Università degli Studi di Padova

DIPARTIMENTO DI MATEMATICA "TULLIO LEVI-CIVITA"

Corso di Laurea Magistrale in Matematica

Bose-Hubbard model of cold atoms to higher orders

Candidato:
Laura Rinaldi
Matricola 1207416

Relatore:
Dott.Antonio Ponno

Anno Accademico 2019–2020
25 Settembre 2020

Abstract

The aim of this work is to study the dynamics of cold atoms trapped in a one-dimensional periodic lattice generated by an optical potential. Such a system is described by a standard model in condensed matter, namely the so-called Bose-Hubbard model [7]. Arrays of cold neutral atoms or ions are the basic elements of some proposals of quantum computers, which motivates the interest of understanding their dynamics from a mathematical point of view [10].

The main targets of this Master Thesis are the following. First, starting from a classical Hamiltonian of the Frenkel-Kontorova type and thanks to Perturbation Theory, to derive the discrete Bougolyubov-Gross-Pitaevskii (dBGP) equation. Second, starting from first principle formulation, to provide a systematic, quantum mechanical, perturbative derivation of the Bose-Hubbard (BH) model to orders higher than the first one in the small parameter.

Contents

Introduction

The starting point, is describing the setting and the model from a physical point of view. The first chapter of this thesis is dedicated to such physical description. The main idea is to trap an atom in one dimension, using a laser beam i.e. to send against the atom some photons, of a well defined frequency, in order to decelerate it. Then, as a further step, one can extend the machinery to the three dimensional case sending photons in all directions. From a mathematical point of view, such optical cooling is like applying an (optical) potential to the array of atoms. The interference between two counter propagating laser beams can be represented by an optical standing wave with space period $\lambda/2$, in which the atoms can be trapped and where λ is the wavelength of the laser beam [5].

Such a trapping potential is generated by overlapping two counter propagating laser beams in each direction. The resulting classical Hamiltonian, of the Frenkel-Kontorova type, which is the starting point of our investigation in second chapter, reads

$$H(x,p) = \sum_{j=1}^{N} \left[\frac{{p_j}^2}{2m} + U(x_{j+1} - x_j) + V(x_j) \right] \ , \tag{1}$$

defining a system of N equal particles of mass m pairwise interacting through an inter-particle potential U and subject to a periodic confining potential V of period $d = \lambda/2$. In (1) x_j and p_j denote position and conjugate momentum of the j-th particle of the array. Periodic boundary conditions are chosen in such a way that

$$x_{j+N} = x_j + L \ ; \quad p_{j+N} = p_j \ , \quad j = 1, \ldots, N \ , \tag{2}$$

the space-period of the system being $L = Nd$.

In the specific case considered here the trapping potential $V(x)$ is of the form:

$$V(x) = V_0 \sin^2(kx) \ , \tag{3}$$

where $k = \pi/d$ and $V_0 > 0$ is the maximum amplitude of the trapping potential. Such a potential is generated by counter propagating laser beams (and suitable magnetic traps not included in the model treated here). The inter-particle potential U for neutral atoms, the only case considered here, is of the attractive Van der Waals form:

$$U(x) = -\frac{C}{x^6} \ , \tag{4}$$

where C is a suitable positive, dimensional constant. See e.g. [7].

The Hamiltonian system (1) can be treated both form the classical and from the quantum point of view. In both cases, the perturbative setting consists in studying the small nonlinear motions of the system close to ideal crystal equilibrium: $\bar{x}_j = jd$ ($j \in \mathbb{Z}$). By setting $x_j = \bar{x}_j + q_j$ and expanding the potentials V about 0, and U about d, the Hamiltonian (1) takes on the form:

$$H(q,p) = h(q,p) + \ P_1(q) + P_2(q) + \dots \ , \tag{5}$$

where

$$h(q,p) := \sum_{j=1}^{N} \left(\frac{{p_j}^2}{2m} + \frac{m\omega^2}{2} q_j^2 \right) \ ; \tag{6}$$

$$P_1(q) := \sum_{j=1}^{N} \left(-\frac{\Lambda}{4} q_j^4 + \frac{K}{2}(q_{j+1} - q_j)^2 \right) \ ; \tag{7}$$

$$P_2(q) := \sum_{j=1}^{N} \left(\frac{\Gamma}{6} q_j^6 + \frac{\alpha}{3}(q_{j+1} - q_j)^3 \right) \ , \tag{8}$$

the dots in (5) denoting higher order terms $O(|q|^8 + |\Delta q|^4)$. The parameters $\omega, \Lambda, K, \Gamma, \alpha$ appearing in (6)-(8) are linked to the derivatives of V and U in an obvious way.

The Hamiltonian (5) is now regarded as a perturbation of the Hamiltonian h of N non interacting, identical harmonic oscillators whose flow Φ_h^t is $2\pi/\omega$-periodic in time for all initial conditions. In so doing, we are supposing an ordering of the kind $|X_h| \gg |X_{P_1}| \gg |X_{P_2}| \gg \cdots$, where X_G is the Hamiltonian vector field of $G(q,p)$. The central idea of Hamiltonian perturbation theory consists in looking for a change of variables that removes, completely or partially, the perturbations P_i from H, up to some pre-fixed order n. To this purpose, the relevant concept is that of normal form.

Definition *(Normal form) A Hamiltonian of the form* $H = h + \bar{P}_1 + \bar{P}_2 + \dots$ *is said to be in* normal form *to order* n *with respect to* h *if* $\{\bar{P}_i, h\} = 0$ *for any* $i = 1, ..., n$.

We thus look for a smooth, close to the identity, canonical change of variables C_n such that the transformed Hamiltonian $H^{(n)} := H \circ C_n^{-1}$, where H is of the form (5), turns out to be in normal form to order n with respect to h, namely

$$H^{(n)} = h + \bar{P}_1 + \bar{P}_2 + \cdots + \bar{P}_n + R \ , \tag{9}$$

where $\{\bar{P}_i, h\} = 0$ for any $i = 1, \dots, n$ and R is a small remainder (in the sense specified above). The canonical transformation C_n is obtained by composing the time-one Hamiltonian flows $\Phi_{G_1}, \dots, \Phi_{G_n}$ of suitable, unknown generating functions $G_1, \dots, G_n$, namely $C_n = \Phi_{G_n}^{-1} \circ \cdots \circ \Phi_{G_1}^{-1}$. The natural variables for the computation of the normal form (9) in our case are the *complex Birkhoff variables*

$$z_j = \frac{m\omega q_j + \imath p_j}{\sqrt{2m\omega}} \ ; \quad {z_j}^* = \frac{m\omega q_j - \imath p_j}{\sqrt{2m\omega}} \ , \ (\imath^2 = -1) \tag{10}$$

with respect to which the unperturbed Hamiltonian (6) reads $h = \sum_j \omega |z_j|^2$ and the perturbations P_i have a simple computable structure to all orders. The main result, on the classical side, is the following.

Theorem *For any fixed* n*, there exists a close to the identity, canonical transformation* $C_n : (z, z^*) \mapsto (a, a^*)$ *such that* $H^{(n)}(a, a^*) = H(C_n^{-1}(a, a^*))$ *is in normal form to order* n *with respect to* h*. In particular,*

$$\begin{aligned} \bar{P}_1(a, a^*) &= \frac{\omega}{2\pi} \int_0^{2\pi/\omega} P_1(\Phi_h^\tau(a, a^*)) \mathrm{d}\tau = \\ &= W \sum_{j=1}^N |a_j|^2 + J \sum_{j=1}^N a_j^* (a_{j+1} + a_{j-1}) + U \sum_{j=1}^N |a_j|^4 \ , \end{aligned} \tag{11}$$

with suitable real parameters W*,* J *and* U*.*

The Hamiltonian $h + \bar{P}_1$ is that of the discrete Nonlinear Schrödinger (dNLS), or discrete Bogolyubov-Gross-Pitaevskii (dBGP) equation, a complex equation which is guessed to describe the dynamics of the atomic array at extremely low temperatures. The first few normalized perturbations $\bar{P}_2$, $\bar{P}_3$ and so on, are explicitly computable, though their link with the original perturbations $P_1, P_2 \dots$ is not as easy as (11). The Theorem above implies that the classical dynamics of the atomic array is well described, to any fixed perturbative order, i.e. on arbitrarily large time-scales, by a suitable

deformation of the dBGP, if the amplitude of the initial conditions is small enough.

The third chapter is focused on the term of remainder, in particular on the estimate of its effects.

Of course, an atomic array of cold atoms is a quantum-mechanical system, so that its dynamics must be studied in the framework of quantum mechanics analyzed in chapter four. This is done transforming the Hamiltonian (1) into a differential operator $\boldsymbol{H}$ by the procedure of canonical quantization, which amounts to set $\boldsymbol{H} := H(x, -\imath\hbar\partial_x)$, where $\partial_x := (\partial_{x_1}, \ldots, \partial_{x_N})$ and $\hbar$ is the Planck constant (actually $\hbar = h/2\pi$ is the so called normalized Planck constant). The state of the system is then described by the Schrödinger equation $\imath\hbar\psi_t = \boldsymbol{H}\psi$, where $\psi(t, x)$ is the complex valued wave function of the system defined on the configuration space. The formal solution of the equation is given by $\psi(t) = \boldsymbol{U}_{\boldsymbol{H}}(t)\psi(0)$, where $\boldsymbol{U}_{\boldsymbol{H}}(t) := \exp(-\imath\boldsymbol{H}t/\hbar)$ is the unitary time evolution operator associated to the quantum Hamiltonian $\boldsymbol{H}$. As is well known, one can regard everything in the equivalent representation of the dynamics, due to Heisenberg, where any quantized operator $\boldsymbol{F}$ evolves along the flow of $\boldsymbol{H}$ by unitary conjugation, namely $\boldsymbol{F}(t) := \boldsymbol{U}_{\boldsymbol{H}}(t)^\dagger \boldsymbol{F} \boldsymbol{U}_{\boldsymbol{H}}(t)$ (a dagger here denotes the adjoint). In such a way, the algebra of operators $\boldsymbol{F}, \boldsymbol{G}, \ldots$ defined on the configuration space of a given system becomes a Poisson algebra with Poisson bracket given by $\{\boldsymbol{F}, \boldsymbol{G}\} := -\imath[\boldsymbol{F}, \boldsymbol{G}]/\hbar$, where $[\ ,\ ]$ denotes the standard commutator. Since the formal properties of Hamiltonian perturbation theory depends only on the algebraic properties of the Poisson structure, one can extend the classical results listed above to the quantum case.

One thus canonically quantizes the Hamiltonian (1) and gets the quantum Hamiltonian $\boldsymbol{H}$, or its equivalent expansion (5)-(8), that can be rewritten in terms of the Dirac, Boson or ladder operators

$$\boldsymbol{b}_j := \frac{m\omega q_j + \hbar\partial_{q_j}}{\sqrt{2m\omega\hbar}} \ ; \quad \boldsymbol{b}_j^\dagger := \frac{m\omega q_j - \hbar\partial_{q_j}}{\sqrt{2m\omega\hbar}} \ , \tag{12}$$

the quantum version of the Birkhoff variables (10) up to a scale factor $1/\sqrt{\hbar}$. The quantum Hamiltonian $\boldsymbol{H} = \boldsymbol{h} + \boldsymbol{P}_1 + \boldsymbol{P}_2 + \ldots$ thus obtained can now be brought into normal form to any order n through a suitable canonical transformation (i.e. unitary conjugation).

Definition *A quantum Hamiltonian of the form* $\boldsymbol{H} = \boldsymbol{h} + \bar{\boldsymbol{P}}_1 + \bar{\boldsymbol{P}}_2 + \ldots$ *is said to be in normal form to order* n *with respect to* $\boldsymbol{h}$ *if* $[\bar{\boldsymbol{P}}_i, \boldsymbol{h}] = 0$ *for any* $i = 1, \ldots, n$.

Theorem *For any fixed n, there exists a close to the identity, canonical (unitary) transformation $\boldsymbol{C}_n : (\boldsymbol{b}, \boldsymbol{b}^\dagger) \mapsto (\boldsymbol{a}, \boldsymbol{a}^\dagger)$ such that $\boldsymbol{H}^{(n)} = \boldsymbol{C}_n^\dagger \boldsymbol{H} \boldsymbol{C}_n$ is in normal form to order n with respect to $\boldsymbol{h}$. In particular,*

$$\begin{aligned} \bar{\boldsymbol{P}}_1(a, a^*) &= \frac{\omega}{2\pi} \int_0^{2\pi/\omega} \boldsymbol{U}_{\boldsymbol{h}}^\dagger(\tau) \boldsymbol{P}_1 \boldsymbol{U}_{\boldsymbol{h}}(\tau) \mathrm{d}\tau = \\ &= \mathcal{W} \sum_{j=1}^N \boldsymbol{a}_j \boldsymbol{a}_j^\dagger + \mathcal{J} \sum_{j=1}^N \boldsymbol{a}_j^\dagger (\boldsymbol{a}_{j+1} + \boldsymbol{a}_{j-1}) + \mathcal{U} \sum_{j=1}^N \boldsymbol{a}_j^{\dagger 2} \boldsymbol{a}_j^2 \end{aligned} \quad (13)$$

with suitable real parameters $\mathcal{W}$, $\mathcal{J}$ and $\mathcal{U}$.

The quantum Hamiltonian $\boldsymbol{h} + \bar{\boldsymbol{P}}_1$ is that of the standard BH model. Successive corrections $\bar{\boldsymbol{P}}_2, \bar{\boldsymbol{P}}_3$ and so on, are computable as well. Notice that the BH Hamiltonian is just the quantum version of the dBGP Hamiltonian.

As a matter of fact, the classical mechanics describes well both the dynamics and the statistical properties of condensed matter at high temperatures. On the other hand, the surprising feature of trapped cold atoms is that the lower their temperature is, the closer their dynamics is to that of the "classical" dBGP equation. The reasons of such a behavior are explained in [8], where it is proved that the quantum evolution of any operator $\boldsymbol{F}(\boldsymbol{a}, \boldsymbol{a}^\dagger)$ along the flow of the BH model is close (in a suitable sharp sense) to the evolution of its classical analogue along the flow of the dBGP model, over times that grow exponentially like $e^{\omega/T}$, where T is the temperature of the system. The results listed above may allow to improve such a conclusion extending it, in principle, to any higher order approximation (i.e. BH deformation) of the true Hamiltonian (1).

Chapter 1

Optical Cooling and Trapping of Atoms

A laser beam is a monochromatic wave with a specific frequency ω_L. The idea of scientists in 80's was that of exploiting the quantum jump and the emission of photons due to the atom-laser interaction, in order to cool down and trap atoms in laboratory.
The idea of this chapter is to illustrate how to construct a trap for an array of atoms with a laser beam. For precision measurements it is desirable to keep atoms inside the observation region as long as possible, free from interactions with other particles or with the wall of the vacuum chamber. In order to reach this goal, one has to reduce the atom velocity and trap the atoms for a sufficiently long time in a small and well-defined volume away from any wall of the vacuum vessel. This is possible due to new techniques of optical cooling and trapping, which allows one to reduce the temperature of an atomic gas down to below $1\mu K$ [5]. The first section of this chapter analyzes such technique in dimension one, instead in the second section we extend the method of trapping atoms in the three dimensional space.

1.1 One-dimensional Cooling

In order to illustrate the above technique, let's consider the following:

I) An atom, of mass m, which is moving with the velocity v along the $\hat{x}$ direction, in the ground state, where ΔE is the energy difference between the first excited state level and the ground one.

II) A photon with the specific frequency $\omega_L = \omega = \Delta E/\hbar$ and momentum

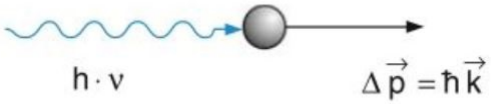

Figure 1.1: The image illustrates the first step of collision. The photon is represented by the blue arrow and it has momentum $p_L = \hbar k = h\nu/c$, instead the ball represents the atom, whose momentum varies by $\Delta p = p_L$.

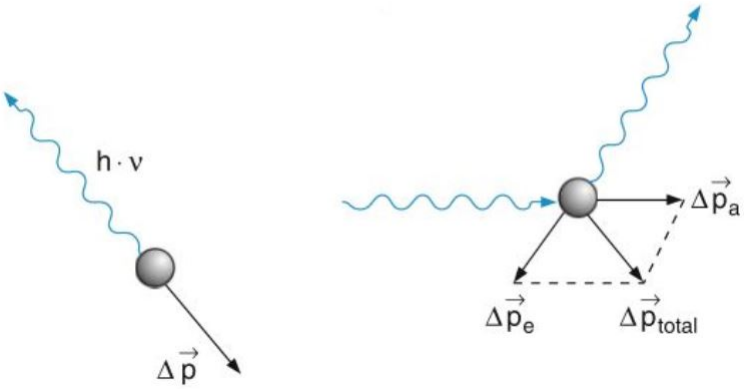

Figure 1.2: On the left side the second step of collision: emission of a fluorescence photon and recoil. On the right side: a complete collision.

$p_L = \hbar k$, traveling in the opposite direction of the atom $-\hat{x}$.
During the collision between these particles, the photon is absorbed by the atom and the total momentum $p = mv + \hbar k$ must be conserved (Figure 1.1). After photon absorption, the atom becomes excited and has a lower velocity $v' = v - (\hbar k)/m$ even if the speed variation is very small:

$$|\Delta v| = |v' - v| = |\hbar \frac{k}{m}| = h \frac{\nu}{mc}.$$

If instead of a photon one takes a laser beam, for conservation of energy and momentum, the atom slows down till it stops.
After absorption, the excited atom emits photon with frequency ω_L in a random direction and comes back to its ground state. Due to momentum conservation, the atom recoils in the opposite direction (Figure 1.2).

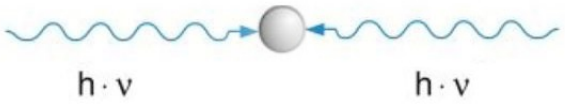

Figure 1.3: The image represents two photons sent against the atom, when the motion takes place along the $\hat{x}$ axis.

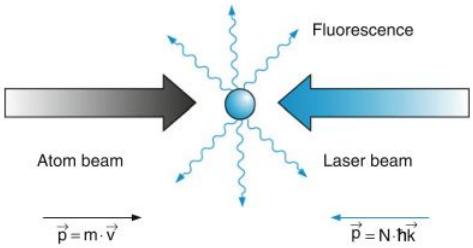

Figure 1.4: For many absorption-emission cycles, the average recoil of the fluorescence photons is zero and the net momentum transfer for N absorbed photons is $\Delta p = N\hbar k$.

Now let us assume the motion taking place along the $\hat{x}$ axis.
Suppose to send two photons against the atom, which is in its ground state, in opposite directions. The photons have frequency ω_L smaller than ω in order to trap the atom: $\omega_L < \omega = \Delta E/\hbar$ where ΔE is the energy difference between the first excited state and the ground one. If the atom is stationary then it remains stationary because ω_L is not large enough for atom to jump to its first excited level (Figure 1.3).
Instead, if the atom is moving with a velocity v then, by Doppler shift, it stops. Indeed due to its velocity, the atom perceives the photon (in the opposite direction of its motion) with a sufficient frequency $\omega'_L = \omega$ allowing the quantum jump. Then if it emits in any of the two possible directions, thus recoiling in the opposite one, the process starts again until the atom reaches a minimal velocity (kinetic energy), i.e. a minimal temperature.

1.2 Three-dimensional Cooling

In the previous section, it was discussed how to decelerate only one velocity component of atoms. The experimental goal is the deceleration of all the three velocity components resulting in a real three-dimensional cooling and

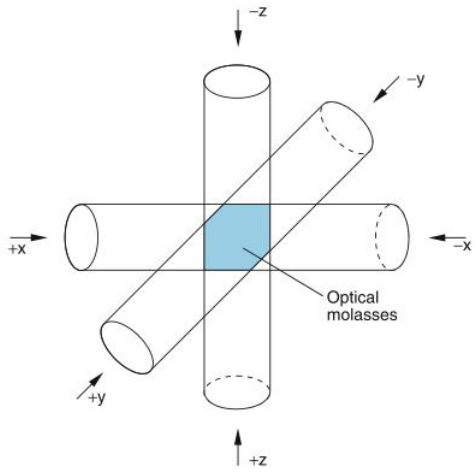

Figure 1.5: Optical molasses with six pair-wise counter propagating laser beams.

a corresponding reduction of the gas temperature. So one should decelerate and almost stop a single atom by extending this optical trap in the three dimensional space. When an atom in a gas cell is irradiated from six laser beams pointing into the $\hat{x}$, $\hat{y}$, $\hat{z}$ directions, the atom suffers a recoil if it absorbs photons from the six beams. The total recoil vanishes on (statistical) average and so the atom is trapped (Figure 1.5). When the laser frequency ω_L is slightly smaller than the resonance frequency ω atoms moving towards a laser beam have a larger probability to absorb a photon than those atoms that move in the direction of the beam. Therefore in this case the atoms are pushed towards the overlap region of the six laser beams. This method of trapping atoms is called "*Laser cooling*".

Often a magnetic field is used in order to box the array of atoms and isolate them from the outside. For this reason the trap is also call "Magneto-optical trap" (MOT) (Figure 1.6). Atoms can be trapped in a magneto-optical trap which consists of an anti-Helmholtz pair of coils, producing a cylindrically symmetric, homogeneous magnetic field which causes a Zeeman splitting of the absorption line that increases with increasing distance from the trap center. The trapping is caused by atomic recoil, due to photon absorption which depends on the distance from the trap center [5].

