Ultracold atoms in a 1D optical lattice: Mott-Superfluid transition

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Abstract: In this project, the transition between different quantum phases of ultracold bosonic systems trapped in an optical lattice is studied using the exact diagonalization method. First, the Mott Insulator to Superfluid transition is analyzed. Afterwards, the Density Wave phase is also considered. Specifically, a Julia programming language code is used to find the ground state of a system defined by a Bose-Hubbard Hamiltonian and the phase of this state is determined by means of specific observables derived from the occupation levels.

I. INTRODUCTION

Ultracold atomic gases are physical systems composed of identical atoms at near zero temperatures. If the atoms in these systems are bosons, they can freely occupy the same single-particle quantum state. This means that, as they cool down, all but an infinitesimally small number of atoms will settle into the same single-particle ground state [1]. In this situation, the system reaches what is known as Bose-Einstein condensation, a new state of matter in which the wave functions of the bosons overlap [1]. The Bose-Einstein condensate, first experimentally realized in 1995 by Eric Cornell and Carl Wieman at University of Colorado Boulder [2] and Wolfgang Ketterle at MIT [3], possesses interesting properties not present in any classical system, exhibiting quantum phenomena on a macroscopic scale.

Neutral bosons do not readily interact with static electric fields, but they can be manipulated using optical lattices. These can be created with counter-propagating laser beams, resulting in standing waves that can trap atoms in different separated wells due to the Stark shift [4]. By tuning the amplitude and the spacing of the different optical wells, also called "sites", the chances of quantum tunneling between neighbor sites can be modified. Moreover, the strength of interatomic interactions can be tuned experimentally.

Since the temperatures are close to zero, classical phase transitions do not play a role in ultracold atomic gases, as there are no thermal excitations to affect the system's behavior. However, quantum fluctuations play a central role, leading to the formation of distinct quantum phases. The interactions between particles and their relative strength depend on certain parameters of the optical lattice, such as the depth of the potential wells and the geometry of the sites.

By studying how the behavior of the ground state of the system changes as the parameters are tuned, these phases can be identified and classified, along with their phase transitions. Among the quantum phases that ultracold bosonic systems can exhibit in optical lattices, two of the most notable are the superfluid phase (SF) and the Mott Insulator phase (MI) [5].

Superfluidity is a property of quantum fluids with zero viscosity, which can flow without losing kinetic energy, allowing for the formation of persistent currents and quantized vortices. In the case of an optically-trapped system, superfluidity is characterized by a single wavefunction spanning all sites, with a well defined phase. This means that there is long-range coherence between the atoms, and the individual particles are delocalized over the entire optical lattice [4]. This leads to non-zero number fluctuation as well as non-zero compressibility at all sites.

Mott Insulators are solid materials that are expected to conduct electricity in electron band theory, but present very strong Coulomb interactions between electrons that block the electric current from flowing. This phase can be realized in optically-trapped ultracold bosonic systems when the repulsive contact interatomic interaction is strong enough to stop tunneling between sites. When the tunneling vanishes, the wavefunction becomes localized in each site with a fixed number of atoms per well. For this reason, the Mott Insulator phase lacks global phase coherence and presents an energy gap corresponding to the energy needed to create a particle-hole pair [4].

Another interesting phase that can be explored with ultracold bosons in optical lattices is the so-called Density Wave (DW) [6]. It appears when the atoms interact repulsively with nearest neigbour sites. When the atoms are charged or neutral, it is also known as charge density wave (CDW) or mass density wave (MDW), respectively. Due to the repulsion between neighboring sites, it is characterized by an alternating occupation pattern over the sites [1].

