_1, c_2, \dots$ such that, for any $N \geq 0$,

$$A(\varepsilon) = c_0 I + c_1 \varepsilon I + \dots + c_N \varepsilon^N I + \mathcal{O}(\varepsilon^{N+1}).$$

By the Borel Lemma, there exists a C^∞ function $\lambda(\varepsilon)$ whose Taylor series at $\varepsilon = 0$ is

$$\lambda(\varepsilon) \sim c_0 + c_1\varepsilon + c_2\varepsilon^2 + \cdots + c_N\varepsilon^N + \dots$$

which means $\forall N, A(\varepsilon) - \lambda(\varepsilon)I = \mathcal{O}(\varepsilon^N)$. Thus, $A(\varepsilon) = \lambda(\varepsilon)I + \mathcal{O}(\varepsilon^\infty)$, which gives the result. \square

3 Birkhoff-Gustavson normal form in near resonance

In this section, we shall discuss the Birkhoff normal form procedure for Schrödinger operators \hat{P}_ε which depend on small parameters $\hbar > 0$ and ε , and we will then apply the general ideas to the near Fermi resonance.

3.1 ε -Birkhoff-Gustavson normal form theorem

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

$$\hat{P}_\varepsilon = -\frac{\hbar^2}{2}\Delta_x + V_\varepsilon(x),$$

where $\Delta = \Delta_x$ is the n dimensional Laplacian and V_ε is a smooth real potential depending smoothly on ε . We wish to perform a local (and microlocal) analysis near the origin $x = 0$. To this effect, we assume that for $\varepsilon = 0$, the potential V_0 has a non-degenerate minimum at the origin:

$$V_0(0) = 0, V_0'(0) = 0, V_0''(0) > 0.$$

Using the implicit function theorem to $F(\varepsilon, x) = V_\varepsilon'(x)$, we obtain a smooth map $\varepsilon \mapsto x_\varepsilon$ near the origin such that $x_0 = 0$ and $V_\varepsilon'(x_\varepsilon) = 0$, for $\varepsilon > 0$ small enough. So, there exists $\varepsilon_0 > 0$ such that for all $|\varepsilon| \leq \varepsilon_0$, the point x_ε is a non-degenerate minimum for V_ε . Using the translation $x \mapsto \tilde{x} = x - x_\varepsilon$, which yields a unitary map τ_ε on $L^2(\mathbb{R}^n)$, given by $\tau_\varepsilon f(\tilde{x}) = f(\tilde{x} + x_\varepsilon)$, \hat{P}_ε is transformed into

$$\tau_\varepsilon \hat{P}_\varepsilon \tau_\varepsilon^{-1} = -\frac{\hbar^2}{2}\Delta_{\tilde{x}} + W_\varepsilon(\tilde{x}),$$

where $W_\varepsilon(\tilde{x}) = V_\varepsilon(\tilde{x} + x_\varepsilon)$. We have

$$W_\varepsilon(0) = V_\varepsilon(x_\varepsilon), \quad W_\varepsilon'(0) = V_\varepsilon'(x_\varepsilon) = 0,$$

and the symmetric matrix $W_\varepsilon''(0)$ is positive definite, for $\varepsilon > 0$ sufficiently small.

Using theorem 2.1, we can smoothly diagonalize $W_\varepsilon''(0)$ modulo $\mathcal{O}(\varepsilon^\infty)$, via a change of variables $y = U_\varepsilon^* \tilde{x}$, with $U_\varepsilon \in O(n)$. Let $(\omega_{1,\varepsilon}^2, \dots, \omega_{n,\varepsilon}^2)$ be

its approximate eigenvalues: they are positive and depend in a C^∞ way on ε .

The change of variables U_ε induces a unitary map g_ε on $L^2(\mathbb{R}^n)$ given by $g_\varepsilon f(y) = f(U_\varepsilon y)$. Since U_ε is orthogonal, $g_\varepsilon \Delta_{\tilde{x}} g_\varepsilon^{-1} = \Delta_y$ and hence the transformed operator is

$$g_\varepsilon \tau_\varepsilon \hat{P}_\varepsilon \tau_\varepsilon^{-1} g_\varepsilon^{-1} = -\frac{\hbar^2}{2} \Delta_y + W_\varepsilon(U_\varepsilon y),$$

Since $W_\varepsilon(\tilde{x}) = \frac{1}{2} \langle W_\varepsilon''(0) \tilde{x}, \tilde{x} \rangle + \mathcal{O}(\tilde{x}^3)$, we obtain

$$W_\varepsilon(U_\varepsilon y) = W_\varepsilon(0) + \frac{1}{2} \sum_{j=1}^n \omega_{j,\varepsilon}^2 y_j^2 + \mathcal{O}(\varepsilon^\infty \|y\|^2) + \mathcal{O}(y^3). \quad (3)$$

The rescaling $y_j \mapsto \tilde{y}_j := \sqrt{\omega_{j,\varepsilon}} y_j$, giving rise to the unitary map $\Lambda_\varepsilon : f \mapsto (\tilde{y} \mapsto \frac{1}{(\omega_{1,\varepsilon} \dots \omega_{n,\varepsilon})^{n/2}} f(\frac{\tilde{y}_1}{\sqrt{\omega_{1,\varepsilon}}}, \dots, \frac{\tilde{y}_n}{\sqrt{\omega_{n,\varepsilon}}}))$ transforms \hat{P}_ε into a perturbation of the harmonic oscillator $\hat{H}_{2,\varepsilon}$:

$$\Lambda_\varepsilon g_\varepsilon \tau_\varepsilon \hat{P}_\varepsilon \tau_\varepsilon^{-1} g_\varepsilon^{-1} \Lambda_\varepsilon^{-1} = W_\varepsilon(0) + \hat{H}_{2,\varepsilon} + R_\varepsilon(\tilde{y}), \quad (4)$$

where,

$$\hat{H}_{2,\varepsilon} = \sum_{j=1}^n \frac{\omega_{j,\varepsilon}}{2} \left(-\hbar^2 \frac{\partial^2}{\partial \tilde{y}_j^2} + \tilde{y}_j^2 \right) + \mathcal{O}(\varepsilon^\infty \|\tilde{y}\|^2),$$

and $R_\varepsilon(\tilde{y})$ is a smooth function of order $\mathcal{O}(\tilde{y}^3)$ at the origin, uniformly with respect to ε .

From now on, to simplify notation, we switch back to x , and assume that

$$\hat{P}_\varepsilon = W_\varepsilon(0) + \hat{H}_{2,\varepsilon} + R_\varepsilon(x),$$

with

$$\hat{H}_{2,\varepsilon} = \sum_{j=1}^n \frac{\omega_{j,\varepsilon}}{2} \left(-\hbar^2 \frac{\partial^2}{\partial x_j^2} + x_j^2 \right) + \mathcal{O}(\varepsilon^\infty \|x^2\|).$$

Let

$$\hat{H}_{2,0} = \sum_{j=1}^n \frac{\omega_{j,0}}{2} \left(-\hbar^2 \frac{\partial^2}{\partial x_j^2} + x_j^2 \right),$$

The eigenvalues $\omega_{j,\varepsilon}$ being smooth in ε , we have

$$\omega_{j,\varepsilon} = \omega_{j,0} + \varepsilon \omega_{j,1} + \varepsilon^2 \tilde{\omega}_{j,2}(\varepsilon).$$

Therefore,

$$\hat{P}_\varepsilon = W_\varepsilon(0) + \hat{H}_{2,0} + \varepsilon \hat{L}_2 + \varepsilon^2 \hat{M}_{2,\varepsilon} + R_\varepsilon(x) + \mathcal{O}(\varepsilon^\infty \|x^2\|),$$

where

$$\hat{L}_2 = \sum_{j=1}^n \frac{\omega_{j,1}}{2} \left(-\hbar^2 \frac{\partial^2}{\partial x_j^2} + x_j^2 \right) \text{ and } \hat{M}_{2,\varepsilon} = \sum_{j=1}^n \frac{\tilde{\omega}_{j,2}(\varepsilon)}{2} \left(-\hbar^2 \frac{\partial^2}{\partial x_j^2} + x_j^2 \right), \quad (5)$$

Because the symbol of \hat{L}_2 is quadratic, it cannot be reduced by the usual Birkhoff-Gustavson procedure; in order to deal with this issue, we have to add ε to the set of formal variables, so that $\varepsilon \hat{L}_2$ becomes of order 3.

Thus, we introduce the space

$$\mathcal{E} = \mathbb{C}[[x, \xi, \varepsilon, \hbar]] = \mathbb{C}[[x_1, \dots, x_n, \xi_1, \dots, \xi_n, \varepsilon, \hbar]],$$

of formal power series of $(2n+2)$ variables with complex coefficients, where the degree of the monomial $x^\alpha \xi^\beta \varepsilon^m \hbar^\ell$ is defined to be $|\alpha| + |\beta| + m + 2\ell$, $\alpha, \beta \in \mathbb{N}^n, \ell, m \in \mathbb{N}$. 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, then $(\mathcal{O}_N)_{N \in \mathbb{N}}$ is a filtration:

$$\mathcal{E} \supset \mathcal{O}_0 \supset \mathcal{O}_1 \supset \dots, \quad \bigcap_N \mathcal{O}_N = \{0\}.$$

This filtration will be used for all formal convergences in this section. We shall also need to discuss the degree in (x, ξ, \hbar) only; to this aim, we denote by $\mathcal{O}_N(x, \xi, \hbar)$ the subspace of \mathcal{E} spanned by monomials $x^\alpha \xi^\beta \varepsilon^m \hbar^\ell$ such that $|\alpha| + |\beta| + 2\ell \geq N$.

Let $d, m \in \mathbb{R}$, the symbol class $S^d(m)$ is the set of the smooth functions $a_\varepsilon(\cdot, \hbar) : \mathbb{R}^{2n} \times]0, 1] \rightarrow \mathbb{C}$ such that, for all $\alpha \in \mathbb{N}^n$,

$$|\partial_{(x,y)}^\alpha a_\varepsilon(x, \xi, \hbar)| \leq C_\alpha \hbar^d (1 + |x|^2 + |\xi|^2)^{\frac{m}{2}}$$

for some constant $C_\alpha > 0$, uniformly in $\hbar \in (0, \hbar_0]$ and $\varepsilon \in [-\varepsilon_0, \varepsilon_0]$, where \hbar_0 and ε_0 are small enough. $S^d(m)$ is called the space of symbols of order d and degree m .

For $a_\varepsilon \in S^d(m)$ and $u \in C_0^\infty(\mathbb{R}^{2n})$, the Weyl quantization of a_ε acting on u is given by the oscillatory integral

$$(Op_\hbar^W(a_\varepsilon)u)(x) = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} e^{\frac{i}{\hbar}\langle x-y, \xi \rangle} a_\varepsilon\left(\frac{x+y}{2}, \xi, \hbar\right) u(y) |dy d\xi|.$$

In general, $Op_h^W(a_\varepsilon)$ is an unbounded linear operator on $L^2(\mathbb{R}^n)$, and a_ε is called its Weyl symbol. For example, the Weyl symbol of the harmonic oscillator $\hat{H}_{2,0}$ is the polynomial

$$H_{2,0} = \sum_{j=1}^n \frac{\omega_{j,0}}{2} (\xi_j^2 + x_j^2), \quad (6)$$

and the Weyl symbol of the operator of multiplication by a function $f(x)$ is the function f itself or, more precisely, the function $(x, \xi) \mapsto f(x)$.

In this article, we use the Weyl bracket $[f, g]_W$ defined on \mathcal{E} by the formal Taylor series of the Weyl symbol of the commutator

$$Op_h^W \tilde{f} \circ Op_h^W \tilde{g} - Op_h^W \tilde{g} \circ Op_h^W \tilde{f},$$

where \tilde{f} and \tilde{g} are smooth symbols whose formal Taylor series is equal to f and g , respectively. From now on, when $f = f(x, \xi, \varepsilon, \hbar)$ is a smooth function, we shall allow us to write $f \in \mathcal{E}$ to signify that its Taylor series at the origin belongs to \mathcal{E} .

