Exact Diagonalization of the one-dimensional Bose-Hubbard model

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Abstract: The Bose-Hubbard model was introduced to describe the behaviour of ultracold bosons trapped in an optical lattice. Such systems present a quantum phase transition of the ground state between two phases: the Mott Insulator and the superfluid phase. We characterise the ground state phases of one-dimensional systems for different lattice sizes with the unit filling. To do so, we use the Exact Diagonalisation method. The computation of the exact ground state energy and eigenvectors enable the study of different relevant physical quantities that will help us portrait such phase transition.

I. INTRODUCTION

The study of many-body quantum physics has an important legacy on fundamental discoveries such as novel states of matter or the observation of unseen phase transitions [1]. Since the experimental discovery of the Bose-Einstein condensation in 1995, a lot of effort has been put into understanding the physics beyond ultra-cold quantum many-body systems [1].

Remarkably, ultra-cold dilute atomic gases offer an unprecedented degree of experimental control [2]. Optical lattices allow us to tune effective parameters of the system, such as the potential depth or its geometry. The Bose-Hubbard model provides an accurate description of the physics on ultra-cold atomic systems in optical lattices [3], first introduced for model studies related to ^4He liquids in porous media and granular superconductors [13].

The experimentation with Bose-Einstein condensates in optical lattices give access to new regimes dominated by strong correlations, not reachable with magnetic traps [13]. Such correlations bring to light quantum phase transitions (QPT) that could not be studied before.

The Bose-Hubbard model shows a quantum phase transition between a Mott Insulator phase and a superfluid (SF) phase due to the interplay of kinetic energy and interactions at zero temperature [4]. This transitions are of great importance in understanding superconductivity. The system shifts from having all the atoms localized with no phase coherence, to a long-range phase coherence, where each atom is spread out over the entire lattice.

Many-body systems are numerically challenging, generally due to the scaling of the systems. Mean-field theories are widely used to solve these problems, but the introduction of such approximations can lead to loss of information about the system. Amongst the various methods used for the study of quantum many-body systems, Exact Diagonalization (ED) offers a unique position. It allows total access to the eigenstates and eigenvalues of the Hamiltonain with no approximations, and thus an exact calculation of different observables.

ED is used as a benchmark of state-of-the-art computational methods such as Tensor Networks, widely used in recent years. It does not rely on any assumptions or approximations, thus providing exact results. Such results are unlikely to be obtained via other analytical or numerical approaches. The deep understanding of this method is a first step towards the understanding of other computational methods and the physics beyond the Bose-Hubbard model.

II. THEORETICAL BACKGROUND

A. The Bose-Hubbard model

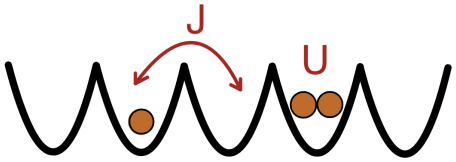

FIG. 1: Graphical representation of particles in the Bose-Hubbard model considering hopping between adjacent sites (J) and interaction between particles (U).

The one-dimensional Bose-Hubbard model can be thought as interacting bosons trapped in a 1D optical lattice by a periodic potential, assuming that the lattice wells are deep enough (Fig. 1) [7]. It uses the tight binding model, which approximates the wave function to a set of wave functions for isolated atoms in each lattice site. The use of this approximation incorporates short-range interactions and neglects the long-range ones on Hubbard models. Optical lattices are prepared in a way that they fulfil the tight-binding approximation.

The Bose-Hubbard model is a single band model, it only includes the lowest band states. Therefore, this model is only valid for low enough temperatures and tight enough potentials. The Hamiltonian can be written in terms of the particle creation and annihilation operators,

$a_i^\dagger$, a_i, within second quantisation formalism [1] :

$$\mathcal{H}_{BH} = -J \sum_{<ij>} \left(a_i^\dagger a_j + a_j^\dagger a_i \right) + \frac{U}{2} \sum_{i=1}^{M} \hat{n_j}(\hat{n_j} - 1), \quad (1)$$

where the system contains M sites labelled by the index i, and contains N particles. The particle creation operator is defined as $a_i^\dagger |n+1\rangle = \sqrt{n+1}|n+1\rangle$ and the particle annihilation operator is its adjoint. They follow the basic commutation relations for bosons, *i.e.* $\left[\hat{a}_\alpha, \hat{a}_\beta^\dagger\right] = \delta_{\alpha,\beta}, [\hat{a}_\alpha, \hat{a}_\beta] = 0, \left[\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger\right] = 0$, [8]. $\hat{n_i} = \hat{a}_i^\dagger \hat{a}_i$ is the atomic number operator and it is defined as $\hat{n}_i|n_1, n_2, ..., n_M\rangle = n_i|n_1, n_2, ..., n_M\rangle$.

