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Ultracold atoms trapped in optical lattice

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Introduction

Every day we encounter macroscopic systems formed by many constituents: the air in a room, the particles in a glass of water or the photons ejected by a lamp are system formed by a huge number of particles (that is more than an Avogadro's number), referred at as many-body systems. Classically, we could treat a many-body system as components are massive points. For example, if we aim to analyze how the molecules of H_2O interact with each other in a glass of water, we could use the thermodynamic or statistical methods. We obtain a good model that well describes the system.

Now we assume to simulate the H_2O system as a quantum system. We must solve differential equations (like Schrödinger equation) and exponentiate matrices to obtain a description of the evolution of the model. In general, study the quantum many-body system is complicated and the numerical simulations have a computational cost that increases exponentially with the size of the system. An example, we suppose to analyze the evolution of a system formed by N particles with spin $1/2$. The spin state can be 'up' $|\uparrow\rangle$ or 'down' $|\downarrow\rangle$, thus we have two possibilities for a single particle. The total system can be in 2^N different configurations. The temporal evolution is defined by the exponential $\exp\{-(iH_{sys})/\hbar\}$, where H_{sys} is the Hamiltonian operator of the system. H_{sys} consists in a $2^N \times 2^N$ matrix. For example, assuming $N = 50$, the classical computer must calculate $2^{50} \times 2^{50} \approx 10^{30}$ matrix elements. For a classical computer, it would require several million Gigabytes of memory and 10^{13} of years at Gigahertz speed, namely we have an 'exponential explosion' of required sources (like time or memory) [1, 2].

Richard Philips Feynman, in 1982, thought that a quantum system could be simulated by another quantum system. In his words, "Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws." [1]. Following this idea, in the last years, some machines have been built based on the rules of quantum mechanics, such as coherent superposition of states. The calculation becomes more efficient and we can bypass the exponential scaling of the required resources. The idea behind it is simple: we have a controlled system and we know how it evolves and its proprieties; We consider a model that we want investigate and we map it into our controlled system [2, 3, 4, 5].

Quantum simulators are 'digital' or 'analog'. The first one is a universal machine formed by reconfigurable registers of qubits and programmable gates to realize the simulation. It is a quantum computer. The second one consists of a physical system that can simulate a specific model [6, 7].

In this thesis, we study a possible implementation of an analog quantum simulator, namely ultracold atoms in an optical lattice. The system consists of an ultracold atomic gas placed in an optical potential, which forms the trap for the atoms. The lattice is formed by three pairs of counter-propagating lasers orthogonal to each other. According to the frequency, number and position, and intensity of the lasers, the geometry of the optical trap may be different. Near zero Kelvin temperature, we can consider the atoms standing still in the potential well.

In the first chapter of this thesis, we briefly describe how the quantum simulator works and the difference between digital and analog quantum simulation. Then, we describe the optical lattice and how it interacts with the atoms. Describing the Hamiltonian for a system of bosons, we introduce the potential for two bosons in the condition of weakly interaction.

In the second chapter of the thesis, we introduce the formalism of second quantization. Passing through the quantum harmonic oscillator, we derive the ladder operators. Then, we switch to the quantum field theory for global description of the system. We use the ladder operators to decompose the field and to derive the Bose-Hubbard Hamiltonian. Analyzing it, we introduce and characterize the Mott insulator and the superfluid phase for a system of atoms.

In the last part of the thesis, we report a numerical simulation for a chain with two sites. We determine the fluctuation for the number of particles in one site to establish the passages between the two phases.

Chapter 1

Cold atoms in periodic potential

1.1 Quantum simulator

Quantum simulators are based on quantum laws and they are helpful to analyze quantum many-body systems. In general, we have a set of quantum objects placed in a controlled apparatus and we determine the model for that system: we can achieve information. We can apply this data to another set of particles using the model of the controlled apparatus and know its proprieties.

Assuming we have a set of N quantum objects and we want to determine its evolution or its energy. The total system can be defined by a state $|\Phi\rangle$, given by

$$|\Phi\rangle \equiv |\phi\rangle_1 \otimes |\phi\rangle_2 \otimes \dots \otimes |\phi\rangle_N \equiv |\phi\rangle_1 |\phi\rangle_2 \dots |\phi\rangle_N, \quad (1.1)$$

where, $\{|\phi\rangle_i\}_{i=1}^N$ represents the single particle state. The temporal evolution is determined by Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\Phi(t)\rangle = H_{sys} |\Phi(t)\rangle, \quad (1.2)$$

whose solutions is

$$|\Phi(t)\rangle = e^{-i\frac{H_{sys}}{\hbar}t} |\Phi(0)\rangle = U(t) |\Phi(0)\rangle, \quad (1.3)$$

where $|\Phi(0)\rangle$ is the initial state, at $t = 0$. The operator $U(t) = \exp\{-(iH_{sys}t)/\hbar\}$ is a unity operator and it determines the temporal evolution. The exact dynamics is in general hard to computes. Feynman said, "I don't want to have an explosion." [7].

Now we supposed to have a quantum simulator. This kind of machine consists of a controlled system how can simulate the system that we want to study. A set of quantum objects is placed in a specific configuration and we use the model given by the controlled system to derive proprieties about the other system. If the controlled system is in the state $|\Psi\rangle$ and is define by H_{con} , its evolution is given by (1.3) with $U'(t) = \exp\{-(iH_{con}t)/\hbar\}$. So temporal evolution is

$$|\Psi(t)\rangle = e^{-i\frac{H_{con}}{\hbar}t} |\Psi(0)\rangle = U'(t) |\Psi(0)\rangle. \quad (1.4)$$

There are two principal types of quantum simulator: Digital quantum simulator and Analog quantum simulator.

Digital quantum simulator (DQS) is a universal machine that can emulate the evolution of a quantum system. The DQS is the Feynman thought about the quantum machine. This is nothing but a quantum computer: it is formed by reconfigurable registers of the qubit and programmable gates to realize the simulation. Its development is not to make quantum algorithms, such as Shor factorization or Grover search¹. It is thought for optimization of the problem, as the determination of ground state for a given system described by a Hamiltonian H_{sys} . The system is defined by wave function $|\phi\rangle$, which is encoded by a computational basis in an overlap of binary strings of qubit $|0\rangle$ and $|1\rangle$. To emulate the evolution of $|\psi(0)\rangle \rightarrow |\psi(t)\rangle$, we need to implement a sequence of gates which represent the unitary operator. The simulation consists in three steps: the initial-state preparation in which we use some quantum algorithms to define an initial state as $|000\dots\rangle$; the unitary evolution in which we configure some gates to reproduce the unitary evolution $U(t)$; the measurement in which we obtain the information about controlled system [3, 8].

Analog quantum simulation (AQS) consists of a physical system that can simulate a specific model. The idea is to create an ensemble of elements with a specific configuration. For example, if we want to simulate a set of particles with spin 1/2, we must consider a system with two well-defined states, such the polarization of photons or two internal states of atom and use them to represent the spin state, we must engineer the system in agreement with the Hamiltonian H_{sys} we want to simulate. We create a map between the Hamiltonian of the system that we want to analyze and the Hamiltonian of the controlled system, H_{sys} corresponding to H_{con} .

¹They are used for factorization big prime number and search a string in a non-structured database respectively.

If we want to describe a system in the initial state $|\phi(0)\rangle$ described by H_{sys} , we prepare a system in the initial state $|\psi(0)\rangle$ described by H_{con} such that an operator f which maps $|\psi(0)\rangle = f|\phi(0)\rangle$. The final state $|\psi(t)\rangle$ is mapped back to $|\phi(t)\rangle$ via f^{-1} . The choice for the map depends on what we need to simulate and on the capabilities of the simulator. AQS is helpful in the presence of errors: if we have an appreciable noise in the controlled system, we also can obtain the answer without the full quantitative details. Some of the experimental setups most analog simulator, on ultracold quantum gases, artificial ion crystals, photonic system or superconducting circuits [3, 8]. In the following, we talk about the AQS given by ultracold atoms trapped in an optical lattice.