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[1] For example, for $N = M$ we may observe an occupation pattern $2 - 0 - 2 - 0 - \cdots$

II. MODEL AND IMPLEMENTATION

A. The system

An ultracold atomic gas with N atoms trapped in an optical lattice with M sites at zero temperature can be described by means of the Bose-Hubbard (BH) framework, with the following Hamiltonian:

$$\mathcal{H} = -t\sum_i \left(\hat{b}_i^\dagger \hat{b}_{i+1} + H.c.\right) + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - \mu\sum_i \hat{n}_i + V\sum_i \hat{n}_i\hat{n}_{i+1}\,, \tag{1}$$

where $\hat{b}_i^\dagger$, $\hat{b}_i$ and $\hat{n}_i$ are the creation, annihilation and number operators of one atom at the site i, respectively. The tunneling strength is given by t, U corresponds to the on-site interatomic interaction, V is the interaction between neighboring sites, and μ is the chemical potential.

This Hamiltonian encodes different interactions the atoms may have with each other. We distinguish the different terms in the following way [7]: $\mathcal{H}_t = -t\sum_i \left(\hat{b}_i^\dagger \hat{b}_{i+1} + H.c.\right)$ is the tunneling term, restricted here only to first-neighbor interactions, which accounts for the tunneling of an atom from one of the potential wells to the next one. $\mathcal{H}_U = \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1)$ is the on-site interaction between particles, which for positive values of U penalizes multiple atoms occupying the same site. For a given total amount of particles N and sites M, these two terms are enough to allow for the observation of the MI and SF phases, and would represent the minimal BH Hamiltonian with $V = 0$. The on-site chemical potential term $\mathcal{H}_\mu = -\mu\sum_i \hat{n}_i$ is fixed for a given amount of particles N, and penalizes low total occupation. The last term we consider is $\mathcal{H}_V = V\sum_i \hat{n}_i\hat{n}_{i+1}$. When $V > 0$, it corresponds to a repulsive first-neighbors density-density interaction [8]. This last term V is not present in the simplest form of the BH Hamiltonian, as it arises due to a power-law interaction that depends on the presence of an external magnetic or electrical field to polarize the bosons and vanishes as the distance between sites increases. However, as we will show, this term is needed in order to observe the DW phase. Additional terms can be added to the Hamiltonian to include more sophisticated interactions [7], such as the density assisted hopping term and the pair-hopping term. These terms give rise to other phases not considered here, such as Staggered Super Fluids and Haldane Insulators [8].

While the M sites in optical lattices can be arranged in a variety of ways, here we will only consider the following three geometries: an open 1D array with unconnected ends (line geometry), a cycle such that the first and last sites are connected (ring geometry), and an M-simplex in which the M sites are all connected to each other (simplex geometry). It is worth noting that this last configuration only has physical sense for $M < 5$, but is still interesting to study, as it showcases an extreme case of full connectivity in which all sites are first neighbors. The different geometries are represented in Fig. 1.

FIG. 1: Schematic representation of line, ring and simplex geometries for $M = 4$.

The differences in these geometries give rise to differences in the connectivity of the sites. As such, we expect phases characterized by more particle-particle correlations to emerge more readily at the highly connected simplex geometry rather than in the less connected line geometry.

B. Observables

While many properties can be used to distinguish between SF, MI and DW phases, in this work we will consider the compressibility and the static structure form factor, as in Ref. [8]. They are defined as [2]:

$$\Delta n_j = \langle \hat{n}_j^2 \rangle - \langle \hat{n}_j \rangle^2\,, \tag{2}$$

$$S(q) = \frac{1}{M^2}\sum_{j,k}^{M} \langle \hat{n}_j \hat{n}_k \rangle\, e^{-iq(j-k)}\,. \tag{3}$$

Compressibility, which we calculate through the number fluctuation Δn_j in Eq. (2), as in [9], allows us to distinguish between SF and MI phases, as the former is compressible and the latter is not. To identify the DW phase, we use the peaks of the static structure form factor $S(q)$ calculated using Eq. (3), as the alternating occupation pattern results in a peak at the Fourier component $q = \pi$ not present in the other two phases.