The filtration \mathcal{E} has a nice behaviour with respect to the Weyl bracket: if $N_1 + N_2 \geq 2$, then, $\hbar^{-1}[\mathcal{O}_{N_1}, \mathcal{O}_{N_2}]_W \subset \mathcal{O}_{N_1+N_2-2}$.

The Weyl symbol $H_{2,\varepsilon}$ of $\hat{H}_{2,\varepsilon}$ is:

$$\begin{aligned} H_{2,\varepsilon} &= H_{2,0} + \varepsilon L_2 + \varepsilon^2 M_{2,\varepsilon} + \mathcal{O}(\varepsilon^\infty \|x\|^2) \\ &= \sum_{j=1}^n \frac{\omega_{j,0}}{2} (\xi_j^2 + x_j^2) + \varepsilon \sum_{j=1}^n \frac{\omega_{j,1}}{2} (\xi_j^2 + x_j^2) + \varepsilon^2 M_{2,\varepsilon} + \mathcal{O}(\varepsilon^\infty \|x\|^2), \end{aligned} \quad (7)$$

with

$$L_2 = \sum_{j=1}^n \frac{\omega_{j,1}}{2} (\xi_j^2 + x_j^2),$$

where $M_{2,\varepsilon}$ is the Weyl symbol of $\hat{M}_{2,\varepsilon}$ and L_2 is the Weyl symbol of \hat{L}_2 .

To summarize, we have proven the following.

Proposition 3.1 *Let \hat{P}_ε be the Schrodinger operator defined in (1). Then there exists an explicit unitary operator U_ε on $L^2(\mathbb{R}^n)$ ($U_\varepsilon = \Lambda_\varepsilon g_\varepsilon \tau_\varepsilon$ is composed of a translation, a unitary transform, and a scaling, all in the position variable x) such that the differential operator $U_\varepsilon \hat{P}_\varepsilon U_\varepsilon^*$ has the following Weyl symbol:*

$$\begin{aligned} \sigma_W(U_\varepsilon \hat{P}_\varepsilon U_\varepsilon^*) &= \min_{\mathbb{R}^n} V_\varepsilon + H_{2,0} + \varepsilon L_2 + L'_\varepsilon, \\ &= \min_{\mathbb{R}^n} V_\varepsilon + H_{2,0} + L_\varepsilon, \end{aligned}$$

where $H_{2,0}$ and L_2 are defined in (7), $L_2 \in \mathcal{D}_2$, $L'_\varepsilon = \varepsilon^2 M_{2,\varepsilon} + R_\varepsilon(x) + \mathcal{O}(\varepsilon^\infty \|x\|^2) \in \mathcal{O}_3$, $L_\varepsilon = \varepsilon L_2 + L'_\varepsilon \in \mathcal{O}_3$, $M_{2,\varepsilon}$ is the Weyl symbol of $\hat{M}_{2,\varepsilon}$ defined in (5), and $R_\varepsilon(x)$ is a smooth function of order $\mathcal{O}(x^3)$ at the origin, uniformly with respect to ε .

Let $A \in \mathcal{E}$, we define the adjoint operator $\text{ad}_A(P) := [A, P]_W$, $P \in \mathcal{E}$. The crucial properties of $\text{ad}_{H_{2,0}}$ are given in the next proposition, for more details see [3].

Proposition 3.2 1. Let $\omega_0 = (\omega_{1,0}, \dots, \omega_{n,0})$, and let $z_j = x_j + i\xi_j$; then $\text{ad}_{H_{2,0}}$ is diagonal on the family $\{z^\alpha \bar{z}^\beta, z \in \mathbb{C}^n, \alpha, \beta \in \mathbb{N}^n\}$ of $\mathbb{C}[[z, \bar{z}]] = \mathbb{C}[[x, \xi]]$ and

$$\text{ad}_{H_{2,0}}(z^\alpha \bar{z}^\beta) = \hbar \langle \beta - \alpha, \omega_0 \rangle z^\alpha \bar{z}^\beta.$$

2. We have

$$\mathcal{D}_N = \ker(\hbar^{-1} \text{ad}_{H_{2,0}}) \oplus \text{Im}(\hbar^{-1} \text{ad}_{H_{2,0}}). \quad (8)$$

We are now ready to state the formal ε -Birkhoff-Gustavson normal form, which is a natural extension of the usual Birkhoff-Gustavson case. Note that we prove here the result for a general perturbation $L_\varepsilon \in \mathcal{O}_3$, which does not need to be equal to the particular form obtained above when one reduces a Schrödinger operator.

Theorem 3.3 Let $H_{2,0}$ be as in (6), and let $L_\varepsilon \in \mathcal{O}_3$, then there exist $A_\varepsilon \in \mathcal{O}_3$ and $K_\varepsilon \in \mathcal{O}_3$ such that,

$$\begin{aligned} e^{i\hbar^{-1} \text{ad}_{A_\varepsilon}}(H_{2,0} + L_\varepsilon) &= H_{2,0} + K_\varepsilon, \\ [H_{2,0}, K_\varepsilon]_W &= 0. \end{aligned} \quad (9)$$

Moreover, the following properties hold.

1. K_ε is unique, and A_ε is unique modulo $\ker \text{ad}_{H_{2,0}}$.
2. if $H_{2,0}$ and L_ε have real coefficients (i.e. belong to $\mathbb{R}[[x, \xi, \varepsilon, \hbar]]$) then $K_\varepsilon \in \mathbb{R}[[x, \xi, \varepsilon, \hbar]]$, and A_ε can be chosen to have real coefficients as well.
3. If $L_\varepsilon \in \varepsilon^m \mathbb{C}[[x, \xi, \varepsilon, \hbar]]$, for some $m \in \mathbb{N}$, then $K_\varepsilon \in \varepsilon^m \mathbb{C}[[x, \xi, \varepsilon, \hbar]]$ as well.
4. If $L_\varepsilon \in \hbar^\ell \mathbb{C}[[x, \xi, \varepsilon, \hbar]]$, for some $\ell \in \mathbb{N}$, then $K_\varepsilon \in \hbar^\ell \mathbb{C}[[x, \xi, \varepsilon, \hbar]]$ as well.

5. If $L_\varepsilon \in \mathcal{O}_N(x, \xi, \hbar)$ for some $N \geq 0$, then $K_\varepsilon \in \mathcal{O}_N(x, \xi, \hbar)$ as well.

Notice that the sum :

$$e^{i\hbar^{-1}\text{ad}_{A_\varepsilon}}(H_{2,0} + L_\varepsilon) = \sum_{\ell=0}^{\infty} \frac{1}{\ell!} \left(\frac{i}{\hbar} \text{ad}_{A_\varepsilon} \right)^\ell (H_{2,0} + L_\varepsilon),$$

is usually not convergent in the analytic sense, even if P_ε is analytic, but it is always convergent in the formal topology of \mathcal{E} , because the map $B \mapsto \frac{i}{\hbar} \text{ad}_A(B) = \frac{i}{\hbar} [A, B]_W$ sends \mathcal{O}_N into \mathcal{O}_{N+1} .

Proof of the Theorem. We construct A_ε and K_ε inductively, by successive approximations with respect to the filtration \mathcal{E} .

Let $N \geq 1$, we suppose that there exists $A_{N,\varepsilon} \in \mathcal{O}_3$ and $K_{N,\varepsilon} \in \mathcal{O}_3$ such:

$$e^{i\hbar^{-1}\text{ad}_{A_{N,\varepsilon}}}(H_{2,0} + L_\varepsilon) = H_{2,0} + K_{3,\varepsilon} + \cdots + K_{N+1,\varepsilon} + R_{N+2,\varepsilon} + \mathcal{O}_{N+3} \quad (10)$$

where $K_{j,\varepsilon} \in \mathcal{D}_j$ commutes with $H_{2,0}$ and $R_{N+2,\varepsilon} \in \mathcal{D}_{N+2}$. We look for $A'_\varepsilon \in \mathcal{D}_{N+2}$, and $K_{N+2,\varepsilon} \in \mathcal{D}_{N+2}$ that commutes with $H_{2,0}$, such that :

$$e^{i\hbar^{-1}\text{ad}_{A_{N,\varepsilon} + A'_\varepsilon}}(H_{2,0} + L_\varepsilon) = H_{2,0} + K_{3,\varepsilon} + \cdots + K_{N+1,\varepsilon} + K_{N+2,\varepsilon} + \mathcal{O}_{N+3}.$$

This is equivalent to

$$R_{N+2,\varepsilon} - \frac{i}{\hbar} [H_{2,0}, A'_\varepsilon]_W = K_{N+2,\varepsilon}.$$

Since $H_{2,0}$ satisfies (8), we have $R_{N+2,\varepsilon} = R'_{N+2,\varepsilon} + \frac{i}{\hbar} [H_{2,0}, R''_{N+2,\varepsilon}]_W$, where $R'_{N+2,\varepsilon} \in \mathcal{D}_{N+2}$ commutes with $H_{2,0}$ (and is unique) and $R''_{N+2,\varepsilon} \in \mathcal{D}_{N+2}$, unique modulo $\ker \text{ad}_{H_{2,0}}$. Thus, we must (and can) choose $K_{N+2,\varepsilon} = R'_{N+2,\varepsilon}$ and, we may choose $A'_\varepsilon = R''_{N+2,\varepsilon}$. This shows that (10) holds at order $N+1$, proving (9), and the first property.

The second property follows from Moyal's formula

$$i[f, g]_W(x, \xi, \hbar) = 2 \sin\left(\frac{\hbar}{2} \square\right) (f(x_1, \xi_1, \hbar) g(x_2, \xi_2, \hbar)) \Big|_{\substack{x=x_1=x_2, \\ \xi=\xi_1=\xi_2}}$$

where

$$\square = \sum_{j=1}^n \partial_{\xi_1^j} \partial_{x_2^j} - \partial_{x_1^j} \partial_{\xi_2^j}.$$

Properties 3 and 4 are due to the fact that ε and \hbar are central elements in \mathcal{E} (they commute with everything). The last properties holds because $\text{ad}_{H_{2,0}}$ preserves the (x, ξ, \hbar) -order. \square

3.2 Normalizing the near Fermi resonance

A vector of n frequencies $(\omega_1, \dots, \omega_n)$ is called *resonant* if the coefficients $\omega_1, \dots, \omega_n$ are linearly dependent over the rationals.

In the extreme case where the rank of these coefficients over \mathbb{Q} is one, the frequencies $(\omega_1, \dots, \omega_n)$ are called *completely resonant*, and there exist co-prime integers p_1, \dots, p_n and $\lambda \in \mathbb{R}$ such that $\omega_j = p_j \lambda$. In this case, we say that $(\omega_1, \dots, \omega_n)$ (or the harmonic oscillator $\sum_{j=1}^n \frac{\omega_j}{2} (-\hbar^2 \frac{\partial^2}{\partial x_j^2} + x_j^2)$) exhibits a $p_1 : \dots : p_n$ resonance.

More generally, if there exist an integer $r \in \{1, \dots, n\}$, a number $\lambda \in \mathbb{R}$, and co-prime integers p_{j_1}, \dots, p_{j_r} such that $\omega_{j_i} = p_{j_i} \lambda$, then we say that $(\omega_1, \dots, \omega_n)$ exhibits a $p_{j_1} : \dots : p_{j_r}$ resonance.

In this paper, we are interested in *near resonances*, which we define as follows.

Definition 3.4 Let $\omega_\varepsilon = (\omega_{1,\varepsilon}, \dots, \omega_{n,\varepsilon})$ be the frequencies of the harmonic oscillator $\hat{H}_{2,\varepsilon}$. One says that ω_ε admits a near resonance of type $p_{j_1} \approx \dots \approx p_{j_r}$ if the map $\varepsilon \rightarrow \omega_\varepsilon$ is C^∞ and ω_0 admits a resonance of type $p_{j_1} : \dots : p_{j_r}$.