1.2 Geometry of optical trap

The Hamiltonian of an atom of mass m is given by

$$H_a = \frac{\mathbf{p}^2}{2m} + \sum_j \epsilon_j |j\rangle \langle j|, \quad (1.5)$$

where the first term is the kinetic energy formed by centre of mass momentum \mathbf{p} and the second denotes the internal energy ϵ_j for the state $|j\rangle$. The principal interactions between atoms and laser consists in an absorptive and a dispersive part. In the absorptive part, a photon hits and excites the atom to a higher state. For example, if the atom is in the ground state, such as $j = 0$, next to absorptive event, it rises its state from $|0\rangle$ to $|j\rangle$, with $j \neq 0$ [9, 10]. The result is a spontaneous emission of a photon with frequency $\nu = (E_j - E_0)/h$. This process transfer momentum carried by photon to atom [11]. In our discussion we neglect this interaction considering cooled atoms. The dispersive part is due the interaction between the atoms and the electric field that induce a dipole momentum. If the laser produces an electric field

$$\mathbf{E}(\mathbf{x}, t) = \bar{E}_0 e^{-i(\omega t + \mathbf{k} \cdot \mathbf{x})} \hat{\mathbf{e}} + c.c., \quad (1.6)$$

where $\hat{\mathbf{e}}$ is the unit polarization vector, \bar{E}_0 is the field amplitude, ω is the pulsation and finally we have the scalar product between wave number $\mathbf{k} = \frac{2\pi}{\lambda} \hat{\mathbf{e}}$ and the position \mathbf{x} . The λ is the wavelength. The abbreviation *c.c.* means ‘complex conjugate’ and it is used to take the real part of them. The electric field induces a dipole momentum to the atom, such as

$$\mathbf{p}(\mathbf{x}, t) = \bar{p}_0 e^{-i\omega t + \mathbf{k} \cdot \mathbf{x}} \hat{\mathbf{e}} + c.c., \quad (1.7)$$

where the amplitude of the dipole momentum \bar{p}_0 is related by \bar{E}_0 through the complex polarizability α

$$\bar{p}_0 = \alpha(\omega) \bar{E}_0. \quad (1.8)$$

The electric field varies slowly in time t compared to $1/\omega$ and in space \mathbf{x} compared to the size of atom. Doing so, the interaction is well described within the dipole approximation². We obtain an interaction potential

$$V_{dip}(\mathbf{x}) = -\frac{1}{2} \langle \mathbf{p}(\mathbf{x}, t) \cdot \mathbf{E}(\mathbf{x}, t) \rangle_t = -\frac{1}{2} \alpha(\omega) \langle |\mathbf{E}(\mathbf{x}, t)|^2 \rangle_t, \quad (1.9)$$

where the angular brackets denote the time average over the rapid oscillating terms [9, 10, 12]. The dipole interaction depends only by the time-average of the laser intensity $I(\mathbf{x}) \propto |\mathbf{E}(\mathbf{x})|^2$. If the laser uses a frequency near to the resonance frequency ω_0 to pass from the ground state $|0\rangle$ to an excited state $|n\rangle$, we can approximate the polarizability as

$$\alpha(\omega) \approx \frac{|\langle n | d_{\mathbf{E}} | 0 \rangle|^2}{\hbar(\omega - \omega_0)}, \quad (1.10)$$

where we have introduced the dipole operator $d_{\mathbf{E}}$ in the direction of the field. Depending on the sing of $(\omega - \omega_0)$, the atoms are attracted to the nodes or to the anti-nodes of the laser intensity [13]. The equation (1.9) lead us to generic interaction $H_{dip} = -d_{\mathbf{E}} \mathbf{E} + h.c.$ for atoms-laser system where the abbreviation *h.c.* means ‘hermitian conjugated’ and it is necessary to make H_{dip} hermitian [12].

For next discussion, we can assume that the laser is far detuned from the atom, thus the potential H_{dip} do not produces any particular transition from a state to another. In doing so, we find also the AC Stark effect: the internal state $|n\rangle$ shifts and it form a conservative potential $V(\mathbf{x})$. Its intensity is given by the dipole operator $d_{\mathbf{E}}$ and the proprieties of the laser light.

The set-up of the optical lattice is provided by superimposing two counter propagating laser beams which produce an electric field as in (1.6). If we place two pairs of laser beams along the x, y and z directions, we will obtain an optical trap. The optimal choise of the electric field polarization is the one in which the polarizations are mutually orthogonal. In this way, we create a cubic lattice. The potential formed by the standing waves of counter propagator

²We can approximate the dipole as two charge separated instead an object in which the charge is distributed.

laser beams has a gaussian shape in the x, y and z directions. Since, we made the time-average, we can consider the optical potential as

$$V(\mathbf{x}) = -V_{0x}e^{-2\frac{y^2+z^2}{\omega_x^2}}\cos^2(k_x x) - V_{0y}e^{-2\frac{x^2+z^2}{\omega_y^2}}\cos^2(k_y y) - V_{0z}e^{-2\frac{x^2+y^2}{\omega_z^2}}\cos^2(k_z z). \quad (1.11)$$

In the last relation, we assume that $V_{0x,0y,0z}$ includes all the constants appearing in (1.9) and they give us the potential depths. In the centre of the trap, for distances much smaller than the beam waist, the three dimension potential is well approximate by the sum of periodic potential and harmonic potential. Starting from (1.11) we can expand the exponential factor into $x, y, z = 0$ respectively. We obtain, for example, $\exp\{-2(x^2 + y^2)/\omega_z^2\} \simeq 1 - 2(x^2 + y^2)/\omega_z^2$. Thus, we can write

$$V(\mathbf{x}) \simeq -V_{0x}\left(1 - 2\frac{y^2 + z^2}{\omega_x^2}\right)\cos^2(k_x x) - V_{0y}\left(1 - 2\frac{x^2 + z^2}{\omega_y^2}\right)\cos^2(k_y y) - V_{0z}\left(1 - 2\frac{x^2 + y^2}{\omega_z^2}\right)\cos^2(k_z z). \quad (1.12)$$

The $\cos^2(x)$ function changes between 0 and 1; We must describe atoms near the center of the well and so, for the quadratic term in (1.12) we can approximate $\cos^2(k_i i) \simeq 1$ where $i = x, y$, and z and obtain

$$V(x) \simeq -V_{0x}\cos^2(k_x x) - V_{0y}\cos^2(k_y y) - V_{0z}\cos^2(k_z z) + \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2), \quad (1.13)$$

where $\omega_{x,y,z}^2$ are the squares of the effective trapping frequencies of the external harmonic confinement. They are defined by $\omega_x^2 = 4/m(V_y/\omega_y^2 + V_z/\omega_z^2)$ and permutation of the index x, y and z , where m is the mass of the particle in the lower lying. For the next discussion we consider the periodic term as V_{lat} and harmonic term as V_{ext} [18]. Now we can determine the state of a particle in potential well. For the Bloch Theorem³, the eigenfunction for particles trapped in a periodic potential is

$$\psi_{\mathbf{q}}^{(n)}(\mathbf{x}) = u_{\mathbf{q}}^{(n)}(\mathbf{x})e^{i\mathbf{q}\cdot\mathbf{x}} \quad (1.14)$$

and they are known as Bloch functions. They are multiplied by a pure phase factors, thus with a translation of the vector \mathbf{x} we can extend them over all the lattice [13, 14]. The function $u_{\mathbf{q}}^{(n)}(x)$ is a periodic function and quantity \mathbf{q} is the quasi-momentum⁴. Bloch function are the eigenstate for an atom in a lattice site [19]. n is the band index and it needs because we can have wave the same eigenenergy $E_{\mathbf{q}}^{(n)}$ for different band. The index n is similar to the principal quantum number and it individuates a specific band. A well approximation for a particle in the lowest lying is considering it as a harmonic oscillator, in which a particle swings with frequency ω_t around the minimal point \mathbf{x}_j . By solving this problem as a classical harmonic oscillator, we find $\omega_t = \sqrt{4V_0 E_R}$, where V_0 is the depth of the lattice and E_R is the recoil energy. Recoil energy is a natural measure of energy scales in optical lattice potentials (when a resting atom absorbs a photon, it acquires an energy E_R) [13, 15]. In this assumption, the bands are well separated, and we can consider every minimum point as isolated by each other.

The dynamics of a particle trapped in a potential well can be described by the Wannier functions. They are linked with Bloch function through the discrete Fourier transform⁵ as

$$\omega_{\mathbf{q}}^{(n)}(\mathbf{x} - \mathbf{x}_j) = \Theta^{-\frac{1}{2}} \sum_i e^{-i\mathbf{q}\cdot\mathbf{x}_i} \psi_{\mathbf{q}}^{(n)}(\mathbf{x}_j) = \Theta^{-\frac{1}{2}} \sum_i e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}_i)} u_{\mathbf{q}}^{(n)}(\mathbf{x}_j), \quad (1.15)$$

where $\Theta^{-1/2}$ a normalization constant and the index j refers to the site in which the function is localized. We will use the Wannier function to describe the particles in potential well sited in \mathbf{x}_j . They depend only on the relative distance $\mathbf{x} - \mathbf{x}_j$ and, in the lowest band, they are centred on the lattice site \mathbf{x}_j [13]. They obey the orthonormality relation, such as

$$\int d^3\mathbf{x} \omega_{\mathbf{q}}^{(n)*}(\mathbf{x} - \mathbf{x}_i) \omega_{\mathbf{q}}^{(n')}(\mathbf{x} - \mathbf{x}_j) = \delta_{n,n'} \delta_{\mathbf{x}_i, \mathbf{x}_j}, \quad (1.16)$$

for different band index n and different site \mathbf{x}_i [13].