The basis used is the occupation number basis. It represents single particle orbitals occupied by an n_i number of particles. It is defined as the set of Fock states $|\{n_1, n_2, ..., n_M\}\rangle$ that contain all possible combinations of bosons all over the lattice, following the constraint $\sum_{l=1}^{M} n_l = N$. In this basis, the eigenstates are expressed as:

$$|\psi_\nu\rangle = \sum_{i=1}^{D} \lambda_i^\nu |\{n_1, ..., n_M\}_i\rangle, \quad (2)$$

Where (λ_i) are the corresponding eigenvector coefficients and $i = 1, ..., D$ labels the different basis Fock states.

The first term of the Hamiltonian (1) is the hopping term. It quantifies the probability of a particle tunneling between two adjacent sites [1]. We set $U > 0$, as we treat systems with repulsive interaction. For information about the Bose-Hubbard model with attractive interactions, check [6] . Long-range tunneling, which would involve hopping over many lattice sites and long-range interactions, is neglected in this model.

B. Analitical considerations

In the Bose-Hubbard model there is an ongoing "competition" between the on-site interactions U and the tunneling J which is nicely captured by the modification of only one parameter: U/J. To do so, we study the behaviour of $\hat{\mathcal{H}}'_{BH} = \mathcal{H}_{BH}/J$. In order to characterise the QPT between SF and MI, we study the following observables.

The first one, is the ground state energy, which is given by the lowest eigenvalue resulting from the diagonalization of the Hamiltonian.

The Single-Particle Density Matrix (SPDM) gives us information on the probability of finding a particle in each state of the system. It is defined as:

$$\rho_{ij} = \frac{\langle\psi|a_i^\dagger a_j|\psi\rangle}{\sqrt{\langle\psi|a_i^\dagger a_i|\psi\rangle\langle\psi|a_j^\dagger a_j|\psi\rangle}}, \quad (3)$$

The off-diagonal terms of the SPDM correspond to the correlation values for two different sites. The diagonal terms provide the mean occupation number for a given site, which is the density, defined as $\rho_{ii} = \langle\psi|\hat{n}_i|\psi\rangle$.

To study the fluctuations of the occupation number of the i-th site, we study it's variance, defined as:

$$\sigma_i = \sqrt{\langle\psi|\hat{n}_i^2|\psi\rangle - \langle\psi|\hat{n}_i|\psi\rangle^2}. \quad (4)$$

If a state can be described with a single Fock state, the fluctuations on the occupation number are small, or can even disappear. Contrary to this, if a state needs several Fock states to be described (2) it means that the occupation number has large fluctuations.

Another interesting observable is the condensate fraction. According to Penrose-Onstager definition [12], it reads:

$$f_c = \frac{\lambda_1}{N}, \quad (5)$$

where λ_1 is the highest eigenvalue obtained from the diagonalization of the SPDM. If λ_1 is macroscopic, f_c is about the order of the unity and it is considered a BEC [10],[12]. This means that if one of the natural orbitals is macroscopically occupied, a BEC is present. The term macroscopically occupied, strictly means the ratio between the occupation number and the total particle number. This ratio remains finite for any M, so we cannot determine the absence of a BEC [10]. Note that a BEC and the SF phase are not the same. The SF phase definition is connected to flow properties. Macroscopcically, the SF phase is defined as that flowing system that doesn't move in the presence of moving boundaries [13].

This observables help us to characterize the nature of the ground state [13]. If the kinetic energy, *i.e.* the hopping term, of the particles is much greater than the interaction term, the particles become delocalized within the lattice. So, in this limit $(U/J \to 0)$ the ground state is stated as [3]:

$$|\psi_{SF}\rangle = \left(\frac{1}{\sqrt{N}} \sum_{i=1}^{M} \hat{a}_i^\dagger \right)^N |0\rangle, \quad (6)$$

which is the so called SF phase, with long-range coherence and characterised by maximal correlations and variance, as the particles are completely delocalized in the lattice. The condensate fraction of the SF phase is one, so it is also considered as a BEC [10].

On the other hand, if the interaction term is much greater than the hopping term $(J/U \to 0)$, the kinetic energy drops. As a result, the atoms are totally localized in the lattice sites. This results in the MI phase, ground state of which is:

$$|\psi_{MI}\rangle = \prod_{i=1}^{M} \left(\hat{a}_i^\dagger \right)^n |0\rangle. \quad (7)$$

It presents no phase coherence across the lattice, which results in a low correlation. Characterized by a zero energy and a small variance.