For example, we say that there is a near resonance relation of the form $p \approx q$, where $p, q \in \mathbb{N}^*$, if there exist $j_0, k_0 \in \{1, \dots, n\}$ such that $q\omega_{j_0,0} = p\omega_{k_0,0}$.

This concept of near resonance was introduced in molecular spectroscopy, where such a phenomenon is extremely common among small molecules, see [13].

In order to better understand the non-quadratic terms $K_{j,\varepsilon}$ obtained in Theorem 3.3 from the Hamiltonian \hat{P}_ε in near resonance, we suggest in this paper to study the typical case of the near Fermi resonance in dimension 2, denoted by $1 \approx 2$ (i.e. $\omega_{2,0} = 2\omega_{1,0}$), and we will give an explicit computation of the first non trivial term of the ε -Birkhoff normal form. Physically, the near Fermi resonance is known to affect the spectroscopy of many molecules, among which we find famous ones such as carbon dioxide CO_2 and carbon disulfide CS_2 , see [12]. The physics or chemical literature on Fermi resonance is enormous; interestingly, in a very recent work, the $1 \approx 2$ resonance of the CO_2 molecule was demonstrated to have a direct effect on global warming [20]. From the point of view of classical mechanics, the Fermi resonance and its bifurcations have been extensively studied, see for instance [5, 10] and references therein.

Consider on $L^2(\mathbb{R}^2)$ the semiclassical Schrödinger operator which is transformed according to Proposition 3.1 into a perturbation of the harmonic

oscillator $\hat{H}_{2,0}$, which we denote by $\hat{P}_\varepsilon(\hbar)$ again:

$$\hat{P}_\varepsilon(\hbar) = W_\varepsilon(0) + \hat{H}_{2,0} + \varepsilon \hat{L}_2 + \varepsilon^2 \hat{M}_{2,\varepsilon} + R_\varepsilon(x) + \mathcal{O}(\varepsilon^\infty \|x\|^2),$$

where

$$\begin{aligned} \hat{H}_{2,0} &= \frac{\omega_{1,0}}{2} \left(-\hbar^2 \frac{\partial^2}{\partial x_1^2} + x_1^2 \right) + \frac{\omega_{2,0}}{2} \left(-\hbar^2 \frac{\partial^2}{\partial x_2^2} + x_2^2 \right), \\ \hat{L}_2 &= \frac{\omega_{1,1}}{2} \left(-\hbar^2 \frac{\partial^2}{\partial x_1^2} + x_1^2 \right) + \frac{\omega_{2,1}}{2} \left(-\hbar^2 \frac{\partial^2}{\partial x_2^2} + x_2^2 \right), \\ \hat{M}_{2,\varepsilon} &= \frac{\tilde{\omega}_{1,2}(\varepsilon)}{2} \left(-\hbar^2 \frac{\partial^2}{\partial x_1^2} + x_1^2 \right) + \frac{\tilde{\omega}_{2,2}(\varepsilon)}{2} \left(-\hbar^2 \frac{\partial^2}{\partial x_2^2} + x_2^2 \right), \end{aligned}$$

and $R_\varepsilon(x) = \mathcal{O}(x^3)$ at the origin. The associated symbol is

$$P_\varepsilon = W_\varepsilon(0) + H_{2,0} + \varepsilon L_2 + L'_\varepsilon,$$

where for $z_j = x_j + i\xi_j, j = 1, 2$,

$$\begin{aligned} H_{2,0} &= \frac{1}{2} (\omega_{1,0}|z_1|^2 + \omega_{2,0}|z_2|^2), & L_2 &= \frac{1}{2} (\omega_{1,1}|z_1|^2 + \omega_{2,1}|z_2|^2), \\ L'_\varepsilon &= \varepsilon^2 M_{2,\varepsilon} + R_\varepsilon(x) + \mathcal{O}(\varepsilon^\infty), \text{ and } & M_{2,\varepsilon} &= \frac{1}{2} (\tilde{\omega}_{1,2}(\varepsilon)|z_1|^2 + \tilde{\omega}_{2,2}(\varepsilon)|z_2|^2). \end{aligned}$$

We now consider the associated Taylor series (which we denote by the same symbols). Thus, $L'_\varepsilon \in \mathcal{O}_3$, and notice that $\varepsilon L_2 \in \mathcal{D}_3$ and commutes with $H_{2,0}$. By applying Theorem 3.3, there exist $A_{1,\varepsilon} \in \mathcal{O}_3$ and $K_{3,\varepsilon} \in \mathcal{D}_3$ such that $K_{3,\varepsilon} \in \mathcal{O}_2(x, \xi, \hbar)$ and

$$e^{i\hbar^{-1} \text{ad}_{A_{1,\varepsilon}}} (H_{2,0} + \varepsilon L_2 + L'_\varepsilon) = H_{2,0} + K_{3,\varepsilon} + \mathcal{O}_4,$$

hence

$$\varepsilon L_2 + L'_\varepsilon + \frac{i}{\hbar} [A_{1,\varepsilon}, H_{2,0} + \varepsilon L_2 + L'_\varepsilon]_W - K_{3,\varepsilon} \in \mathcal{O}_4.$$

Let us write the expansion

$$R_\varepsilon(x) = R_0(x) + \varepsilon R_1(x) + \varepsilon^2 R_2(x) + \dots,$$

where $R_j(x) = \mathcal{O}(x^3)$, and we can write $R_0(x) = R_{3,0} + \mathcal{O}(x^4)$ with $R_{3,0} \in \mathcal{D}_3$. Since $\varepsilon^2 M_{2,\varepsilon} \in \mathcal{O}_4$, we have $L'_\varepsilon = R_{3,0} + \mathcal{O}(4)$. We obtain:

$$\varepsilon L_2 + R_{3,0} = \frac{i}{\hbar} [H_{2,0}, A_{1,\varepsilon}]_W + K_{3,\varepsilon} + \mathcal{O}_4.$$

Since $R_{3,0} \in \mathcal{D}_3 = \ker(i\hbar^{-1}\text{ad}_{H_{2,0}}) \oplus \text{Im}(i\hbar^{-1}\text{ad}_{H_{2,0}})$, we can write

$$R_{3,0} = \tilde{R}_{3,0} + \frac{i}{\hbar} \left[H_{2,0}, \tilde{\tilde{R}}_{3,0} \right]_W, \quad (11)$$

where $\tilde{R}_{3,0} \in \mathcal{D}_3$ and commutes with $H_{2,0}$, and $\tilde{\tilde{R}}_{3,0} \in \mathcal{D}_3$. Consequently,

$$K_{3,\varepsilon} = \varepsilon L_2 + \tilde{R}_{3,0}.$$

Notice that, because $H_{2,0}$ is quadratic, Equation (11) is equivalent to $R_{3,0} = \tilde{R}_{3,0} + \{H_{2,0}, \tilde{\tilde{R}}_{3,0}\}$; therefore, $\tilde{R}_{3,0}$ does not depend on \hbar nor ε . Hence, in order to make the condition that $\tilde{R}_{3,0}$ commutes with $H_{2,0}$ explicit, we may use the known results from the classical normal form, see for instance [5]. Let us recall the arguments. By Proposition 3.2, we have

$$\tilde{R}_{3,0} = \sum_{\substack{|\alpha|+|\beta|=3 \\ \langle \omega_0, \beta-\alpha \rangle=0}} c_{\alpha\beta}^{(3)} z^\alpha \bar{z}^\beta.$$

According to the definition 3.4, a near Fermi resonance for $\omega_\varepsilon = (\omega_{1,\varepsilon}, \omega_{2,\varepsilon})$ means an exact Fermi resonance for $\omega_0 = (\omega_{1,0}, \omega_{2,0})$, that is:

$$\omega_{2,0} = 2\omega_{1,0}.$$

Therefore,

$$\langle \omega_0, \beta - \alpha \rangle = 0 \Leftrightarrow (\alpha_1 + 2\alpha_2) = (\beta_1 + 2\beta_2), \quad (12)$$

where $\alpha = (\alpha_1, \alpha_2) \in \mathbb{N}^2$ and $\beta = (\beta_1, \beta_2) \in \mathbb{N}^2$. Now, to obtain $\tilde{R}_{3,0}$, it is necessary to look for all monomials of order 3 that satisfy the Fermi resonance relation (12). Thus, $\tilde{R}_{3,0}$ is generated by the monomials $\bar{z}_1^2 z_2, z_1^2 \bar{z}_2$. Since $\tilde{R}_{3,0}$ is real,

$$\begin{aligned} \tilde{R}_{3,0} &= \mu \text{Re}(z_1^2 \bar{z}_2) + \nu \text{Im}(z_1^2 \bar{z}_2) \\ &= \frac{\mu}{2} (\bar{z}_1^2 z_2 + z_1^2 \bar{z}_2) + \frac{\nu}{2i} (\bar{z}_1^2 z_2 - z_1^2 \bar{z}_2), \quad \mu, \nu \in \mathbb{R}. \end{aligned}$$

Determination of the coefficients μ and ν : We Taylor expand $R_{3,0}$ at the origin:

$$\begin{aligned} R_{3,0}(x_1, x_2) &= \frac{1}{3!} \left[\frac{\partial^3 R_{3,0}(0)}{\partial x_1^3} x_1^3 + 3 \frac{\partial^3 R_{3,0}(0)}{\partial x_1^2 \partial x_2} x_1^2 x_2 \right. \\ &\quad \left. + 3 \frac{\partial^3 R_{3,0}(0)}{\partial x_2^2 \partial x_1} x_2^2 x_1 + \frac{\partial^3 R_{3,0}(0)}{\partial x_2^3} x_2^3 \right]. \end{aligned}$$

Recall that, due to (8), $\tilde{R}_{3,0}$ is obtained by writing $R_{3,0}$ in the $(z^\alpha \bar{z}^\beta)$ basis and keeping only the resonant coefficients, *i.e.* the coefficients of $z_1^2 \bar{z}_2$ and $\bar{z}_1^2 z_2$. Since $x_j = \frac{1}{2}(z_j + \bar{z}_j)$, we remark first that only the coefficient of $x_1^2 x_2$ in $R_{3,0}(x_1, x_2)$ contributes to $\tilde{R}_{3,0}$ (by homogeneity considerations), and second, that the expansion of $R_{3,0}$ in the $(z^\alpha \bar{z}^\beta)$ basis has only *real* coefficients (which would not be the case for a general Hamiltonian depending also on ξ). More precisely, we have

$$x_1^2 x_2 = \frac{1}{8} (z_1^2 z_2 + z_1^2 \bar{z}_2 + \bar{z}_1^2 z_2 + \bar{z}_1^2 \bar{z}_2 + 2|z_1|^2 z_2 + 2|z_1|^2 \bar{z}_2),$$

which gives

$$\begin{aligned} \tilde{R}_{3,0} &= \frac{1}{16} \frac{\partial^3 R_{3,0}(0)}{\partial x_1^2 \partial x_2} (z_1^2 \bar{z}_2 + \bar{z}_1^2 z_2) \\ &= \frac{1}{8} \frac{\partial^3 R_{3,0}(0)}{\partial x_1^2 \partial x_2} \operatorname{Re} (z_1^2 \bar{z}_2). \end{aligned}$$

So, $\nu = 0$, and we obtain the following result,

Theorem 3.5 *In dimension 2, the quantum ε -Birkhoff-Gustavson normal form of the operator $H_{2,\varepsilon} + R_\varepsilon(x)$ in near Fermi resonance $1 \approx 2$, is equal to $H_{2,0} + K_{3,\varepsilon} + \mathcal{O}_4$ with*

$$K_{3,\varepsilon} = \frac{\omega_{1,1}}{2} \varepsilon |z_1|^2 + \frac{\omega_{2,1}}{2} \varepsilon |z_2|^2 + \mu \operatorname{Re} (z_1^2 \bar{z}_2),$$

where

$$\mu = \frac{1}{8} \frac{\partial^3 R_{3,0}(0)}{\partial x_1^2 \partial x_2}. \quad (13)$$

Moreover, the remainder in \mathcal{O}_4 also belongs to $\mathcal{O}_2(x, \xi, \hbar)$.