The position of the lattice site determines the geometry of optical lattice. If we prepare three pairs of counter lasers beams, we have a cubic lattice. But if we set the pair of lasers with an angle φ respect a plane, for example, xy , we obtain a different optical lattice. We can use the angles between the pairs of laser beams to make a two- or a one-dimension lattice model, as shown in Fig.1.1.

³The eigenfunctions of the wave equation for a periodic potential are the product of a plane wave $\exp(i\mathbf{k} \cdot \mathbf{x})$ and a function $u_{\mathbf{k}}(\mathbf{x})$ with the periodicity of the crystal lattice.

⁴If every particle has a momentum $p = h/\lambda = \hbar k$, in vectorial term is $\mathbf{p} = \hbar \mathbf{k}$. We assume $\mathbf{p} \equiv \mathbf{q}$.

⁵It is defined as $X(\omega) = \sum_{n=-\infty}^{+\infty} x(n)e^{-i\omega n}$ and it is used for function with discrete values.

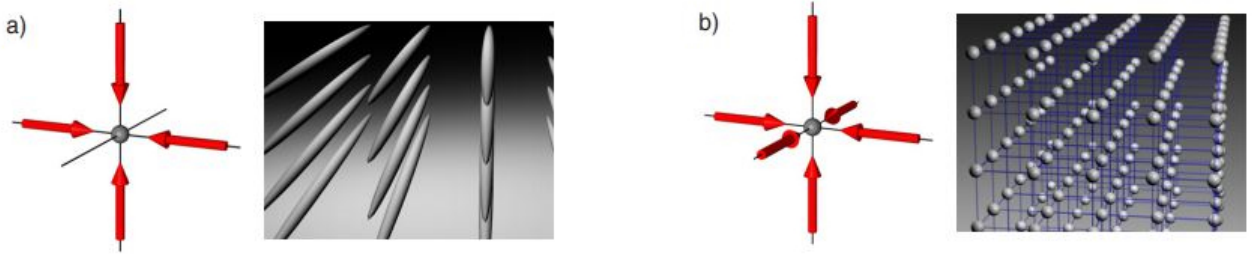


Figure 1.1: Different configuration for the optical lattice. In a) two standing waves orthogonal to each other form an array that is a one-dimension lattice; in b) a three-dimensional lattice potential can be created by superimposing three standing waves [18].

1.3 Bosons in optical potential

Particles in quantum mechanics are identical. We cannot mark a particle: after the interaction with other particles, we cannot find it. It has profound consequences: the state $|\psi\rangle$ that describes the particles must be symmetric or anti-symmetric for the exchange of particles. Particles that respect the first are the bosons and particles which respect the second are the fermions. Bosons obey the Bose-Einstein statistic and they can create a condensate under special conditions; fermions obey the Fermi-Dirac statistic and they obey the Pauli exclusion principle⁶. As a consequence, bosons can stay all in the same state, while instead, fermions cannot. Furthermore, bosons have integer spin $s = 0, 1, 2, \dots$ instead fermions have semi-integer spin $s = 1/2, 3/2, \dots$.

In this section we consider a system formed by ultracold bosons in order to have a controlled system. The Hamiltonian for general system of N bosons is

$$H = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} V(\mathbf{x}_i - \mathbf{x}_j) + \sum_{i=1}^N U(\mathbf{x}_i), \quad (1.17)$$

where \mathbf{p}_i is the momentum of the i -particle, $V(\mathbf{x}_i - \mathbf{x}_j)$ is the interaction potential between the i -particle and the j -particle and $U(\mathbf{x}_i)$ is a potential imposed by the system to the particle in \mathbf{x}_i , as in (1.13). In the Hamiltonian we assume that the particles have the same mass m because they are indistinguishable. If we neglect the dependence by the time t , we call $|\psi_i\rangle \equiv |i\rangle$, with $\{|i\rangle\}_{i=1}^N$.

Classically, we can follow the evolutions of single particle defined by the position \mathbf{x}_i and momentum \mathbf{p}_i . We can define a space phase for the particles, defined by $(\mathbf{x}, \mathbf{p}) = (\mathbf{x}_1, \mathbf{p}_1; \mathbf{x}_2, \mathbf{p}_2; \dots; \mathbf{x}_N, \mathbf{p}_N)$ and described the trajectory of i -particles by its position and momentum without ambiguities. In quantum mechanics we cannot do that. For the Heisenberg uncertainty principle, a single quantum objects must respect

$$\Delta \mathbf{x} \Delta \mathbf{p} \geq \frac{\hbar \cdot \hbar \cdot \hbar}{2 \cdot 2 \cdot 2} = \frac{\hbar^3}{8}, \quad (1.18)$$

because we are in 3-dimension. It implies that we cannot treat a system as an ensemble of singular objects but as unique system. Doing so, the probability $|\psi(\mathbf{x}_1, \dots, \mathbf{x}_N)|^2$ is the conjoint probability to find the 1-particle in the position \mathbf{x}_1 , the 2-particle in the position \mathbf{x}_2 and so on. The system obeys to the Schrödinger equation. The solution to this equation is not easy in general. We need approximation methods or statistic method or simulator to resolve it.

We can define a generic particle through the quantum numbers. Usually they are n the principal quantum number who defines if the system is in excited state or not; l is the orbital quantum number and it quantifies the angular momentum of the particles; m is the magnetic quantum number and it corresponds to the projections of z -momentum on the z -axis; s is the spin quantum number and it refers to the internal spin momentum projected on the z -axis. If we neglect the interaction and mark a generic state for a single particle with the quantum number k_j , with $j = 1, 2, \dots, r$, a generic wave function for a bosons system is given by the sum over all permutation of position for the particles, as

$$\psi(\mathbf{x}_1, \dots, \mathbf{x}_N) = \left(\frac{N_1! N_2! \dots N_r!}{N!} \right)^{1/2} \sum_{perm. \mathbf{x}_i} \psi_{k_1}(\mathbf{x}_1) \psi_{k_2}(\mathbf{x}_2) \dots \psi_{k_r}(\mathbf{x}_N), \quad (1.19)$$

where $N_1 + N_2 + \dots + N_r = N$ is the total number of particles, instead N_i is the number of particles in the state k_i [11].

⁶It is impossible to have a system formed by fermions with two particles the same quantum numbers.

In our discussion, we have to consider the interaction between bosons. They are cooled and so we can consider they have low energies. The low interaction is given by scattering between close atoms. It is a short-range interaction between two bodies. We call *s*-wave the interaction between atoms characterized by angular quantum number *l* equal to zero. We can assume that because we are in a system of ultracold atoms and it means the classical motions, like rotations, are freeze [16]. In this condition, the interaction is given by the Fermi pseudopotential

$$U(\mathbf{x}_i - \mathbf{x}_j) = \frac{2\pi\hbar^2}{m} a_s \delta(\mathbf{x}_i - \mathbf{x}_j), \quad (1.20)$$

in which $\mathbf{x}_i, \mathbf{x}_j$ are the position of the two atoms, a_s are scattering length, δ are the Dirac function [17]. This approximation is valid until the de Broglie wavelength⁷ of the atoms is much larger than the range of the interatomic interaction potential [9].

A set of ultracold bosons can be described by the Hamiltonian in (1.17). The potential terms are given by the sum of (1.13) and (1.20) [18]. We obtain:

$$H = \sum_{i=1}^N \left(-\frac{\hbar^2}{2m} \nabla_i^2 + V_{lat}(\mathbf{x}_i) + V_{ext}(\mathbf{x}_i) \right) + \frac{1}{2} \sum_{i \neq j} U(\mathbf{x}_i - \mathbf{x}_j). \quad (1.21)$$

This is the Hamiltonian that we use in the next discussion for derive the Bose-Hubbard model. The Hamiltonian is formed by the kinetic and the optical potential whose will form tunneling term of the model; the external potential will describe the energy for the system; the interaction potential will describe the possibility that two or more bosons stay in the same potential well [18]. In Fig.(1.2) there is a representation how optical lattice can trap a system of bosons.

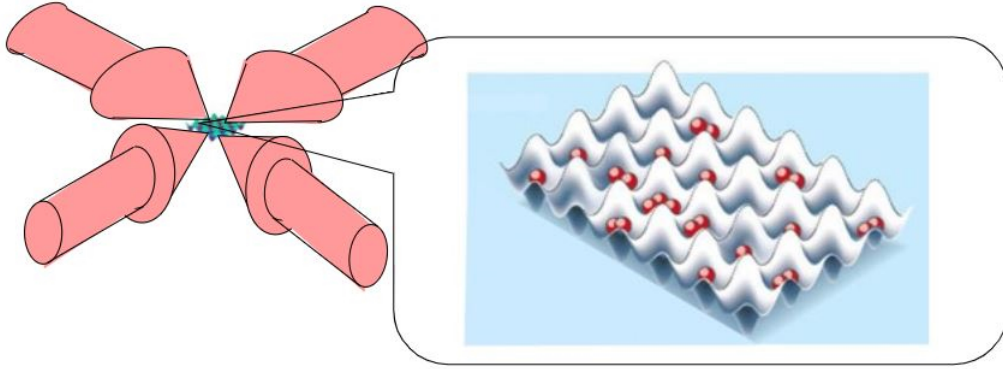


Figure 1.2: Schematic representation of two-dimensional optical lattice. Laser beams (arrow in figure) force the atoms to stay in optical lattice. They cannot stay or can stay more than one in the lattice [20].