1.3 Optical Lattice

Trapping of atoms can be expressed by a confining periodic potential V. The interference between two counter propagating laser beams can be represented

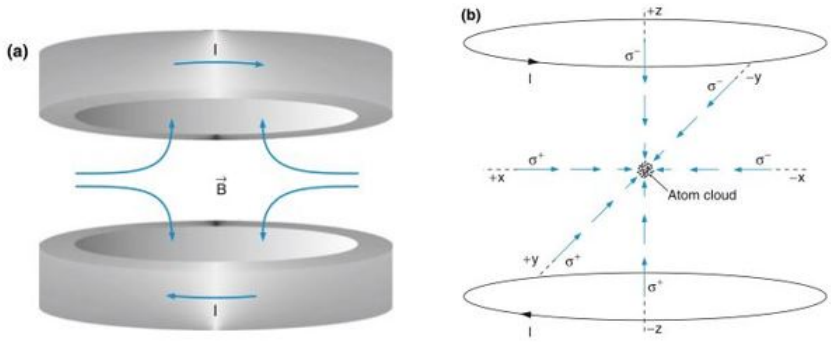

Figure 1.6: Principal arrangement of the magneto-optical trap MOT.

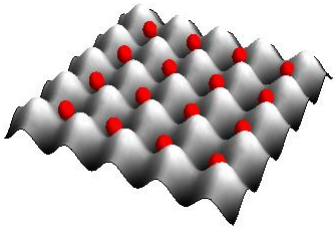

Figure 1.7: Optical lattice: in this case each atom occupies a well of the potential.

by an optical standing wave with period $\lambda/2$, in which atoms can be trapped and where $\lambda = c/\nu$ is the wavelength and ν is the frequency of the laser.
Such potential is generated by overlapping two counter propagating laser beams for each axis direction. Atoms thus trapped are often called **Cold Atoms** because their low kinetic energy. The potential minima form an optical lattice with a lattice constant $d = \lambda/2$. Neutral atoms can be trapped in such potential minima of the lattice. Depending on the atomic density in the condensate the different minima can be populated with N atoms ($N = 0; 1; 2; \dots$). This allows to study interactions between atoms in the same minimum or in neighboring minima.
It's experimentally possible to construct an atomic array with up to about hundred cold atoms each staying in the bottom of the well of effective periodic potential $V(x)$ (Figure 1.7). From now on we assume a periodic potential of the following form:

$$V(x) = V_0 \sin^2(kx) = V_0 \frac{1 - \cos(2kx)}{2}, \tag{1.1}$$

where $k = 2\pi/\lambda$ is the wave vector of the laser light and V_0 is the maximum depth of lattice potential. The period d of the potential is obtained by setting

$2kd = 2\pi$ so that $d = \pi/k$. In atomic array $d = \pi/k = \lambda/2$ represents the space between two consecutive atoms where each of them occupies a well of the potential. Recall that holds $\lambda\nu = c$ where $\nu = \omega/2\pi$ and $d = \pi c/\omega$; moreover $\omega = \Delta E/\hbar$ so that:

$$d = \frac{\pi c\hbar}{\Delta E}. \tag{1.2}$$

Such relation tells that the distance d is related to ΔE which changes according to the given atom. Often scientists use Rubidium 87 with a suitable laser light. The choice of the atom and laser depends by the ability to reproduce the experiment in laboratory. Sometimes instead of atoms are used ions whose interaction is different with respect to neutral atoms. The different interaction influences the choice of the potential U which appears in the Hamiltonian.

Coulomb's force expresses the interaction between two ions (of charge q_1 and q_2):

$$F(d) = k\frac{q_1 q_2}{d^2}\ ; \qquad U(d) = \frac{q_1 q_2}{d}. \tag{1.3}$$

The interaction between two neutral atoms is expressed by the Lennard-Jones's potential (Figure 1.8):

$$U(d) = \frac{B}{d^n} - \frac{C}{d^6}\ , \tag{1.4}$$

where:

- B and C are positive constants for the repulsive and attractive component, respectively.
- $n \geq 12$ is a phenomenology parameter, useful for describing Pauli exclusion principle.

In experiments Rubidium atoms have $\lambda \approx 780$ nm so: $d_{ca} = \lambda/2 \approx 4 \cdot 10^{-5}$ cm. Instead in condensed matter the dimension of atoms is $\dot{A} = 10^{-8}$cm and the distance between them is almost the same $d_{cm} \approx 10^{-8}$ cm. This implies that the distance between cold trapped atoms is much larger than that in ordinary condensed matter: $d_{ca} = 10^3 d_{cm}$. From now on, due to the distance between particles, the repulsive part of potential will be omitted and we will considered only the Van der Waals component $-C/d^6$. The possibility of tunneling effect (that would bring two atoms into the same well) is inhibited by the low temperature of the atoms.

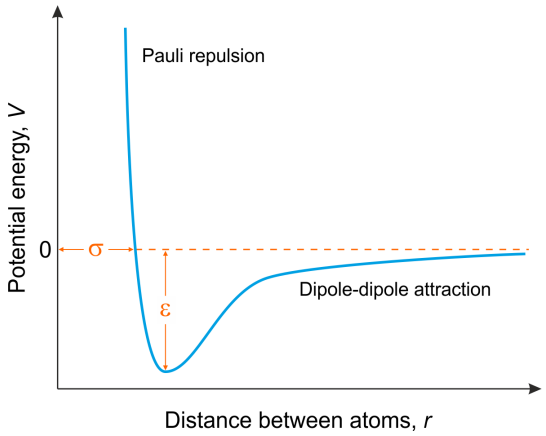

Figure 1.8: U is the intermolecular potential between two neutral atoms or molecules, ε is the well depth and a measure of how strongly the two particles attract each other, σ is the distance at which the intermolecular potential between the two particles is zero, r is the distance of separation between centers of both particles.

The Van der Waals form potential energy U_1 of a single neutral atom due to its interaction with the other ones, that are equally spaced, is:

$$\begin{aligned} U_1 &= 2\Big(-\frac{C}{d^6}-\frac{C}{(2d)^6}-\frac{C}{(3d)^6}+\dots\Big)= \\ &= -\frac{2C}{d^6}\Big(1+\frac{1}{2^6}+\frac{1}{3^6}+\dots\Big). \end{aligned} \tag{1.5}$$

Note that the Van der Waals interaction quickly vanishes at large distances between interacting atoms. It's a generalized harmonic series, which always converges. One can neglect terms of order higher than first one (which means retaining only the nearest neighbor interaction), because they give only a small correction to the value of the series. On the other hand, consider an array of equally spaced ions of charge q. The Coulomb potential energy of one of them is:

$$\begin{aligned} U_1 &= 2\Big(\frac{q^2}{d}+\frac{q^2}{2d}+\frac{q^2}{3d}+\dots\Big)= \\ &= \frac{2q^2}{d}\Big(1+\frac{1}{2}+\frac{1}{3}+\dots\Big). \end{aligned} \tag{1.6}$$

If the number of ions is infinite the previous expression is a harmonic series, that is logarithmically divergent. Condensed matter ions have alternating charges so for the Leibniz's criterion the sum converges.

The energy is infinite. In such cases we speak about long range forces because the contribution of interactions between distant ions cannot be neglected.

Chapter 2

Classical-Mechanical System

The central idea of this chapter is to analyze the problem from the point of view of classical mechanics. In the first part we will write the classical Hamiltonian and study the boundary conditions due to the periodicity of the model. The next section consists in studying the small nonlinear motions of the system close to ideal crystal equilibrium expanding the potentials V about 0, and U about d, and then to apply perturbation theory. The Hamiltonian is now regarded as a perturbation of the Hamiltonian h of N non interacting, identical harmonic oscillators. The central idea of Hamiltonian perturbation theory consists in looking for a change of variables that removes, partially, the perturbations up to some pre-fixed order n. We will compute the normal form to second order. The Hamiltonian $h + \bar{P}_1$ is that of the discrete Nonlinear Schrödinger (dNLS), or discrete Bogolyubov-Gross-Pitaevskii (dBGP) equation, a complex equation which is guessed to describe the dynamics of the atomic array at extremely low temperatures.

2.1 Model and Classical Hamiltonian

The most general classical Hamiltonian for a N array of neutral atoms interacting through a two-body potential U while moving in an external potential

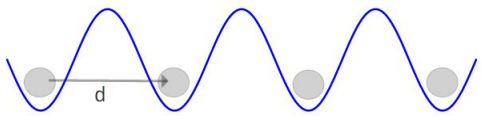

Figure 2.1: The image represents a sketch of the array of atoms confined by the periodic potential V. Each atom occupies a well of the potential.

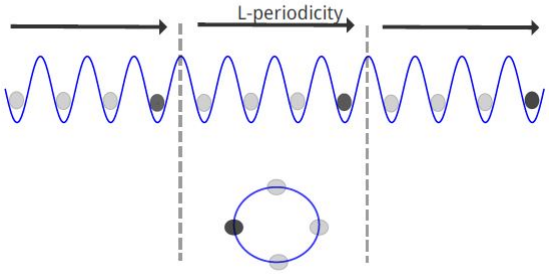

Figure 2.2: Extended the model by periodicity.

V is described by the Frenkel-Kontorova model:

$$H(x,p) = \sum_{j=1}^{N} \left[\frac{{p_j}^2}{2m} + U(x_{j+1} - x_j) + V(x_j) \right], \tag{2.1}$$

where m is the atom mass and

- ${p_j}^2/2m$ is the kinetic energy for single particle;
- $U(x_{j+1} - x_j) = -C/(x_{j+1} - x_j)^6$ is the interaction potential between two consecutive particles;
- $V(x_j) = V_0 \sin^2(kx_j)$ is the periodic potential due to the laser.

2.1.1 Boundary Conditions

A priori such model could be constructed with an infinite number of atoms. The period of the optical potential V is d and we suppose to have the system to be periodic of period L where $L >> d$. Now we consider, in such infinite L-periodic model, only one period (Figure 2.2). The topology (but not geometry), where such periodic model lives in, is the same of the circle in which, roughly speaking, the first particle is identified with the last one.

Of course the fundamental period d of the optical potential is related with the number of particles N by $L = dN$ which will be justified in the next section. Boundary conditions for positions and momenta result by imposing L-periodicity:

$$x_{j+N} = x_j + L; \qquad j = 1 \dots N, \tag{2.2}$$

$$p_{j+N} = p_j; \qquad j = 1 \dots N. \tag{2.3}$$

Remark 1 *The interaction potential between the consecutive particles which occupy x_0 and x_1 positions is the same as the ones between x_N and x_{N+1}, indeed:*

$$U(x_{N+1} - x_N) = U(x_1 + L - x_N) = U(x_1 + L - (x_0 + L)) = U(x_1 - x_0).$$

The periodic boundary conditions are equivalent to study the problem in $\mathbb{Z} \mod N$, denoted by $\mathbb{Z}_N$. For this reason the sum which appears in the Hamiltonian is denoted, from now on, by $\sum_{j\in\mathbb{Z}_N}$.

2.1.2 Classical Hamiltonian Equations

The classical Hamiltonian equations of the system (2.1) are:

$$\begin{aligned}
\dot{x_j} &= \frac{\partial H}{\partial p_j} = \frac{p_j}{m} \ ; \\
\dot{p_j} &= -\frac{\partial H}{\partial x_j} = \\
&= -\Big[\frac{\partial U(x_{j+1} - x_j)}{\partial x_j} + \frac{\partial U(x_j - x_{j-1})}{\partial x_j} + \frac{\partial V(x_j)}{\partial x_j}\Big] = \\
&= -\Big[\frac{-6C}{(x_{j+1} - x_j)^7} + \frac{6C}{(x_j - x_{j-1})^7} + V_0\frac{1}{2}\Big(2k\sin(2kx_j)\Big)\Big] = \\
&= \frac{6C}{(x_{j+1} - x_j)^7} - \frac{6C}{(x_j - x_{j-1})^7} - kV_0\sin(2kx_j).
\end{aligned}$$

2.1.3 Crystal Equilibrium

Let us now consider the equilibrium solutions obtained by solving the system:

$$\begin{aligned}
0 &= \frac{\partial H}{\partial p_j} = \frac{p_j}{m} \implies p_j = 0 \ ; \\
0 &= -\frac{\partial H}{\partial x_j} = \Big[\frac{\partial U(x_j - x_{j-1})}{\partial x_j} - \frac{\partial U(x_{j+1} - x_j)}{\partial x_j} - \frac{\partial V(x_j)}{\partial x_j}\Big].
\end{aligned}$$

The first equation expresses a stationary condition for the j-th particle. Now we focus our attention on equally spaced equilibria, which means:

$$x_{j+1} - x_j = d \qquad \forall j \in \mathbb{Z}. \tag{2.4}$$

In this particular case one gets:

$$\frac{\partial U(x_{j+1} - x_j)}{\partial x_j} = \frac{\partial U(d)}{\partial x_j} = 0, \tag{2.5}$$

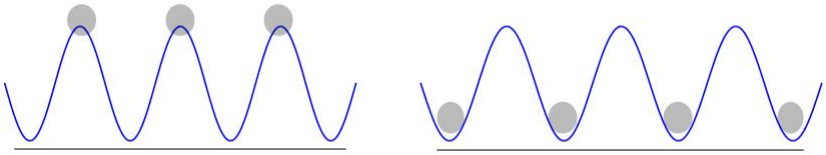

Figure 2.3: Two examples of equally spaced particles.

so solving the second equation one obtains:

$$0 = -\frac{\partial V(x_j)}{\partial x_j} = kV_0 \sin(2kx_j), \tag{2.6}$$

$$2k\bar{x}_j = \pi s \Longrightarrow \bar{x}_j = \frac{\pi}{2k}s = \frac{\lambda}{4}s \quad \forall s \in \mathbb{Z}, \tag{2.7}$$

where $k = \lambda/2$.
Assuming $s = 2j$ means that the particles are in the bottom of each well (Figure 2.3).

$$\bar{x}_j = \frac{\lambda}{2}j = dj \qquad \forall j \in \mathbb{Z}. \tag{2.8}$$

Such type of equilibria are referred to **Crystal Equilibria**. If one now imposes periodic boundary conditions then, the number of particles N, considering only a period L, is related to the fundamental period d by the following formula that holds for all $j \in \mathbb{Z}$:

$$\bar{x}_{j+N} \quad = \quad \bar{x}_j + L \tag{2.9}$$

which, due to (2.8), becomes $(j+N)d = jd + L$ and implies $Nd = L$.

2.1.4 Analysis of Potentials

The perturbative setting consists in studying the small non linear motions of the systems close to the crystal equilibrium. In order to reach this goal one has to first perform a simple translation of the position variables:

$$x_j = \bar{x}_j + q_j = jd + q_j; \qquad p_j = p_j. \tag{2.10}$$

The periodic boundary conditions satisfied by the canonical variables q_j and p_j are:

$$q_{j+N} = q_j \ ; \qquad\qquad j = 1 \dots N, \tag{2.11}$$

$$p_{j+N} = p_j \ ; \qquad\qquad j = 1 \dots N. \tag{2.12}$$

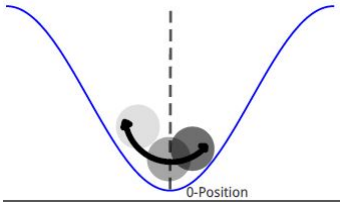

Figure 2.4: The image represents small motions of neutral atoms around their crystal equilibrium.

Consider such translation and re-write the expression of potentials with this change of variables:

$$U(x_{j+1} - x_j) = U(\bar{x}_{j+1} + q_{j+1} - \bar{x}_j - q_j) = U(d + q_{j+1} - q_j); \tag{2.13}$$
$$V(x_j) = V(\bar{x}_j + q_j) = V(jd + q_j) = V(q_j). \tag{2.14}$$

Now, assuming that the atoms perform small oscillations around their ideal equilibrium position, one can make a Taylor expansion of V (Figure 2.4). The periodicity of the potential implies that:

$$V(jd) = V(d) = V(0) = 0 \text{ and } V'(jd) = V'(0) = 0,$$

$$V(q_j) = V(0) + V'(0)q_j + \frac{1}{2}V''(0){q_j}^2 + \frac{1}{6}V'''(0){q_j}^3 + \dots. \tag{2.15}$$

In the specific case of the periodic potential $V(q_j) = V_0 \sin^2(kq_j)$, the Taylor expansion has the form:

$$\begin{aligned}
V(q_j) &= \frac{V_0}{2}[1 - \cos(2kq_j)] = \\
&= \frac{V_0}{2}\Big[1 - \Big(1 - \frac{1}{2!}(2kq_j)^2 + \frac{1}{4!}(2kq_j)^4 - \frac{1}{6!}(2kq_j)^6 + \dots\Big)\Big] = \\
&= \frac{V_0}{2}\Big[\frac{1}{2}4(kq_j)^2 - \frac{1}{24}16(kq_j)^4 + \frac{1}{720}64(kq_j)^6 + \dots\Big] = \\
&= V_0\Big[(kq_j)^2 - \frac{1}{3}(kq_j)^4 + \frac{2}{45}(kq_j)^6 + \dots\Big] = \\
&= V_0\Big[\Big(\frac{\pi}{d}q_j\Big)^2 - \frac{1}{3}\Big(\frac{\pi}{d}q_j\Big)^4 + \frac{2}{45}\Big(\frac{\pi}{d}q_j\Big)^6 + \dots\Big],
\end{aligned}$$

where $k = \pi/d$ and $q_j/d << 1$, which means that the Taylor expansion holds only for small displacements from the equilibrium position thus

$$V_{tot}(q) = \sum_{j\in\mathbb{Z}_N} V(q_j) = \sum_{j\in\mathbb{Z}_N} V_0\Big[\Big(\frac{\pi}{d}q_j\Big)^2 - \frac{1}{3}\Big(\frac{\pi}{d}q_j\Big)^4 + \frac{2}{45}\Big(\frac{\pi}{d}q_j\Big)^6 + \dots\Big]. \tag{2.16}$$

Notice that the optical potential is periodic of period d with an even axial symmetry so that: $V(x) = V(-x)$ and $V(0) = 0$.
In addition if the interaction force between particles is weak, then one can Taylor expanded the potential U around d:

$$\begin{aligned} U(d + q_{j+1} - q_j) &= U(d) + U'(d)(q_{j+1} - q_j) + \frac{1}{2!}U''(d)(q_{j+1} - q_j)^2 + \\ &+ \frac{1}{3!}U'''(d)(q_{j+1} - q_j)^3 + \dots . \end{aligned} \tag{2.17}$$

The potential energy due to the sum of all interactions has the following expression:

$$\begin{aligned} U_{tot}(q) &= \sum_{j\in\mathbb{Z}_N} U(d + q_{j+1} - q_j) = \\ &= NU(d) + U'(d)\sum_{j\in\mathbb{Z}_N}(q_{j+1} - q_j) + \frac{U''(d)}{2}\sum_{j\in\mathbb{Z}_N}(q_{j+1} - q_j)^2 + \\ &+ \frac{U'''(d)}{6}\sum_{j\in\mathbb{Z}_N}(q_{j+1} - q_j)^3 + \cdots = \\ &= NU(d) + \frac{U''(d)}{2}\sum_{j\in\mathbb{Z}_N}(q_{j+1} - q_j)^2 + \frac{U'''(d)}{6}\sum_{j\in\mathbb{Z}_N}(q_{j+1} - q_j)^3 + \dots , \end{aligned}$$

where the last equality holds because the first sum $\sum_{j=1}^{N}(q_{j+1} - q_j) = q_{N+1} - q_1 = 0$.
In the specific case of the Van der Walls interaction, derivatives of different orders are:

$$U(d) = -\frac{C}{d^6}, \quad U''(d) = -\frac{42C}{d^8}, \quad U'''(d) = \frac{336C}{d^9},$$

and the Taylor expansion is given by:

$$\begin{aligned} U_{tot}(q) &= -\frac{NC}{d^6} - \frac{21C}{d^8}\sum_{j\in\mathbb{Z}_N}(q_{j+1} - q_j)^2 + \frac{56C}{d^9}\sum_{j\in\mathbb{Z}_N}(q_{j+1} - q_j)^3 + \cdots = \\ &= -\frac{C}{d^6}\Big[N + \frac{21}{d^2}\sum_{j\in\mathbb{Z}_N}(q_{j+1} - q_j)^2 - \frac{56}{d^3}\sum_{j\in\mathbb{Z}_N}(q_{j+1} - q_j)^3 + \dots\Big]. \end{aligned} \tag{2.18}$$

Now, the Hamiltonian, takes on the following form:

$$H(q,p) = \sum_{j\in\mathbb{Z}_N} \Big[\frac{{p_j}^2}{2m} + V(q_j) + U(q_{j+1}-q_j)\Big] =$$
$$= \sum_{j\in\mathbb{Z}_N} \Big[\frac{{p_j}^2}{2m} + V_0\Big((kq_j)^2 - \frac{1}{3}(kq_j)^4 + \frac{2}{45}(kq_j)^6\Big) +$$
$$+ \Big(\frac{U''(d)}{2}(q_{j+1}-q_j)^2 + \frac{U'''(d)}{6}(q_{j+1}-q_j)^3\Big) + \dots\Big]. \qquad (2.19)$$

In order to have an easier writing of the Hamiltonian rename some constants, linked to the derivatives of V and U, and replace them into H.

- $\omega := \sqrt{\frac{2V_0k^2}{m}} \to V_0k^2 = \frac{m\omega^2}{2}$;
- $\Lambda := \frac{4V_0k^4}{3} \to \frac{V_0k^4}{3} = \frac{\Lambda}{4}$;
- $\Gamma := \frac{4V_0k^6}{15} \to \frac{\Gamma}{6} = \frac{2V_0k^6}{45}$;
- $K := U''(d)$;
- $\alpha := \frac{U'''(d)}{2}$.