In order to obtain a fully satisfactory result for the original Schrödinger operator (1), let us now express μ in terms of the potential V_0 .

Theorem 3.6 *Expressed in terms of the original potential V_0 , the coefficient μ of Theorem 3.5 is given as follows.*

$$\begin{aligned} \mu &= \frac{1}{8\sqrt{2}\omega_{1,0}^{3/2}(1+z^2)^{\frac{3}{2}}} \left(z \partial_{x_1}^3 V_0(0) + (1-2z^2) \partial_{x_1^2 x_2}^3 V_0(0) \right. \\ &\quad \left. + (z^3 - 2z) \partial_{x_1 x_2^2}^3 V_0(0) + z^2 \partial_{x_2^3}^3 V_0(0) \right) \end{aligned}$$

with

$$\omega_{1,0} = \frac{1}{\sqrt{3}} \left[\left(\partial_{x_1}^2 V_0(0) - \partial_{x_2}^2 V_0(0) \right)^2 + 4 \left(\partial_{x_1 x_2}^2 V_0(0) \right)^2 \right]^{1/4},$$

and

$$z = \frac{2 |\partial_{x_1 x_2}^2 V_0(0)|}{3\omega_{1,0}^2 - \partial_{x_1}^2 V_0(0) + \partial_{x_2}^2 V_0(0)}.$$

Proof. According to Proposition 3.1, see also (4), we can write

$$(\Lambda_\varepsilon g_\varepsilon \tau_\varepsilon V_\varepsilon)(\tilde{y}) = V_\varepsilon(x_\varepsilon) + \sum_{j=1}^n \frac{\omega_{j,\varepsilon}}{2} \tilde{y}_j^2 + R_\varepsilon(\tilde{y}),$$

where the variable \tilde{y} is given by the three successive change of coordinates:

$$\tilde{y} = \Lambda_\varepsilon U_\varepsilon^*(x - x_\varepsilon),$$

where we abuse of the notation $\Lambda_\varepsilon(y_1, \dots, y_n) = (\sqrt{\omega_{1,\varepsilon}}y_1, \dots, \sqrt{\omega_{n,\varepsilon}}y_n)$. Therefore, for all $|\alpha| \geq 3$,

$$\partial_{\tilde{y}}^\alpha R_\varepsilon(\tilde{y}) = \partial_{\tilde{y}}^\alpha (\Lambda_\varepsilon g_\varepsilon \tau_\varepsilon V_\varepsilon)(\tilde{y}).$$

Since $R_\varepsilon(\tilde{y}) = R_{3,0}(\tilde{y}) + \mathcal{O}_4$ (in the sense of the Taylor series at the origin)

$$\frac{\partial^3 R_{3,0}}{\partial \tilde{y}_1^2 \partial \tilde{y}_2}(0) = \frac{\partial^3 R_0}{\partial \tilde{y}_1^2 \partial \tilde{y}_2}(0) + \mathcal{O}_4 = \frac{\partial^3 (\Lambda_0 g_0 \tau_0 V_0)}{\partial \tilde{y}_1^2 \partial \tilde{y}_2}(0) + \mathcal{O}_4,$$

and hence the equality holds without the \mathcal{O}_4 , since the quantities do not depend on $x, \xi, \varepsilon, \hbar$. Moreover, $\tau_0 = \text{Id}$, so

$$\frac{\partial^3 R_{3,0}}{\partial \tilde{y}_1^2 \partial \tilde{y}_2}(0) = \frac{\partial^3 (\Lambda_0 g_0 V_0)}{\partial \tilde{y}_1^2 \partial \tilde{y}_2}(0) = \frac{1}{\omega_{1,0} \sqrt{\omega_{2,0}}} \frac{\partial^3 (g_0 V_0)}{\partial y_1^2 \partial y_2}(0). \quad (14)$$

Let us now compute the derivatives of $(g_0 V_0)(y) = V_0(U_0 y)$. Let (a, b) and (c, d) be an orthonormal basis of eigenvectors of the Hessian matrix $V_0''(0)$ for the eigenvalues $(\omega_{1,0}^2, \omega_{2,0}^2)$, so that we can take

$$U_0 = \begin{pmatrix} a & c \\ b & d \end{pmatrix}.$$

We have

$$\begin{aligned} \frac{\partial^3 (V_0(U_0 y))}{\partial y_1^2 \partial y_2}(0) &= a^2 c \partial_{x_1}^3 V_0(0) + (2abc + a^2 d) \partial_{x_1^2 x_2}^3 V_0(0) \\ &\quad + (b^2 c + 2abd) \partial_{x_1 x_2^2}^3 V_0(0) + b^2 d \partial_{x_2^3}^3 V_0(0). \end{aligned} \quad (15)$$

It remains to express the coefficients a, b, c, d , taking into account the fact that the eigenvalues of the Hessian matrix $V_0''(0)$ are $\omega_{1,0}^2 = \lambda$, $\omega_{2,0}^2 = 4\lambda$; one can check that this implies

$$\lambda := \frac{1}{3} \sqrt{\left(\partial_{x_1}^2 V_0(0) - \partial_{x_2}^2 V_0(0)\right)^2 + 4(\partial_{x_1 x_2}^2 V_0(0))^2}.$$

In fact, it is elementary to check that for a real symmetric positive matrix whose eigenvalues are $(\lambda, 4\lambda)$, the discriminant of the characteristic polynomial is equal to $9\lambda^2$, and the matrix takes the form, for some $x \in \mathbb{R}$,

$$\begin{pmatrix} \frac{x+5\lambda}{2} & \frac{\sqrt{9\lambda^2-x^2}}{2} \\ \frac{\sqrt{9\lambda^2-x^2}}{2} & \frac{5\lambda-x}{2} \end{pmatrix}.$$

Its eigenvectors can be written as

$$(1, -z) \quad \text{and} \quad (z, 1),$$

with $z = \frac{\sqrt{9\lambda^2-x^2}}{3\lambda-x} \geq 0$. Upon normalization, we obtain

$$\begin{aligned} a &= \frac{1}{\sqrt{1+z^2}} & b &= \frac{-z}{\sqrt{1+z^2}} \\ c &= \frac{z}{\sqrt{1+z^2}} & d &= \frac{1}{\sqrt{1+z^2}}. \end{aligned}$$

In our case we have

$$x = \partial_{x_1}^2 V_0(0) - \partial_{x_2}^2 V_0(0),$$

therefore

$$\begin{aligned} z &= \frac{2|\partial_{x_1 x_2}^2 V_0(0)|}{3\lambda - x} \\ &= \frac{2|\partial_{x_1 x_2}^2 V_0(0)|}{\left(\left(\partial_{x_1}^2 V_0(0) - \partial_{x_2}^2 V_0(0)\right)^2 + 4\left(\partial_{x_1 x_2}^2 V_0(0)\right)^2\right)^{1/2} - \partial_{x_1}^2 V_0(0) + \partial_{x_2}^2 V_0(0)}, \end{aligned}$$

and

$$\begin{aligned} a^2c &= \frac{z}{(1+z^2)^{\frac{3}{2}}} \\ 2abc + a^2d &= \frac{1-2z^2}{(1+z^2)^{\frac{3}{2}}} \\ b^2c + 2abd &= \frac{z^3-2z}{(1+z^2)^{\frac{3}{2}}} \\ b^2d &= \frac{z^2}{(1+z^2)^{\frac{3}{2}}}, \end{aligned}$$

which, in view of (13), (14), and (15), proves the theorem. \square

4 Spectral analysis in near Fermi resonance

Theorem 3.3 gives a formal conjugation of the initial Schrödinger Hamiltonian \hat{P}_ε into an operator of the form $c_\varepsilon + \hat{H}_{2,0} + K_\varepsilon$, where $c_\varepsilon = W_\varepsilon(0) = \min V_\varepsilon$, see Proposition 3.1. Therefore, it is expected that, in regimes where E and \hbar are small enough, the spectrum inside $(-\infty, E)$ of the normal form $c_\varepsilon + \hat{H}_{2,0} + K_\varepsilon$, restricted to the spectral subspace of $H_{2,0}$ corresponding to energies in $[0, (1+\eta)E]$, where $\eta > 0$ is fixed, is a good approximation of the spectrum of \hat{P}_ε in the interval $(-\infty, E)$, see [3].

The goal of this section is to describe the spectrum of the ε -Birkhoff-Gustavson normal form of \hat{P}_ε in the case of a near Fermi resonance, in terms of the original potential V_ε . We shall use the expression of the normal form modulo \mathcal{O}_4 given in the previous section. Since the remainder also belongs to $\mathcal{O}_2(x, \xi, \hbar)$ by Theorem 3.5, it belongs to

$$\mathcal{O}_4(x, \xi, \hbar) + \varepsilon \mathcal{O}_3(x, \xi, \hbar) + \varepsilon^2 \mathcal{O}_2(x, \xi, \hbar).$$

Therefore, using [3, Lemma 4.2], the normal form at order 3, that is to say $c_\varepsilon + \hat{H}_{2,0} + K_{3,\varepsilon}$, is expected to approximate the spectrum of \hat{P}_ε below some energy E with a precision of order $\mathcal{O}(E^2) + \mathcal{O}(\varepsilon E^{3/2}) + \mathcal{O}(\varepsilon^2 E)$. For instance, if we are interested in a fixed number of low-lying eigenvalues, we may take $E = C\hbar$ for some constant $C > 0$ and we obtain a precision of order $\mathcal{O}(\hbar^2) + \mathcal{O}(\varepsilon \hbar^{3/2}) + \mathcal{O}(\varepsilon^2 \hbar)$.

In order to compute the matrix elements of the normal form, we shall

need to understand the Weyl quantization $\hat{K}_{3,\varepsilon}$ of $K_{3,\varepsilon}$, which is

$$\begin{aligned}\hat{K}_{3,\varepsilon} &= \varepsilon \hat{L}_2 + \mu \widehat{\text{Re}(z_1^2 \bar{z}_2)}, \\ &= \varepsilon \hat{L}_2 + \mu \left(x_1^2 x_2 - 2\hbar^2 x_1 \frac{\partial}{\partial x_1} \frac{\partial}{\partial x_2} + \hbar^2 x_2 \frac{\partial^2}{\partial x_1^2} - \hbar^2 \frac{\partial}{\partial x_2} \right).\end{aligned}$$

For that purpose, it will be convenient to pass to the Bargmann representation.

4.1 Creation and annihilation operators

Let us introduce

$$\begin{aligned}a_j(\hbar) &= \frac{1}{\sqrt{2\hbar}} \left(x_j + \hbar \frac{\partial}{\partial x_j} \right); \\ b_j(\hbar) &= \frac{1}{\sqrt{2\hbar}} \left(x_j - \hbar \frac{\partial}{\partial x_j} \right),\end{aligned}\tag{16}$$

which are respectively called the operators of annihilation and creation, acting as unbounded operators on $L^2(\mathbb{R}^n)$ (see for instance [4]).