⁷He thought all the particles as a wavelength $\lambda = h/|\mathbf{p}|$ where \mathbf{p} is the momentum of the particle.

Chapter 2

Second quantization

2.1 Harmonic oscillator

The harmonic oscillator is composed of a particle trapped in a quadratic potential well. We briefly recall it now since permits to introduce special operators used in quantum field theory [11].

Given a particle with mass m in one dimension, its Hamiltonian is

$$\hat{H}_{quan} = \frac{\hat{P}^2}{2m} + \frac{m}{2}\omega^2 \hat{X}^2 = -\frac{\hbar^2}{2m}\nabla^2 + \frac{m}{2}\omega^2 x^2, \quad (2.1)$$

where the last part is written in position representation. The symbol ∇ is the gradient defined as $\nabla = (\partial_x, \partial_y, \partial_z)$ which in one dimension is just ∂_x . We can solve this system analytically. Harmonic potential $V(x) = m\omega^2 x^2/2$ is time-independent and we can write the time-independent Schrödinger equation. If the system is in the state $|\psi\rangle$ we express it in the position representation, we have

$$\hat{H}_{quan}\psi(x) = E\psi(x). \quad (2.2)$$

This is the eigenvalues equation, in fact E is the eigenvalue for Hamiltonian operator if $|\psi\rangle$ is the eigenstate for \hat{H} . In explicit form, the (2.2) is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{m}{2}\omega^2 x^2\psi(x) = E\psi(x) \quad \Rightarrow \quad \frac{\partial^2\psi(x)}{\partial x^2} + \frac{2m}{\hbar}\left(E - \frac{m}{2}\omega^2 x^2\right)\psi(x) = 0. \quad (2.3)$$

We can resolve the equation analytically through the Hermite polynomials and find the eigenvalues and eigenvectors for the system. Every state is determined by quantum number n . $n = 0$ is the ground state, i.e. the low energy. The wave eigenfunctions for the system are

$$\psi_n(x) = C_n H_n(\alpha x) e^{-\frac{1}{2}\alpha^2 x^2}, \quad \text{where} \quad H_n(\alpha x) = (-1)^n \frac{e^{\alpha^2 x^2}}{\alpha^n} \frac{d^n}{dx^n} e^{-\alpha^2 x^2}, \quad C_n = \left(\frac{\alpha}{\pi^{1/2} 2^n n!}\right)^{1/2} \quad (2.4)$$

and $\alpha = \sqrt{\frac{m\omega}{\hbar}}$. We can derive also the energy E_n analytically. Another way to solve this problem is to define the operators

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{X} + i \frac{\hat{P}}{m\omega} \right) \quad \text{and} \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{X} - i \frac{\hat{P}}{m\omega} \right), \quad (2.5)$$

known as ‘ladder’ operators. In particular \hat{a}^\dagger is the ‘raising’ and \hat{a} is the ‘lowering’ operator. Now we can define the position and momentum operators through the \hat{a} and \hat{a}^\dagger operators, such as

$$\hat{X} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^\dagger) \quad \text{and} \quad \hat{P} = -i\sqrt{\frac{m\omega\hbar}{2}} (\hat{a} - \hat{a}^\dagger). \quad (2.6)$$

We introduce the algebra of raising and lowering operators that is helpful for the next treatment. Now we can compute the commutator between \hat{a} and \hat{a}^\dagger using their definition

$$[\hat{a}, \hat{a}^\dagger] = \left[\sqrt{\frac{m\omega}{2\hbar}} \left(\hat{X} + i \frac{\hat{P}}{m\omega} \right), \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{X} - i \frac{\hat{P}}{m\omega} \right) \right] = 1 \quad \Rightarrow \quad [\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1. \quad (2.7)$$

Obviously, the commutators of an operator with itself is zero $[\hat{a}, \hat{a}] = [\hat{a}^\dagger, \hat{a}^\dagger] = 0$. We can use the ladder operators to redefine the Hamiltonian operators \hat{H} . Using the relation in (2.6), we write

$$\begin{aligned}\hat{H} &= \frac{\hat{P}^2}{2m} + \frac{m}{2}\omega^2 \hat{X}^2 = -\frac{1}{2m}\frac{m\omega\hbar}{2}(\hat{a} - \hat{a}^\dagger)^2 + \frac{m}{2}\omega^2 \frac{\hbar}{2m\omega}(\hat{a} + \hat{a}^\dagger)^2 = \\ &= \frac{\hbar\omega}{4}(2\hat{a}^\dagger\hat{a} + 2\hat{a}\hat{a}^\dagger) \frac{\hbar\omega}{4}(4\hat{a}^\dagger\hat{a} + 2) \Rightarrow \hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right).\end{aligned}\quad (2.8)$$

Now we obtain the eigenvalues for the Hamiltonian operator \hat{H} . We start by observing that

$$[\hat{a}^\dagger\hat{a}, \hat{a}^\dagger] = \hat{a}^\dagger = \hat{a}^\dagger(\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}) \quad \text{and} \quad [\hat{a}^\dagger\hat{a}, \hat{a}] = -\hat{a} = (\hat{a}^\dagger\hat{a} - \hat{a}\hat{a}^\dagger)\hat{a}. \quad (2.9)$$

Then, we calculate the eigenvalue equation for $\hat{H}\hat{a}^{(\dagger)}$ for a generic eigenstate $|n\rangle$. If $|n\rangle$ is an eigenvector for \hat{H} , we obtain

$$\hat{H}\hat{a}^\dagger|n\rangle = (E_n + \hbar\omega)\hat{a}^\dagger|n\rangle \quad \text{and} \quad \hat{H}\hat{a}|n\rangle = (E_n - \hbar\omega)\hat{a}|n\rangle. \quad (2.10)$$

This means that both $\hat{a}|n\rangle$ and $\hat{a}^\dagger|n\rangle$ are also eigenstates for the Hamiltonian operator \hat{H} . We define

$$\hat{\mathcal{N}} = \hat{a}^\dagger\hat{a}; \quad (2.11)$$

called ‘number’ operator. Thus, the Hamiltonian operator is $\hat{H} = \hbar\omega(\hat{\mathcal{N}} + 1/2)$. The eigenvalues for raising and lowering operators are

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \quad \text{and} \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \quad (2.12)$$

We achieve

$$\hat{a}^\dagger\hat{a}|n\rangle = \hat{a}\hat{a}^\dagger|n\rangle - [\hat{a}, \hat{a}^\dagger]|n\rangle = \hat{a}\sqrt{n+1}|n+1\rangle - |n\rangle = n|n\rangle \Rightarrow \hat{\mathcal{N}}|n\rangle = n|n\rangle. \quad (2.13)$$

Thus, the eigenvalues for Hamiltonian operator, in a generic eigenstate $|n\rangle$ are given by

$$\hat{H}|n\rangle = \hbar\omega\left(\hat{\mathcal{N}} + \frac{1}{2}\right)|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle = E_n|n\rangle. \quad (2.14)$$

To understand which values n can assume, we start from the ground state $|0\rangle$ which corresponds to the energy $E_0 = \frac{\hbar\omega}{2}$ and we apply the lower operator \hat{a} ; from (2.12) we obtain

$$\hat{a}|0\rangle = 0. \quad (2.15)$$

Vice versa, if we apply the raising operator \hat{a}^\dagger , we obtain $\hat{a}^\dagger|0\rangle = |1\rangle$. If we apply a second time the ladder operator to the ground state the raising operator, we obtain $\hat{a}^{\dagger 2}|0\rangle = \hat{a}^\dagger|1\rangle = \sqrt{2}|2\rangle$, understanding that the operator $\hat{\mathcal{N}}$ has natural number as eigenvalues. It can be shown that the eigenstates $|n\rangle$ are