The Hamiltonian now reads:

$$H(q,p) = \sum_{j\in\mathbb{Z}_N} \Big[\Big(\frac{{p_j}^2}{2m} + \frac{m\omega^2}{2}q_j^2\Big) + \Big(-\frac{\Lambda}{4}q_j^4 + \frac{K}{2}(q_{j+1}-q_j)^2\Big)$$
$$+ \Big(\frac{\Gamma}{6}q_j^6 + \frac{\alpha}{3}(q_{j+1}-q_j)^3\Big) + \dots\Big]. \qquad (2.20)$$

2.2 Perturbation Theory

The idea of this section is to write H in the form:

$$H(q,p) = h(q,p) + P_1(q) + P_2(q) + \dots \qquad (2.21)$$

where h is an integrable unperturbed Hamiltonian and $P := H - h$ is called the **Perturbation** split into ordered perturbation terms P_1 (first order perturbation), P_2 (second order perturbation), and so on, with the following property

$$||X_h|| >> ||X_{P_1}|| >> ||X_{P_2}|| >> \dots$$

in the sense of vector fields.

In our particular case the unperturbed Hamiltonian h is given by the Hamiltonian of N independent identical harmonic oscillators, so that:

$$h(q,p) := \sum_{j\in\mathbb{Z}_N} \Big(\frac{{p_j}^2}{2m} + \frac{m\omega^2}{2} q_j^2\Big); \tag{2.22}$$

$$P_1(q) := \sum_{j\in\mathbb{Z}_N} \Big(-\frac{\Lambda}{4} q_j^4 + \frac{K}{2}(q_{j+1}-q_j)^2\Big); \tag{2.23}$$

$$P_2(q) := \sum_{j\in\mathbb{Z}_N} \Big(\frac{\Gamma}{6} q_j^6 + \frac{\alpha}{3}(q_{j+1}-q_j)^3\Big). \tag{2.24}$$

2.2.1 Hamiltonian Normal Form

The central idea of Hamiltonian perturbation theory, which goes back to Lagrange and Poincaré and has then be developed by Birkhoff, Bogoliubov and Kolmogorov, consists in looking for a change of variables that removes, completely or partially, the perturbation P_i from H, up to some pre-fixed order. Complete removal of the perturbation, already at first order (i.e. the complete removal of P_1) is not possible, in general.

Definition 2 *(Normal form). A Hamiltonian $H^{(n)}$ of the form*

$$H^{(n)} = h + \sum_{j=1}^{n} \bar{P}_j + R_{n+1}, \tag{2.25}$$

*where $\{\bar{P}_j, h\} = 0$ for any $j = 1,\dots,n$ is said to be in **Normal Form** to order n with respect to h.*

The perturbations terms $\bar{P}_j$ are first integrals of h, which includes also the case of absence of perturbation of order j that is $\bar{P}_j = 0$.

The aim of Hamiltonian perturbation theory is finding a suitable change of variables that maps the quasi-integrable Hamiltonian (2.21) into its normal form to some fixed order. Then one looks for a smooth, close to the identity, canonical change of variables of the type

$$C : (p,q) \longmapsto (Q,P)$$

such that $H \circ C^{-1}$ is in normal form:

$$H(C^{-1}(Q,P)) = h(Q,P) + \bar{P}_1(Q,P) + \bar{P}_2(Q,P) + \dots. \tag{2.26}$$

in which $\bar{P}_1, \bar{P}_2, \dots$ are first integrals of h.

Remark 3 *A precise formulation of Lagrange's theory of perturbation shows that $\bar{P}_1$ is the time average of P_1 on the unperturbed flow of h, instead $\bar{P}_2$ is the time average on the unperturbed Hamiltonian flow of h of P_2 plus another term depending on P_1.*

The canonical transformation C is very conveniently made by composing the Hamiltonian flows of suitable generating Hamiltonians at unit times. Each generating Hamiltonian defines a flow whose composition gives the canonical transformation:

$$C = \Phi^{-1}_{G_n} \circ \Phi^{-1}_{G_{n-1}} \circ \cdots \circ \Phi^{-1}_{G_1}.$$

Where $\Phi^{-1}_{G_j}$ is the flow of the Hamiltonian G_j at time -1.
The $G_1, \ldots, G_n$ are called the **Generating Hamiltonians** of the canonical transformation, to be determined order by order. An Averaging theorem ensures that given a Hamiltonian H there is always a (local) canonical transformation C for a suitable choice of $G_1, \ldots, G_n$.

2.2.2 Birkhoff Variables

Let us introduce the complex coordinates (z, z^*) known as **Complex Birkhoff Variables**:

$$z_j := \frac{m\omega q_j + \imath p_j}{\sqrt{2m\omega}} \; ; \qquad {z_j}^* := \frac{m\omega q_j - \imath p_j}{\sqrt{2m\omega}}, \tag{2.27}$$

where $\imath$ is the imaginary unit ($\imath^2 = -1$).
In terms of such coordinates the previous variables p_j and q_j become:

$$q_j = \frac{z_j + {z_j}^*}{\sqrt{2m\omega}} \; ; \qquad p_j = \sqrt{2m\omega}\frac{z_j - {z_j}^*}{2\imath}. \tag{2.28}$$

One also gets:

$$|z_j|^2 = z_j \cdot z_j^* = \frac{(m\omega q_j)^2 + {p_j}^2}{2m\omega} = \frac{1}{\omega} h. \tag{2.29}$$

The next steps are: to express H in terms of the complex Birkhoff variables, to compute its normal form, to some prefixed order with respect to the unperturbed Hamiltonian (2.22). We obtain such Hamiltonian replacing the expressions (2.28)-(2.29) in the (2.20):

$$H(z, z^*) = h(z, z^*) + P_1(z, z^*) + P_2(z, z^*) + \ldots \tag{2.30}$$

The unperturbed Hamiltonian h and the first two order perturbations P_1 and P_2 in terms of Birkhoff variables become:

$$h(z,z^*) := \sum_{j\in\mathbb{Z}_N} \omega|z_j|^2; \tag{2.31}$$

$$P_1(z,z^*) := \sum_{j\in\mathbb{Z}_N} \Big\{ \frac{-\Lambda}{16m^2\omega^2}(z_j + {z_j}^*)^4 + \frac{K}{4m\omega}\Big[(z_{j+1} + {z_{j+1}}^*) - (z_j + {z_j}^*)\Big]^2 \Big\}; \tag{2.32}$$

$$P_2(z,z^*) := \sum_{j\in\mathbb{Z}_N} \Big\{ \frac{\Gamma}{48m^3\omega^3}(z_j + z_j^*)^6 + \frac{\alpha}{3\sqrt{2m\omega}^3}\Big[(z_{j+1} + z_{j+1}^*) - (z_j + z_j^*)\Big]^3 \Big\}. \tag{2.33}$$

The Poisson bracket of two functions F and G on the phase space reads:

$$\{F,G\}_{pq} \;=\; \sum_j \Big(\frac{\partial F}{\partial q_j}\frac{\partial G}{\partial p_j} - \frac{\partial F}{\partial p_j}\frac{\partial G}{\partial q_j}\Big), \tag{2.34}$$

which, in terms of the Birkhoff variables becomes:

$$\{F,G\}_{zz^*} \;=\; -\imath\sum_j \Big(\frac{\partial F}{\partial z_j}\frac{\partial G}{\partial z_j^*} - \frac{\partial F}{\partial z_j^*}\frac{\partial G}{\partial z_j}\Big). \tag{2.35}$$

The fundamental Poisson brackets are:

$$\{z_j, z_k^*\} = -\imath\delta_{j,k} \;\text{ and }\; \{z_j, z_k\} = \{z_j^*, z_k^*\} = 0. \tag{2.36}$$

Let's focus on the Hamiltonian given by the sum of N harmonic independent oscillator Hamiltonians, i.e. $h = \sum_j \omega|z_j|^2$ to which there correspond the Hamiltonian equations:

$$\dot{z_j} = \{z_j, h\} = -\imath\sum_k \frac{\partial z_j}{\partial z_k}\frac{\partial h}{\partial z_k^*} = -\imath\frac{\partial h}{\partial z_j^*} = -\imath\omega z_j, \tag{2.37}$$

and similarly

$$\dot{z_j^*} = \{z_j^*, h\} = \imath\sum_k \frac{\partial z_j^*}{\partial z_k^*}\frac{\partial h}{\partial z_k} = \imath\frac{\partial h}{\partial z_j} = \imath\omega z_j^*. \tag{2.38}$$

Thus, with respect to the Birkhoff vector $(z,z^*)^T$, the equations of motion of the harmonic Hamiltonian are:

$$\begin{pmatrix} \dot{z} \\ \dot{z^*} \end{pmatrix} = \begin{pmatrix} -\imath\omega & 0 \\ 0 & \imath\omega \end{pmatrix}\begin{pmatrix} z \\ z^* \end{pmatrix}. \tag{2.39}$$

The flow Φ_h^s of the Hamiltonian h is the solution of the Hamiltonian equations at time s, corresponding to any given initial condition $(z_0, z_0^*)^T$ at $s = 0$. The explicit expression of the flow is:

$$\Phi_h^s(z_0, z_0^*)^T = \exp(sA)(z_0, z_0^*)^T = (z_0 e^{-\imath\omega s}, z_0^* e^{\imath\omega s})^T. \tag{2.40}$$

2.2.3 Averaging Theory [4]

A canonical change of variables leaves the Hamiltonian equations invariant in form. A very convenient way of performing the canonical transformations is to do it through Hamiltonian flows. To such a purpose, let us consider a Hamiltonian $h(x)$ and its associated Hamiltonian equations $\dot{x} = X_h(x)$. Let Φ_h denote the flow of h, so that $\Phi_h^s(y)$ is the solution of the Hamiltonian equations at time s, corresponding to the initial condition y at $s = 0$. We also denote by

$$L_h := \{, h\} = (J\nabla h) \circ \nabla = X_h \circ \nabla, \tag{2.41}$$

the Lie derivative along the Hamiltonian vector field X_h; notice that $L_h F = \{F, h\}$.

Lemma 4 *For any function F one has*

$$F \circ \Phi_h^s = e^{sL_h} F.$$

Proof. Set $\tilde{F}(s) := F \circ \Phi_h^s$ and notice that $\tilde{F}(0) = F$. Then

$$\frac{d}{ds}\tilde{F}(0) = \{F, h\} = L_h F.$$

Then

$$\begin{aligned}\frac{d}{ds}\tilde{F}(s) &= \lim_{\varepsilon\to 0}\frac{\tilde{F}(s+\varepsilon) - \tilde{F}(s)}{\varepsilon} = \lim_{\varepsilon\to 0}\frac{\tilde{F}(s)\circ\Phi_h^\varepsilon - \tilde{F}(s)}{\varepsilon} = \\ &= \frac{d}{ds}\tilde{F}(s)\circ\Phi_h^\varepsilon\Big|_{\varepsilon=0} = \{\tilde{F}(s), h\} = L_h\tilde{F}(s)\end{aligned}$$

whose solution is

$$\tilde{F}(s) = e^{sL_h}\tilde{F}(0) = e^{sL_h}F.$$

■

Definition 5 *Given the Hamiltonian h, for any real function F on the phase space, its time-average $\langle F\rangle_h$ along the flow of h and its deviation from the average $\delta_h F$ are defined by:*

$$\langle F\rangle_h := \lim_{t\to+\infty}\frac{1}{t}\int_0^t (F\circ\Phi_h^s)\mathrm{d}s; \tag{2.42}$$

$$\delta_h F := F - \langle F\rangle_h. \tag{2.43}$$

In the particular case in which the Hamiltonian h is periodic, of period τ, one has

$$\langle F\rangle_h := \frac{1}{\tau}\int_0^\tau (F\circ\Phi_h^s)\mathrm{d}s. \tag{2.44}$$

Lemma 6 *The time-average $\langle\cdot\rangle_h$ is invariant with respect to the flow of h, i.e. for any function F one has*

$$\langle F\rangle_h \circ \Phi_h^s = \langle F\rangle_h \, \forall s \;\Leftrightarrow\; L_h \langle F\rangle_h = 0.$$

Proof. Two equivalent proofs of the statement are given. The first one starts by writing down explicitly $\langle F\rangle_h \circ \Phi_h^s$ and making use of the group property of the flow, namely $\Phi_h^r \circ \Phi_h^s = \Phi_h^{r+s}$, which yields:

$$\langle F\rangle_h \circ \Phi_h^s = \lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau (F\circ\Phi_h^{s+r})\mathrm{d}r = \lim_{\tau\to\infty}\frac{1}{\tau}\int_s^{\tau+s}(F\circ\Phi_h^u)\mathrm{d}u.$$

Now, by splitting $\int_s^{\tau+s}\mathrm{d}u = \int_s^0\mathrm{d}u + \int_0^\tau \mathrm{d}u + \int_\tau^{\tau+s}\mathrm{d}u$, observing that the first and the third integral are on bounded intervals, and making use of the boundedness hypothesis on Φ_h^t, the thesis of the Lemma follows. The second proof starts from the chain of identities

$$\frac{d}{ds}F\circ\Phi_h^s = L_hF\circ\Phi_h^s = \{F,h\}\circ\Phi_h^s = \{F\circ\Phi_h^s, h\}.$$

Now, integrating the above identity (left and rightmost members) from 0 to t and dividing by t, one gets

$$\frac{F\circ\Phi_h^t - F}{t} = \frac{1}{t}\int_0^t \{F\circ\Phi_h^s, h\}\mathrm{d}s = \left\{\frac{1}{t}\int_0^t F\circ\Phi_h^s\mathrm{d}s, h\right\}$$

where the second equality follows by the bi-linearity of the Poisson bracket (think of computing the integral as the limit of Riemann sums). The thesis of the lemma, right form, follows in the limit as $t\to+\infty$, by observing that the left hand side of above identity vanishes in the limit (recall the boundedness of the flow). ■

Lemma 7 *For any function F, the solution of the equation*

$$L_hG = \delta_hF \Leftrightarrow \{G,h\} = F - \langle F\rangle_h,$$

is given by

$$G = K + L_h^{-1}\delta_h(F) := K + \lim_{t\to+\infty}\frac{1}{t}\int_0^t (s-t)(\delta_hF\circ\Phi_h^s)\mathrm{d}s \qquad (2.45)$$

where K is an arbitrary element of $\ker L_h$.

Proof. Taking into account the Homological equation $L_hG = \delta_h(F)$

$$\begin{aligned}
L_hG &= \delta_h(F) \\
\lim_{t\to+\infty}\frac{1}{t}\int_0^t (s-t)e^{sL_h}L_hG\mathrm{d}s &= \lim_{t\to+\infty}\frac{1}{t}\int_0^t (s-t)e^{sL_h}\delta_h(F)\mathrm{d}s \\
\lim_{t\to+\infty}\frac{1}{t}\int_0^t (s-t)\frac{d}{ds}(e^{sL_h}G)\mathrm{d}s &= \lim_{t\to+\infty}\frac{1}{t}\int_0^t (s-t)e^{sL_h}\delta_h(F)\mathrm{d}s \\
\lim_{t\to+\infty}\frac{1}{t}\Big\{\Big[(s-t)(e^{sL_h}G)\Big]_0^t - \int_0^t e^{sL_h}G\mathrm{d}s\Big\} &= \lim_{t\to+\infty}\frac{1}{t}\int_0^t (s-t)e^{sL_h}\delta_h(F)\mathrm{d}s \\
G - \lim_{t\to+\infty}\frac{1}{t}\int_0^t e^{sL_h}G\mathrm{d}s &= \lim_{t\to+\infty}\frac{1}{t}\int_0^t (s-t)e^{sL_h}\delta_h(F)\mathrm{d}s
\end{aligned}$$

$$G = K + \lim_{t\to+\infty}\frac{1}{t}\int_0^t (s-t)\Big(\delta_hF\circ\Phi_h^s\Big)\mathrm{d}s.$$

The choice of $K = \lim_{t\to+\infty}\frac{1}{t}\int_0^t e^{sL_h}G\mathrm{d}s$ is not unique thanks to $K \in \ker L_h$. ■

Notice that in the particular case in which the Hamiltonian h is periodic, of period τ one has

$$G - K = \frac{1}{\tau}\int_0^\tau s\Big(\delta_hF\circ\Phi_h^s\Big)\mathrm{d}s. \tag{2.46}$$

Theorem 1 *(Averaging principle). Consider a quasi integrable Hamiltonian $H_\lambda = h + \lambda P_1 + \lambda^2 P_2 + \dots$ where $H_0 = h$ is integrable and its flow bounded in some norm. Here λ denotes the small parameter. Then*
I) For any choice of the generating Hamiltonians $G_1, ..., G_n$ defining the canonical transformation $C_\lambda = \Phi_{G_n}^{\lambda^{-n}}\circ\Phi_{G_{n-1}}^{\lambda^{-(n-1)}}\circ\cdots\circ\Phi_{G_1}^{\lambda^{-1}}$, one has

$$H_\lambda^{(n)} = H_\lambda\circ C_\lambda^{-1} = h + \sum_{j=1}^n \lambda^j\bar{P}_j + R_{n+1},$$

where, for $j = 1, \dots, n$ and starting with $F_1 = 0$,

$$\bar{P}_j = -L_hG_j + P_j + F_j[h, P_1, \dots, P_{j-1}, G_1, \dots, G_{j-1}];$$

$$R_{n+1} = \sum_{j\geq n+1}\lambda^j(P_j + F_j[h, P_1, \dots, P_{j-1}, G_1, \dots, G_n]).$$

II) The perturbation at order $j = 1, \dots, n$ of the normal form is given by

$$\bar{P}_j = \langle P_j + F_j\rangle_h.$$

III) The n normalizing, generating Hamiltonians $G_1, \dots, G_n$ are given by

$$G_j = K_j + L_h^{-1}\delta_h(P_j + F_j), \quad K_j \in \ker L_h.$$

In particular, the normal form Hamiltonian to second order reads explicitly

$$H_\lambda^{(2)} = h + \lambda \bar{P}_1 + \lambda^2 \bar{P}_2 + R_3$$

where:

$$\bar{P}_1 = \langle P_1 \rangle_h ; \tag{2.47}$$

$$\bar{P}_2 = \langle P_2 \rangle_h + \frac{1}{2} \langle \{\delta_h P_1, \delta_h G_1\} \rangle_h + \{\bar{P}_1, K_1\}. \tag{2.48}$$

2.2.4 Application to the Hamiltonian (2.30)

In order to apply the perturbative theory to our specific Hamiltonian and compute the normal form, recall the flow of h, which is $\Phi_h^s = (ze^{-i\omega s}, z^* e^{i\omega s})$ and which has period $\tau = 2\pi/\omega$. By definition (2.42) and thanks to the formula,

$$\frac{\omega}{2\pi} \int_0^{2\pi/\omega} e^{\imath m\omega s} \mathrm{d}s = \delta_{m,0} = \begin{cases} 1 & \text{if } m = 0, \\ 0 & \text{if } m \in \mathbb{Z} \setminus \{0\}, \end{cases} \tag{2.49}$$

one can compute the Hamiltonian normal form as follows.

Remark 8 *The average theory has been conveniently exposed making use of the small parameters λ. In our application to the cold atoms problem, the actual small parameter is the amplitude of the displacement q_j and as a matter of fact $\lambda = 1$.*

Theorem 2 *The Hamiltonian of cold atoms problem, in normal form to the first order is:*

$$H^{(1)}(a, a^*) = H(C_1^{-1}(a, a^*)) = h(a, a^*) + \bar{P}_1(a, a^*) + R_2,$$

where

$$\begin{aligned} \bar{P}_1(a, a^*) &= \frac{\omega}{2\pi} \int_0^{2\pi/\omega} P_1(\Phi_h^\tau(a, a^*)) \mathrm{d}\tau = \\ &= W \sum_{j=1}^N |a_j|^2 + J \sum_{j=1}^N a_j^* (a_{j+1} + a_{j-1}) + U \sum_{j=1}^N |a_j|^4, \end{aligned} \tag{2.50}$$

with suitable real parameters W, J and U.