C. Method

Since the object of our study is a quantum system at zero temperature, the quantum states considered must always be those with the smallest energy. For this, the ground state of the Bose-Hubbard Hamiltonian must be calculated. With this aim, we implemented a direct diagonalization method in the programming language Julia.

There are two ways in which the Bose-Hubbard Hamiltonian can be constructed and diagonalized,

[2] Notice that Δn_j^2 may be more mathematically rigorous. We are using the notation of Ref. [8].

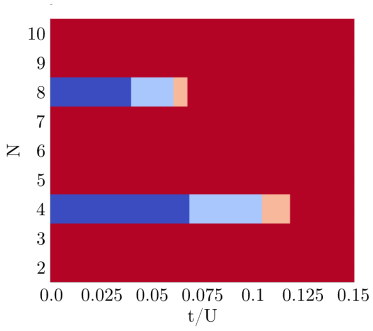

FIG. 2: MI-SF transition for $M = 4$ sites and varying N, with $U = 1$, $V = 0$ and $\mu = 0$. The system forms a MI in the dark blue region for all geometries, in the light blue region for line and ring geometries, and in the orange region for line geometry. Where it's not in an MI phase for a given geometry it is in a SF phase. In the red region, all systems are in SF.

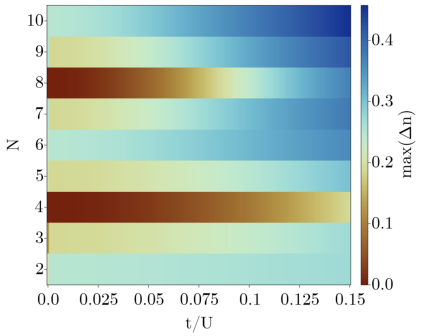

FIG. 3: Value of $\max(\Delta n)$ for $M = 4$ sites in ring geometry at different values of N as a function of t/U, with $V = 0$ and $\mu = 0$.

depending on whether or not the total amount of particles in the system is fixed or variable. When it is fixed, such that the total amount of particles is N, all the eigenstates of the Hamiltonian correspond to a state of N particles. If N is not fixed, but the total amount of particles is bounded by N_{max}, a new block-diagonal Hamiltonian must be constructed $\mathcal{H} = \text{Diag}(\mathcal{H}_1, \mathcal{H}_2, \dots)$ where $\mathcal{H}_i$ is the BH Hamiltonian with $N = i$. Since the eigenstates of a block-diagonal matrix correspond bijectively to the eigenstates of the individual blocks, the ground state of $\mathcal{H}$ will be the ground state of a certain $\mathcal{H}_i$, fixing $N = i$ as the amount of particles that minimize the Hamiltonian with those coefficients.

Since all matrices involved are sparse, they are stored as sparse arrays using the *SparseArrays* Julia package to save memory. The BH hamiltonians need not be fully diagonalized, as only the eigenstate with the lowest eigenvalue is needed, so the *Arpack* package is used to return the ground state and its corresponding energy.

III. RESULTS

A. MI-SF transition with $V = 0$

To investigate the MI-SF transition for a system with a fixed number of sites M and a given number of atoms N, we have obtained the ground state of the Hamiltonian for different values of the tunneling strength t/U and vanishing first neighbors interaction $V = 0$. In Fig. 2 we have set $M = 4$, $U \neq 0$ and $\mu = 0$. By calculating the ground state of the Hamiltonian at different values of t/U, we can find the values at which the MI and SF phases form for any given N. To find the transition between these two phases, we have used the compressibility in Eq. (2). More specifically, we assume that the system is in the MI phase if $\max(\Delta n) < 0.1$. This threshold is arbitrary, as is explained below.

Fig. 2 shows that the low-compressibility MI phase can only form if the number of bosons N is a multiple of the number of sites M. This is explained by the fact that if the number of particles does not divide the number of sites, at least one particle is left free to hop between sites, remaining delocalized over the lattice. Moreover, as the connectivity between the sites increases by changing the geometry of the sites, the SF phase can appear at lower values of the tunneling strength t/U. This is due to the fact that for a more connected site geometry, the chances of the boson tunneling to another site increase.