Formally, the operators $a_j(\hbar)$ and $b_j(\hbar)$ satisfy the following properties:

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

Using $a_j(\hbar)$ and $b_j(\hbar)$ to rewrite $\hat{H}_{2,0}$, we have

$$\begin{aligned}\hat{H}_{2,0} &= \hbar \left(\omega_{1,0} (a_1(\hbar) b_1(\hbar) - \tfrac{1}{2}) + \omega_{2,0} (a_2(\hbar) b_2(\hbar) - \tfrac{1}{2}) \right), \\ \hat{L}_2 &= \hbar \left(\omega_{1,1} (a_1(\hbar) b_1(\hbar) - \tfrac{1}{2}) + \omega_{2,1} (a_2(\hbar) b_2(\hbar) - \tfrac{1}{2}) \right),\end{aligned}$$

and $\hat{K}_{3,\varepsilon}$ is given by

$$\begin{aligned}\hat{K}_{3,\varepsilon} &= \hbar \varepsilon \left(\omega_{1,1} (a_1(\hbar) b_1(\hbar) - \tfrac{1}{2}) + \omega_{2,1} (a_2(\hbar) b_2(\hbar) - \tfrac{1}{2}) \right) \\ &\quad + \sqrt{2} \mu \hbar^{3/2} (a_2(\hbar) b_1^2(\hbar) + a_1^2(\hbar) b_2(\hbar)).\end{aligned}\tag{17}$$

4.2 Bargmann representation

In this section, we review several fundamental results relating to the Bargmann transform and the space $\mathcal{B}_{\mathcal{F}}$ of Bargmann-Fock, also known as the Bargmann space [1]. For further details see [4]. Let us consider the space

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

where $d\mu_n(\zeta)$ is the Gaussian measure defined by $d\mu_n(\zeta) = e^{-|\zeta|^2/\hbar} d^n\zeta$, $\zeta_j = \frac{x_j - i\xi_j}{\sqrt{2}} = \bar{z}_j/\sqrt{2}$, and $d^n\zeta$ is the Lebesgue measure in (x, ξ) . $\mathcal{B}_{\mathcal{F}}$ is a Hilbert space equipped with natural inner product

$$\langle f, g \rangle = \int_{\mathbb{C}^n} f(\zeta) \overline{g(\zeta)} d\mu_n(\zeta).$$

The semiclassical scaling that we use here can be found, for instance, in [4, Proposition 7].

Theorem 4.1 ([1]) *There is a unitary mapping $T_{\mathcal{B}}$ from $L^2(\mathbb{R}^n)$ to $\mathcal{B}_{\mathcal{F}}$ defined by*

$$(T_{\mathcal{B}}f)(\zeta) = \frac{1}{2^{\frac{n}{2}}(\pi\hbar)^{\frac{3n}{4}}} \int_{\mathbb{R}^n} f(x) e^{-\frac{1}{\hbar}[\frac{1}{2}(\zeta^2 + x^2) + \sqrt{2}x\zeta]} dx,$$

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

The Bargmann representation is particularly suited for studying harmonic approximations, as creation and annihilation operators become expressible in a very simple way.

Proposition 4.1 ([1]) *We have*

$$T_{\mathcal{B}}(a_j(\hbar))T_{\mathcal{B}}^{-1} = \frac{\partial}{\partial \zeta_j} \quad \text{and} \quad T_{\mathcal{B}}(b_j(\hbar))T_{\mathcal{B}}^{-1} = \zeta_j,$$

where ζ_j represents the operator of multiplication by ζ_j .

Thus, the harmonic oscillator's Bargmann transform is,

$$\hat{H}_{2,0}^{\mathcal{B}} := T_{\mathcal{B}}(\hat{H}_{2,0})T_{\mathcal{B}}^{-1} = \hbar \sum_{j=1}^n \omega_{j,0} \left(\zeta_j \frac{\partial}{\partial \zeta_j} + \frac{1}{2} \right).$$

It is then standard to prove that the functions $\left\{ \varphi_{\alpha} := \frac{\zeta^{\alpha}}{(2\pi\hbar)^{n/2}\sqrt{\alpha!}} \right\}_{\alpha \in \mathbb{N}^n}$ form an orthonormal Hilbertian basis of $\mathcal{B}_{\mathcal{F}}$, on which $\hat{H}_{2,0}^{\mathcal{B}}$ is diagonal. It follows that $\hat{H}_{2,0}^{\mathcal{B}}$ is essentially self-adjoint with a discrete spectrum which consists of the eigenvalues λ_{α} , $\alpha \in \mathbb{N}^n$ given by:

$$\sigma(\hat{H}_{2,0}^{\mathcal{B}}) = \left\{ \lambda_{\alpha} = \hbar \left(u + \frac{|\omega_0|}{2} \right), \quad u = \langle \omega_0, \alpha \rangle = \sum_{j=1}^n \omega_{j,0} \alpha_j, \quad \alpha \in \mathbb{N}^n \right\},$$

(repeated with their multiplicities) where $\omega_0 = (\omega_{1,0}, \dots, \omega_{n,0})$, $\alpha = (\alpha_1, \dots, \alpha_n)$ and $|\omega_0| = \sum_{j=1}^n \omega_{j,0}$. The corresponding eigenspaces are

$$\mathcal{H}_u^{\mathcal{B}} = \text{Span} \left\{ \frac{\zeta^{\alpha}}{(2\pi\hbar)^{n/2}\sqrt{\alpha!}}, \quad \langle \omega_0, \alpha \rangle = u \right\}.$$

4.3 Spectrum in near Fermi resonance

The authors in [3] give a detailed study of the spectrum of semiclassical pseudodifferential operators whose harmonic approximation possesses an exact complete resonance; the idea was to restrict the Birkhoff normal form to the eigenspaces of the resonant harmonic oscillator. In this section, we extend this result to the case of a near Fermi resonance, using the ε -Birkhoff-Gustavson normal form $H_{2,0} + K_{3,\varepsilon} + \mathcal{O}(4)$ of Theorem 3.3.

First, let us rewrite this normal form in the Bargmann representation. According to (17), we have

$$\begin{aligned} \hat{K}_{3,\varepsilon}^{\mathcal{B}} &:= \mathrm{T}_{\mathcal{B}}(\hat{K}_{3,\varepsilon})\mathrm{T}_{\mathcal{B}}^{-1} = \hbar\varepsilon\omega_{1,1} \left(\zeta_1 \frac{\partial}{\partial \zeta_1} + \frac{1}{2} \right) + \hbar\varepsilon\omega_{2,1} \left(\zeta_2 \frac{\partial}{\partial \zeta_2} + \frac{1}{2} \right) \\ &\quad + \sqrt{2}\mu\hbar^{3/2} \left(\zeta_2 \frac{\partial^2}{\partial \zeta_1^2} + \zeta_1^2 \frac{\partial}{\partial \zeta_2} \right). \end{aligned} \quad (18)$$

Thus, in order to obtain a good approximation of the spectrum of our Schrödinger operator \hat{P}_ε , we shall compute the spectrum of the restriction of $\hat{K}_{3,\varepsilon}^{\mathcal{B}}$ to the eigenspaces of $\hat{H}_{2,0}^{\mathcal{B}}$ (recall that $\hat{H}_{2,0}^{\mathcal{B}}$ commutes with $\hat{K}_{3,\varepsilon}^{\mathcal{B}}$). To this aim, we calculate the matrix elements of $\hat{K}_{3,\varepsilon}^{\mathcal{B}}$ in the basis φ_α of $\mathcal{H}_N^{\mathcal{B}}$, where $N \in \mathbb{N}$ and

$$\mathcal{H}_N^{\mathcal{B}} = \mathrm{Span} \left\{ \varphi_\alpha = \frac{\zeta^{\alpha_1} \zeta^{\alpha_2}}{2\pi\hbar\sqrt{\alpha_1!\alpha_2!}}; \quad \alpha = (\alpha_1, \alpha_2) \in \mathbb{N}^2, \alpha_1 + 2\alpha_2 = N \right\}. \quad (19)$$

As in [8], we use

$$\begin{aligned} \frac{\partial \varphi_{(\alpha_1, \alpha_2)}}{\partial \zeta_1} &= \sqrt{\alpha_1} \varphi_{(\alpha_1-1, \alpha_2)}, \\ \frac{\partial^2 \varphi_{(\alpha_1, \alpha_2)}}{\partial \zeta_1^2} &= \sqrt{\alpha_1} \sqrt{\alpha_1-1} \varphi_{(\alpha_1-2, \alpha_2)}, \\ \frac{\partial \varphi_{(\alpha_1, \alpha_2)}}{\partial \zeta_2} &= \sqrt{\alpha_2} \varphi_{(\alpha_1, \alpha_2-1)}, \\ \frac{\partial^2 \varphi_{(\alpha_1, \alpha_2)}}{\partial \zeta_2^2} &= \sqrt{\alpha_2} \sqrt{\alpha_2-1} \varphi_{(\alpha_1, \alpha_2-2)}, \\ \frac{\partial^2 \varphi_{(\alpha_1, \alpha_2)}}{\partial \zeta_1 \partial \zeta_2} &= \sqrt{\alpha_1} \sqrt{\alpha_2} \varphi_{(\alpha_1-1, \alpha_2-1)}, \end{aligned} \quad (20)$$

and

$$\begin{aligned}
\zeta_1 \varphi_{(\alpha_1, \alpha_2)} &= \sqrt{\alpha_1 + 1} \varphi_{(\alpha_1+1, \alpha_2)}, \\
\zeta_1^2 \varphi_{(\alpha_1, \alpha_2)} &= \sqrt{\alpha_1 + 2} \sqrt{\alpha_1 + 1} \varphi_{(\alpha_1+2, \alpha_2)}, \\
\zeta_2 \varphi_{(\alpha_1, \alpha_2)} &= \sqrt{\alpha_2 + 1} \varphi_{(\alpha_1, \alpha_2+1)}, \\
\zeta_2^2 \varphi_{(\alpha_1, \alpha_2)} &= \sqrt{\alpha_2 + 2} \sqrt{\alpha_2 + 1} \varphi_{(\alpha_1, \alpha_2+2)}, \\
\zeta_1 \zeta_2 \varphi_{(\alpha_1, \alpha_2)} &= \sqrt{\alpha_1 + 1} \sqrt{\alpha_2 + 1} \varphi_{(\alpha_1+1, \alpha_2+1)}.
\end{aligned}$$

According to (18), we obtain, with $\alpha = (\alpha_1, \alpha_2)$,

$$\begin{aligned}
\hat{K}_{3,\varepsilon}^{\mathcal{B}} \varphi_\alpha &= \hbar \varepsilon \omega_{1,1} \left(\zeta_1 \partial_{\zeta_1} \varphi_\alpha + \frac{1}{2} \varphi_\alpha \right) + \hbar \varepsilon \omega_{2,1} \left(\zeta_2 \partial_{\zeta_2} \varphi_\alpha + \frac{1}{2} \varphi_\alpha \right) \\
&\quad + \sqrt{2} \mu \hbar^{3/2} \left(\zeta_2 \sqrt{\alpha_1} \sqrt{\alpha_1 - 1} \varphi_{(\alpha_1-2, \alpha_2)} + \zeta_1^2 \sqrt{\alpha_2} \varphi_{(\alpha_1, \alpha_2-1)} \right), \\
&= \hbar \left(\varepsilon \omega_{1,1} \left(\alpha_1 + \frac{1}{2} \right) + \varepsilon \omega_{2,1} \left(\alpha_2 + \frac{1}{2} \right) \right) \varphi_\alpha \\
&\quad + \sqrt{2} \mu \hbar^{3/2} \left(\sqrt{(\alpha_2 + 1) \alpha_1 (\alpha_1 - 1)} \varphi_{(\alpha_1-2, \alpha_2+1)} \right. \\
&\quad \left. + \sqrt{(\alpha_1 + 2)(\alpha_1 + 1) \alpha_2} \varphi_{(\alpha_1+2, \alpha_2-1)} \right).
\end{aligned}$$

We can confirm on these formulas that the space $\mathcal{H}_N^{\mathcal{B}}$ is stable by $\hat{K}_{3,\varepsilon}^{\mathcal{B}}$ because:

$$\alpha_1 - 2 + 2(\alpha_2 + 1) = \alpha_1 + 2\alpha_2 = N \text{ and } \alpha_1 + 2 + 2(\alpha_2 - 1) = \alpha_1 + 2\alpha_2 = N.$$

We can also confirm the Hermitian symmetry of the matrix $\hat{K}_{3,\varepsilon}^{\mathcal{B}}$. Indeed, let us order the basis φ_α according to $\ell = 0, 1, \dots, E \left[\frac{N}{2} \right]$ and $\alpha_\ell = (N - 2\ell, \ell)$. The image of φ_{α_ℓ} is a vector with three components, on φ_{α_ℓ} , $\varphi_{\alpha_{\ell-1}}$, and $\varphi_{\alpha_{\ell+1}}$. Thus, the matrix is symmetric if and only if the coefficient of $\hat{K}_{3,\varepsilon}^{\mathcal{B}}(\varphi_{\alpha_\ell})$ on $\varphi_{\alpha_{\ell+1}}$ is equal to the coefficient of $\hat{K}_{3,\varepsilon}^{\mathcal{B}}(\varphi_{\alpha_{\ell+1}})$ on φ_{α_ℓ} . The first one is equal to

$$\sqrt{2} \mu \hbar^{3/2} \sqrt{(\alpha_2 + 1) \alpha_1 (\alpha_1 - 1)}$$

with $\alpha_1 = \ell$, $\alpha_2 = N - 2\ell$, and the second one is

$$\sqrt{2} \mu \hbar^{3/2} \sqrt{(\alpha'_1 + 2)(\alpha'_1 + 1) \alpha'_2}$$

with $\alpha'_1 = \alpha_1 - 2$, $\alpha'_2 = \alpha_2 + 1$, so the equality of these coefficients is clear.