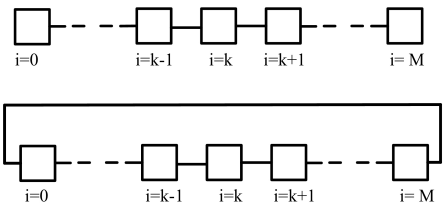

FIG. 2: Graphic representation for the PBC (top) and the PBC (bottom).

We consider two different sets of boundary conditions: the open boundary conditions (OBC) and the periodic boundary conditions (PBC). They indicate how to consider the pairs $< ij >$ of the first term of the Hamiltonian (1. In the OPB the first and last lattice only interact with the lattice neighbouring them and the wavefunction is set to zero on the extremes. In the PBC these two lattices can interact with each other and the lattice can be pictured as a ring (see Fig. 2).

The Bose-Hubbard model presents three important symmetries [9]:

- U(1) symmetry: Associated with the conservation of the total atom number $\hat{N} = \sum_{i=1}^{m} \hat{n_i}$. The Hamiltonian (1) is invariant under the transform $(a_i^\dagger, a_i) = (a_i^\dagger e^{i\theta}, a_i e^{i\theta})$.
- Reflection symmetry: The Hamiltonian is invariant under transformations $(\hat{a}_i^\dagger, \hat{a}_i) \rightarrow (\hat{a}_{M-i}^\dagger, \hat{a}_{M-i})$. As a consequence all the observables, for both OBC and PBC, are symmetric around the centre of the lattice.
- Translation symmetry: Since the potential has a periodicity of $V_{opt}(x + a) = V_{opt}(x)$, the Hamiltonian has translational symmetry which means it is invariant under the transform $(a_i^\dagger, a_i) = (a_{i+1}^\dagger, a_{i+1})$, which is associated with the quasi-momentum's conservation. It only applies to PBC. It makes the boson density constant all over the lattice and the correlation is the same for each site when keeping the same distance, *i.e.* $\rho_{ij}^{(N)} = \rho_{i+k,j+k}^{(N)}$. That is also the main reason why the boson density for OBC is not constant within U/J.

III. NUMERICAL METHOD - ED

We use the numerical ED. Its basic lies with the representation of the Hamiltonian matrix, $H_{ij} = \langle n_i|\hat{\mathcal{H}}|n_j\rangle$, in a convenient and appropriated Fock space basis. Then, we diagonalize it to obtain the eigenvalues and eigenvectors. Note that the off-diagonal terms are given by the hopping term and the diagonal terms by the interacting term.

Solving systems through this method can be a challenge computationally, since the size of the many-body systems scales exponentially. The number of possible states scales as [9]:

$$D = \frac{(N + M - 1)!}{N!\,(M - 1)!}, \tag{8}$$

Where D is the number of basis' states needed to describe the system. For larger systems, other methods such as Tensor Networks appear, as they are computationally more favourable. Nevertheless, the validity of their results is commonly compared with the ones obtained from ED. The most valuable characteristic of the ED is that it provides all the eigenstates and eigenvalues of the system, as the matrix is purely numerically diagonalized.

We create the basis in lexicographic order, which sets that a vector $|n_1, n_2, ..., n_M\rangle$ is superior to $|n'_1, n'_2, ..., n'_M\rangle$ if $n_k > n'_k$, knowing that there is a certain index $1 \leq k \leq M - 1$ for which $n_k \neq n'_k$ while $n_i = n'_i$ for $1 \leq i \leq k - 1$. Using this order, the first vector of our basis is $|N, 0, ..., 0\rangle$ and the last one $|0, 0, ..., N\rangle$ [9].

Once the Hamiltonian is computed analitically, we use the numpy.linalg library, based on LAPACK package [11] to diagonalize it. Note that the result of this diagonalisation is exact, as no approximations are made at any stage of the procedure.

IV. RESULTS AND DISCUSSION

In this section, we focus on the results obtained using ED as explained before. We study the dependence of the quantum phase transition between SF and MI phases as a function of U/J for different system sizes. We consider the systems with the unit filling, *i.e.* $N/M = 1$. This choice is made for the sake of numerical simplicity to show the two behaviours of our system: MI for smaller U/J values, and SF for larger U/J ones.

All the quantities computed below refer to the ground state solution of our system, given by equations (6) and (7), using the eigenvectors related to the lowest eigenvalues and for a given U/J.