An interesting feature of the MI-SF transition for a fixed N, as shown in Fig. 3, is that compressibility does not change drastically with t/U as may be expected in a phase transition, but rather gradually. It is for this reason that the exact value at which the system transitions from one phase to the other has to be arbitrarily chosen [10]. However, the significant drop-off from $\max(\Delta n) \approx 0.24$ to $\max(\Delta n) = 0$ at $t/U = 0$ for $N = 4$ and $N = 8$ confirms that commensurability between the number of sites and the number of bosons is a key factor for the formation of a Mott Insulator.

We can study how the chemical potential μ/U affects the occupation density of the system and the MI-SF transition when the number of bosons is not fixed. Given a chemical potential μ/U and a tunneling strength t/U, the ground state of the system settles into a number of particles N. Fig. 4 shows the occupation density $n = N/M$ at different values of $t/U, \mu/U$ for $M = 4$ sites and $V = 0$. One can see that, for large values of t/U, the occupation density increases almost linearly with μ/U and t/U. For low values of t/U, conversely, integer values of occupation density appear more prevalently. In the $t/U = 0$ limit, only integer occupation density is possible. As seen above, the MI phase can only form in these regions of integer occupation density.

In Fig. 5 we plot the compressibility along the $t - \mu$ plane, finding differentiated regions where the ultracold bosonic gas forms a MI. These are the well-known Mott lobes of the 1D Bose-Hubbard model [7, 10]. The thin strips of increasing occupation density on the right side of Fig. 4 get progressively thinner with M, making

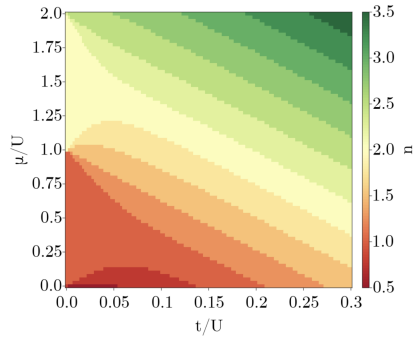

FIG. 4: Occupation density n for $M = 4$ sites with ring geometry, $V = 0$ and $N_{max} = 14$.

the MI-SF transition more evident and sharp. Fig. 6 shows the first of these lobes for different values of $N = M$ superimposed on one another. The range of μ/U values at any given t/U decreases with the number of particles and sites added. In the high M limit, the lobe closes down completely, as seen in Ref. [10], but this is computationally impossible to calculate using the direct diagonalization method.

By changing the geometry of the sites, the values of t/U at which the system forms a MI change. The same pattern as in Fig. 2 is found here, with compressibility being always lower for line geometry than for ring geometry, and it being the lowest for simplex geometry. As expected, along a given Mott lobe, the compressibility values are the same as in Fig. 3.

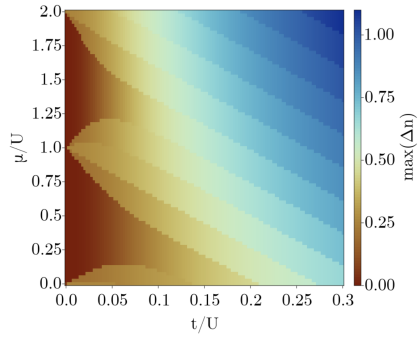

FIG. 5: max(Δn) for $M = 4$ sites with ring geometry, $V = 0$ and $N_{max} = 14$.