In matrix form, we obtain

Theorem 4.2 For any $N \geq 0$, in the basis (φ_α) of the space $\mathcal{H}_N^{\mathcal{B}}$ given in (19), ordered by α_2 , of size $\lfloor \frac{N}{2} \rfloor + 1$, the matrix of the operator $\hat{K}_{3,\varepsilon}^{\mathcal{B}}$ is

$$\mathcal{M}_{\varepsilon,N} = \begin{pmatrix} d_{N,0} & A_{N,0} & & & & \\ A_{N,0} & d_{N,1} & \ddots & & & \mathbf{0} \\ & \ddots & \ddots & \ddots & & \\ & & A_{N,\ell-1} & d_{N,\ell} & A_{N,\ell} & \\ & \mathbf{0} & & A_{N,\ell} & d_{N,\ell+1} & \ddots \\ & & & & A_{N,\ell+1} & \ddots & \ddots \\ & & & & & \ddots & \ddots \end{pmatrix},$$

where for $\ell = 0, 1, \dots, \lfloor \frac{N}{2} \rfloor$:

$$\begin{cases} A_{N,\ell} = \sqrt{2\mu\hbar^{3/2}} \sqrt{(\ell+1)(N-2\ell)(N-2\ell-1)} \\ d_{N,\ell} = \hbar\varepsilon\omega_{1,1} \left(N-2\ell+\frac{1}{2}\right) + \hbar\varepsilon\omega_{2,1} \left(\ell+\frac{1}{2}\right), \end{cases}$$

and μ is defined in Theorem 3.6.

Finally, note that the spectrum of $\hat{H}_{2,0}^{\mathcal{B}} + \hat{K}_{3,\varepsilon}^{\mathcal{B}}$ restricted to $\mathcal{H}_N^{\mathcal{B}}$ is exactly

$$\bigcup_{N \in \mathbb{N}} \left\{ \hbar\omega_{1,0} \left(N + \frac{3}{2}\right) + \mu_{\varepsilon,N,j}; \quad j = 0, \dots, \lfloor \frac{N}{2} \rfloor \right\},$$

where $(\mu_{\varepsilon,N,0}, \dots, \mu_{\varepsilon,N,\lfloor \frac{N}{2} \rfloor})$ are the eigenvalues of the matrix $\mathcal{M}_{\varepsilon,N}$ of Theorem 4.2.

5 Numerical simulations for the near Fermi resonance

We now illustrate our results numerically for the following family of potentials:

$$V_\varepsilon(x_1, x_2) = \left(\frac{1}{2} + \varepsilon\right)x_1^2 + (2 + 2c\varepsilon)x_2^2 + x_1^3 + \frac{1}{2}x_1x_2^2 + \gamma x_1^2x_2 + x_1^4 + x_2^4,$$

where $c \in \mathbb{R}$ and γ are fixed, and $\varepsilon \in \mathbb{R}$ is such that

$$\frac{1}{2} + \varepsilon > 0 \quad \text{and} \quad 1 + c\varepsilon > 0. \quad (21)$$

In view of the normalization (3), this potential corresponds to $W_\varepsilon(0) = 0$, $\omega_{1,\varepsilon} := \sqrt{1+2\varepsilon}$ and $\omega_{2,\varepsilon} = 2\sqrt{1+c\varepsilon}$. Therefore,

$$\omega_{1,0} = 1, \omega_{2,0} = 2, \omega_{1,1} = 1, \omega_{2,1} = c.$$

Since the quadratic part of the potential is already diagonalized, we can take $U = \text{Id}$, and hence it is easy to compute $z = 0$ and

$$\mu = \frac{\gamma}{4\sqrt{2}} \quad (22)$$

from Theorem 3.6.

Due to the term $x_1^4 + x_2^4$, the potential V_ε is confining, and hence $\hat{P}_\varepsilon := -\frac{\hbar^2}{2}\Delta + V_\varepsilon$ has a discrete spectrum, bounded from below, and whose eigenvalues form a non-decreasing sequence tending to $+\infty$. We are interested in the eigenvalues that belong to the interval $(-\infty, E)$, where $E \rightarrow 0$ as $\hbar \rightarrow 0$.

5.1 Numerical computation of the spectrum of \hat{P}_ε

In order to numerically compute the spectrum of \hat{P}_ε without any *a priori*, we use a general spectral method, not specially adapted to the 1 : 2 resonance. Namely, we consider the Hermite functions $H_{\alpha_1, \alpha_2}(x_1, x_2)$, which correspond via the Bargmann transform to the functions $\varphi_{\alpha_1, \alpha_2}$ from (19). We order them according, first, to the energy level $\hbar(\alpha_1 + \alpha_2 + 1)$ of the usual harmonic oscillator $-\frac{\hbar^2}{2}\Delta + \frac{1}{2}(x_1^2 + x_2^2)$, and then according to α_1 . In other words, the first few pairs (α_1, α_2) in increasing order are:

$$(0, 0), (0, 1), (1, 0), (0, 2), (1, 1), (2, 0), (0, 3), (1, 2), (2, 1), (3, 0), \text{ etc.}$$

The next step of the numerical method is to truncate the basis (H_α) into a finite family adapted to the chosen spectral window; according to the semi-classical theory, for a given E , eigenfunctions corresponding to eigenvalues less than E must be microlocalized in the phase space region Ω_ε given by $\frac{1}{2}\|\xi\|^2 + V_\varepsilon(x) \leq E$. Assume that the parameters γ, c are chosen such that V_ε admits a unique minimum at $x = 0$, for ε small enough (see Proposition 5.1 below). By construction, we have

$$\frac{1}{2}\|\xi\|^2 + V_\varepsilon(x) = \frac{1}{2}(x_1^2 + \xi_1^2) + 2x_2^2 + \frac{1}{2}\xi_2^2 + \mathcal{O}(\varepsilon x^2) + \mathcal{O}(x^3).$$

Therefore, if E and ε are small enough, Ω_ε is contained in the ball of radius $\sqrt{3E}$ in phase space. (The number 3 could be replaced by any number larger than 2. For large E , one could do better by using the confinement gained by

the quartic term x^4 , but in this work we are mainly interested in small E). Taking into account that a wave function localized inside a ball may extend slightly beyond the ball, typically at a distance of order $\mathcal{O}(\sqrt{\hbar})$, we can decide to truncate the basis for (α_1, α_2) satisfying $\hbar(\alpha_1 + \alpha_2 + 1) \leq \frac{3}{2}E + \sqrt{\hbar}$; thus we shall take $\alpha_1 + \alpha_2 \leq M$ with

$$M = \frac{3E}{2\hbar} + \frac{1}{\sqrt{\hbar}}. \quad (23)$$

We obtain a basis \mathcal{B}_M of cardinal $(M+1)(M+2)/2$ which, when E is bounded and \hbar is small, is $\mathcal{O}(\frac{E^2}{\hbar^2})$.

On this basis, the action of differential operators with polynomial coefficients can be explicitly computed, similarly to (20); namely, from (16) and Proposition 4.1, we have

$$x_j H_\alpha = \sqrt{\frac{\hbar}{2}} (\sqrt{\alpha_j} H_{\alpha-1_j} + \sqrt{\alpha_j+1} H_{\alpha+1_j})$$

and

$$\hbar \partial_{x_j} H_\alpha = \sqrt{\frac{\hbar}{2}} (\sqrt{\alpha_j} H_{\alpha-1_j} - \sqrt{\alpha_j+1} H_{\alpha+1_j}),$$

where we have denoted by $(1_1, 1_2)$ the canonical basis of \mathbb{Z}^2 . In order to implement the operator of multiplication by x_j^2 , instead of writing the explicit formula, we may also simply square the truncated matrix for x_j ; by doing so, of course we introduce an error due to the fact that matrix truncation does not commute with matrix multiplication. The wrong columns concern the images of H_α when $\alpha + 1_j \notin [0, M] \times [0, M]$, *i.e.* $\alpha_1 + \alpha_2 + 1 > M$. In other words, in order to obtain a correct matrix, we need to delete the “highest energy level”, which means truncating the computed matrix to the smaller basis \mathcal{B}_{M-1} . Similarly, since the matrix for x_j^2 has a band structure of width 5 (instead of 3 for x_j), when computing x_j^3 we need to reduce M by 2 more. Finally, the truncated matrix for x_j^4 will be exact if we reduce M by 3 more. The analogous discussion holds for $\hbar \partial_{x_j}$. Consequently, in order to obtain the matrix for \hat{P}_ε on \mathcal{B}_M , we need to start from the larger basis \mathcal{B}_{M+6} .

In view of the above discussion, we can now implement, explicitly, the matrix of \hat{P}_ε on the basis $\mathcal{B}_M = \{H_\alpha, |\alpha| \leq M\}$, and call a standard diagonalization routine for real symmetric matrices. On a standard laptop, this can be easily done for a matrix of size 1000×1000 , which means $M \leq 43$.

Our first experiment is to test the validity of the truncation (23). Taking $\hbar = 0.01$ and $E = 10\hbar$, Formula (23) gives $M = 25$, which corresponds to

a matrix of size 351×351 . In Figure 1, we vary M around that value, and plot the ℓ_∞ norm of the difference between the spectrum below E computed with the given M value (that is, using the matrix obtained from the basis \mathcal{B}_M) and the spectrum computed using the largest M (here $M_{\max} = 35$). This experiment confirms that the value predicted by (23) is large enough to obtain a very good accuracy.

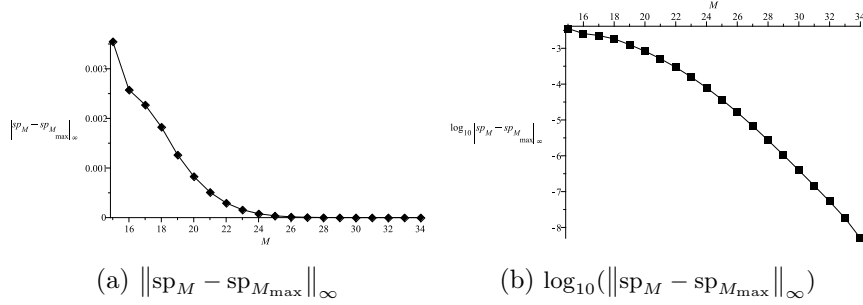


Figure 1: Quality of the numerical spectrum in terms of M . With $\hbar = 0.01$, $\varepsilon = 0$, and $E = 10\hbar$, the value given by (23) is $M = 25$. We plot here $\|\text{sp}_M - \text{sp}_{M_{\max}}\|_\infty$ with $M_{\max} = 35$, and sp_M is the spectrum below E obtained by diagonalizing the truncated matrix of \hat{P}_ε in the basis \mathcal{B}_M . The same data with a \log_{10} scale is plotted on the right picture. We see that, at $M \geq 25$, the error is indeed negligible. Interestingly, we also see that simply choosing $M = \frac{3E}{2\hbar} = 15$ would *not* be sufficient.