Proof. The specific computation for $\bar{P}_1 = \langle P_1 \rangle_h$ is

$$\begin{aligned}
\langle P_1 \rangle_h (a, a^*) &= \frac{\omega}{2\pi} \int_0^{2\pi/\omega} P_1(\Phi_h^s(a, a^*)) \mathrm{d}s = \\
&= \frac{\omega}{2\pi} \int_0^{2\pi/\omega} \sum_{j \in \mathbb{Z}_N} \Big\{ -\frac{\Lambda}{16m^2\omega^2} (a_j e^{-i\omega s} + {a_j}^* e^{i\omega s})^4 + \\
&+ \frac{K}{4m\omega} \Big[(a_{j+1} e^{-i\omega s} + {a_{j+1}}^* e^{i\omega s}) - (a_j e^{-i\omega s} + {a_j}^* e^{i\omega s}) \Big]^2 \Big\} \mathrm{d}s = \\
&= \sum_{j \in \mathbb{Z}_N} \Big\{ \frac{K}{2m\omega} \Big[(a_{j+1} - a_j)({a_{j+1}}^* - {z_j}^*) \Big] - \frac{3\Lambda}{8m^2\omega^2} (a_j {a_j}^*)^2 \Big\} = \\
&= \sum_{j \in \mathbb{Z}_N} \Big\{ \frac{K}{2m\omega} \Big[|a_{j+1}|^2 + |a_j|^2 - a_{j+1} a_j^* - a_j a_{j+1}^* \Big] - \frac{3\Lambda}{8m^2\omega^2} |a_j|^4 \Big\} = \\
&= \sum_{j \in \mathbb{Z}_N} \Big\{ \frac{K}{2m\omega} \Big[2|a_j|^2 - a_{j+1} a_j^* - a_{j-1} a_j^* \Big] - \frac{3\Lambda}{8m^2\omega^2} |a_j|^4 \Big\} = \\
&= \sum_{j \in \mathbb{Z}_N} \frac{K}{m\omega} |a_j|^2 - \sum_{j \in \mathbb{Z}_N} \frac{K}{2m\omega} \Big[a_{j+1} a_j^* + a_{j-1} a_j^* \Big] - \sum_{j \in \mathbb{Z}_N} \frac{3\Lambda}{8m^2\omega^2} |a_j|^4 = \\
&= \sum_{j \in \mathbb{Z}_N} \frac{K}{m\omega} |a_j|^2 - \sum_{j \in \mathbb{Z}_N} \frac{K}{2m\omega} a_j^* \Big[a_{j+1} + a_{j-1} \Big] - \sum_{j \in \mathbb{Z}_N} \frac{3\Lambda}{8m^2\omega^2} |a_j|^4 = \\
&= W \sum_{j \in \mathbb{Z}_N} |a_j|^2 + J \sum_{j \in \mathbb{Z}_N} a_j^* \Big[a_{j+1} + a_{j-1} \Big] + U \sum_{j \in \mathbb{Z}_N} |a_j|^4.
\end{aligned}$$

So the Hamiltonian in normal form to the first order is:

$$H^{(1)}(a, a^*) = h(a, a^*) + \bar{P}_1(a, a^*) + R_2, \tag{2.51}$$

where

$$\bar{P}_1(a, a^*) = W \sum_{j \in \mathbb{Z}_N} |a_j|^2 + J \sum_{j \in \mathbb{Z}_N} a_j^* \Big[a_{j+1} + a_{j-1} \Big] + U \sum_{j \in \mathbb{Z}_N} |a_j|^4, \tag{2.52}$$

with

$$W := \frac{K}{m\omega}; \tag{2.53}$$

$$J := -\frac{K}{2m\omega}; \tag{2.54}$$

$$U := -\frac{3\Lambda}{8m^2\omega^2}. \tag{2.55}$$

■

The truncated normal form

$$H^{(1)} - R_2 = h + \bar{P}_1 = \\ = (W+\omega)\sum_{j\in\mathbb{Z}_N} |a_j|^2 + J\sum_{j\in\mathbb{Z}_N} a_j^*\Big[a_{j+1}+a_{j-1}\Big] + U\sum_{j\in\mathbb{Z}_N}|a_j|^4$$

is the Hamiltonian of the discrete Bogolyubov-Gross-Pitaevskii (dBGP) or the discrete Nonlinear Schrödinger (dNLS) equation namely:

$$\imath\dot{a}_j = (W+\omega)a_j + J(a_{j+1}+a_{j-1}) + 2U|a_j|^2 a_j. \tag{2.56}$$

An equation of this form describes the dynamics of the trapped atoms at low temperature [8].

The first few normalized perturbations $\bar{P}_2$, $\bar{P}_3$ and so on are explicitly computable, though their link with the original perturbations $P_1, P_2 \dots$ is not as easy as (2.50). Theorem 2 implies that the classical dynamics of the atomic array is well described, to any fixed perturbative order, i.e. on arbitrarily large time-scales, by a suitable deformation of the dBGP, if the amplitude of the initial conditions is small enough.

In order to compute $\bar{P}_2$, according to formula (2.48) one has to compute the generating Hamiltonian G_1. To such a purpose we first need:

$$\delta_h P_1 = P_1 - \langle P_1\rangle_h = \sum_{j\in\mathbb{Z}_N}\Big[\frac{K}{4m\omega}\Big((z_{j+1}-z_j)^2 + ({z_{j+1}}^* - z_j^*)^2\Big) + \\ -\frac{\Lambda}{16m^2\omega^2}\Big(z_j^4 + z_j^{*4} + 4z_j z_j^{*3} + 4z_j^3 z_j^*\Big)\Big]. \tag{2.57}$$

Morevore we will make use of the formula:

$$\frac{\omega}{2\pi}\int_0^{2\pi/\omega} s e^{\imath m\omega s}\mathrm{d}s \;=\; \frac{1}{\imath m\omega} \quad \forall m\in\mathbb{Z}\setminus\{0\}. \tag{2.58}$$

The computation of G_1 follows:

$$\begin{aligned}
G_1(z,z^*) &= \frac{\omega}{2\pi}\int_0^{2\pi/\omega} s\delta_h P_1(\Phi_h^s(z,z^*))\mathrm{d}s = \\
&= \sum_{j\in\mathbb{Z}_N}\frac{\omega}{2\pi}\int_0^{2\pi/\omega} s\Big\{\frac{K}{4m\omega}\Big[e^{-2i\omega s}(z_{j+1}-z_j)^2 + e^{2i\omega s}({z_{j+1}}^*-z_j^*)^2\Big] + \\
&- \frac{\Lambda}{16m^2\omega^2}\Big(e^{-4i\omega s}z_j^4 + e^{4i\omega s}z_j^{*4} + 4e^{2i\omega s}z_j z_j^{*3} + 4e^{-2i\omega s}z_j^3 z_j^*\Big)\Big\}\mathrm{d}s = \\
&= \sum_{j\in\mathbb{Z}_N}\Big[\frac{K}{4m\omega}\Big(\frac{({z_{j+1}}^*-z_j^*)^2}{2i\omega} - \frac{(z_{j+1}-z_j)^2}{2i\omega}\Big) + \\
&- \frac{\Lambda}{16m^2\omega^2}\Big(-\frac{z_j^4}{4i\omega} + \frac{z_j^{*4}}{4i\omega} + \frac{4z_j z_j^{*3}}{2i\omega} - \frac{4z_j^3 z_j^*}{2i\omega}\Big)\Big].
\end{aligned}$$

Choosing $K_1 = 0$ as a kernel element in (2.46), compute the second order perturbation term in normal form:

$$\bar{P}_2 = \langle P_2\rangle_h + \frac{1}{2}\langle\{\delta_h P_1, G_1\}\rangle_h \tag{2.59}$$

where we observe that $\delta_h G_1 = G_1$ when $K_1 = 0$.

By an easy computation one gets:

$$\langle P_2\rangle_h(a,a^*) = \frac{\omega}{2\pi}\int_0^{2\pi/\omega} P_2(\Phi_h^s(a,a^*))\mathrm{d}s = \sum_{j\in\mathbb{Z}_N}\frac{5\Gamma}{12m^3\omega^3}|a_j|^6. \tag{2.60}$$

In order to compute the Poisson bracket between $\delta_h P_1$ and G_1 using the formula

$$\{\delta_h P_1, G_1\} = -\imath\sum_{j\in\mathbb{Z}_N}\Big(\frac{\partial\delta_h P_1}{\partial z_j}\frac{\partial G_1}{\partial z_j^*} - \frac{\partial\delta_h P_1}{\partial z_j^*}\frac{\partial G_1}{\partial z_j}\Big),$$

one has to compute first the derivatives with respect to z_j and z_j^* and then the products between them.

$$\begin{aligned}
\frac{\partial\delta_h P_1}{\partial z_j} &= \frac{K}{2m\omega}\Big[(z_j - z_{j-1}) - (z_{j+1}-z_j)\Big] - \frac{\Lambda}{4m^2\omega^2}\Big(z_j^3 + {z_j^*}^3 + 3z_j^2 z_j^*\Big);\\
\frac{\partial\delta_h P_1}{\partial z_j^*} &= \frac{K}{2m\omega}\Big[(z_j^* - z_{j-1}^*) - (z_{j+1}^*-z_j^*)\Big] - \frac{\Lambda}{4m^2\omega^2}\Big({z_j^*}^3 + {z_j}^3 + 3{z_j^*}^2 z_j\Big);\\
\frac{\partial G_1}{\partial z_j} &= -\frac{K}{4m\imath\omega^2}\Big[(z_j - z_{j-1}) - (z_{j+1}-z_j)\Big] - \frac{\Lambda}{16m^2\imath\omega^3}\Big(-z_j^3 + 2{z_j^*}^3 - 6z_j^2 z_j^*\Big);\\
\frac{\partial G_1}{\partial z_j^*} &= -\frac{K}{4m\imath\omega^2}\Big[({z_{j+1}}^* - z_j^*) - ({z_j}^* - z_{j-1}^*)\Big] - \frac{\Lambda}{16m^2\imath\omega^3}\Big({z_j^*}^3 + 6z_j{z_j^*}^2 - 2z_j^3\Big).
\end{aligned}$$

$$\begin{aligned}
\frac{\partial \delta_h P_1}{\partial z_j}\frac{\partial G_1}{\partial z_j^*} &= -\frac{K^2}{8m^2\imath\omega^3}\Big[(z_j - z_{j-1}) - (z_{j+1} - z_j)\Big]\Big[({z_{j+1}}^* - z_j^*) - ({z_j}^* - z_{j-1}^*)\Big] + \\
&+\frac{K\Lambda}{16m^3\imath\omega^4}\Big(z_j^3 + {z_j^*}^3 + 3z_j^2 z_j^*\Big)\Big[({z_{j+1}}^* - z_j^*) - ({z_j}^* - z_{j-1}^*)\Big] + \\
&- \frac{\Lambda K}{32m^3\imath\omega^4}\Big[(z_j - z_{j-1}) - (z_{j+1} - z_j)\Big]\Big({z_j^*}^3 + 6z_j{z_j^*}^2 - 2z_j^3\Big) + \\
&+ \frac{\Lambda^2}{64m^4\imath\omega^5}\Big(z_j^3 + {z_j^*}^3 + 3z_j^2 z_j^*\Big)\Big({z_j^*}^3 + 6z_j{z_j^*}^2 - 2z_j^3\Big). \\
\frac{\partial \delta_h P_1}{\partial z_j^*}\frac{\partial G_1}{\partial z_j} &= -\frac{K^2}{8m^2\imath\omega^3}\Big[(z_j^* - z_{j-1}^*) - (z_{j+1}^* - z_j^*)\Big]\Big[(z_j - z_{j-1}) - (z_{j+1} - z_j)\Big] + \\
&+\frac{\Lambda K}{16m^3\imath\omega^4}\Big({z_j^*}^3 + {z_j}^3 + 3{z_j^*}^2 z_j\Big)\Big[(z_j - z_{j-1}) - (z_{j+1} - z_j)\Big] + \\
&- \frac{\Lambda K}{32m^3\imath\omega^4}\Big[(z_j^* - z_{j-1}^*) - (z_{j+1}^* - z_j^*)\Big]\Big(- z_j^3 + 2{z_j^*}^3 - 6z_j^2 z_j^*\Big) + \\
&+ \frac{\Lambda^2}{64m^4\imath\omega^5}\Big({z_j^*}^3 + {z_j}^3 + 3{z_j^*}^2 z_j\Big)\Big(- z_j^3 + 2{z_j^*}^3 - 6z_j^2 z_j^*\Big).
\end{aligned}$$

The explicit expression of the bracket is:

$$\begin{aligned}
\{\delta_h P_1, G_1\} = \sum_{j\in\mathbb{Z}_N}\Big\{ &- \frac{K^2}{4m^2\omega^3}\Big[(z_j^* - z_{j-1}^*) - (z_{j+1}^* - z_j^*)\Big]\Big[(z_j - z_{j-1}) - (z_{j+1} - z_j)\Big] + \\
&- \frac{\Lambda K}{32m^3\omega^4}\Big[\Big((z_j - z_{j-1}) - (z_{j+1} - z_j)\Big)\Big(- 3{z_j^*}^3 - 12{z_j^*}^2 z_j\Big) + \\
&- \Big((z_j^* - z_{j-1}^*) - (z_{j+1}^* - z_j^*)\Big)\Big(3z_j^3 + 12z_j^* z_j^2\Big)\Big] + \\
&- \frac{\Lambda^2}{64m^4\omega^5}\Big[34z_j^3{z_j^*}^3 - {z_j^*}^6 - z_j^6 + 15z_j^4{z_j^*}^2 + 3{z_j^*}^4 z_j^2\Big]\Big\}.
\end{aligned}$$

So now one can compute the average of the previous Poisson bracket along the unperturbed flow of h:

$$\begin{aligned}
\langle\{\delta_h P_1, G_1\}\rangle_h(a, a^*) &= \frac{\omega}{2\pi}\int_0^{2\pi/\omega}\{\delta_h P_1, G_1\}(\Phi_h^s(a, a^*))\mathrm{d}s = \\
&= \sum_{j\in\mathbb{Z}_N}\Big\{ - \frac{17\Lambda^2}{32m^4\omega^5}|a_j|^6 + \frac{3\Lambda K}{2m^3\omega^4}|a_j|^4 + \\
&- \frac{3\Lambda K}{8m^3\omega^4}\Big[{a_j^*}^2 a_j\Big(a_{j-1} + a_{j+1}\Big) + a_j^2 a_j^*\Big(a_{j-1}^* + a_{j+1}^*\Big)\Big] + \\
&+ \frac{K^2}{4m^2\omega^3}|a_{j+1} + a_{j-1} - 2a_j|^2\Big\}. \qquad (2.61)
\end{aligned}$$

Finally the perturbation term of second order $\bar{P}_2$ has the form:

$$\bar{P}_2(a,a^*) = \tilde{U}\sum_{j\in\mathbb{Z}_N}|a_j|^6 + \tilde{M}\sum_{j\in\mathbb{Z}_N}|a_j|^4 + \tilde{J}\sum_{j\in\mathbb{Z}_N}|a_{j+1}+a_{j-1}-2a_j|^2 + \\ +\tilde{N}\sum_{j\in\mathbb{Z}_N}\Big[a_j^{*2}a_j(a_{j-1}+a_{j+1}) + a_j^2a_j^*(a_{j-1}^*+a_{j+1}^*)\Big] \tag{2.62}$$

where

$$\tilde{U} := -\frac{17\Lambda^2}{64m^4\omega^5} + \frac{5\Gamma}{12m^3\omega^3}; \tag{2.63}$$

$$\tilde{J} := -\frac{K^2}{8m^2\omega^3}; \tag{2.64}$$

$$\tilde{M} := \frac{3\Lambda K}{4m^3\omega^4}; \tag{2.65}$$

$$\tilde{N} := -\frac{3\Lambda K}{16m^3\omega^4}. \tag{2.66}$$

We have thus proved the following:

Theorem 3 *The Hamiltonian of the cold atoms problem in normal form to the second order is*

$$H^{(2)}(a,a^*) = h(a,a^*) + \bar{P}_1(a,a^*) + \bar{P}_2(a,a^*) + R_3, \tag{2.67}$$

where $\bar{P}_1$ and $\bar{P}_2$ are given in (2.50) and (2.62) respectively.

2.3 Summary of the Classical Part

We summarize the model obtained in the classical case in order to have a general and complete point of view.
The starting Hamiltonian before the canonical transformation is the following:

$$H(q,p) = \sum_{j\in\mathbb{Z}_N} \Big[\Big(\frac{{p_j}^2}{2m} + \frac{m\omega^2}{2}q_j^2\Big) + \Big(-\frac{\Lambda}{4}q_j^4 + \frac{K}{2}(q_{j+1}-q_j)^2\Big) + \Big(\frac{\Gamma}{6}q_j^6 + \frac{\alpha}{3}(q_{j+1}-q_j)^3\Big)\Big]. \tag{2.68}$$

The Hamiltonian in normal form, to second order is:

$$H^{(2)} = h + \bar{P}_1 + \bar{P}_2 + R_3 \tag{2.69}$$

where h is the unperturbed Hamiltonian and $\bar{P}_1$ and $\bar{P}_2$ are the first and second term of perturbation.

$$h = \sum_{j\in\mathbb{Z}_N} \omega|a_j|^2; \tag{2.70}$$

$$\bar{P}_1 = W\sum_{j\in\mathbb{Z}_N}|a_j|^2 + J\sum_{j\in\mathbb{Z}_N} a_j^*(a_{j+1}+a_{j-1}) + U\sum_{j\in\mathbb{Z}_N}|a_j|^4; \tag{2.71}$$

$$\bar{P}_2 = \tilde{U}\sum_{j\in\mathbb{Z}_N}|a_j|^6 + \tilde{M}\sum_{j\in\mathbb{Z}_N}|a_j|^4 + \tilde{J}\sum_{j\in\mathbb{Z}_N}|a_{j+1}+a_{j-1}-2a_j|^2 + \\ +\tilde{N}\sum_{j\in\mathbb{Z}_N}\Big[a_j^{*2}a_j(a_{j-1}+a_{j+1}) + a_j^2a_j^*(a_{j-1}^*+a_{j+1}^*)\Big], \tag{2.72}$$

where the coefficients are $W := \frac{K}{m\omega}$, $J := -\frac{K}{2m\omega}$, $U := -\frac{3\Lambda}{8m^2\omega^2}$ instead $\tilde{U} = -\frac{17\Lambda^2}{64m^4\omega^5} + \frac{5\Gamma}{12m^3\omega^3}$, $\tilde{J} = -\frac{K^2}{8m^2\omega^3}$, $\tilde{M} = \frac{3\Lambda K}{4m^3\omega^4}$, $\tilde{N} = -\frac{3\Lambda K}{16m^3\omega^4}$.

The explicit expression of the truncated normal form is

$$\begin{aligned} H^{(2)} - R_3 &= h + \bar{P}_1 + \bar{P}_2 = \\ &= \sum_{j\in\mathbb{Z}_N}\Big\{(W+\omega)|a_j|^2 + Ja_j^*\Big[a_{j+1}+a_{j-1}\Big] + \\ &+ (U+\tilde{M})|a_j|^4 + \tilde{U}|a_j|^6 + \tilde{J}|a_{j+1}+a_{j-1}-2a_j|^2 + \\ &+ \tilde{N}\Big[a_j^{*2}a_j(a_{j-1}+a_{j+1}) + a_j^2a_j^*(a_{j-1}^*+a_{j+1}^*)\Big]\Big\}. \end{aligned}$$

The corresponding discrete Bogolyubov-Gross-Pitaevskii (dBGP) or discrete Nonlinear Schrödinger (dNLS) equation, corrected to second order is:

$$\begin{aligned} \imath\dot{a}_j &= (W+\omega)a_j + J(a_{j+1}+a_{j-1}) + 2(U+\tilde{M})|a_j|^2 a_j + 3\tilde{U}|a_j|^4 a_j + \\ &+ \tilde{J}\Big[(a_j + a_{j-2} - 2a_{j-1}) - 2(a_{j+1}+a_{j-1}-2a_j) + (a_{j+2}+a_j-2a_{j+1})\Big] + \\ &+ \tilde{N}\Big[2a_j^* a_j(a_{j-1}+a_{j+1}) + a_j^2(a_{j-1}^* + a_{j+1}^*) + a_{j+1}^2 a_{j+1}^* + a_{j-1}^2 a_{j-1}^*\Big]. \quad (2.73) \end{aligned}$$

Chapter 3

The Remainder Term

In the previous chapter one, thanks to the canonical transformation, we wrote the original Hamiltonian in normal form, which looks like a perturbation of the dBGP equation. Now focus our attention on the remainder R_{n+1} appearing in the Hamiltonian normal form of order n.

3.1 Estimate of the Remainder

The idea of this section is to find an explicit estimate of the effects of remainder term in

$$H^{(n)} = h + \lambda \bar{P}_1 + \lambda^2 \bar{P}_2 + \cdots + \lambda^n \bar{P}_n + R_{n+1} \ . \tag{3.1}$$

In general consider a vector field X and its integral curve ϕ^s which solves the following problem, for any given starting point x_0

$$\frac{d}{ds}\phi^s = X \circ \phi^s$$

that is

$$\dot{x} = X(x) \Longrightarrow x(s) = \phi^s(x_0).$$

Now consider any function $f(x(s))$

$$\begin{aligned}\frac{d}{ds}f(x(s)) &= \sum_j \frac{\partial}{\partial x_j} f(x(s)) \frac{d}{ds} x_j(s) = \\ &= \sum_j \frac{\partial}{\partial x_j} f(x(s)) X_j(x(s)) = \\ &= (L_X f)(x(s)).\end{aligned}$$

where $L_X f = X \cdot \nabla f = f'X$ is the Lie derivative of f along X.

$$\begin{aligned}\frac{d}{ds}(f \circ \phi^s) &= f'(\phi^s)\frac{d}{ds}\phi^s = \\ &= f' \circ \phi^s X \circ \phi^s = \\ &= (f'X) \circ \phi^s = \\ &= (L_X f) \circ \phi^s.\end{aligned}$$

Integrating from 0 to $\lambda > 0$ the previous equality:

$$\int_0^\lambda \frac{d}{ds}(f \circ \phi^s)\mathrm{d}s = \int_0^\lambda (L_X f) \circ \phi^s \mathrm{d}s \Longrightarrow f \circ \phi^\lambda - f = \int_0^\lambda (L_X f) \circ \phi^s \mathrm{d}s.$$

Solving the integral on the left side and iterating the procedure:

$$\begin{aligned}f \circ \phi^\lambda &= f + \int_0^\lambda (L_X f) \circ \phi^{s_0} \mathrm{d}s_0 = \\ &= f + \int_0^\lambda \Big[(L_X f) + \int_0^{s_0} (L_X^2 f) \circ \phi^{s_1} \mathrm{d}s_1\Big]\mathrm{d}s_0 = \\ &= f + \lambda(L_X f) + \int_0^\lambda \mathrm{d}s_0 \int_0^{s_0} \mathrm{d}s_1 (L_X^2 f) \circ \phi^{s_1} = \\ &= f + \lambda(L_X f) + \frac{\lambda^2}{2}(L_X^2 f) + \int_0^\lambda \mathrm{d}s_0 \int_0^{s_0} \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 (L_X^3 f) \circ \phi^{s_2} = \\ &= \cdots = \\ &= f + \lambda(L_X f) + \frac{\lambda^2}{2}(L_X^2 f) + \cdots + \frac{\lambda^n}{n!}(L_X^n f) + \bar{R}_{n+1} = \\ &= e^{\lambda L_X} f. \end{aligned} \tag{3.2}$$

The previous computation is the Taylor expansion where the term of remainder at order $n+1$ has an integral form:

$$\bar{R}_{n+1} = \int_0^\lambda \mathrm{d}s_0 \int_0^{s_0} \mathrm{d}s_1 \cdots \int_0^{s_{n-1}} \mathrm{d}s_n (L_X^{n+1} f) \circ \phi^{s_n}. \tag{3.3}$$

In the specific case in which $f = H = h + \lambda P_1 + \lambda^2 P_2 + \ldots$, $\phi^s = \Phi^\lambda_{G_1}$ where G_1 is a Hamiltonian and $L_X = L_1$, one has:

$$\begin{aligned} H \circ \Phi^\lambda_{G_1} &= h \circ \Phi^\lambda_{G_1} + \lambda P_1 \circ \Phi^\lambda_{G_1} + \lambda^2 P_2 \circ \Phi^\lambda_{G_1} = \\ &= h + \lambda(L_1 h) + \frac{\lambda^2}{2}(L_1^2 h) + \bar{R}_3^{(h)} + \\ &\quad + \lambda P_1 + \lambda^2 (L_1 P_1) + \lambda \bar{R}_2^{(P_1)} + \\ &\quad + \lambda^2 P_2 + \lambda^2 \bar{R}_1^{(P_2)} = \\ &= h + \lambda(L_1 h + P_1) + \lambda^2 (\frac{1}{2} L_1^2 h + L_1 P_1 + P_2) + \tilde{R}_3 \end{aligned} \tag{3.4}$$

where

$$\tilde{R}_3 = \bar{R}_3^{(h)} + \lambda \bar{R}_2^{(P_1)} + \lambda^2 \bar{R}_1^{(P_2)}. \tag{3.5}$$

In order to be in normal to the first order

$$H \circ \Phi^\lambda_{G_1} = h + \bar{P}_1 + R_2$$

which means

$$L_1 h + P_1 \in \ker L_h.$$

In particular the reminder of the normal form

$$R_2 = \lambda^2 (\frac{1}{2} L_1^2 h + L_1 P_1 + P_2) + \tilde{R}_3$$

is determined by a specific G_1. Clearly it's possible to use this machinery to compute the Hamiltonian normal form to any order n with its remainder R_{n+1}.