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle. \quad (2.16)$$

The ladder operators and the $\hat{\mathcal{N}}$ can be defined through their matrix elements and give us the representations in matricial terms. Considering that the eigenstates for the system belong to an orthonormal basis which respects $\langle m|n\rangle = \delta_{n,m}$, where $\delta_{n,m}$ is the Kronecker delta, who is equal to 1 if $n = m$ and 0 in all other cases. The matrix elements for an operator are $\hat{a}_{mn} = \langle m|\hat{a}|n\rangle$. The representation for the operators is

$$\hat{a} = \begin{pmatrix} 0 & \sqrt{1} & & & \\ 0 & 0 & \sqrt{2} & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & 0 & \sqrt{n} \\ & & & 0 & 0 \end{pmatrix}, \quad \hat{a}^\dagger = \begin{pmatrix} 0 & 0 & & & \\ \sqrt{1} & 0 & & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{n-1} & 0 & 0 \\ & & & \sqrt{n} & 0 \end{pmatrix}, \quad \hat{\mathcal{N}} = \begin{pmatrix} 0 & 0 & & & \\ 0 & 1 & 0 & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & n-1 & 0 \\ & & & 0 & n \end{pmatrix}. \quad (2.17)$$

The objects \hat{a} and \hat{a}^\dagger are used to raise or to lower the number of excitations of the harmonic oscillator. The physical interpretation for this operator shows up thinking about \hat{H} and its eigenvalue problems. Assuming that energy levels are equidistant by $\hbar\omega$, we consider \hat{H} as a Hamiltonian who describes a system of indistinguishable particles. Because each particle stays in the same dynamical state corresponds to energy $\hbar\omega$, every value of N corresponding to well-defined energy for the total system. Thus, we can consider the state $|n\rangle$ as the state constituted with n particles, and the state $|0\rangle$ as the vacuum state, i.e. without particles. According to this picture, the operator $\hat{\mathcal{N}}$ gives us the number of particles in the state $|n\rangle$ and it can take all the natural values: from 0 to ∞ . The application of \hat{a}^\dagger to the state $|n\rangle$ gives us the state $|n+1\rangle$, formed by $n+1$ particles. For this reason, the raising operator in quantum field theory is called ‘creation operator’. Similar, the lower operator gives us a state formed by $n-1$ particles, so, in quantum field theory, it is known as ‘destruction operator’ [11, 21, 22].

2.2 Second quantization for bosons

In quantum mechanics a particle state is described by a wave function $\psi(\mathbf{x}, t)$, where \mathbf{x} is the position. It obeys the Schrödinger equation and we can determine the evolution. This formalism is known as ‘first quantization’. In quantum field theory the description of particles set is given by the fields operators, which contain all the information about the system. The state of a system is defined, for example, by the action of the field in the position \mathbf{x} . Replacing wave function with fields operators is known as ‘second quantization’. The wave function $\psi(\mathbf{x}, t)$ and $\psi^*(\mathbf{x}, t)$ are replaced by the operators $\hat{\psi}(\mathbf{x}, t)$ and $\hat{\psi}^\dagger(\mathbf{x}, t)$, in which complex conjugated ψ^* is replaced by its hermitian adjoint $\hat{\psi}^\dagger$. In this formalism, the Hamiltonian for a generic system is given by

$$\hat{H} = \int_{\mathcal{V}} d^3\mathbf{x} \hat{\mathcal{H}} = \int_{\mathcal{V}} d^3\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}, t) \left(-\frac{\hbar}{2m} \nabla^2 + V(\mathbf{x}, t) \right) \hat{\psi}(\mathbf{x}, t), \quad (2.18)$$

where $\hat{\mathcal{H}}$ is called Hamilton density and $\hat{\psi}^\dagger(\mathbf{x}, t)$ is the adjoint of $\hat{\psi}(\mathbf{x}, t)$. The integration on a volume \mathcal{V} is necessary because we do not matter the dependence by the position \mathbf{x} but we only matter the dependence from the field. These operators satisfy the equal time commutation relation (ETCR):

$$[\hat{\psi}(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)] = \delta^{(3)}(\mathbf{x} - \mathbf{x}'), \quad \text{and} \quad [\hat{\psi}(\mathbf{x}, t), \hat{\psi}(\mathbf{x}', t)] = [\hat{\psi}^\dagger(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)] = 0, \quad (2.19)$$

where $\delta^{(3)}(\mathbf{x} - \mathbf{x}')$ is the Dirac delta function. It is equal to $+\infty$ if $\mathbf{x} = \mathbf{x}'$ and 0 in all other cases. These relations are true only for bosonic particles. The evolution of the field operators is given by Heisenberg picture

$$\dot{\hat{\psi}} = \frac{1}{i\hbar} [\hat{\psi}, \hat{H}] \quad \text{and} \quad \dot{\hat{\psi}}^\dagger = \frac{1}{i\hbar} [\hat{\psi}^\dagger, \hat{H}]. \quad (2.20)$$

The field operators $\hat{\psi}$ and $\hat{\psi}^\dagger$ are operators in abstract space called ‘Fock space’, defined in the next section. We want to rewrite the Hamiltonian in (2.18) in term of ladder operators. We assume that $u_i(\mathbf{x})$ is a set of orthonormal wave functions that form an orthonormal basis for the eigenfunction of \hat{H} . We can decompose the field operators with this set of wave functions and obtain

$$\hat{\psi}(\mathbf{x}, t) = \sum_i \hat{b}_i(t) u_i(\mathbf{x}) \quad \text{and} \quad \hat{\psi}^\dagger(\mathbf{x}, t) = \sum_i \hat{b}_i^\dagger(t) u_i^*(\mathbf{x}). \quad (2.21)$$

We are decomposing the field operators into a sum of time-dependent operator $\hat{b}_i(t)$ or $\hat{b}_i^\dagger(t)$ and ordinary complex-valued function $u_i(\mathbf{x})$ or $u_i^*(\mathbf{x})$. Since $\hat{\psi}$ and $\hat{\psi}^\dagger$ are bosonic fields, \hat{b} and \hat{b}^\dagger are bosonic operators too and behave as the \hat{a} and \hat{a}^\dagger operators defined for the harmonic oscillator. Indeed, the $u_i(\mathbf{x})$ are a set of complex-valued functions that form an orthogonal system, such as

$$\int_{\mathcal{V}} d^3\mathbf{x} u_i^*(\mathbf{x}) u_j(\mathbf{x}) = \delta_{ij} \quad \text{and} \quad \sum_i u_i(\mathbf{x}) u_i^*(\mathbf{x}') = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (2.22)$$

By inserting the relations (2.21) into (2.19) and obtain

$$[\hat{b}_i(t), \hat{b}_j^\dagger(t)] = \delta_{ij} \quad \text{and} \quad [\hat{b}_i(t), \hat{b}_j(t)] = [\hat{b}_i^\dagger(t), \hat{b}_j^\dagger(t)] = 0. \quad (2.23)$$

This leads to an explicit form for the Hamiltonian operator

$$\hat{H} = \int_{\mathcal{V}} d^3\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}, t) \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) \right) \hat{\psi}(\mathbf{x}, t) = \sum_{i,j} \hat{b}_i^\dagger(t) \hat{b}_j(t) \epsilon_j \int_{\mathcal{V}} d^3\mathbf{x} u_i^*(\mathbf{x}) u_j(\mathbf{x}) = \sum_i \hat{b}_i^\dagger(t) \hat{b}_i(t) \epsilon_i, \quad (2.24)$$

where in the last step we use the orthogonality of the u_i functions. We can demonstrate that the temporal evolution for operator $\hat{b}_i(t)$ is given by the definitions in (2.20) and (2.24), obtaining

$$i\hbar \dot{\hat{b}}_i(t) = \epsilon_i \hat{b}_i(t) \quad \Rightarrow \quad \hat{b}_i(t) = e^{-\frac{i\epsilon_i t}{\hbar}} \hat{b}_i(0) \quad (2.25)$$

and in similar way we treat $\hat{b}_i^\dagger(t)$. Using an eigenfunction basis for the decomposition make the time dependence for $\hat{b}_i(t)$ trivial being characterized by a phase factor. Thus, for the construction of state vector, we can assume \hat{b}_i time-independence.

We can use the definition in (2.11) to define the total number of particles

$$\hat{\mathcal{N}} = \sum_i \hat{n}_i = \sum_i \hat{b}_i^\dagger \hat{b}_i, \quad \text{where} \quad \hat{n}_i = \hat{b}_i^\dagger \hat{b}_i. \quad (2.26)$$

This operator is known as ‘particles-number operator’ and it counts the number of particles for the system. The operators \hat{n}_i count the number of particles in the state i , thus the Hamiltonian in (2.24) describes the total energy of a collection of particles distributed over the states u_i , with energy ϵ_i . The algebra for these operators is

$$[\hat{n}_i, \hat{n}_j] = 0, \quad [\hat{n}_i, \hat{b}_j] = -\hat{b}_i \quad \text{and} \quad [\hat{n}_i, \hat{b}_j^\dagger] = \hat{b}_i^\dagger. \quad (2.27)$$

We can understand that the number of particles is constant. The number of objects cannot change for a system if we do not make any operation. We have $\hat{N} = -i/\hbar[\hat{N}, \hat{H}] = 0$.