In Figure 2, we compare the spectrum of \hat{P}_ε obtained with the above numerical method to the spectrum of the unperturbed harmonic oscillator $H_{2,0}$. Recall that the oscillator spectrum is explicit

$$\text{sp}(H_{2,0}) = \left\{ \hbar\omega_{1,0}(\alpha_1 + 2\alpha_2 + \tfrac{3}{2}), \quad (\alpha_1, \alpha_2) \in \mathbb{N}^2 \right\} \quad (24)$$

and features the famous phenomenon of *clustering* of eigenvalues on the ladder $\hbar\omega_{1,0}(N + \frac{3}{2})$, $N \geq 0$, which correspond to *polyads* in the chemistry literature. While we can recognize the footprints of these polyads on the spectrum of \hat{P}_ε , we notice that much of the structure is lost, even for relatively small ε .

5.2 V_ε has a global minimum

Our goal is to compare the spectrum of P_ε with what the ε -Birkhoff-Gustavson normal form gives. In order to apply our results, let us first check that V_ε has a unique non-degenerate minimum, when the constants γ, c, ε are properly chosen.

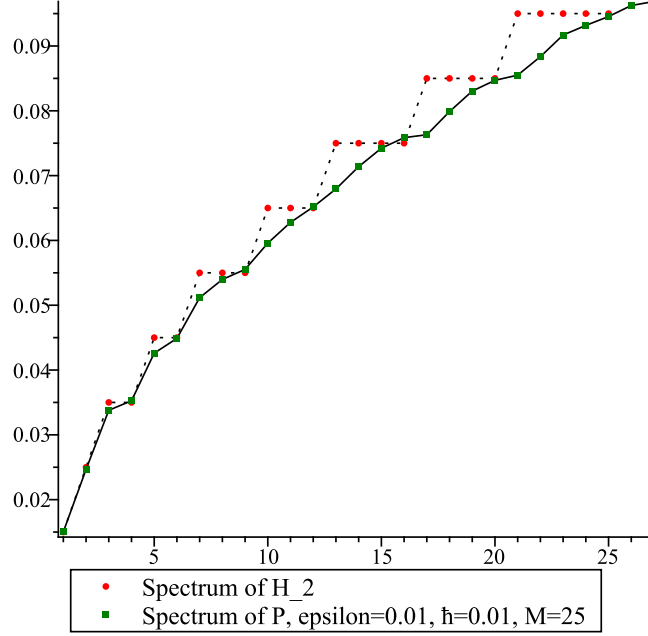


Figure 2: Spectrum of \hat{P}_ϵ (green boxes, solid line) on top of the spectrum of the 1 : 2 harmonic oscillator $H_{2,0}$ (red discs, dotted line).

Proposition 5.1 *Assume that, in addition to (21), the following conditions hold:*

$$1 - \frac{\gamma^2}{8(1 + c\epsilon)} > 0$$

$$\frac{7}{16} + \epsilon - \frac{1}{4 \left(1 - \frac{\gamma^2}{8(1 + c\epsilon)} \right)} > 0.$$

Then, the potential V_ϵ admits a unique non-degenerate minimum at the origin. In particular, if $|\gamma| < \sqrt{\frac{24}{7}}$ and $|\epsilon|$ is small enough, then V_ϵ admits a unique non-degenerate minimum at the origin.

Proof. We simply complete three squares: first, we write

$$\frac{1}{2}x_1x_2^2 + x_4^4 = \left(x_2^2 + \frac{x_1}{4}\right)^2 - \frac{x_1^2}{16}.$$

Then, we use

$$(2 + 2c\varepsilon)x_2^2 + \gamma x_1^2 x_2 = 2(1 + c\varepsilon) \left(x_2 + \frac{\gamma x_1^2}{4(1 + c\varepsilon)} \right)^2 - \frac{\gamma^2 x_1^4}{8(1 + c\varepsilon)}.$$

Incorporating the last term with the monomial x_1^4 from V_ε , we finally write, with $\kappa := 1 - \frac{\gamma^2}{8(1+c\varepsilon)}$,

$$\kappa x_1^4 + x_1^3 = x_1^2 \left(\kappa \left(x_1 + \frac{1}{2\kappa} \right)^2 - \frac{1}{4\kappa} \right).$$

This finally gives

$$\begin{aligned} V_\varepsilon = & \left(\frac{1}{2} + \varepsilon - \frac{1}{16} - \frac{1}{4\kappa} \right) x_1^2 + 2(1 + c\varepsilon) \left(x_2 + \frac{\gamma x_1^2}{4(1 + c\varepsilon)} \right)^2 \\ & + \kappa x_1^2 \left(x_1 + \frac{1}{2\kappa} \right)^2 + \left(x_2^2 + \frac{x_1}{4} \right)^2. \end{aligned}$$

Thus, under the conditions of the proposition, we have a sum of four non-negative terms; the sum vanishes if and only if all terms vanish, which is equivalent to $x_1 = x_2 = 0$.

Now, if γ and c are fixed, the two conditions take the form

$$\begin{aligned} 1 - \frac{\gamma^2}{8} + \mathcal{O}(\varepsilon) &> 0 \\ \frac{7}{16} - \frac{1}{4(1 - \frac{\gamma^2}{8})} + \mathcal{O}(\varepsilon) &> 0 \end{aligned}$$

which holds, if ε is small enough, as soon as

$$\frac{7}{16} - \frac{1}{4(1 - \frac{\gamma^2}{8})} > 0 \quad \text{i.e.} \quad \gamma^2 < \frac{24}{7},$$

which is stronger than the first condition $\gamma^2 < 8$. □

Remark 5.2 We don't claim that the two conditions of Proposition 5.1 are necessary. But they allow for a simple proof, and they are sufficient for our numerical purposes $\gamma = 0$ and $\gamma = 1$. △

5.3 Joint spectrum of $\hat{H}_{2,0}$ and $\hat{K}_{3,\varepsilon}$

Let us apply the ε -Birkhoff-Gustavson normal form of Theorem 3.3 to order 3: we conjugate the initial Schrödinger operator \hat{P}_ε to an operator of the form $H_{2,0} + K_{3,\varepsilon} + \mathcal{O}_4$, and our goal is perform numerical computations neglecting the \mathcal{O}_4 term.

The operator $K_{3,\varepsilon}$ can be explicitly implemented thanks to Theorem 3.5, Theorem 3.6 and Theorem 4.2. For any given $N \geq 0$, we obtain the exact matrix for $K_{3,\varepsilon}$ in the orthonormal basis (19), of cardinal $\lfloor \frac{N}{2} \rfloor + 1$.

In order to obtain an approximation of the spectrum of \hat{P}_ε , following Section 4, we fix some energy $E > 0$, and we compute the spectrum of $H_{2,0} + K_{3,\varepsilon}$ restricted to the spectral subspace of $H_{2,0}$ corresponding to energies in $[0, (1+\eta)E]$, where $\eta > 0$ is fixed. In view of the Bargmann representation of Section 4.2, this is equivalent to computing the spectrum of the restriction of $\hat{H}_{2,0}^\mathcal{B} + \hat{K}_{3,\varepsilon}^\mathcal{B}$ to the space $\oplus_{n=0}^N \mathcal{H}_n^\mathcal{B}$, see (19), for some N large enough. Specifically, the integer N has to be chosen such that $\hbar(\tilde{n} + \frac{3}{2}) + \sigma((\hat{K}_{3,\varepsilon}^\mathcal{B})|_{\mathcal{H}_{\tilde{n}}^\mathcal{B}})$ does not intersect the interval $(0, E)$ for all $\tilde{n} > N$.

A nice way of displaying this computation is to plot the *joint spectrum* of the commuting operators $\hbar^{-1}\hat{H}_{2,0}$ and $\hat{K}_{3,\varepsilon}$: this is the set of pairs $(\lambda_1, \lambda_2) \in \mathbb{R}^2$ such that, with the notation of Theorem 4.2,

$$\begin{aligned}\lambda_1 &= \omega_{1,0}(N + \tfrac{3}{2}) \\ \lambda_2 &= \mu_{\varepsilon,N,j} \text{ for some } j = 0, \dots, \lfloor \tfrac{N}{2} \rfloor,\end{aligned}$$

see Figure 7. Then, the spectrum $H_{2,0} + K_{3,\varepsilon}$ is obtained from the joint spectrum by applying the map $(\lambda_1, \lambda_2) \mapsto \hbar\lambda_1 + \lambda_2$.

Notice that the computation of the joint spectrum is much faster than the computation of the spectrum of \hat{P}_ε from Section 5.1, since instead of a matrix of size at least $\mathcal{O}(\frac{E^2}{\hbar^2} \times \frac{E^2}{\hbar^2})$, we have $N = \mathcal{O}(\frac{E}{\hbar})$ matrices of sizes $\mathcal{O}(\frac{E}{\hbar} \times \frac{E}{\hbar})$, so we gain (at least) an order of magnitude in $\frac{E}{\hbar}$. For instance, with $M = 41$, instead of a 903×903 matrix, we have 10 matrices of sizes $1 \times 1, 2 \times 2, 2 \times 2, \dots, 6 \times 6$.

5.4 The case $\gamma = 0$

The case $\gamma = 0$ is interesting because the remaining terms of order 3 in the potential V_ε , namely x_1^3 and $x_1x_2^2$, are completely cancelled out by the Birkhoff normal form: we have $\mu = 0$ in Theorem 3.6. Therefore, the spectrum of \hat{P}_ε is approximated up to \mathcal{O}_4 merely by the quadratic term $\hat{H}_{2,0} + \varepsilon\hat{L}_2$,

whose spectrum is explicit:

$$\{\hbar(\omega_{1,0}(\alpha_1 + 2\alpha_2 + \tfrac{3}{2})) + \hbar\varepsilon(\omega_{1,1}(\alpha_1 + \tfrac{1}{2}) + \omega_{2,1}(\alpha_2 + \tfrac{1}{2}))\}, \quad (\alpha_1, \alpha_2) \in \mathbb{N}^2\}$$

When $\varepsilon = 0$, the theoretical results of [3] apply. In particular, in the regime $E = C\hbar$, the spectrum should converge to the polyads of (24), with an error of order $\mathcal{O}(\hbar^2)$. This is clearly illustrated in Figures 3 and 4.

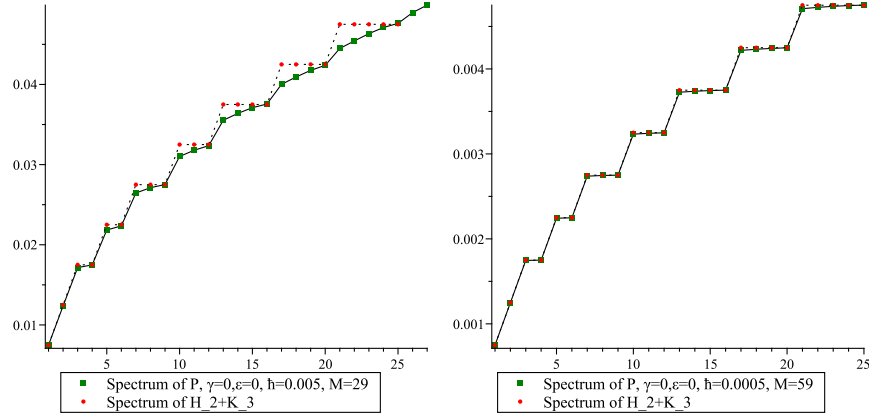


Figure 3: Comparison of the spectrum of \hat{P}_ε with the eigenvalues obtained from the Birkhoff normal form $H_{2,0} + K_{3,\varepsilon}$. Here $\hbar = 0.005$ (left) or $\hbar = 0.0005$ (right), and $\gamma = 0, \varepsilon = 0$, hence $K_{3,\varepsilon} = 0$.

In order to experiment the case $\varepsilon \neq 0$, we chose the regime $\varepsilon = \sqrt{\hbar}$, where we still expect an error of order $\mathcal{O}(\hbar^2)$, which is confirmed by the numerics, see Figures 5 and 6.