3.2 Effects of the Remainder

The advantage to get a normal form to high order in the small parameters is easily seen to be in the longer time of preservation of approximate first integrals, or "adiabatic invariants" of the system.

Consider a function J which commutes with all terms in the Hamiltonian (3.1):

$$\{h, J\} = 0 = \{\bar{P}_j, J\}. \tag{3.6}$$

The evolution of J along the flow of $H^{(n)}$ is given by

$$\dot{J} = \{J, H^{(n)}\} = \{J, R_{n+1}\} \tag{3.7}$$

that is $\{J, H^{(n)} - R_{n+1}\} = 0$.

If $R_{n+1} = \lambda^{n+1} r_n$, with $r_n = O(1)$ then

$$\frac{dJ}{dt} = \{J, \lambda^{n+1} r_n\} = \lambda^{n+1} \{J, r_n\}. \tag{3.8}$$

If moreover $|\{J, r_n\}| \leq C_n$, one obtains the following estimate:

$$|J(t) - J_0| = |\lambda^{n+1} \int_0^t \{J, r_n\} \mathrm{d}t| \leq \lambda^{n+1} C_n |t|. \tag{3.9}$$

Thus for times as long as $|t| < 1/\lambda^n$ one has

$$|J(t) - J_0| \leq C_n \lambda. \tag{3.10}$$

In general, due to the growth of C_n with n, there's an optimal value of n in this scheme, as shown first by Nekhoroshev.

In this conclusive section we use perturbation theory, and in particular the Hamiltonian normal form, to construct approximate solutions of the original problem and we will show in which sense they are actually close to exact solutions [9]. The original problem is given by the equations of motion with Hamiltonian

$$H = h + \lambda P_1 + \lambda^2 R$$

$$\begin{cases} \dot{z}_j = -\imath \frac{\partial H}{\partial z_j^*} \\ \dot{z}_j^* = \imath \frac{\partial H}{\partial z_j} \end{cases}$$

By defining the vector $u := (z, z^*)^T$, one can rewrite such equations as

$$\dot{u} = Au + \lambda X_1(u) + \lambda^2 X_R(u) \tag{3.11}$$

where A is the linear operator linked to h: $Au = J\nabla h(u)$ and $X_1 = J\nabla P_1$. The Hamiltonian normal form to first order is obtained by a coordinate transformation $u := T_\lambda(v) = \Phi_{G_1}^\lambda(v)$.

$$H^{(1)} = h + \lambda \bar{P}_1 + \lambda^2 \bar{R}$$

with corresponding equations:

$$\dot{v} = Av + \lambda N(v) + \lambda^2 \mathcal{R}(v) \tag{3.12}$$

where $N = X_{\bar{P}_1}$ instead $\mathcal{R}$ is a remainder. The truncated, or simplified system, instead is:

$$\dot{w} = Aw + \lambda N(w). \tag{3.13}$$

The solutions w of the simplified system are expected to approximate well the solutions of the complete problem v. However, depending on the remainder $\mathcal{R}$ then it could happen that the solutions of the equation (3.13) and solutions of the equation (3.12) are very different. In order to ensure that they are close to each other one should be able to prove some a priori estimate of $\mathcal{R}$ and get an estimate of the time scale on which this happens. To reach this goal consider a solution $w(t)$ of (3.13) and construct an approximate solution $\bar{u}$ of the original system:

$$\bar{u}(t) := T_\lambda(w(t)). \tag{3.14}$$

The error $r(t)$ is defined as the difference between the true solution u and the approximate one $\bar{u}$:

$$r(t) := u(t) - \bar{u}(t). \tag{3.15}$$

Such error fulfills the equation:

$$\begin{aligned}
\dot{r}(t) &= \dot{u}(t) - \dot{\bar{u}}(t) = \\
&= Au + \lambda X_1(u) + \lambda^2 X_R(u) - T'_\lambda \dot{w} = \\
&= Au + \lambda X_1(u) + \lambda^2 X_R(u) - T'_\lambda \Big(Aw + \lambda N(w) \Big) = \\
&= Ar + A\bar{u} + \lambda X_1(r+\bar{u}) + \lambda^2 X_R(r+\bar{u}) - T'_\lambda \Big(Aw + \lambda N(w) \Big) = \\
&= Ar + A\bar{u} + \lambda X_1(r+\bar{u}) + \lambda^2 X_R(r+\bar{u}) - A\bar{u} - \lambda X_1(\bar{u}) - \lambda^2 X_R(\bar{u}) + \\
&\quad + \lambda^2 T'_\lambda(w)\mathcal{R}(w) = \\
&= Ar + \lambda[X_1(r+\bar{u}) - X_1(\bar{u})] + \lambda^2[X_R(r+\bar{u}) - X_R(\bar{u})] + \lambda^2 T'_\lambda(w)\mathcal{R}(w)
\end{aligned}$$

where the following equivalence which holds for every v has been used:

$$AT_\lambda(v) + \lambda X_1(T_\lambda(v)) + \lambda^2 X_R(T_\lambda(v)) = \dot{u} = T'_\lambda(v)[Av + \lambda N(v) + \lambda^2 \mathcal{R}(v)]. \tag{3.16}$$

The equation satisfied by the error is:

$$\dot{r} = Ar + \lambda[X_1(r+\bar{u}) - X_1(\bar{u})] + \lambda^2[X_R(r+\bar{u}) - X_R(\bar{u})] + \lambda^2 T'_\lambda(w)\mathcal{R}(w). \tag{3.17}$$

The main point is that the reminder is evaluated on the approximate solution w, so this gives a small contribution if some control on the approximate solutions is available. Assume that $\mathcal{R}(w)$ is bounded, then in order to control the norm of r one has just to apply Gronwall's lemma (that follows) to estimate solutions of (3.17).

Lemma 9 ***Gronwall's Inequality*** *Let I denote an interval of the real line of the form $[0, T)$. Let α, β and u be real-valued functions defined on I. Assume that β and u are continuous and that the negative part of α is integrable on every closed and bounded sub interval of I. If β is non-negative, α is non-decreasing and if u satisfies the integral inequality*

$$u(t) \leq \alpha(t) + \int_0^t \beta(s)u(s)\,\mathrm{d}s, \qquad \forall t \in I \tag{3.18}$$

then

$$u(t) \leq \alpha(t) \exp\left(\int_0^t \beta(s)\,\mathrm{d}s\right), \qquad \forall t \in I. \tag{3.19}$$

Let us now define $\rho(t) := e^{-At} r(t)$. Notice that the evolution of h is unitary which means $|e^{-At}| = 1$ so $|r(t)| = |\rho(t)|$. Thus, $\rho(t)$ satisfies the equation

$$\dot{\rho}(t) = e^{-At}[\lambda \Delta X + \lambda^2 T' \mathcal{R}(w)], \tag{3.20}$$

where $\Delta X = \Delta X_1 + \lambda \Delta X_R$. Supposing that $X = X_1 + \lambda X_R$ is a Lipschitz vector field of constant L and $T'\mathcal{R}$ is bounded then:

$$\begin{aligned}
r(t) &= \int_0^t \frac{dr}{ds}(s)\mathrm{d}s; \\
|r(t)| = |\rho(t)| &\leq \int_0^t |\dot{\rho}(s)|\mathrm{d}s \\
&\leq \int_0^t (\lambda|\Delta X| + \lambda^2 |T'\mathcal{R}|)\mathrm{d}s \\
&\leq \int_0^t (\lambda L|r(s)| + \lambda^2 |T'\mathcal{R}(w(s))|)\mathrm{d}s \\
&= \lambda L \int_0^t |r(s)|\mathrm{d}s + \lambda^2 C t.
\end{aligned}$$

Now apply the Gronwall's lemma with $u = |\rho|$, $\alpha(t) = \lambda^2 C t$ and $\beta(t) = \lambda L$ one gets the estimate:

$$|\rho(t)| \leq \lambda^2 C t e^{\lambda L t}. \tag{3.21}$$

Such estimate shows that the distance $|\rho(t)|$ between the true and the approximate solutions of the problem, is small of order λ on a time scale of order $1/\lambda$ that cannot be increased.

Chapter 4

Quantum-Mechanical System

The central idea of this chapter is to describe the model of an atomic array of cold atoms from the point of view of quantum mechanics. In the first part we will transform the Hamiltonian H into a differential operator $\boldsymbol{H}$ by the procedure of canonical quantization. Then we will represent the dynamics of the system defined by $\boldsymbol{H}$ using Heisenberg picture, where any quantized operator $\boldsymbol{F}$ evolves along the flow of $\boldsymbol{H}$ by unitary conjugation, namely $\boldsymbol{F}(t) := \boldsymbol{U_H}(t)^\dagger \boldsymbol{F} \boldsymbol{U_H}(t)$. In such a way, the algebra of operators $\boldsymbol{F}, \boldsymbol{G}, \ldots$ defined on the configuration space of a given system becomes a Poisson algebra with Poisson bracket given by $\{\boldsymbol{F}, \boldsymbol{G}\} := -\imath[\boldsymbol{F}, \boldsymbol{G}]/\hbar$, where $[\ ,\ ]$ denotes the standard commutator, namely $[\boldsymbol{F}, \boldsymbol{G}] := \boldsymbol{F}\boldsymbol{G} - \boldsymbol{G}\boldsymbol{F}$. Since the formal properties of Hamiltonian perturbation theory depend only on the algebraic properties of the Poisson structure, we will extend the classical results listed above to the quantum case.

4.1 Model and Quantum Hamiltonian

Recall the classical Hamiltonian obtained in the previous chapter:

$$H(q,p) = \sum_{j=1}^{N} \Big[\Big(\frac{{p_j}^2}{2m} + \frac{m\omega^2}{2} q_j^2 \Big) + \Big(-\frac{\Lambda}{4} q_j^4 + \frac{K}{2}(q_{j+1} - q_j)^2 \Big) + \Big(\frac{\Gamma}{6} q_j^6 + \frac{\alpha}{3}(q_{j+1} - q_j)^3 \Big) \Big].$$

In order to work in a quantum setting one has to apply canonical quantization to each variable involved in the model. Such procedure is described in the next section.

4.1.1 Canonical Quantization

In physics, quantization is the procedure to transform a classical Hamiltonian system into a quantum mechanical model. This procedure is basic to theories of particle physics, nuclear physics, condensed matter physics, and quantum optics.

Quantization converts classical functions defined on the phase space into operators acting on some Hilbert space.

Definition 10 *In quantum mechanics one defines* $\boldsymbol{q}$ *as the* ***Position Operator*** *and* $\boldsymbol{p}$ *as the* ***Momentum Operator****. By definition they act on some function* ϕ *and work as follows:*

$$\boldsymbol{q} := q \implies \boldsymbol{q}\phi = q\phi \ ; \tag{4.1}$$

$$\boldsymbol{p} := -\imath\hbar\frac{\partial}{\partial q} \implies \boldsymbol{p}\phi = -\imath\hbar\frac{\partial\phi}{\partial q}. \tag{4.2}$$

The fundamental commutation relation:

$$[\boldsymbol{q}, \boldsymbol{p}] = \imath\hbar. \tag{4.3}$$

Roughly speaking the position operator multiplies the function ϕ for the q variable, instead the momentum operator takes the derivative of the function ϕ with respect to the q variable and multiplies the result by the constant $(-\imath\hbar)$. The explicit computation of the commutator between $\boldsymbol{q}$ and $\boldsymbol{p}$ is:

$$\begin{aligned}
[\boldsymbol{q}, \boldsymbol{p}]\phi(q) &= (\boldsymbol{qp} - \boldsymbol{pq})\phi(q) = \\
&= q\Big(-\imath\hbar\frac{\partial\phi(q)}{\partial q}\Big) - \Big(-\imath\hbar\frac{\partial}{\partial q}\Big)q\phi(q) = \\
&= -\imath\hbar q\frac{\partial\phi(q)}{\partial q} - \Big(-\imath\hbar\phi(q) - \imath\hbar q\frac{\partial\phi(q)}{\partial q}\Big) = \\
&= \imath\hbar\phi(q).
\end{aligned}$$

The quantum Hamiltonian operator has the same structure of the classical one where the p and q variables are substituted by the operators $\boldsymbol{p}$ and $\boldsymbol{q}$:

$$\begin{aligned}
\boldsymbol{H}(\boldsymbol{q}, \boldsymbol{p}) &= H(q, -\imath\hbar\frac{\partial}{\partial q}) = \\
&= \sum_{j\in\mathbb{Z}_N}\Big[\Big(\frac{m\omega^2}{2}q_j^2 - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2}\Big) + \Big(-\frac{\Lambda}{4}q_j^4 + \frac{K}{2}(q_{j+1} - q_j)^2\Big) + \\
&+ \Big(\frac{\Gamma}{6}q_j^6 + \frac{\alpha}{3}(q_{j+1} - q_j)^3\Big)\Big].
\end{aligned} \tag{4.4}$$

Notice that it is equivalent to do quantization before or after the translation of the original variables (2.10).

4.2 Heisenberg Picture [6]

We now examine the effect of applying time translation to operators, as well as to wave functions. The transformed operators are called Heisenberg-picture operators:

$$\boldsymbol{Q_H}(t) = \boldsymbol{U}^\dagger(t)\boldsymbol{Q}\boldsymbol{U}(t). \tag{4.5}$$

In the Schrödinger picture, the wave function ψ evolves in time according to the Schrödinger equation:

$$\boldsymbol{H}\Psi(q,t) = \imath\hbar\frac{\partial}{\partial t}\Psi(q,t). \tag{4.6}$$

The solution of the latter equation, if the Hamiltonian is independent of time, is

$$\Psi(q,t) = \boldsymbol{U}(t)\Psi(q,0)\ ; \quad \boldsymbol{U}(t) := e^{-\frac{\imath}{\hbar}\boldsymbol{H}t}. \tag{4.7}$$

The operators $\boldsymbol{q}$ and $\boldsymbol{p}$ have no time dependence of their own, and the time dependence of expectation values (or, more generally, matrix elements) comes from the time dependence of the wave function:

$$\langle \boldsymbol{Q} \rangle = \langle \Psi(t)|\boldsymbol{Q}|\Psi(t)\rangle\,. \tag{4.8}$$

In the Heisenberg picture, the wave function $\Psi_{\boldsymbol{H}}(q) = \Psi(q,0)$ is constant in time, and the operators evolve in time according to Equation (4.5). The time dependence of expectation values (or matrix elements) is carried by the operators.

$$\langle \boldsymbol{Q} \rangle = \langle \Psi_{\boldsymbol{H}}|\boldsymbol{Q_H}(t)|\Psi_{\boldsymbol{H}}\rangle\,. \tag{4.9}$$

Of course, the two pictures are entirely equivalent since:

$$\langle \Psi(t)|\boldsymbol{Q}|\Psi(t)\rangle = \big\langle \Psi(0)|\boldsymbol{U}^\dagger(t)\boldsymbol{Q}\boldsymbol{U}(t)|\Psi(0)\big\rangle = \langle \Psi_{\boldsymbol{H}}|\boldsymbol{Q_H}(t)|\Psi_{\boldsymbol{H}}\rangle\,. \tag{4.10}$$

If the Hamiltonian is time-dependent one can still write the formal solution to the Schrödinger equation in terms of the time-translation operator, $\boldsymbol{U}$:

$$\Psi(q,t) = \boldsymbol{U}(t,t_0)\Psi(q,t_0) \tag{4.11}$$

but $\boldsymbol{U}(t,t_0)$ no longer takes on the simple form $e^{-\frac{\imath}{\hbar}\boldsymbol{H}t_0}$; however, for an infinitesimal time interval δ

$$\boldsymbol{U}(t_0+\delta,t_0) \approx 1 - \frac{\imath}{\hbar}\boldsymbol{H}(t_0)\delta. \tag{4.12}$$

Due to (4.5), the time evolution of $\boldsymbol{Q_H}(t)$ is given by

$$\frac{d}{dt}\boldsymbol{Q_H} = -\frac{\imath}{\hbar}[\boldsymbol{Q_H},\boldsymbol{H}] + \frac{\partial}{\partial t}\boldsymbol{Q_H}. \tag{4.13}$$

As a consequence, if $\boldsymbol{Q}_{\boldsymbol{H}}(t) = \boldsymbol{H}(t)$ and

$$\frac{\partial \boldsymbol{H}}{\partial t} = 0$$

then:

$$\frac{d}{dt}\boldsymbol{H} = -\frac{\imath}{\hbar}[\boldsymbol{H}, \boldsymbol{H}] = 0. \tag{4.14}$$

From now on, we work in the Heisenberg picture omitting everywhere the subscript $\boldsymbol{H}$ for the operators.

4.3 Perturbation Theory in Quantum Mechanics

The formalism of Hamiltonian perturbation theory developed in the classical context can be applied to quantum mechanics once one identifies the relevant quantum objects such as Hamiltonian flows and canonical transformations. To such a purpose, we start by observing that unitary transformations of the wave function, the unknown of the Schrödinger equation, are canonical transformations of the latter equation. Indeed, given any unitary operator $\boldsymbol{U}$ independent of time, and defining $\Psi' := \boldsymbol{U}^\dagger \Psi$ and $\boldsymbol{H}' = \boldsymbol{U}^\dagger \boldsymbol{H} \boldsymbol{U}$, one has

$$\imath\hbar\Psi_t = \boldsymbol{H}\Psi \Longleftrightarrow \imath\hbar\Psi'_t = \boldsymbol{H}'\Psi', \tag{4.15}$$

where $\boldsymbol{U}^\dagger \boldsymbol{U} = 1$, the equation on the right hand side being identical in form to that on the left one. The idea of this section is to write the quantum Hamiltonian of (4.4) in the form:

$$\boldsymbol{H}(\boldsymbol{q}, \boldsymbol{p}) = \boldsymbol{h}(\boldsymbol{q}, \boldsymbol{p}) + \boldsymbol{P}_1(\boldsymbol{q}) + \boldsymbol{P}_2(\boldsymbol{q}) + \dots, \tag{4.16}$$

where $\boldsymbol{h}$ is the unperturbed Hamiltonian and $\boldsymbol{P} := \boldsymbol{H} - \boldsymbol{h}$ is the perturbation split into ordered terms $\boldsymbol{P}_1$, $\boldsymbol{P}_2$, and so on.
In our particular case holds:

$$\boldsymbol{h}(\boldsymbol{q}, \boldsymbol{p}) := \sum_{j \in \mathbb{Z}_N} \Big(\frac{m\omega^2}{2} q_j^2 - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} \Big); \tag{4.17}$$

$$\boldsymbol{P}_1(\boldsymbol{q}) := \sum_{j \in \mathbb{Z}_N} \Big(-\frac{\Lambda}{4} q_j^4 + \frac{K}{2} (q_{j+1} - q_j)^2 \Big); \tag{4.18}$$

$$\boldsymbol{P}_2(\boldsymbol{q}) := \sum_{j \in \mathbb{Z}_N} \Big(\frac{\Gamma}{6} q_j^6 + \frac{\alpha}{3} (q_{j+1} - q_j)^3 \Big). \tag{4.19}$$

in complete analogy with the classical case.