2.3 Fock Space

We define the Hilbert space on which field operators act, namely the ‘Fock space’. This space is a Hilbert space for second quantization in particle number representation. If we have N particles, we can define a set of eigenstates fully characterized by the number of occupations for the single state i . The generic state has the form $|N\rangle = |n_1, n_2, \dots, n_i \dots\rangle$. If we apply the operator \hat{n}_i to this state, it returns the number of particles in the state i . Similar, if we apply the particle-number operator \hat{N} , we obtain the total number of particles for the system.

We can define the scalar product in Fock space as

$$\langle n'_1, n'_2, \dots | n_1, n_2 \dots \rangle = \delta_{n_1, n'_1} \delta_{n_2, n'_2} \dots \quad (2.28)$$

We define now the action of the ladder operators to a generic state $|N\rangle$: applying \hat{b}_i^\dagger the number of particles in the state i increases by 1 and applying \hat{b}_i the number of particles decreases by 1. This justifies why they are called ‘creation’ and ‘annihilation’ operators. In analogy with the harmonic oscillator, they obey the relation:

$$\hat{b}_i^\dagger |n_1, n_2, \dots, n_i \dots\rangle = \sqrt{n_i + 1} |n_1, n_2, \dots, n_i + 1 \dots\rangle \quad (2.29)$$

and

$$\hat{b}_i |n_1, n_2, \dots, n_i + 1 \dots\rangle = \sqrt{n_i} |n_1, n_2, \dots, n_i \dots\rangle. \quad (2.30)$$

The state without particles, is called vacuum $|0\rangle$. The application of annihilation operator to the vacuum state gives us zero $\hat{b}_i |0, 0, \dots\rangle \equiv \hat{b}_i |0\rangle = 0$ for all the sites i . We can start from the vacuum state to build a generic state, such as

$$|n_1, n_2, \dots\rangle = C_{n_1, n_2, \dots} (\hat{b}_1^\dagger)^{n_1} (\hat{b}_2^\dagger)^{n_2} \dots |0\rangle, \quad C_{n_1, n_2, \dots} = \frac{1}{\sqrt{n_1! n_2! \dots}} \quad (2.31)$$

where $C_{n_1, n_2, \dots}$ is a constant needed to the normalization. This term derives from the fact that we have indistinguishable particles: if we have two particles, the state is $|2\rangle$; it means that the system may be in two different configuration: particles 1 and 2 respectively in position \mathbf{x}_1 and \mathbf{x}_2 or vice versa. We can also represent the ladder operators in matricial terms through its matrix elements

$$\langle n'_1, \dots, n'_i \dots | \hat{b}_i^\dagger | n_1, \dots, n_i, \dots \rangle = \sqrt{n_i + 1} \delta_{n_1, n'_1} \dots \delta_{n_i + 1, n'_i} \dots \quad (2.32)$$

and

$$\langle n'_1, \dots, n'_i \dots | \hat{b}_i | n_1, \dots, n_i, \dots \rangle = \sqrt{n_i} \delta_{n_1, n'_1} \dots \delta_{n_i - 1, n'_i} \dots \quad (2.33)$$

We must link the Fock space a generic Hilbert space in which we have positions or momenta to describe particles. We define a localized state as

$$|\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n; t\rangle = \frac{1}{\sqrt{n!}} \hat{\psi}^\dagger(\mathbf{x}_1, t) \dots \hat{\psi}^\dagger(\mathbf{x}_n, t) |0\rangle, \quad (2.34)$$

which describes a system of n particles at the same time t . This state follows the orthonormality relation

$$\langle \mathbf{x}'_1, \dots, \mathbf{x}'_n; t | \mathbf{x}_1, \dots, \mathbf{x}_n; t \rangle = \frac{1}{n!} \sum_{\text{permutation}} \mathcal{P} \left[\delta^{(3)}(\mathbf{x}_1 - \mathbf{x}'_1) \dots \delta^{(3)}(\mathbf{x}_n - \mathbf{x}'_n) \right], \quad (2.35)$$

where \mathcal{P} is the permutation operator that interchange the order of the index. The equation shows up the indistinguishability of quantum particles. The state shows how many particles are in the position $\mathbf{x}_1, \dots, \mathbf{x}_n$. If we apply the particle-number operator $\hat{N}_\mathcal{V}$, restricted to a volume \mathcal{V} , to the state in (2.35), the eigenvalue is 0 if none a particles are in the position $\mathbf{x}_i \in \mathcal{V}$, where $i = 1, \dots, r$ and r is the number of sites; it may be 1 if there are particles in just one $\mathbf{x}_i \in \mathcal{V}$, where $i = 1, \dots, r$, and so on. The particle-number operator counts how many positions are occupied by particles in a specific volume. From definition of localized state vector in (2.34) we understand that the filed

operator creates a particle in the position \mathbf{x} . If we apply $\hat{\psi}^\dagger(\mathbf{x}, t)$ to a localized state, we start from n particles and we obtain $n + 1$, where the $n + 1$ -th particle is in the position \mathbf{x}

$$\hat{\psi}^\dagger(\mathbf{x}, t) |\mathbf{x}_1, \dots, \mathbf{x}_n; t\rangle = \sqrt{n+1} |\mathbf{x}, \mathbf{x}_1, \dots, \mathbf{x}_n; t\rangle. \quad (2.36)$$

Analogously by applying the field operator $\hat{\psi}(\mathbf{x}, t)$ to the state in (2.34), we destroy a particle in the position \mathbf{x} . Applying the field operator to the vacuum state, we obtain $\hat{\psi}(\mathbf{x}, t) |0\rangle = 0$.

Now we can build a wave function for the state in which field operators act. We define

$$\Phi_{[k_1, k_2, \dots]}^{(n)}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n; t) = \langle \mathbf{x}_1, \dots, \mathbf{x}_n; t | n_1, n_2, \dots \rangle. \quad (2.37)$$

In the definition, n is the total number of particles namely $n = n_1 + n_2 + \dots$. k_i is the i -state, which is occupied or not by particles. The function $\Phi_{[k_1, k_2, \dots]}^{(n)}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n; t)$ is a wave function of n -particles system in space coordinate. The wave functions defined early is symmetric under permutation of coordinates: we are describing a collection of indistinguishable particles that obey the Bose-Einstein statistics.

2.4 Bose-Hubbard model

We can start from the (1.21) and write the Hamiltonian operator in terms of field operators. We write

$$\hat{H} = \int d^3\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}) \left(-\frac{\hbar}{2m} \nabla^2 + V_{latt}(\mathbf{x}) + V_{ext}(\mathbf{x}) \right) \hat{\psi}(\mathbf{x}) + \int d^3\mathbf{x} \int d^3\mathbf{x}' \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}') U(\mathbf{x} - \mathbf{x}') \hat{\psi}(\mathbf{x}) \hat{\psi}(\mathbf{x}'), \quad (2.38)$$

where we use the proprieties of delta function in $U(\mathbf{x} - \mathbf{x}')$ to eliminate second integral in \mathbf{x}' . We obtain

$$\hat{H} = \int d^3\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}) \left(-\frac{\hbar}{2m} \nabla^2 + V_{latt}(\mathbf{x}) + V_{ext}(\mathbf{x}) \right) \hat{\psi}(\mathbf{x}) + \frac{g}{2} \int d^3\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}) \hat{\psi}(\mathbf{x}), \quad (2.39)$$

where we set $g = 4\pi\hbar^2/m$ by (1.20). This Hamiltonian describes a weakly interacting atomic gas trapped in an optical lattice: ultracold atoms are in low energy and we can use the tiny-binding approximation. In this condition, we assume that all the particles are in the lowest energy band. Thus, we can consider the Wannier function (1.21) only for the lowest band and use them to expand the field operators. We are in the band defined by $n = 0$ and so we neglect the index. We can write

$$\hat{\psi}(\mathbf{x}) = \sum_{i=1}^r \hat{b}_i \omega(\mathbf{x} - \mathbf{x}_i) \quad \text{and} \quad \hat{\psi}^\dagger(\mathbf{x}) = \sum_{i=1}^r \hat{b}_i^\dagger \omega^*(\mathbf{x} - \mathbf{x}_i), \quad (2.40)$$

in which we assume to have r lattice site. The decomposition is expanded on the basis formed by the Wannier functions. The operators \hat{b}_i^\dagger and \hat{b}_i are respectively the creation and annihilation operators. They can create or destroy a particle whose probability distribution is relative to the function $\omega_i \equiv \omega(\mathbf{x} - \mathbf{x}_i)$. By replacing (2.40) into (2.39), we obtain

$$\hat{H} = - \sum_{i,j} J_{ij} \hat{b}_i^\dagger \hat{b}_j + \frac{1}{2} \sum_{i,j,k,l} U_{ijkl} \hat{b}_i^\dagger \hat{b}_j^\dagger \hat{b}_k \hat{b}_l \quad (2.41)$$

where we define

$$J_{ij} = - \int d^3\mathbf{x} \omega(\mathbf{x} - \mathbf{x}_i) \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{lat}(\mathbf{x}) + V_{ext}(\mathbf{x}) \right) \omega(\mathbf{x} - \mathbf{x}_j) \quad (2.42)$$

and

$$U_{ijkl} = g \int d^3\mathbf{x} \omega^*(\mathbf{x} - \mathbf{x}_i) \omega^*(\mathbf{x} - \mathbf{x}_j) \omega(\mathbf{x} - \mathbf{x}_k) \omega(\mathbf{x} - \mathbf{x}_l). \quad (2.43)$$