The joint spectrum of the commuting operators $(\hbar^{-1}\hat{H}_{2,0}, \hat{K}_{3,\varepsilon})$ is depicted in Figure 7.

5.5 The case $\gamma = 1$

The case $\gamma = 1$ corresponds to the heart of our result, since the Birkhoff term of order 3, $K_{3,\varepsilon}$ is not trivial, due to (22).

When $\varepsilon = 0$, as above, the theoretical results of [3] apply and we observe the expected $\mathcal{O}(\hbar^2)$ error in Figures 8 and 9. The clear agreement with $\mathcal{O}(\hbar^2)$ is a strong confirmation of the validity of the Birkhoff procedure, and in particular of the correctness of the value of μ from (22), because any other value of μ would lead to an error of the order of the eigenvalues of $K_{3,0}$ on the given spectral subspace, which is known to be $\mathcal{O}(\hbar^{3/2})$.

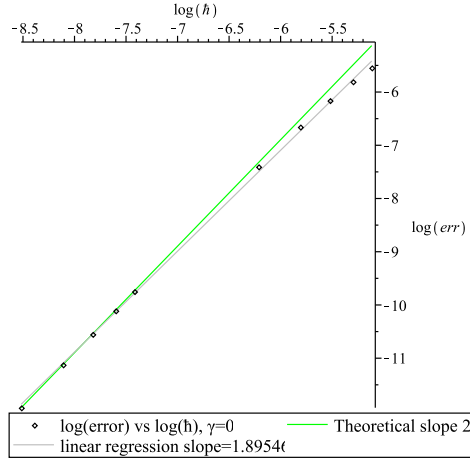


Figure 4: Error(log scale) between the spectrum of \hat{P}_ε and that of $H_{2,0} + K_{3,\varepsilon}$. Here $\gamma = 0, \varepsilon = 0$. When \hbar is small enough, we observe the theoretical slope of 2 (green line), corresponding to an error of order $\mathcal{O}(\hbar^2)$.

The new results correspond to $\varepsilon \neq 0$. As in the case $\gamma = 0$ we experiment the regime $\varepsilon = \sqrt{\hbar}$, and, in spite of this perturbation, the ε -Birkhoff-Gustavson procedure suggests that the error should still be $\mathcal{O}(\hbar^2)$. This is confirmed by Figures 10 and 11.

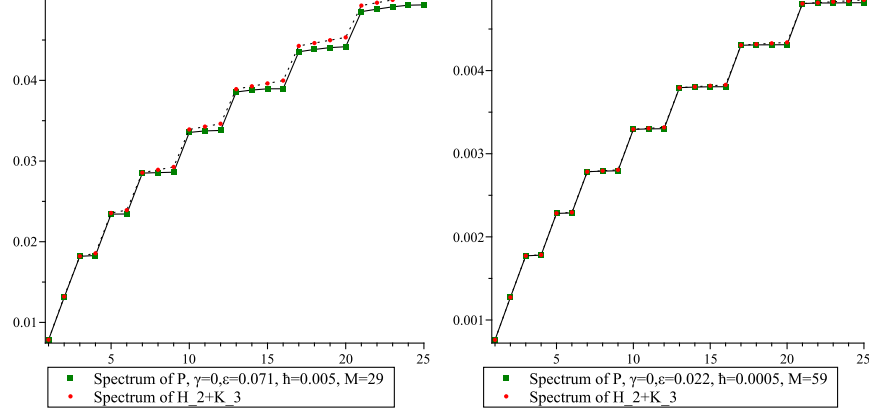


Figure 5: Comparison of the spectrum of \hat{P}_ε with the eigenvalues obtained from the Birkhoff normal form $H_{2,0} + K_{3,\varepsilon}$. Here $\hbar = 0.005$ (left) or $\hbar = 0.0005$ (right), and $\gamma = 0, \varepsilon = \sqrt{\hbar}$, hence $K_{3,\varepsilon} = 0$.

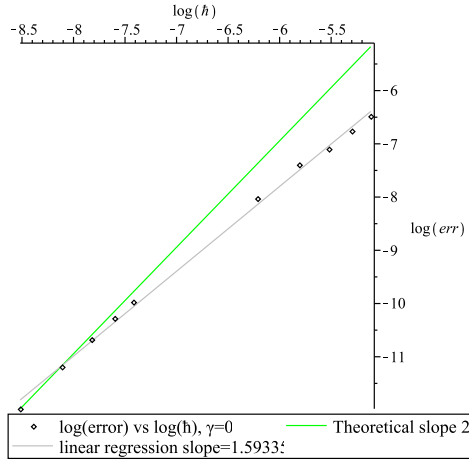


Figure 6: Error(log scale) between the spectrum of \hat{P}_ε and that of $H_{2,0} + K_{3,\varepsilon}$. Here $\gamma = 0, \varepsilon = \sqrt{\hbar}$. When \hbar is small enough, we tend to the theoretical slope of 2 (green line), corresponding to an error of order $\mathcal{O}(\hbar^2)$, though it seems slower than in the case $\varepsilon = 0$ (Figure 4); on the other hand, for the larger \hbar , the absolute error is quite smaller here than for the case $\varepsilon = 0$.

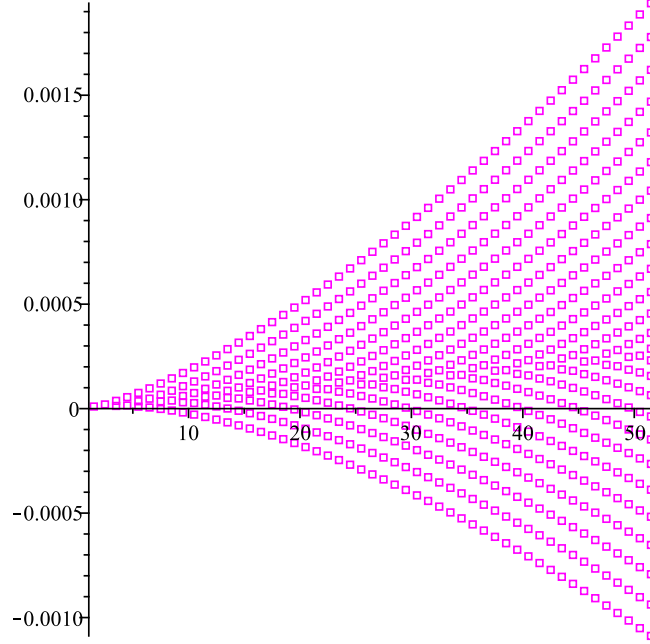


Figure 7: Joint spectrum of $(\hbar^{-1} \hat{H}_{2,0}, \hat{K}_{3,\varepsilon})$. The abscissae are $n + \frac{3}{2}$, $n \geq 0$. Here $\gamma = 1, c = 1, \varepsilon = 0.01, \hbar = 0.001$.

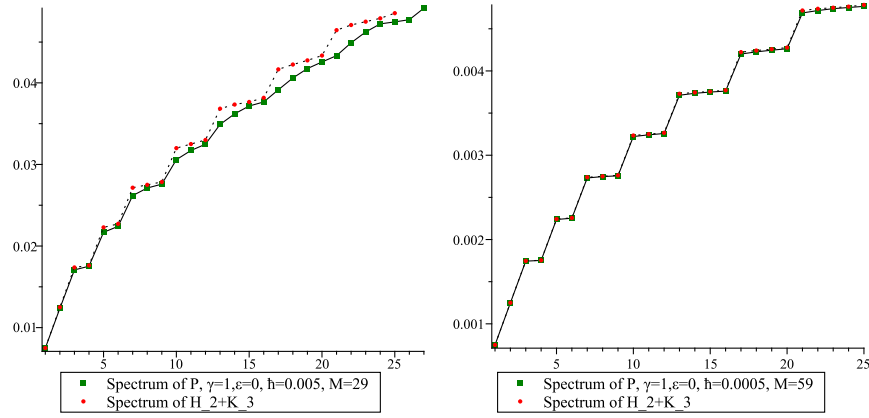


Figure 8: Comparison of the spectrum of \hat{P}_ε with the eigenvalues obtained from the Birkhoff normal form $H_{2,0} + K_{3,\varepsilon}$. Here $\hbar = 0.005$ (left) or $\hbar = 0.0005$ (right), and $\gamma = 1, \varepsilon = 0$.

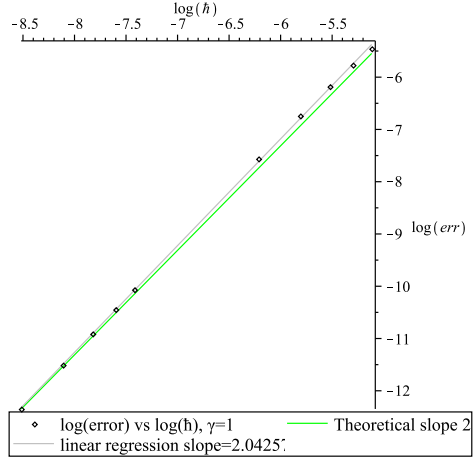


Figure 9: Error(log scale) between the spectrum of \hat{P}_ε and that of $H_{2,0} + K_{3,\varepsilon}$. Here $\gamma = 1, \varepsilon = 0$. We observe a nice fit with the theoretical slope of 2 (green line), corresponding to an error of order $\mathcal{O}(\hbar^2)$.

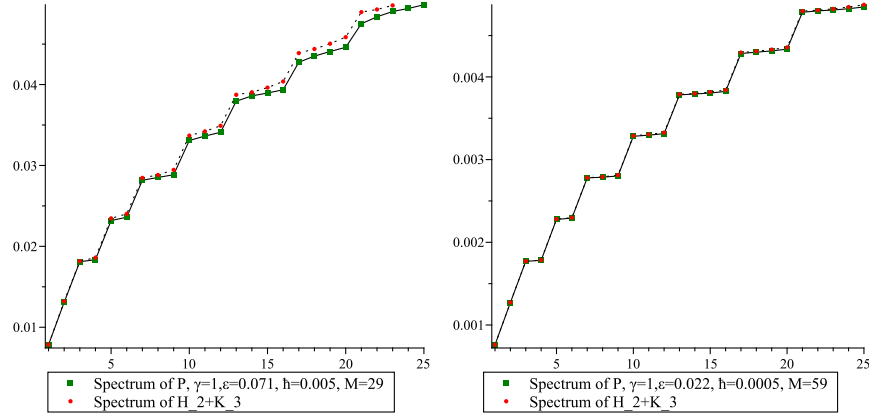


Figure 10: Comparison of the spectrum of \hat{P}_ε with the eigenvalues obtained from the Birkhoff normal form $H_{2,0} + K_{3,\varepsilon}$. Here $\hbar = 0.005$ (left) or $\hbar = 0.0005$ (right), and $\gamma = 1, \varepsilon = \sqrt{\hbar}$.

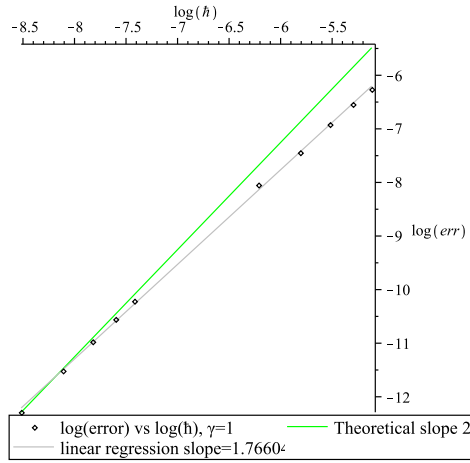


Figure 11: Error(log scale) between the spectrum of \hat{P}_ε and that of $H_{2,0} + K_{3,\varepsilon}$. Here $\gamma = 1, \varepsilon = \sqrt{h}$. When h is small enough, we tend to the theoretical slope of 2 (green line), corresponding to an error of order $\mathcal{O}(h^2)$, though it seems slower than in the case $\varepsilon = 0$ (Figure 9); on the other hand, for the larger h , the absolute error is quite smaller here than for the case $\varepsilon = 0$.

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