4.3.1 Hamiltonian Normal Form in Quantum Mechanics

In the perturbative context one can try to remove the leading order perturbation $\boldsymbol{P}_1$ (and then the higher order contributions as well) by looking for a particular unitary operator $\mathbf{U}$ that conjugates $\boldsymbol{H}$ to its normal form, to leading order.

Definition 1 *A quantum Hamiltonian $\boldsymbol{H}^{(n)}$ of the form*

$$\boldsymbol{H}^{(n)} = \boldsymbol{h} + \sum_{j=1}^{n} \bar{\boldsymbol{P}}_j + \boldsymbol{R}_{n+1}, \tag{4.20}$$

*where $[\bar{\boldsymbol{P}}_j, \boldsymbol{h}] = 0$ for any $j = 1, \ldots, n$ is said to be in **Normal Form** to order n with respect to $\boldsymbol{h}$.*

4.3.2 Ladder Operators

Creation and **annihilation** operators $\boldsymbol{b}_j^\dagger$ and $\boldsymbol{b}_j$, also called Dirac, Boson or ladder operators, are defined by the following formulas:

$$\boldsymbol{b}_j := \frac{m\omega q_j + \imath p_j}{\sqrt{2m\hbar\omega}}; \qquad\qquad \boldsymbol{b}_j^\dagger := \frac{m\omega q_j - \imath p_j}{\sqrt{2m\hbar\omega}}. \tag{4.21}$$

They are the quantum version of the Birkhoff variables (2.27) up to the scale factor $1/\sqrt{\hbar}$ with the property

$$[\boldsymbol{b}_i, \boldsymbol{b}_j^\dagger] = \delta_{i,j}. \tag{4.22}$$

A dagger above and in the sequel denotes the adjoint.

One thus canonically quantizes the Hamiltonian (2.20) and gets the quantum Hamiltonian $\boldsymbol{H}$, or its equivalent expansion (4.17)-(4.19), that can be rewritten in terms of the ladder operators. Due to the definition (4.21) and to the commutation relation (4.22) one gets

$$\begin{aligned}
\boldsymbol{b}_j^\dagger \boldsymbol{b}_j &= \frac{m^2\omega^2 \boldsymbol{q}_j^2 + \boldsymbol{p}_j^2 + \imath m\omega(\boldsymbol{q}_j \boldsymbol{p}_j - \boldsymbol{p}_j \boldsymbol{q}_j)}{2m\hbar\omega} = \\
&= \frac{m^2\omega^2 \boldsymbol{q}_j^2 + \boldsymbol{p}_j^2 + \imath m\omega \imath\hbar}{2m\hbar\omega} = \\
&= \frac{1}{\hbar\omega}\Big(\frac{m\omega^2}{2}\boldsymbol{q}_j^2 + \frac{\boldsymbol{p}_j^2}{2m} - \frac{\omega\hbar}{2}\Big) = \\
&= \frac{1}{\hbar\omega}\Big(\frac{m\omega^2}{2}\boldsymbol{q}_j^2 + \frac{\boldsymbol{p}_j^2}{2m}\Big) - \frac{1}{2} = \\
&= \frac{1}{\hbar\omega}\Big(\boldsymbol{h}_j\Big) - \frac{1}{2}.
\end{aligned}$$

Thus, the unperturbed Hamiltonian $\boldsymbol{h}$ which is the sum of N Hamiltonians of single harmonic oscillators reads:

$$\boldsymbol{h}(\boldsymbol{b},\boldsymbol{b}^\dagger) := \sum_{j\in\mathbb{Z}_N} \hbar\omega(\boldsymbol{b}_j^\dagger \boldsymbol{b}_j + \frac{1}{2}) = \sum_{j\in\mathbb{Z}_N} \hbar\omega(\boldsymbol{b}_j \boldsymbol{b}_j^\dagger - \frac{1}{2}). \tag{4.23}$$

Clearly one can also express the operators of position and momentum in terms of creation and annihilation operators and then replace them into the Hamiltonian like we've done in the classical case:

$$\boldsymbol{q}_j = \sqrt{\frac{\hbar}{2m\omega}}(\boldsymbol{b}_j + \boldsymbol{b}_j^\dagger); \qquad \boldsymbol{p}_j = -\imath\sqrt{\frac{m\omega\hbar}{2}}(\boldsymbol{b}_j - \boldsymbol{b}_j^\dagger). \tag{4.24}$$

The next steps are: to express $\boldsymbol{H}$ in terms of the ladder operators and to compute its normal form to some prefixed order with respect to the unperturbed Hamiltonian (4.23). We obtain such Hamiltonian replacing the expressions (4.24) in (4.4):

$$\boldsymbol{H}(\boldsymbol{b},\boldsymbol{b}^\dagger) = \boldsymbol{h}(\boldsymbol{b},\boldsymbol{b}^\dagger) + \boldsymbol{P}_1(\boldsymbol{b},\boldsymbol{b}^\dagger) + \boldsymbol{P}_2(\boldsymbol{b},\boldsymbol{b}^\dagger) + \dots. \tag{4.25}$$

The two order perturbations $\boldsymbol{P}_1$ and $\boldsymbol{P}_2$ in terms of ladder operators become:

$$\boldsymbol{P}_1(\boldsymbol{b},\boldsymbol{b}^\dagger) := \sum_{j\in\mathbb{Z}_N} \Big\{ \frac{-\Lambda\hbar^2}{16m^2\omega^2}(\boldsymbol{b}_j + \boldsymbol{b}_j^\dagger)^4 + \frac{K\hbar}{4m\omega}\Big[(\boldsymbol{b}_{j+1} + \boldsymbol{b}_{j+1}^\dagger) - (\boldsymbol{b}_j + \boldsymbol{b}_j^\dagger)\Big]^2 \Big\};$$

$$\boldsymbol{P}_2(\boldsymbol{b},\boldsymbol{b}^\dagger) := \sum_{j\in\mathbb{Z}_N} \Big\{ \frac{\Gamma\hbar^3}{48m^3\omega^3}(\boldsymbol{b}_j + \boldsymbol{b}_j^\dagger)^6 + \frac{\alpha}{3}\sqrt{\frac{\hbar}{2m\omega}}^3 \Big[(\boldsymbol{b}_{j+1} + \boldsymbol{b}_{j+1}^\dagger) - (\boldsymbol{b}_j + \boldsymbol{b}_j^\dagger)\Big]^3 \Big\}.$$

Definition 11 *Given the creation and annihilation operators $\boldsymbol{b}_j^\dagger$ and $\boldsymbol{b}_j$ the* ***Number Operator*** *$\boldsymbol{n}_j$ is defined by*

$$\boldsymbol{n}_j = \boldsymbol{b}_j^\dagger \boldsymbol{b}_j, \tag{4.26}$$

with the property $[\boldsymbol{n}_j, \boldsymbol{n}_k] = 0 \ \forall j,k$.

The number operator is the observable that counts the number of "quasi-particles". The Hamiltonian $\boldsymbol{h}$ in terms of the number operators becomes:

$$\boldsymbol{h} = \sum_{j\in\mathbb{Z}_N} \hbar\omega(\boldsymbol{n}_j + \frac{1}{2}). \tag{4.27}$$

Notice that, instead of $\boldsymbol{h}$, one can study $\boldsymbol{h} = \sum_{j\in\mathbb{Z}_N} \hbar\omega\boldsymbol{n}_j$ because constants don't influence the dynamics.

The evolution of any operator $\boldsymbol{Q}$ with respect to the flow of a Hamiltonian $\boldsymbol{h}$ is given by:

$$\dot{\boldsymbol{Q}} = \frac{1}{\imath\hbar}[\boldsymbol{Q}, \boldsymbol{h}] := L_{\boldsymbol{h}}\boldsymbol{Q} \implies \boldsymbol{Q}(t) = e^{tL_{\boldsymbol{h}}}\boldsymbol{Q}(0). \tag{4.28}$$

It follows that the evolution of $\boldsymbol{b}_j$ and $\boldsymbol{b}_j^\dagger$ trough $\boldsymbol{h}$ is given by:

$$\begin{aligned}\imath\hbar\dot{\boldsymbol{b}}_j = [\boldsymbol{b}_j, \boldsymbol{h}] = [\boldsymbol{b}_j, \sum_{k\in\mathbb{Z}_N} \hbar\omega \boldsymbol{b}_k^\dagger \boldsymbol{b}_k] = \sum_{k\in\mathbb{Z}_N} \hbar\omega[\boldsymbol{b}_j, \boldsymbol{b}_k^\dagger\boldsymbol{b}_k] = \hbar\omega[\boldsymbol{b}_j, \boldsymbol{b}_j^\dagger]\boldsymbol{b}_j \\ = \hbar\omega\boldsymbol{b}_j,\end{aligned}$$

hence it holds

$$\dot{\boldsymbol{b}}_j = -\imath\omega\boldsymbol{b}_j \implies \boldsymbol{b}_j(t) = e^{-\imath\omega t}\boldsymbol{b}_j(0), \tag{4.29}$$

and similarly for creation operators, one has:

$$\boldsymbol{b}_j^\dagger(t) = e^{\imath\omega t}\boldsymbol{b}_j^\dagger(0). \tag{4.30}$$

One should obtain the same result using Taylor expansion for $e^{L_{\boldsymbol{h}}t}$ in the following way:

$$\begin{aligned}\boldsymbol{b}_j(t) &= e^{L_{\boldsymbol{h}}t}\boldsymbol{b}_j(0) = \\ &= (1 + tL_{\boldsymbol{h}} + \frac{t^2}{2}L_{\boldsymbol{h}}^2 + \dots)\boldsymbol{b}_j(0) = \\ &= \boldsymbol{b}_j(0) + tL_{\boldsymbol{h}}\boldsymbol{b}_j(0) + \frac{t^2}{2}L_{\boldsymbol{h}}^2\boldsymbol{b}_j(0) + \cdots = \\ &= \boldsymbol{b}_j(0) + t\frac{1}{\imath\hbar}[\boldsymbol{b}_j(0), \boldsymbol{h}] + \frac{t^2}{2}(\frac{1}{\imath\hbar})^2[[\boldsymbol{b}_j(0), \boldsymbol{h}], \boldsymbol{h}] + \cdots = \\ &= \boldsymbol{b}_j(0) + t\frac{1}{\imath\hbar}\hbar\omega\boldsymbol{b}_j(0) + \frac{t^2}{2}\Big(\frac{1}{\imath\hbar}\Big)^2(\hbar\omega)^2\boldsymbol{b}_j(0) + \cdots = \\ &= \boldsymbol{b}_j(0) + t\frac{\omega}{\imath}\boldsymbol{b}_j(0) + \frac{t^2}{2}\Big(\frac{\omega}{\imath}\Big)^2\boldsymbol{b}_j(0) + \cdots = \\ &= \boldsymbol{b}_j(0) - t\omega\imath\boldsymbol{b}_j(0) - \frac{t^2}{2}\omega^2\boldsymbol{b}_j(0) + \cdots = \\ &= e^{-\imath\omega t}\boldsymbol{b}_j(0).\end{aligned}$$

4.3.3 Averaging Theory in Quantum Mechanics

By analogy with the classical case one looks for a unitary operator $\boldsymbol{U}_\lambda$ that is the Schrödinger flow at time λ of some unknown Hamiltonian (Hermitian) operator $\boldsymbol{G}$, namely

$$\boldsymbol{U}_\lambda = e^{-\frac{\imath\lambda\boldsymbol{G}}{\hbar}}. \tag{4.31}$$

To any Hermitian operator $\boldsymbol{G}$ one can associate the operator

$$L_{\boldsymbol{G}} := -\frac{\imath}{\hbar}[,\boldsymbol{G}] \tag{4.32}$$

i.e. the quantum Lie derivative along the flow of $\boldsymbol{G}$. One easily proves the following

Lemma 12 *For any pair of Hermitian operators $\boldsymbol{F}$ and $\boldsymbol{G}$ independent of λ, one has*

$$e^{+\frac{\imath\lambda\boldsymbol{G}}{\hbar}}\boldsymbol{F}e^{-\frac{\imath\lambda\boldsymbol{G}}{\hbar}} = e^{\lambda L_{\boldsymbol{G}}}\boldsymbol{F}. \tag{4.33}$$

In particular, it follows that $\boldsymbol{F}$ is invariant with respect to the flow of $\boldsymbol{G}$ if and only if $[\boldsymbol{F},\boldsymbol{G}] = 0$.

Proof. Define $\boldsymbol{F}(\lambda)$ the left hand side of the previous equation and take its derivative with respect to λ, getting

$$\frac{d}{d\lambda}\boldsymbol{F}(\lambda) = \frac{\imath}{\hbar}(\boldsymbol{G}\boldsymbol{F}(\lambda) - \boldsymbol{F}(\lambda)\boldsymbol{G}) = L_{\boldsymbol{G}}\boldsymbol{F}(\lambda). \tag{4.34}$$

The latter differential equation can be formally integrated with the initial condition $\boldsymbol{F}(0) = \boldsymbol{F}$, to yield the equation. ■

We are interested on normal form up to a fixed order of a Hamiltonian. Let us very quickly see how the classical procedure for finding the normal form is kept conceptually the same up to first order concerning higher orders, it will be evident that there is really nothing different to do with respect to the classical case. Now, supposing that the quantum Hamiltonian has the form

$$\boldsymbol{H} = \boldsymbol{h} + \lambda\boldsymbol{P}_1 + ... \tag{4.35}$$

and transforming it by $\boldsymbol{U}_\lambda = e^{-\frac{\imath\lambda\boldsymbol{G_1}}{\hbar}}$, one obtains

$$\begin{aligned}
\boldsymbol{H}'_\lambda &= \boldsymbol{U}^\dagger_\lambda\boldsymbol{H}\boldsymbol{U}_\lambda = && (4.36)\\
&= e^{\frac{\imath\lambda\boldsymbol{G_1}}{\hbar}}(\boldsymbol{h} + \lambda\boldsymbol{P}_1 + \dots)e^{-\frac{\imath\lambda\boldsymbol{G_1}}{\hbar}} = && (4.37)\\
&= \boldsymbol{h} + \lambda(\boldsymbol{P}_1 + L_{\boldsymbol{G_1}}\boldsymbol{h}) + O(\lambda^2) = && (4.38)\\
&= \boldsymbol{h} + \lambda\bar{\boldsymbol{P}}_1 + O(\lambda^2), && (4.39)
\end{aligned}$$

and one requires that $\bar{\boldsymbol{P}}_1 := \boldsymbol{P}_1 + L_{\boldsymbol{G}_1}\boldsymbol{h}$ is invariant with respect to the flow of $\boldsymbol{h}$, that is $L_{\boldsymbol{h}}\bar{\boldsymbol{P}}_1 = 0$. Similarly to the classical case, one finds:

$$\bar{\boldsymbol{P}}_1 = \langle\boldsymbol{P}_1\rangle_{\boldsymbol{h}}\,.$$

Taking into account that $L_{\boldsymbol{G_1}}\boldsymbol{h} = -L_{\boldsymbol{h}}\boldsymbol{G}_1$ one writes down the **Quantum Homological Equation** (to first order):

$$\bar{\boldsymbol{P}}_1 = \boldsymbol{P}_1 - L_{\boldsymbol{h}}\boldsymbol{G}_1 \tag{4.40}$$

and solves it for $\bar{\boldsymbol{P}}_1$ and $\boldsymbol{G}_1$ exactly as done in the classical case. The result is the following

$$\bar{\boldsymbol{P}}_1 = \langle \boldsymbol{P}_1 \rangle_{\boldsymbol{h}} := \lim_{t\to+\infty} \frac{1}{t} \int_0^t e^{+\frac{\imath s \boldsymbol{h}}{\hbar}} \boldsymbol{P}_1 e^{-\frac{\imath s \boldsymbol{h}}{\hbar}} \mathrm{d}s; \tag{4.41}$$

$$\delta_{\boldsymbol{h}} \boldsymbol{P}_1 := \boldsymbol{P}_1 - \bar{\boldsymbol{P}}_1; \tag{4.42}$$

$$\boldsymbol{G}_1 = \boldsymbol{K}_1 + \lim_{t\to+\infty} \frac{1}{t} \int_0^t (s-t) e^{+\frac{\imath s \boldsymbol{h}}{\hbar}} (\delta_{\boldsymbol{h}} \boldsymbol{P}_1) e^{-\frac{\imath s \boldsymbol{h}}{\hbar}} \mathrm{d}s, \tag{4.43}$$

where $\boldsymbol{K}_1$ is any Hermitian operator such that $[\boldsymbol{K}_1; \boldsymbol{h}] = 0$. The formulas for the next orders can be obtained by using the quantum Averaging Principle. Below is reported the second order perturbation term:

$$\bar{\boldsymbol{P}}_2 = \langle \boldsymbol{P}_2 \rangle_{\boldsymbol{h}} + \frac{1}{2} \left\langle -\frac{\imath}{\hbar} [\delta_{\boldsymbol{h}} \boldsymbol{P}_1, \delta_{\boldsymbol{h}} \boldsymbol{G}_1] \right\rangle_{\boldsymbol{h}} - \frac{\imath}{\hbar} [\bar{\boldsymbol{P}}_1, \boldsymbol{K}_1], \tag{4.44}$$

where $\delta_{\boldsymbol{h}} \boldsymbol{G}_1 = \boldsymbol{G}_1 - \boldsymbol{K}_1$. It follows that the averaging principle, holds in quantum mechanics to all orders, with a formulation that, up to the replacement of the Poisson bracket $\{,\}$ with the commutator $[,]$ divided by $\imath\hbar$, is completely analogous to the classical one. In particular, to first order, the perturbation in normal form is the time average of the perturbation along the flow of the unperturbed system. We have seen, then, that the Hamiltonian perturbation theory represents a powerful tool that can help study quasi-integrable systems, in the sense described before. As observed in the classical case, we will work with $\lambda = 1$ in the sequel.

4.3.4 Application to the Quantum Hamiltonian (4.25)

Theorem 4 *The Hamiltonian of the quantum cold atoms problem, in normal form to the first order is*

$$\boldsymbol{H}^{(1)}(\boldsymbol{a}, \boldsymbol{a}^\dagger) = \boldsymbol{U}_1^\dagger \boldsymbol{H} \boldsymbol{U}_1 = \boldsymbol{h}(\boldsymbol{a}, \boldsymbol{a}^\dagger) + \bar{\boldsymbol{P}}_1(\boldsymbol{a}, \boldsymbol{a}^\dagger) + \boldsymbol{R}_2 \tag{4.45}$$

where,

$$\begin{aligned} \bar{\boldsymbol{P}}_1(\boldsymbol{a}, \boldsymbol{a}^\dagger) &= \frac{\omega}{2\pi} \int_0^{2\pi/\omega} e^{+\frac{\imath \tau \boldsymbol{h}}{\hbar}}(\tau) \boldsymbol{P}_1 e^{+\frac{-\imath \tau \boldsymbol{h}}{\hbar}}(\tau) \mathrm{d}\tau = \\ &= \mathcal{W} \sum_{j=1}^N \boldsymbol{a}_j^\dagger \boldsymbol{a}_j + \mathcal{J} \sum_{j=1}^N \boldsymbol{a}_j^\dagger (\boldsymbol{a}_{j+1} + \boldsymbol{a}_{j-1}) + \mathcal{U} \sum_{j=1}^N \boldsymbol{a}_j^{\dagger 2} \boldsymbol{a}_j^2, \end{aligned} \tag{4.46}$$

with suitable real parameters $\mathcal{W}$, $\mathcal{J}$ and $\mathcal{U}$.