B. MI-SF-DW transitions for $V \neq 0$

Setting the first neighbors interaction $V \neq 0$ in the Hamiltonian, we introduce a new type of interaction in the model. Namely, for $V/U > 0$ a repulsion between particles in neighboring sites can be induced, and we expect to see the DW phase arise. By comparing the value of the Fourier component $q = \pi$ in Eq. (3) to the component $q = 0$, the MI-DW or SF-DW transitions can

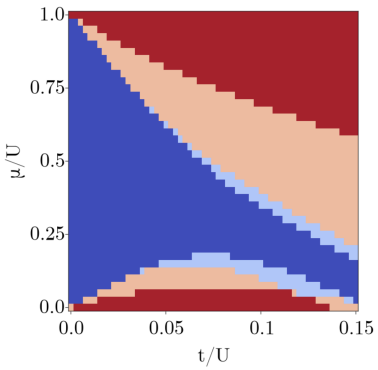

FIG. 6: Contours of the $n = 1$ Mott lobe for $M = 2$ (red-orange interface), $M = 4$ (orange-lightblue interface) and $M = 7$ (lightblue-blue interface), overlapped; for a system with ring geometry.

be observed. This is shown in Fig. 7, where the sharp transition at $V = 0.5\,U$ is evident for $t < 0.05\ U$. For $V/U < 0.5$, the $S(\pi)$ component is much smaller than the $S(0)$ component, indicating the absence of a DW state, while for $V/U > 0.5$ the system can form a DW. This sudden change in behavior is consistent with the results found in [8]. The region $t > 0.05\ U$ also presents a phase transition, but it becomes less sharp.

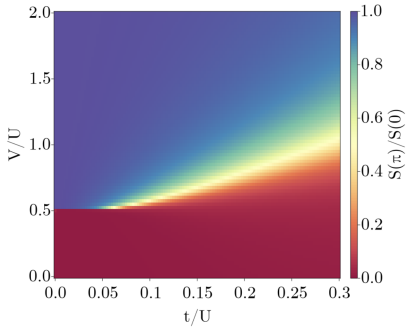

FIG. 7: Ratio $S(\pi)/S(0)$ for $M = 6$ sites and $N = 6$ particles in ring geometry.

Examining the values of the average number density $n = N/M$ in the $t - \mu$ plane for $V \neq 0$, we find that new lobes appear at semi-integer values of n, as shown in Fig. 8. These secondary lobes cannot be Mott lobes, because the ultracold atomic system does not settle into a Mott Insulator phase. This can be verified by calculating the compressibility Δn, resulting in the plot on the left side of Fig. 9. The $n = 0.5$ lobe does not present vanishing compressibility in the low t/U limit characteristic of the Mott Insulator phase. Instead, as shown in the plot on the right side of Fig. 9, the high values of the $S(\pi)/S(0)$ observable identify these half-integer lobes as Density Waves, showing that our two chosen observables are enough to distinguish between the three phases we have studied.

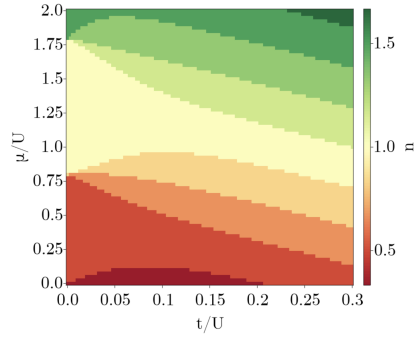

FIG. 8: Average number density $n = N/M$ for a system of $M = 6$ sites arranged in ring geometry with $V = 0.4\ U$. At low t, lobes appear for both integer and half-integer values of n.

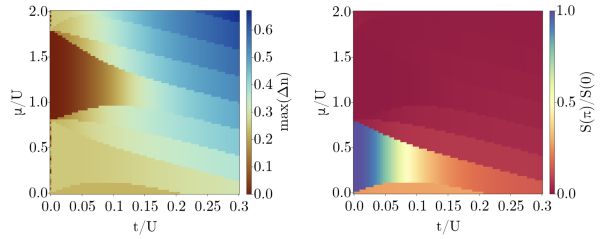

FIG. 9: Left plot: $\max(\Delta n)$ for a system of $M = 6$ sites arranged in ring geometry with $V = 0.4\ U$, showing the $n = 1$ lobe corresponds to a MI. Right plot: $S(\pi)$ for the same system, showing the $n = 0.5$ lobe that corresponds to a DW.