We can make some consideration. The first one is about the interaction term U_{ijkl} . For the atoms we have a short-range interaction, so the matrix elements of U involving Wannier function centred at difference lattice site are insignificant compared to the interaction to the same lattice site. We can neglect them and define $U_{iiii} \equiv U$. The second one is about the term J_{ij} . It can be demonstrated, by using the proprieties of the Wannier functions, that only the passages to the nearest neighbour sites is allowed [10]. It means, if we are in two dimension and we placed in Cartesian plane xy , in the square defined by $(0, 0)$, $(0, 1)$, $(1, 0)$ and $(1, 1)$, an atom in the origin can pass just into $(1, 0)$ or $(0, 1)$ but it is not allowed to pass directly to $(1, 1)$. We can define $J_{i,i+1} \equiv J_{i+1,1} \equiv J$. So, we obtain the standard Bose-Hubbard Hamiltonian

$$\hat{H}_{B-H} = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + h.c. + \frac{U}{2} \sum_i \hat{b}_i^\dagger \hat{b}_i^\dagger \hat{b}_i \hat{b}_i + \sum_i \epsilon_i \hat{b}_i^\dagger \hat{b}_i. \quad (2.44)$$

Using the algebra of ladder operators, we may rewrite the H_{B-H} in terms of the number particle operator \hat{n}_i . In the equation, we can distinguish three terms: the tunneling term, the interaction and an external potential one. We must insert the hermitian conjugated term in (2.44) because we want a hermitian Hamiltonian [10].

The notation $\langle i, j \rangle$ means the sum over the nearest neighbor site. It is called hopping or tunneling term and it describes the process of an atom hops from the i site to the nearest $i + 1$ and it is defined by the matrix elements in (2.42) which satisfy $j = i + 1$. Ladder operators can destroy a particle in a site only to create it in the nearest neighbor site. If we assume to have an ideal gas with $U = 0$ and set the energy $\epsilon_i = 0$, the Hamiltonian eigenvalues are $E_{\mathbf{q}}^{(0)} = -2J \cos(\mathbf{q}a)$, where a is the site size and \mathbf{q} is the quasi-momentum. The highest value for the energy is $4J$ and the lower $-4J$. In this condition, the atoms in the ground state are delocalized over the whole of the lattice. In this limits, the state for N particle in is given by $|\psi\rangle_{SF} \propto (\sum_i \hat{b}_i^\dagger)^N |0\rangle$ and we have a superfluid (SF) [9, 10, 18, 23, 24].

The second term describes an interatomic onsite interaction and it describes the short-range interaction between two atoms in the same lattice site. This term is a repulsive potential ($U > 0$) and it hinders the configuration with more than one boson on the same lattice site. Its values are 0 if the site is not occupied or just one atom it contains. Its matrix elements are given by $U_{iiii} \equiv U = g \int d^3\mathbf{x} |\omega(\mathbf{x} - \mathbf{x}_i)|^4$ and it can be written as $U \sum_i (\hat{n}_i(\hat{n}_i - 1))/2$. If this term dominates on the hopping term, we have a completely different scenario. The long-range correlations cease to exist in the ground state, and we have a Mott insulating (MI). In this case, the state for the system is $|\psi\rangle_{MI} \propto \prod_i \hat{b}_i^\dagger |0\rangle$ and the atoms tend to be localized on the site [9, 10, 18, 23, 24].

The third one is an external potential that gives an energy offset. It reads as $\epsilon_i = \int d^3\mathbf{x} |\omega(\mathbf{x} - \mathbf{x}_i)|^2 V_{ext}(\mathbf{x})$ and it is due by the effects of external potential use to trap the atoms. It can be written as $\epsilon \sum_i \hat{n}_i$.

The Bose-Hubbard Hamiltonian is dominated by the competition between U and J . They are proportional to the lattice deep V_0 and the recoil energy E_R as $U \propto (V_0/E_R)^{3/4}$ and $J \propto (V_0/E_R)^{3/4} \exp\{-2\sqrt{V_0/E_R}\}$. When the potential depth of the optical lattice is increased, the tunneling barrier between neighboring lattice sites is raised and therefore the tunneling matrix element J decreases exponentially. On the other hand, the interaction U is slightly increased in a deeper lattice because the wave function must be confined in a tighter lattice site [9, 13, 18].

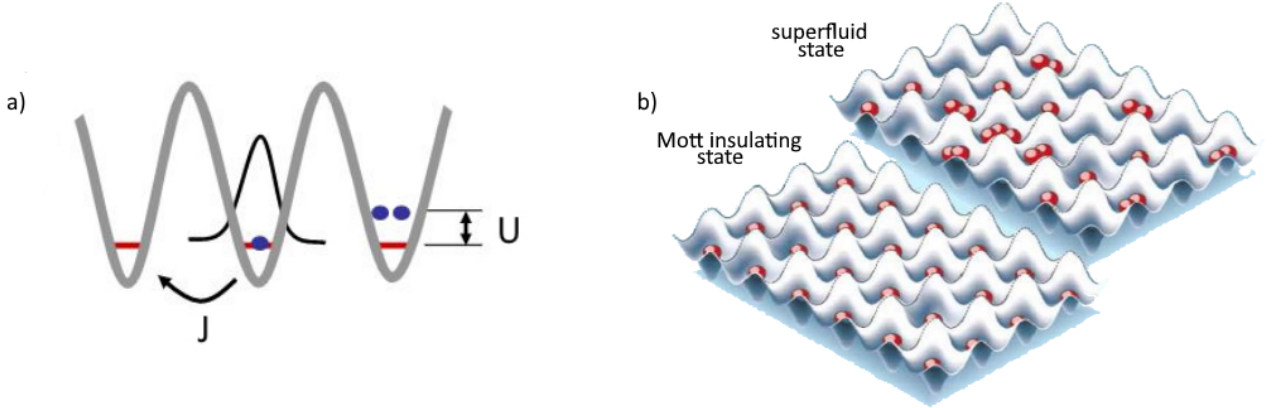


Figure 2.1: a) Pictorial representation of the Bose-Hubbard model. We can distinguish the action of the hopping term J and the interaction term U . The black line is the Wannier function for the site; b) Representation of superfluid and Mott insulating. In the first one the atom is delocalized and in the second one atom are ordered [20].

Chapter 3

Numerical simulation results

Now we analyze numerically a specific case for the system defined by the Bose-Hubbard Hamiltonian: namely a one-dimensional chain formed by two sites. In particular, we will study the behavior of the system for different values of Hamiltonian parameters of (2.44). The quantity we will focus on is the local number of particles n_1 and its fluctuations. The technique used to investigate the ground state is the exact diagonalization for the Hamiltonian in (3.1): we compute the eigenvalues and the eigenvector. The first step is to write the matrix relative to the Hamiltonian in (2.44), namely

$$\hat{H}_{B-H} = J \left(\hat{b}_1^\dagger \hat{b}_2 + \hat{b}_1 \hat{b}_2^\dagger \right) + \frac{U}{2} (\hat{n}_1(\hat{n}_1 - \mathbb{I}) + \hat{n}_2(\hat{n}_2 - \mathbb{I})) - \mu(\hat{n}_1 + \hat{n}_2), \quad (3.1)$$

where we have set $\epsilon_i = 0$ and we consider a uniform chemical potential term proportional to μ . Ladder operators act on infinite-dimensional space, i.e. the Fock space relative to each lattice site. In principle, we can apply the creation operator without limits. Unfortunately, computers cannot store an infinite-dimensional vector. Then, we must impose a truncation: we impose the application of \hat{b}^\dagger to $|n\rangle$ give us 0. In our simulation, we consider, as truncation, two particles.

The Bose-Hubbard Hamiltonian is the sum of three terms. The hopping term allows that a particle moves from the first well to the second and vice versa. The interaction term describes the interaction of particles in the first and second sites; it is 0 for all the states except when there are two particles in one site. Finally, we have the chemical potential whose expression is equal to the external confinement term. The chemical potential μ is necessary to fix the total physical number of particles that we want to consider in our system. Hereafter, we set $\mu = U/2$ which means that are allowed two particles for the total system. In (3.1), we have operators acting on different sites. It implies we must compute the tensor product between operators with different indexes. For example, the chemical potential term for the first site is $\mu(\hat{n}_1 \otimes \mathbb{I}_{3 \times 3})$, in which the identity matrix leaves invariant the second site.