Proof. The specific computation for $\bar{\boldsymbol{P}}_1 = \langle \boldsymbol{P}_1 \rangle_{\boldsymbol{h}}$ is

$$
\begin{aligned}
\langle \boldsymbol{P}_1 \rangle_{\boldsymbol{h}} (\boldsymbol{a}, \boldsymbol{a}^\dagger) &= \frac{\omega}{2\pi} \int_0^{2\pi/\omega} e^{+\frac{\imath\tau \boldsymbol{h}}{\hbar}}(\tau) \boldsymbol{P}_1 e^{+\frac{-\imath\tau \boldsymbol{h}}{\hbar}}(\tau) \mathrm{d}\tau = \\
&= \frac{\omega}{2\pi} \int_0^{2\pi/\omega} \sum_{j \in \mathbb{Z}_N} \Big[- \frac{\Lambda \hbar^2}{16 m^2 \omega^2} (\boldsymbol{a}_j e^{-\imath\omega\tau} + \boldsymbol{a}_j^\dagger e^{\imath\omega\tau})^4 + \\
&+ \frac{K\hbar}{4m\omega} \Big((\boldsymbol{a}_{j+1} e^{-\imath\omega\tau} + \boldsymbol{a}_{j+1}^\dagger e^{\imath\omega\tau}) - (\boldsymbol{a}_j e^{-\imath\omega\tau} + \boldsymbol{a}_j^\dagger e^{\imath\omega\tau}) \Big)^2 \Big] \mathrm{d}\tau = \\
&= \sum_{j \in \mathbb{Z}_N} \Big[- \frac{\Lambda \hbar^2}{16 m^2 \omega^2} (6 \boldsymbol{a}_j^2 \boldsymbol{a}_j^{\dagger 2}) + \\
&+ \frac{K\hbar}{2m\omega} \Big((\boldsymbol{a}_{j+1} \boldsymbol{a}_{j+1}^\dagger + \boldsymbol{a}_j \boldsymbol{a}_j^\dagger) - (\boldsymbol{a}_{j+1} \boldsymbol{a}_j^\dagger + \boldsymbol{a}_{j+1}^\dagger \boldsymbol{a}_j) \Big) \Big] = \\
&= \sum_{j \in \mathbb{Z}_N} \Big[\frac{K\hbar}{2m\omega} (\boldsymbol{a}_{j+1} \boldsymbol{a}_{j+1}^\dagger + \boldsymbol{a}_j \boldsymbol{a}_j^\dagger) - \frac{K\hbar}{2m\omega} (\boldsymbol{a}_j^\dagger \boldsymbol{a}_{j+1} + \boldsymbol{a}_{j+1}^\dagger \boldsymbol{a}_j) + \\
&- \frac{3\Lambda \hbar^2}{8 m^2 \omega^2} (\boldsymbol{a}_j^2 \boldsymbol{a}_j^{\dagger 2}) \Big] = \\
&= \sum_{j \in \mathbb{Z}_N} \frac{K\hbar}{m\omega} \boldsymbol{a}_j \boldsymbol{a}_j^\dagger - \sum_{j \in \mathbb{Z}_N} \frac{K\hbar}{2m\omega} (\boldsymbol{a}_j^\dagger \boldsymbol{a}_{j+1} + \boldsymbol{a}_j^\dagger \boldsymbol{a}_{j-1}) + \\
&- \sum_{j \in \mathbb{Z}_N} \frac{3\Lambda \hbar^2}{8 m^2 \omega^2} (\boldsymbol{a}_j^2 \boldsymbol{a}_j^{\dagger 2}) = \\
&= \frac{K\hbar}{m\omega} \sum_{j \in \mathbb{Z}_N} \boldsymbol{a}_j^\dagger \boldsymbol{a}_j - \frac{K\hbar}{2m\omega} \sum_{j \in \mathbb{Z}_N} \boldsymbol{a}_j^\dagger (\boldsymbol{a}_{j+1} + \boldsymbol{a}_{j-1}) + \\
&- \frac{3\Lambda \hbar^2}{8 m^2 \omega^2} \sum_{j \in \mathbb{Z}_N} (\boldsymbol{a}_j^{\dagger 2} \boldsymbol{a}_j^2) - \frac{3\Lambda \hbar^2}{2 m^2 \omega^2} \sum_{j \in \mathbb{Z}_N} \boldsymbol{a}_j^\dagger \boldsymbol{a}_j .
\end{aligned}
$$

So the quantum Hamiltonian in normal form to first order is:

$$
\boldsymbol{H}^{(1)}(\boldsymbol{a}, \boldsymbol{a}^\dagger) = \boldsymbol{U}_1^\dagger \boldsymbol{H} \boldsymbol{U}_1 = \boldsymbol{h}(\boldsymbol{a}, \boldsymbol{a}^\dagger) + \bar{\boldsymbol{P}}_1(\boldsymbol{a}, \boldsymbol{a}^\dagger) + \boldsymbol{R}_2 \tag{4.47}
$$

where

$$
\bar{\boldsymbol{P}}_1(\boldsymbol{a}, \boldsymbol{a}^\dagger) = \mathcal{W} \sum_{j \in \mathbb{Z}_N} \boldsymbol{a}_j^\dagger \boldsymbol{a}_j + \mathcal{J} \sum_{j \in \mathbb{Z}_N} \boldsymbol{a}_j^\dagger (\boldsymbol{a}_{j+1} + \boldsymbol{a}_{j-1}) + \mathcal{U} \sum_{j \in \mathbb{Z}_N} \boldsymbol{a}_j^{\dagger 2} \boldsymbol{a}_j^2, \tag{4.48}
$$

with

$$\mathcal{W} := \frac{K\hbar}{m\omega} - \frac{3\Lambda\hbar^2}{2m^2\omega^2}; \tag{4.49}$$

$$\mathcal{J} := -\frac{K\hbar}{2m\omega}; \tag{4.50}$$

$$\mathcal{U} := -\frac{3\Lambda\hbar^2}{8m^2\omega^2}. \tag{4.51}$$

■

The truncated quantum normal form

$$\begin{aligned} \boldsymbol{H}^{(1)} - \boldsymbol{R}_2 &= \boldsymbol{h} + \bar{\boldsymbol{P}}_1 = \\ &= (\mathcal{W} + \omega) \sum_{j\in\mathbb{Z}_N} \boldsymbol{a}_j^\dagger \boldsymbol{a}_j + \mathcal{J} \sum_{j\in\mathbb{Z}_N} \boldsymbol{a}_j^\dagger (\boldsymbol{a}_{j+1} + \boldsymbol{a}_{j-1}) + \mathcal{U} \sum_{j\in\mathbb{Z}_N} \boldsymbol{a}_j^{\dagger 2} \boldsymbol{a}_j^2 \end{aligned}$$

defines the so-called Bose-Hubbard (BH) model, the reference standard model in optically trapped cold atom systems. The corresponding BH equation is

$$\imath \dot{\boldsymbol{a}}_j = (\mathcal{W} + \omega)\boldsymbol{a}_j + \mathcal{J}(\boldsymbol{a}_{j+1} + \boldsymbol{a}_{j-1}) + 2\mathcal{U}\boldsymbol{a}_j^\dagger \boldsymbol{a}_j^2. \tag{4.52}$$

Successive corrections $\bar{\boldsymbol{P}}_2, \bar{\boldsymbol{P}}_3$ and so on are computable as well. Notice that the BH Hamiltonian is just the quantum version of the dBGP Hamiltonian. As a matter of fact, the classical mechanics describes well both the dynamics and the statistical properties of condensed matter at high temperatures.

The results listed above allow to improve such a conclusion extending it, in principle, to any higher order approximation (i.e. BH deformation) of the true Hamiltonian.

In order to compute $\bar{\boldsymbol{P}}_2$, like in the classical case, one has to compute $\boldsymbol{G}_1$ but we first need

$$\begin{aligned} \delta_{\boldsymbol{h}} \boldsymbol{P}_1 = \boldsymbol{P}_1 - \langle \boldsymbol{P}_1 \rangle_h = \sum_{j\in\mathbb{Z}_N} \Big[&- \frac{\Lambda\hbar^2}{16m^2\omega^2} (\boldsymbol{b}_j^4 + 4\boldsymbol{b}_j^3 \boldsymbol{b}_j^\dagger + \boldsymbol{b}_j^{\dagger 4} + 4\boldsymbol{b}_j^{\dagger 3} \boldsymbol{b}_j) + \\ &+ \frac{K\hbar}{4m\omega} \Big((\boldsymbol{b}_{j+1} - \boldsymbol{b}_j)^2 + (\boldsymbol{b}_{j+1}^\dagger - \boldsymbol{b}_j^\dagger)^2 \Big) \Big]. \end{aligned} \tag{4.53}$$

The computations of $\boldsymbol{G}_1$ follows:

$$\begin{aligned}\boldsymbol{G}_1(\boldsymbol{b},\boldsymbol{b}^\dagger) &= \frac{\omega}{2\pi}\int_0^{2\pi/\omega} s e^{+\frac{\imath s\boldsymbol{h}}{\hbar}}\delta_{\boldsymbol{h}}\boldsymbol{P}_1 e^{-\frac{\imath s\boldsymbol{h}}{\hbar}}\mathrm{d}s = \\ &= \frac{\omega}{2\pi}\int_0^{2\pi/\omega} s\Big[\sum_{j\in\mathbb{Z}_N} -\frac{\Lambda\hbar^2}{16m^2\omega^2}(\boldsymbol{b}_j^4 e^{-4\imath\omega s} + 4\boldsymbol{b}_j^3 e^{-2\imath\omega s}\boldsymbol{b}_j^\dagger + \boldsymbol{b}_j^{\dagger 4}e^{4\imath\omega s} + \\ &+ 4\boldsymbol{b}_j^{\dagger 3}e^{2\imath\omega s}\boldsymbol{b}_j) + \frac{K\hbar}{4m\omega}\Big((\boldsymbol{b}_{j+1}^2 e^{-2\imath\omega s} + \boldsymbol{b}_j^2 e^{-2\imath\omega s} - 2\boldsymbol{b}_{j+1}\boldsymbol{b}_j e^{-2\imath\omega s}) + \\ &+ (\boldsymbol{b}_{j+1}^{\dagger 2}e^{2\imath\omega s} + \boldsymbol{b}_j^{\dagger 2}e^{2\imath\omega s} - 2\boldsymbol{b}_{j+1}^\dagger\boldsymbol{b}_j^\dagger e^{2\imath\omega s})\Big)\Big]\mathrm{d}s = \\ &= \sum_{j\in\mathbb{Z}_N}\Big[-\frac{\Lambda\hbar^2}{16\imath m^2\omega^3}(-\frac{\boldsymbol{b}_j^4}{4} - \frac{4\boldsymbol{b}_j^3\boldsymbol{b}_j^\dagger}{2} + \frac{\boldsymbol{b}_j^{\dagger 4}}{4} + \frac{4\boldsymbol{b}_j^{\dagger 3}\boldsymbol{b}_j}{2}) + \\ &+ \frac{K\hbar}{8\imath m\omega^2}\Big((-\boldsymbol{b}_{j+1}^2 - \boldsymbol{b}_j^2 + 2\boldsymbol{b}_{j+1}\boldsymbol{b}_j) + (\boldsymbol{b}_{j+1}^{\dagger 2} + \boldsymbol{b}_j^{\dagger 2} - 2\boldsymbol{b}_{j+1}^\dagger\boldsymbol{b}_j^\dagger)\Big)\Big].\end{aligned}$$

Choosing, $\boldsymbol{K}_1 = 0$, as a kernel element in (4.43), compute the second order perturbation term in normal form:

$$\bar{\boldsymbol{P}}_2 = \langle\boldsymbol{P}_2\rangle_{\boldsymbol{h}} + \frac{1}{2}\Big\langle -\frac{\imath}{\hbar}[\delta_{\boldsymbol{h}}\boldsymbol{P}_1, \boldsymbol{G_1}]\Big\rangle_{\boldsymbol{h}}, \tag{4.54}$$

where we observe that $\delta_{\boldsymbol{h}}\boldsymbol{G}_1 = \boldsymbol{G}_1$ when $\boldsymbol{K}_1 = 0$. By an easy computation one gets:

$$\begin{aligned}\langle\boldsymbol{P}_2\rangle_{\boldsymbol{h}}(\boldsymbol{a},\boldsymbol{a}^\dagger) &= \frac{\omega}{2\pi}\int_0^{2\pi/\omega} e^{+\frac{\imath\tau\boldsymbol{h}}{\hbar}}\boldsymbol{P}_2 e^{+\frac{-\imath\tau\boldsymbol{h}}{\hbar}}\mathrm{d}\tau = \\ &= \frac{\omega}{2\pi}\int_0^{2\pi/\omega}\sum_{j\in\mathbb{Z}_N}\Big[\frac{\Gamma}{6}\Big(\frac{\hbar}{2m\omega}\Big)^3(\boldsymbol{a}_j e^{-\imath\omega\tau} + \boldsymbol{a}_j^\dagger e^{\imath\omega\tau})^6 + \\ &+ \frac{\alpha}{3}\sqrt{\frac{\hbar}{2m\omega}}^3[(\boldsymbol{a}_{j+1}e^{-\imath\omega\tau} + \boldsymbol{a}_{j+1}^\dagger e^{\imath\omega\tau}) - (\boldsymbol{a}_j e^{-\imath\omega\tau} + \boldsymbol{a}_j^\dagger e^{\imath\omega\tau})]^3\Big]\mathrm{d}\tau = \\ &= \sum_{j\in\mathbb{Z}_N}\frac{10\Gamma}{6}\Big(\frac{\hbar}{2m\omega}\Big)^3\Big(\boldsymbol{a}_j^3\boldsymbol{a}_j^{\dagger 3} + \boldsymbol{a}_j^{\dagger 3}\boldsymbol{a}_j^3\Big).\end{aligned} \tag{4.55}$$

In order to compute the Lie bracket between $\delta_{\boldsymbol{h}}\boldsymbol{P}_1$ and $\boldsymbol{G}_1$ one has to compute the commutator $[\delta_{\boldsymbol{h}}\boldsymbol{P}_1, \boldsymbol{G}_1] = \delta_{\boldsymbol{h}}\boldsymbol{P}_1\boldsymbol{G}_1 - \boldsymbol{G}_1\delta_{\boldsymbol{h}}\boldsymbol{P}_1$. Notice that holds the following relations:

$$\begin{aligned}[\boldsymbol{b}_j, \boldsymbol{b}_k^{\dagger n}] &= n\boldsymbol{b}_k^{\dagger n-1}\delta_{j,k} = \frac{\partial}{\partial\boldsymbol{b}_j^\dagger}(\boldsymbol{b}_k^{\dagger n}), \\ [\boldsymbol{b}_j^\dagger, \boldsymbol{b}_k^n] &= n\boldsymbol{b}_k^{n-1}\delta_{j,k} = \frac{\partial}{\partial\boldsymbol{b}_j}(\boldsymbol{b}_k^n).\end{aligned}$$

Such relations, allows us to write the commutator between $\boldsymbol{F}$ and $\boldsymbol{G}$ as follows:

$$[\boldsymbol{F}(\boldsymbol{b},\boldsymbol{b}^\dagger),\boldsymbol{G}(\boldsymbol{b},\boldsymbol{b}^\dagger)]=\sum_{j\in\mathbb{Z}_N}\Big(\frac{\partial\boldsymbol{F}}{\partial\boldsymbol{b}_j}\frac{\partial\boldsymbol{G}}{\partial\boldsymbol{b}_j^\dagger}-\frac{\partial\boldsymbol{F}}{\partial\boldsymbol{b}_j^\dagger}\frac{\partial\boldsymbol{G}}{\partial\boldsymbol{b}_j}\Big).$$

So in order to compute $[\delta_{\boldsymbol{h}}\boldsymbol{P}_1,\boldsymbol{G}_1]$ one has to calculate first the derivatives of $\delta_{\boldsymbol{h}}\boldsymbol{P}_1$ and $\boldsymbol{G}_1$ with respect to $\boldsymbol{b}_j$ and $\boldsymbol{b}_j^\dagger$ and then the products between them.

$$\begin{aligned}
\frac{\partial\delta_{\boldsymbol{h}}\boldsymbol{P}_1}{\partial\boldsymbol{b}_j}&=-\frac{\Lambda\hbar^2}{16m^2\omega^2}(4\boldsymbol{b}_j^3+12\boldsymbol{b}_j^2\boldsymbol{b}_j^\dagger+4\boldsymbol{b}_j^{\dagger 3})+\frac{K\hbar}{2m\omega}\Big((\boldsymbol{b}_j-\boldsymbol{b}_{j-1})-(\boldsymbol{b}_{j+1}-\boldsymbol{b}_j)\Big);\\
\frac{\partial\delta_{\boldsymbol{h}}\boldsymbol{P}_1}{\partial\boldsymbol{b}_j^\dagger}&=-\frac{\Lambda\hbar^2}{16m^2\omega^2}(4\boldsymbol{b}_j^3+4\boldsymbol{b}_j^{\dagger 3}+12\boldsymbol{b}_j^{\dagger 2}\boldsymbol{b}_j)+\frac{K\hbar}{2m\omega}\Big((\boldsymbol{b}_j^\dagger-\boldsymbol{b}_{j-1}^\dagger)-(\boldsymbol{b}_{j+1}^\dagger-\boldsymbol{b}_j^\dagger)\Big);\\
\frac{\partial\boldsymbol{G}_1}{\partial\boldsymbol{b}_j}&=-\frac{\Lambda\hbar^2}{16\imath m^2\omega^3}(-\boldsymbol{b}_j^3-6\boldsymbol{b}_j^2\boldsymbol{b}_j^\dagger+2\boldsymbol{b}_j^{\dagger 3})+\frac{K\hbar}{4\imath m\omega^2}\Big((\boldsymbol{b}_{j+1}-\boldsymbol{b}_j)-(\boldsymbol{b}_j-\boldsymbol{b}_{j-1})\Big);\\
\frac{\partial\boldsymbol{G}_1}{\partial\boldsymbol{b}_j^\dagger}&=-\frac{\Lambda\hbar^2}{16\imath m^2\omega^3}(-2\boldsymbol{b}_j^3+\boldsymbol{b}_j^{\dagger 3}+6\boldsymbol{b}_j^{\dagger 2}\boldsymbol{b}_j)+\frac{K\hbar}{4\imath m\omega^2}\Big((\boldsymbol{b}_j^\dagger-\boldsymbol{b}_{j-1}^\dagger)-(\boldsymbol{b}_{j+1}^\dagger-\boldsymbol{b}_j^\dagger)\Big).
\end{aligned}$$

$$\begin{aligned}
\frac{\partial\delta_{\boldsymbol{h}}\boldsymbol{P}_1}{\partial\boldsymbol{b}_j}\frac{\partial\boldsymbol{G}_1}{\partial\boldsymbol{b}_j^\dagger}&=\frac{\Lambda^2\hbar^4}{256\imath m^4\omega^5}(4\boldsymbol{b}_j^3+12\boldsymbol{b}_j^2\boldsymbol{b}_j^\dagger+4\boldsymbol{b}_j^{\dagger 3})(-2\boldsymbol{b}_j^3+\boldsymbol{b}_j^{\dagger 3}+6\boldsymbol{b}_j^{\dagger 2}\boldsymbol{b}_j)+\\
&-\frac{\Lambda K\hbar^3}{64\imath m^3\omega^4}(4\boldsymbol{b}_j^3+12\boldsymbol{b}_j^2\boldsymbol{b}_j^\dagger+4\boldsymbol{b}_j^{\dagger 3})\Big((\boldsymbol{b}_j^\dagger-\boldsymbol{b}_{j-1}^\dagger)-(\boldsymbol{b}_{j+1}^\dagger-\boldsymbol{b}_j^\dagger)\Big)+\\
&-\frac{\Lambda K\hbar^3}{32\imath m^3\omega^4}\Big((\boldsymbol{b}_j-\boldsymbol{b}_{j-1})-(\boldsymbol{b}_{j+1}-\boldsymbol{b}_j)\Big)(-2\boldsymbol{b}_j^3+\boldsymbol{b}_j^{\dagger 3}+6\boldsymbol{b}_j^{\dagger 2}\boldsymbol{b}_j)+\\
&+\frac{K^2\hbar^2}{8\imath m^2\omega^3}\Big((\boldsymbol{b}_j-\boldsymbol{b}_{j-1})-(\boldsymbol{b}_{j+1}-\boldsymbol{b}_j)\Big)\Big((\boldsymbol{b}_j^\dagger-\boldsymbol{b}_{j-1}^\dagger)-(\boldsymbol{b}_{j+1}^\dagger-\boldsymbol{b}_j^\dagger)\Big).
\end{aligned}$$

$$\begin{aligned}
\frac{\partial\delta_{\boldsymbol{h}}\boldsymbol{P}_1}{\partial\boldsymbol{b}_j^\dagger}\frac{\partial\boldsymbol{G}_1}{\partial\boldsymbol{b}_j}&=\frac{\Lambda^2\hbar^4}{256\imath m^4\omega^5}(4\boldsymbol{b}_j^3+4\boldsymbol{b}_j^{\dagger 3}+12\boldsymbol{b}_j^{\dagger 2}\boldsymbol{b}_j)(-\boldsymbol{b}_j^3-6\boldsymbol{b}_j^2\boldsymbol{b}_j^\dagger+2\boldsymbol{b}_j^{\dagger 3})+\\
&-\frac{\Lambda K\hbar^3}{64\imath m^3\omega^4}(4\boldsymbol{b}_j^3+4\boldsymbol{b}_j^{\dagger 3}+12\boldsymbol{b}_j^{\dagger 2}\boldsymbol{b}_j)\Big((\boldsymbol{b}_{j+1}-\boldsymbol{b}_j)-(\boldsymbol{b}_j-\boldsymbol{b}_{j-1})\Big)+\\
&-\frac{\Lambda K\hbar^3}{32\imath m^3\omega^4}\Big((\boldsymbol{b}_j^\dagger-\boldsymbol{b}_{j-1}^\dagger)-(\boldsymbol{b}_{j+1}^\dagger-\boldsymbol{b}_j^\dagger)\Big)(-\boldsymbol{b}_j^3-6\boldsymbol{b}_j^2\boldsymbol{b}_j^\dagger+2\boldsymbol{b}_j^{\dagger 3})+\\
&+\frac{K^2\hbar^2}{8\imath m^2\omega^3}\Big((\boldsymbol{b}_j^\dagger-\boldsymbol{b}_{j-1}^\dagger)-(\boldsymbol{b}_{j+1}^\dagger-\boldsymbol{b}_j^\dagger)\Big)\Big((\boldsymbol{b}_{j+1}-\boldsymbol{b}_j)-(\boldsymbol{b}_j-\boldsymbol{b}_{j-1})\Big).
\end{aligned}$$