IV. CONCLUSIONS

In ultracold atomic systems trapped in optical lattices, different exotic phases of matter arise and their quantum phase transitions can be observed. In particular, bosonic systems at zero temperature present the superfluid, Mott Insulator and Density Wave states, depending on the type of interatomic interactions present in the system. The Bose-Hubbard Hamiltonian can be used to describe the behavior of systems governed by a tunneling strength t, an on-site interaction strength U, a chemical potential μ and a first-neighbors interaction strength V.

Direct diagonalization of the BH Hamiltonian allows us to find detailed information of the ground state of a certain system for a wide range of values of U, t, V and μ. By using observables that depend only on the occupation numbers, namely the compressibility Δn and the static structure form factor $S(q)$, we can distinguish these phases and the transitions among them. However, this method is very computationally costly, scaling superexponentially with both the number of particles N and the number of sites M. Some direct consequences of this limitation are that the Mott lobes do not fully close in the $t - \mu$ plane, so the MI-SF and MI-DW transitions do not appear sharp but smooth, as noted in Ref. [10]. For these reasons, further research has been done in this field with more scalable tensor network methods like Density Matrix Renormalization Group (DMRG) [8].

Certain phases of the Bose-Hubbard Hamiltonian only appear at certain values of $n = N/M$. The Mott Insulator phase requires n to be an integer, while the Density Wave phase requires a half-integer value. Additionally, the geometry affects the values of the parameters at which the phases are found, with more connected geometries favoring the formation of a superfluid.

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Ultracold atoms in a 1D optical lattice: Mott-Superfluid transition

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Resum: En aquest Treball de Fi de Grau s'estudia amb el mètode de diagonalització exacta la transició entre diverses fases quàntiques de sistemes bosònics ultrafreds atrapats en una xarxa òptica. En concret, es fa servir un codi en llenguatge de programació Julia per trobar l'estat fonamental d'un sistema definit per un Hamiltonià de Bose-Hubbard i es determina la fase d'aquest estat mitjançant observables derivats dels nivell d'ocupació.
Paraules clau: Sistemes ultrafreds, Hamiltonià Bose-Hubbard, transicions de fase, Condensat de Bose-Einstein, xarxa òptica.
ODSs: Aquest TFG està relacionat amb els Objectius de Desenvolupament Sostenible (SDGs)

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Objectius de Desenvolupament Sostenible (ODSs o SDGs)

1. Fi de la pobresa		10. Reducció de les desigualtats	
2. Fam zero		11. Ciutats i comunitats sostenibles	
3. Salut i benestar		12. Consum i producció responsables	
4. Educació de qualitat	X	13. Acció climàtica	
5. Igualtat de gènere		14. Vida submarina	
6. Aigua neta i sanejament		15. Vida terrestre	
7. Energia neta i sostenible	X	16. Pau, justícia i institucions sòlides	
8. Treball digne i creixement econòmic		17. Aliança pels objectius	
9. Indústria, innovació, infraestructures	X		

El contingut d'aquest TFG de la carrera de Física a la Universitat de Barcelona es relaciona principalment amb l'ODS 9, "Indústria, innovació, infraestructures", ja que els sistemes atòmics ultrafreds com els estudiats en aquest treball podrien tenir un gran impacte en el desenvolupament tecnològic futur. Per aquest mateix motiu el treball es relaciona amb l'ODS 7, "Energia neta i sostenible". D'una manera més indirecta, el treball es relaciona també amb l'ODS 4, "Educació de qualitat", per ser fruit del treball d'un estudiant de física, supervisat per investigador predoctoral i una professora universitària.