The system can be in nine different state: $\{|0, 0\rangle, |0, 1\rangle, |0, 2\rangle, |1, 0\rangle, |1, 1\rangle, |1, 2\rangle, |2, 0\rangle, |2, 1\rangle, |2, 2\rangle\}$. The numbers in the ket describe the number of particles in the first and second site respectively. For the choice of the chemical potential, we expect only the physical state, like $|0, 2\rangle, |1, 1\rangle$ and $|2, 0\rangle$. To determine the ground state for the system, we have to fix one of the parameters J and U . We choose to set $U = 1$ for simplicity. Then, we can define the parameters in the unit of U , as J/U and μ/U . The choice of $\mu = U/2$ implies that $\mu = 1/2$. By setting different values of the hopping term, we find the ground state by the diagonalization of the Hamiltonian and we can calculate the fluctuation for the operator \hat{n}_1 for each different site.

We start calculating the eigenvalues for H_{B-H} and search the lowest and the corresponding eigenvectors are the ground states. We consider it as the state used for the computation for the fluctuation of \hat{n} . We consider the occupation number for the first site and determine the fluctuation

$$(\Delta n_1)^2 = \langle \psi_{gs} | (\hat{n}_1)^2 | \psi_{gs} \rangle - (\langle \psi_{gs} | \hat{n}_1 | \psi_{gs} \rangle)^2 = \langle \hat{n}_1^2 \rangle_{gs} - (\langle \hat{n}_1 \rangle_{gs})^2, \quad (3.2)$$

where is implicit $\hat{n}_1^2 \equiv \hat{n}_1^2 \otimes \mathbb{I}_{3 \times 3}$ and $\hat{n}_1 \equiv \hat{n}_1 \otimes \mathbb{I}_{3 \times 3}$. For the symmetry of the Hamiltonian, it emerges that the value of Δn_1 and Δn_2 are equal. In the next, we simply call $\Delta n_1 = \Delta n_2 \equiv \Delta n$. In Tab.3.1, we report the chosen values of J/U , the respective state, and Δn . In Fig.3.1 we plot the expectation values and the fluctuations of n_1 .

From the Tab.3.1 and graphic in Fig.3.1, we can see that two different behaviors emerge, corresponding to the Mott insulator and the superfluid phases, while the expectation number $\langle n \rangle$ is independent by the ratio of J/U . When the value of J is smaller than U , the ground state is dominated by the Mott Insulator: the hopping term is dominated by the interaction one and the atoms are disposed of an orderly manner. We have 1 atoms for each site. By increasing the value of J/U , the approximation for the ground state is the superfluid phase in which the hopping term dominates on the interaction one. In this case, the atoms are delocalized on the lattice: the number of particles varies between 0 and 2 for each site and we have $\Delta n \neq 0$. By increasing the value of the hopping term, the states $|2, 0\rangle$ and $|0, 2\rangle$ acquire more probability and the particles are more delocalized.

| J/U | Ground state | (Δn) |
|--------|--|--------------|
| 0 | $ 1, 1\rangle$ | 0 |
| 1/1000 | $-0.001 0, 2\rangle + 0.999 1, 1\rangle - 0.001 2, 0\rangle$ | 0.002 |
| 1/100 | $-0.014 0, 2\rangle + 0.999 1, 1\rangle - 0.014 2, 0\rangle$ | 0.020 |
| 1/10 | $-0.134 0, 2\rangle + 0.981956 1, 1\rangle - 0.134 2, 0\rangle$ | 0.189 |
| 1/5 | $-0.234 0, 2\rangle + 0.944 1, 1\rangle - 0.234 2, 0\rangle$ | 0.331 |
| 1/2 | $-0.372 0, 2\rangle + 0.851 1, 1\rangle - 0.372 2, 0\rangle$ | 0.526 |
| 1 | $-0.435 0, 2\rangle + 0.788 1, 1\rangle - 0.435 2, 0\rangle$ | 0.615 |
| 5 | $-0.487 0, 2\rangle + 0.725 1, 1\rangle - 0.487 2, 0\rangle$ | 0.689 |
| 10 | $-0.494 0, 2\rangle + 0.716 1, 1\rangle - 0.494 2, 0\rangle$ | 0.698 |
| 100 | $-0.499 0, 2\rangle + 0.708 1, 1\rangle - 0.499 2, 0\rangle$ | 0.706 |
| 1000 | $-0.499 0, 2\rangle + 0.708 1, 1\rangle - 0.499 2, 0\rangle$ | 0.707 |

Table 3.1: Data obtained by the simulation of the Bose-Hubbard model for two particles in two sites.

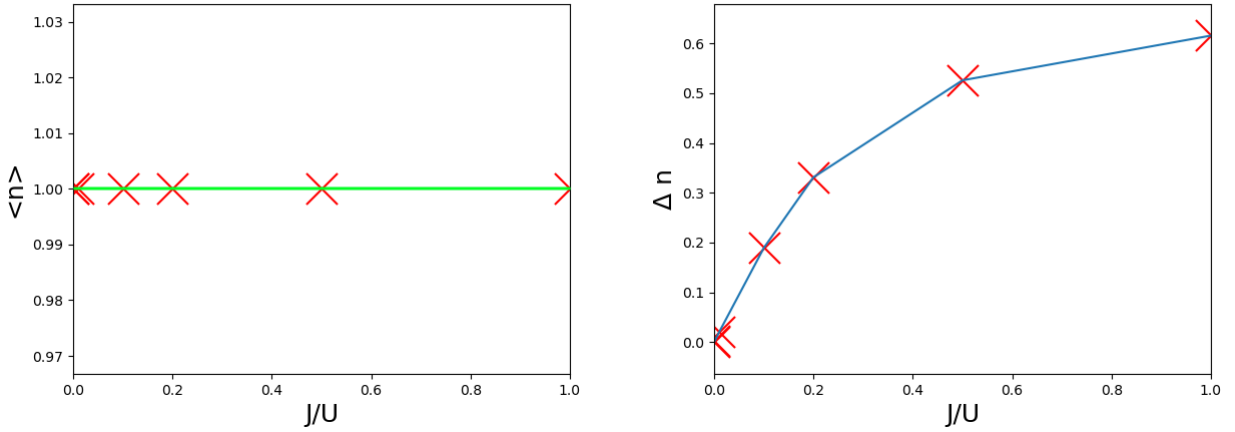


Figure 3.1: On the left: plotting the expectation number for the number of particles. The x-axis is the J/U and the y-axis is $\langle n \rangle$; on the right: plotting of data in Tab.3.1. The x-axis is the J/U and the y-axis is Δn .

Conclusions

We started from the tools necessary to describe ultracold atoms in an optical lattice. In the first chapter, we analyzed the fundamental potentials to write the Hamiltonian for a system of bosons, like the interaction between atoms, the periodic lattice and the external confinement. Here, the introduction of Wannier functions was important for obtaining the Bose-Hubbard Hamiltonian. In the second chapter, we introduced the formalism of second quantization. We introduced the field operators and how they can be decomposed in the Wannier functions base to obtain a picture of the fields in terms of ladder operators. Thanks to this, we obtained the Bose-Hubbard Hamiltonian. This function contains three terms: the hopping, the interaction and the external energy. These terms are multiply by the parameters J , U , and μ respectively. If the hopping term is higher than the interaction one, or vice versa, we could see two different behavior. The first is the superfluid phase, in which the particles are delocalized in all the lattice; the other is the Mott Insulator phase in which the particles are disposed of with the same number for each site. We decide to demonstrate the theory in which the system passes from the superfluid to Mott insulator or vice versa: in the last chapter, we proposed a simulation of two atoms in two sites. Setting the U parameter of the coupling term, we changed the J to obtain a ground state. The truncation that we imposed is given by two particles. We should introduce the chemical potential to fix the number of particles, so we set $\mu = U/2$. For simplicity we assume $U = 1$, thus we have $\mu = 1/2$. Then, we computed the Bose-Hubbard Hamiltonian with different values for the parameters J , U and μ , where we changed the value of J . Using the ground state, we established the expectation values of the number of particles in each site. By the value of $\langle \Delta n \rangle$ we could determine in which state the system is: if J is higher than U , we have a Mott Insulator; if J is lower than U we have a superfluid. To confirm this theory, we computed different values of J . The simulation showed us when the hopping term is dominated by the interaction, the system is in the insulating phase and, when the hopping term dominated to the interaction one, the atoms perform like a superfluid.

In conclusion, the behavior of the system of ultracold atoms is well described by the Bose-Hubbard model. Depending on the set parameters, we confirmed and distinguished the system phase.

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