The explicit expression of the bracket is:

$$
\begin{aligned}
[\delta_{\boldsymbol{h}}\boldsymbol{P}_1, \boldsymbol{G}_1] = \sum_{j\in\mathbb{Z}_N} \Big\{ & \frac{\Lambda^2\hbar^4}{256\imath m^4\omega^5}\Big[(4\boldsymbol{b}_j^3 + 12\boldsymbol{b}_j^2\boldsymbol{b}_j^\dagger + 4\boldsymbol{b}_j^{\dagger 3})(-2\boldsymbol{b}_j^3 + \boldsymbol{b}_j^{\dagger 3} + 6\boldsymbol{b}_j^{\dagger 2}\boldsymbol{b}_j) + \\
& - (4\boldsymbol{b}_j^3 + 4\boldsymbol{b}_j^{\dagger 3} + 12\boldsymbol{b}_j^{\dagger 2}\boldsymbol{b}_j)(-\boldsymbol{b}_j^3 - 6\boldsymbol{b}_j^2\boldsymbol{b}_j^\dagger + 2\boldsymbol{b}_j^{\dagger 3})\Big] + \\
& - \frac{\Lambda K\hbar^3}{64\imath m^3\omega^4}\Big[(4\boldsymbol{b}_j^3 + 12\boldsymbol{b}_j^2\boldsymbol{b}_j^\dagger + 4\boldsymbol{b}_j^{\dagger 3})\Big((\boldsymbol{b}_j^\dagger - \boldsymbol{b}_{j-1}^\dagger) - (\boldsymbol{b}_{j+1}^\dagger - \boldsymbol{b}_j^\dagger)\Big) + \\
& - (4\boldsymbol{b}_j^3 + 4\boldsymbol{b}_j^{\dagger 3} + 12\boldsymbol{b}_j^{\dagger 2}\boldsymbol{b}_j)\Big((\boldsymbol{b}_{j+1} - \boldsymbol{b}_j) - (\boldsymbol{b}_j - \boldsymbol{b}_{j-1})\Big)\Big] + \\
& - \frac{\Lambda K\hbar^3}{32\imath m^3\omega^4}\Big[\Big((\boldsymbol{b}_j - \boldsymbol{b}_{j-1}) - (\boldsymbol{b}_{j+1} - \boldsymbol{b}_j)\Big)(-2\boldsymbol{b}_j^3 + \boldsymbol{b}_j^{\dagger 3} + 6\boldsymbol{b}_j^{\dagger 2}\boldsymbol{b}_j) + \\
& - \Big((\boldsymbol{b}_j^\dagger - \boldsymbol{b}_{j-1}^\dagger) - (\boldsymbol{b}_{j+1}^\dagger - \boldsymbol{b}_j^\dagger)\Big)(-\boldsymbol{b}_j^3 - 6\boldsymbol{b}_j^2\boldsymbol{b}_j^\dagger + 2\boldsymbol{b}_j^{\dagger 3})\Big] + \\
& + \frac{K^2\hbar^2}{8\imath m^2\omega^3}\Big[\Big((\boldsymbol{b}_j - \boldsymbol{b}_{j-1}) - (\boldsymbol{b}_{j+1} - \boldsymbol{b}_j)\Big)\Big((\boldsymbol{b}_j^\dagger - \boldsymbol{b}_{j-1}^\dagger) - (\boldsymbol{b}_{j+1}^\dagger - \boldsymbol{b}_j^\dagger)\Big) + \\
& - \Big((\boldsymbol{b}_j^\dagger - \boldsymbol{b}_{j-1}^\dagger) - (\boldsymbol{b}_{j+1}^\dagger - \boldsymbol{b}_j^\dagger)\Big)\Big((\boldsymbol{b}_{j+1} - \boldsymbol{b}_j) - (\boldsymbol{b}_j - \boldsymbol{b}_{j-1})\Big)\Big]\Big\}.
\end{aligned}
$$

So now one can compute the average of the previous Lie bracket along the unperturbed flow of $\boldsymbol{h}$:

$$
\begin{aligned}
\Big\langle -\frac{\imath}{\hbar}[\delta_{\boldsymbol{h}}\boldsymbol{P}_1, \boldsymbol{G}_1]\Big\rangle_{\boldsymbol{h}}(\boldsymbol{a}, \boldsymbol{a}^\dagger) = \frac{\omega}{2\pi}\int_0^{2\pi/\omega} e^{+\frac{\imath s\boldsymbol{h}}{\hbar}} - \frac{\imath}{\hbar}[\delta_{\boldsymbol{h}}\boldsymbol{P}_1, \boldsymbol{G}_1]e^{-\frac{\imath s\boldsymbol{h}}{\hbar}}(\boldsymbol{a}, \boldsymbol{a}^\dagger)\mathrm{d}s = \\
= \sum_{j\in\mathbb{Z}_N} \Big\{ & - \frac{17\Lambda^2\hbar^3}{64m^4\omega^5}\Big[\boldsymbol{a}_j^3\boldsymbol{a}_j^{\dagger 3} + \boldsymbol{a}_j^{\dagger 3}\boldsymbol{a}_j^3\Big] + \\
& - \frac{27\Lambda^2\hbar^3}{32m^4\omega^5}\Big[\boldsymbol{a}_j^2\boldsymbol{a}_j^{\dagger 2} + \boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j^2\Big] + \\
& + \frac{3\Lambda K\hbar^2}{4m^3\omega^4}\Big[\boldsymbol{a}_j^2\boldsymbol{a}_j^{\dagger 2} + \boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j^2\Big] + \frac{3\Lambda K\hbar^2}{4m^3\omega^4}\Big[\boldsymbol{a}_j\boldsymbol{a}_j^\dagger + \boldsymbol{a}_j^\dagger\boldsymbol{a}_j\Big] \\
& - \frac{3\Lambda K\hbar^2}{16m^3\omega^4}\Big[\boldsymbol{a}_j^2\boldsymbol{a}_j^\dagger(\boldsymbol{a}_{j-1}^\dagger + \boldsymbol{a}_{j+1}^\dagger) + (\boldsymbol{a}_{j-1}^\dagger + \boldsymbol{a}_{j+1}^\dagger)\boldsymbol{a}_j^2\boldsymbol{a}_j^\dagger + \\
& + \boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j(\boldsymbol{a}_{j-1} + \boldsymbol{a}_{j+1}) + (\boldsymbol{a}_{j-1} + \boldsymbol{a}_{j+1})\boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j\Big] \\
& - \frac{K^2\hbar}{8m^2\omega^3}\Big[\Big(2\boldsymbol{a}_j - \boldsymbol{a}_{j-1} - \boldsymbol{a}_{j+1}\Big)\Big(2\boldsymbol{a}_j^\dagger - \boldsymbol{a}_{j-1}^\dagger - \boldsymbol{a}_{j+1}^\dagger\Big) + \\
& + \Big(2\boldsymbol{a}_j^\dagger - \boldsymbol{a}_{j-1}^\dagger - \boldsymbol{a}_{j+1}^\dagger\Big)\Big(2\boldsymbol{a}_j - \boldsymbol{a}_{j-1} - \boldsymbol{a}_{j+1}\Big)\Big]\Big\}.
\end{aligned}
$$

Finally the perturbation term of second order $\bar{\boldsymbol{P}}_2$ has the form:

$$\begin{aligned}\bar{\boldsymbol{P}}_2(\boldsymbol{a},\boldsymbol{a}^\dagger) = \tilde{\mathcal{U}} \sum_{j\in\mathbb{Z}_N} \left[\boldsymbol{a}_j^3\boldsymbol{a}_j^{\dagger 3} + \boldsymbol{a}_j^{\dagger 3}\boldsymbol{a}_j^3\right] + \tilde{\mathcal{M}} \sum_{j\in\mathbb{Z}_N} \left[\boldsymbol{a}_j^2\boldsymbol{a}_j^{\dagger 2} + \boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j^2\right] + \tilde{\mathcal{W}} \sum_{j\in\mathbb{Z}_N} \boldsymbol{a}_j^\dagger\boldsymbol{a}_j + \\ + \tilde{\mathcal{N}} \sum_{j\in\mathbb{Z}_N} \Big[\boldsymbol{a}_j^2\boldsymbol{a}_j^\dagger(\boldsymbol{a}_{j-1}^\dagger + \boldsymbol{a}_{j+1}^\dagger) + (\boldsymbol{a}_{j-1}^\dagger + \boldsymbol{a}_{j+1}^\dagger)\boldsymbol{a}_j^2\boldsymbol{a}_j^\dagger + \\ + \boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j(\boldsymbol{a}_{j-1} + \boldsymbol{a}_{j+1}) + (\boldsymbol{a}_{j-1} + \boldsymbol{a}_{j+1})\boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j\Big] + \\ + \tilde{\mathcal{J}} \sum_{j\in\mathbb{Z}_N} \Big[(2\boldsymbol{a}_j - \boldsymbol{a}_{j-1} - \boldsymbol{a}_{j+1})(2\boldsymbol{a}_j^\dagger - \boldsymbol{a}_{j-1}^\dagger - \boldsymbol{a}_{j+1}^\dagger) + \\ + (2\boldsymbol{a}_j^\dagger - \boldsymbol{a}_{j-1}^\dagger - \boldsymbol{a}_{j+1}^\dagger)(2\boldsymbol{a}_j - \boldsymbol{a}_{j-1} - \boldsymbol{a}_{j+1})\Big] \qquad (4.56)\end{aligned}$$

where

$$\tilde{\mathcal{U}} := -\frac{17\Lambda^2\hbar^3}{128m^4\omega^5} + \frac{5\Gamma\hbar^3}{24m^3\omega^3}; \qquad (4.57)$$

$$\tilde{\mathcal{J}} := -\frac{K^2\hbar}{16m^2\omega^3}; \qquad (4.58)$$

$$\tilde{\mathcal{M}} := \frac{3\Lambda K\hbar^2}{8m^3\omega^4} - \frac{27\Lambda^2\hbar^3}{64m^4\omega^5}; \qquad (4.59)$$

$$\tilde{\mathcal{N}} := -\frac{3\Lambda K\hbar^2}{32m^3\omega^4}; \qquad (4.60)$$

$$\tilde{\mathcal{W}} := \frac{3\Lambda K\hbar^2}{4m^3\omega^4}. \qquad (4.61)$$

We have thus proved the following:

Theorem 5 *The quantum Hamiltonian of the cold atoms problem in normal form to the second order is*

$$\boldsymbol{H}^{(2)}(\boldsymbol{a},\boldsymbol{a}^\dagger) = \boldsymbol{h}(\boldsymbol{a},\boldsymbol{a}^\dagger) + \bar{\boldsymbol{P}}_1(\boldsymbol{a},\boldsymbol{a}^\dagger) + \bar{\boldsymbol{P}}_2(\boldsymbol{a},\boldsymbol{a}^\dagger) + \boldsymbol{R}_3, \qquad (4.62)$$

where $\bar{\boldsymbol{P}}_1$ and $\bar{\boldsymbol{P}}_2$ are given in (4.46) and (4.56) respectively.

4.4 Summary of the Quantum Part

In this section we summarize the model obtained in the quantum case in order to have a general and complete point of view and also to compare with the results obtained in the classical case.
The starting quantum Hamiltonian before the unitary transformation is:

$$\begin{aligned}\boldsymbol{H}(\boldsymbol{q},\boldsymbol{p}) &= H(q,-\imath\hbar\frac{\partial}{\partial q}) = \\ &= \sum_{j\in\mathbb{Z}_N}\Big[\Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2}+\frac{m\omega^2}{2}q_j^2\Big)+\Big(-\frac{\Lambda}{4}q_j^4+\frac{K}{2}(q_{j+1}-q_j)^2\Big) \\ &+\Big(\frac{\Gamma}{6}q_j^6+\frac{\alpha}{3}(q_{j+1}-q_j)^3\Big)\Big]. \end{aligned} \tag{4.63}$$

The quantum Hamiltonian in normal form to second order is:

$$\boldsymbol{H}^{(2)} = \boldsymbol{h}+\bar{\boldsymbol{P}}_1+\bar{\boldsymbol{P}}_2+\boldsymbol{R}_3 \tag{4.64}$$

where $\boldsymbol{h}$ is the unperturbed Hamiltonian and $\bar{\boldsymbol{P}}_1$, $\bar{\boldsymbol{P}}_2$ are the first and the second term of perturbation.

$$\boldsymbol{h} = \sum_{j\in\mathbb{Z}_N}\hbar\omega\boldsymbol{a}_j^\dagger\boldsymbol{a}_j; \tag{4.65}$$

$$\bar{\boldsymbol{P}}_1 = \mathcal{W}\sum_{j\in\mathbb{Z}_N}\boldsymbol{a}_j^\dagger\boldsymbol{a}_j+\mathcal{J}\sum_{j\in\mathbb{Z}_N}\boldsymbol{a}_j^\dagger(\boldsymbol{a}_{j+1}+\boldsymbol{a}_{j-1})+\mathcal{U}\sum_{j\in\mathbb{Z}_N}\boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j^2; \tag{4.66}$$

$$\begin{aligned}\bar{\boldsymbol{P}}_2 =& \tilde{\mathcal{U}}\sum_{j\in\mathbb{Z}_N}\Big[\boldsymbol{a}_j^3\boldsymbol{a}_j^{\dagger 3}+\boldsymbol{a}_j^{\dagger 3}\boldsymbol{a}_j^3\Big]+\tilde{\mathcal{M}}\sum_{j\in\mathbb{Z}_N}\Big[\boldsymbol{a}_j^2\boldsymbol{a}_j^{\dagger 2}+\boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j^2\Big]+\tilde{\mathcal{W}}\sum_{j\in\mathbb{Z}_N}\boldsymbol{a}_j^\dagger\boldsymbol{a}_j+ \\ &+\tilde{\mathcal{N}}\sum_{j\in\mathbb{Z}_N}\Big[\boldsymbol{a}_j^2\boldsymbol{a}_j^\dagger(\boldsymbol{a}_{j-1}^\dagger+\boldsymbol{a}_{j+1}^\dagger)+(\boldsymbol{a}_{j-1}^\dagger+\boldsymbol{a}_{j+1}^\dagger)\boldsymbol{a}_j^2\boldsymbol{a}_j^\dagger+ \\ &+\boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j(\boldsymbol{a}_{j-1}+\boldsymbol{a}_{j+1})+(\boldsymbol{a}_{j-1}+\boldsymbol{a}_{j+1})\boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j\Big]+ \\ &+\tilde{\mathcal{J}}\sum_{j\in\mathbb{Z}_N}\Big[(2\boldsymbol{a}_j-\boldsymbol{a}_{j-1}-\boldsymbol{a}_{j+1})(2\boldsymbol{a}_j^\dagger-\boldsymbol{a}_{j-1}^\dagger-\boldsymbol{a}_{j+1}^\dagger)+ \\ &+(2\boldsymbol{a}_j^\dagger-\boldsymbol{a}_{j-1}^\dagger-\boldsymbol{a}_{j+1}^\dagger)(2\boldsymbol{a}_j-\boldsymbol{a}_{j-1}-\boldsymbol{a}_{j+1})\Big], \end{aligned} \tag{4.67}$$

where the coefficients are $\mathcal{W} := \frac{K\hbar}{m\omega}-\frac{3\Lambda\hbar^2}{2m^2\omega^2}$, $\mathcal{J} := -\frac{K\hbar}{2m\omega}$, $\mathcal{U} := -\frac{3\Lambda\hbar^2}{8m^2\omega^2}$ instead, $\tilde{\mathcal{U}} = -\frac{17\Lambda^2\hbar^3}{128m^4\omega^5}+\frac{5\Gamma\hbar^3}{24m^3\omega^3}$, $\tilde{\mathcal{M}} = \frac{3\Lambda K\hbar^2}{8m^3\omega^4}-\frac{27\Lambda^2\hbar^3}{64m^4\omega^5}$, $\tilde{\mathcal{N}} = \frac{3\Lambda K\hbar^2}{32m^3\omega^4}$, $\tilde{\mathcal{J}} = -\frac{K^2\hbar}{16m^2\omega^3}$, $\tilde{\mathcal{W}} = \frac{3\Lambda K\hbar^2}{4m^3\omega^4}$.

The explicit expression of truncated quantum normal form is

$$\begin{aligned}\boldsymbol{H}^{(2)} - \boldsymbol{R}_3 = \boldsymbol{h} + \bar{\boldsymbol{P}}_1 + \bar{\boldsymbol{P}}_2 = \\ = \sum_{j\in\mathbb{Z}_N} \Big\{ (\hbar\omega + \mathcal{W} + \tilde{\mathcal{W}})\boldsymbol{a}_j^\dagger \boldsymbol{a}_j + \mathcal{J}\boldsymbol{a}_j^\dagger(\boldsymbol{a}_{j+1} + \boldsymbol{a}_{j-1}) + \mathcal{U}\boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j^2 + \\ + \tilde{\mathcal{U}}\Big[\boldsymbol{a}_j^3\boldsymbol{a}_j^{\dagger 3} + \boldsymbol{a}_j^{\dagger 3}\boldsymbol{a}_j^3\Big] + \tilde{\mathcal{M}}\Big[\boldsymbol{a}_j^2\boldsymbol{a}_j^{\dagger 2} + \boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j^2\Big] + \\ + \tilde{\mathcal{N}}\Big[\boldsymbol{a}_j^2\boldsymbol{a}_j^\dagger(\boldsymbol{a}_{j-1}^\dagger + \boldsymbol{a}_{j+1}^\dagger) + (\boldsymbol{a}_{j-1}^\dagger + \boldsymbol{a}_{j+1}^\dagger)\boldsymbol{a}_j^2\boldsymbol{a}_j^\dagger + \\ + \boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j(\boldsymbol{a}_{j-1} + \boldsymbol{a}_{j+1}) + (\boldsymbol{a}_{j-1} + \boldsymbol{a}_{j+1})\boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j\Big] + \\ + \tilde{\mathcal{J}}\Big[(2\boldsymbol{a}_j - \boldsymbol{a}_{j-1} - \boldsymbol{a}_{j+1})(2\boldsymbol{a}_j^\dagger - \boldsymbol{a}_{j-1}^\dagger - \boldsymbol{a}_{j+1}^\dagger) + \\ + (2\boldsymbol{a}_j^\dagger - \boldsymbol{a}_{j-1}^\dagger - \boldsymbol{a}_{j+1}^\dagger)(2\boldsymbol{a}_j - \boldsymbol{a}_{j-1} - \boldsymbol{a}_{j+1})\Big]\Big\}.\end{aligned}$$

The corresponding Bose-Hubbard (BH) equation, corrected to second order is:

$$\begin{aligned}\imath\dot{\boldsymbol{a}}_j = (\hbar\omega + \mathcal{W} + \tilde{\mathcal{W}})\boldsymbol{a}_j + \mathcal{J}(\boldsymbol{a}_{j+1} + \boldsymbol{a}_{j-1}) + 2\mathcal{U}\boldsymbol{a}_j^\dagger\boldsymbol{a}_j^2 + 3\tilde{\mathcal{U}}\Big[\boldsymbol{a}_j^3\boldsymbol{a}_j^{\dagger 2} + \boldsymbol{a}_j^{\dagger 2}\boldsymbol{a}_j^3\Big] + \\ + 2\tilde{\mathcal{M}}\Big[\boldsymbol{a}_j^2\boldsymbol{a}_j^\dagger + \boldsymbol{a}_j^\dagger\boldsymbol{a}_j^2\Big] + \tilde{\mathcal{N}}\Big[\boldsymbol{a}_j^2(\boldsymbol{a}_{j-1}^\dagger + \boldsymbol{a}_{j+1}^\dagger) + 2\boldsymbol{a}_{j+1}^2\boldsymbol{a}_{j+1}^\dagger + 2\boldsymbol{a}_{j-1}^2\boldsymbol{a}_{j-1}^\dagger + \\ + (\boldsymbol{a}_{j-1}^\dagger + \boldsymbol{a}_{j+1}^\dagger)\boldsymbol{a}_j^2 + 2\boldsymbol{a}_j^\dagger\boldsymbol{a}_j(\boldsymbol{a}_{j-1} + \boldsymbol{a}_{j+1}) + 2(\boldsymbol{a}_{j-1} + \boldsymbol{a}_{j+1})\boldsymbol{a}_j^\dagger\boldsymbol{a}_j\Big] + \\ + 2\tilde{\mathcal{J}}\Big[2(2\boldsymbol{a}_j - \boldsymbol{a}_{j-1} - \boldsymbol{a}_{j+1}) - (2\boldsymbol{a}_{j+1} - \boldsymbol{a}_j - \boldsymbol{a}_{j+2}) - (2\boldsymbol{a}_{j-1} - \boldsymbol{a}_{j-2} - \boldsymbol{a}_j)\Big].\end{aligned} \tag{4.68}$$

Bibliography

[1] I.Bloch, J.Dalibadr, W.Zwerger, *Many-body physics with ultracold gases*, Reviews of Modern Physics, Vol 80, (July-September 2008).

[2] M. A. Cazalilla, R. Citro, T. Giamarchi, M. Rigol , *One dimensional Bosons: From Condensed Matter Systems to Ultracold Gases*, (January 28, 2011).

[3] N.Marzari, A.A. Mostofi, J.R. Yates, I.Souza, D.Vanderbilt, *Maximally localized Wannier functions: Theory and applications*, (May 12, 2012).

[4] A.Ponno, *Analytical mechanics: Lecture Notes*, (January 10, 2019).

[5] W.Demtröder, *Atoms, Molecules and Photons. An introduction to Atomic, Molecular and Quantum Physics*, Springer Third Edition, (2018).

[6] David J. Griffiths, Darrell F. Schroeter, *Introduction to Quantum Mechanics*, Cambridge University Press Third Edition, (2018).

[7] I. Bloch, J. Dalibard and W. Zwerger, *Many-body physics with ultracold gases*, Rev. Mod. Phys. 80, 885-964 (2008).

[8] A. Maiocchi, E. Picari, A. Ponno and L. Zanelli, *Long time stability coherent motions in cold atoms*; preprint 2020.

[9] D.Bambusi, A. Carati, A.Ponno, *The nonlinear Scrhödinger equation as a resonant normal form.*

[10] J.I.Cirac, P.Zoller, *A scalable quantum computer with ions in an array of microtraps*, Institute for Theoretical Physics, University of Inbsbruck, Austria, NATURE vol 404, Macmillan Magazine Ltd, (April 6, 2000).

Acknowledgments

First of all, I want to express my sincere gratitude to my advisor Prof. Antonio Ponno for his explanations and patient answers. Although from far, he made me understand and love the topic. In addition I would like to thank Prof.ssa Olga Bernardi for her constant support and her teachings that have proved to be useful.

I would like to thank my boyfriend Alfredo for always being on my side and encouraging me to do my best.

Finally, a big thank-you goes to my parents and my sister for supporting me in every situation.