A. Ground state Energy

In Fig. 3, we compute the ground state energy per particle for different system sizes as a function of U/J. We can see that the system behaves in a similar way for both open and PBC. For small values of U/J, the hopping term on eq. (1) dominates over the interaction on the system, hence the negative value of the energy. Also, the presence of a superfluid phase increases the total energy of the system [13]. This corresponds to the SF phase.

As the interaction increases over the kinetic energy, the bosons become more localised in the lattice sites. For larger values, $U \rightarrow \infty$, the ground state has zero

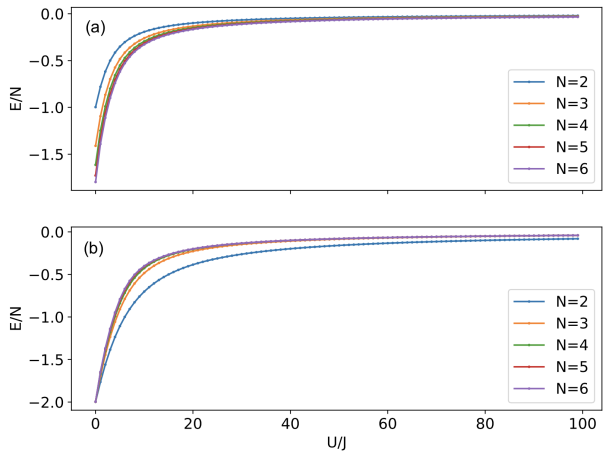

FIG. 3: Ground state energy per particle (E/N) as a function of the rate U/J for OBC (a) and PBC (b).

energy. The system corresponds to a MI phase, in which the bosons are completely localised.

B. Single-particle density matrix

1. *Correlation*

In Fig. (4) we compute the correlation (Eq. (3)), evaluated for $i = 0$ and $j = M/2$ for both OBC and PBC (for odd values of the site, $M/2$ is rounded up to the next integer value). By computing $\rho_{0,[M/2]}$, we check the correlation between the particles in the middle of the lattice and the particles in the first one. As in the SF phase there

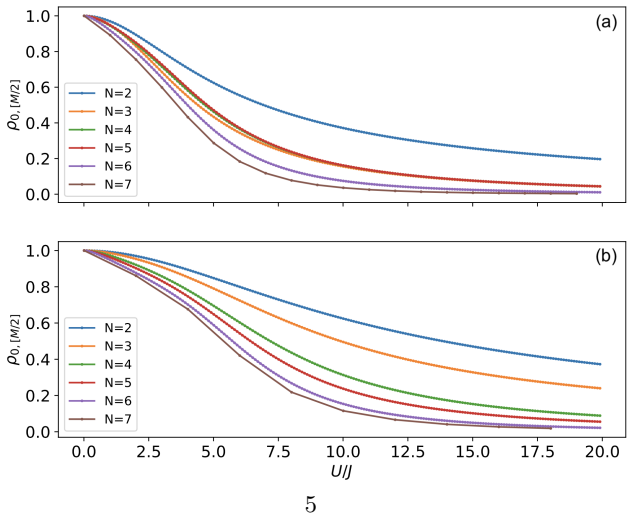

FIG. 4: $\rho_{0,[M/2]}$ as a function of U/J for OBC (a) and PBC (b).

is long-range coherence, particles on the first site and in the middle of the lattice are correlated. That is the reason why $\rho_{0,[M/2]} \to 1$ as $U/J \to 0$. On the other hand, as the interaction decreases, this long-range coherence is lost and as a consequence the correlation decays. In the limit $J/U \to 0$, the particles are completely uncorrelated and the system is found in the MI phase.

2. *Density*

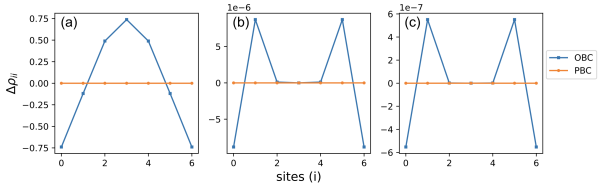

FIG. 5: Deviation from one boson/site ($\Delta\rho_{ii} = \rho_{ii} - 1$) of the expected occupation number on each site for the system N=M=7. OBC (squares) and PBC (dots) for U/J= 0.01 (a), 40.01 (b), 80.01 (c).

As we can see in Fig. (5), for PBC the density is constant with $n_i = 1$ on each site, as expected. The distribution of bosons for the OBC decreases in the extremes, as there the wavefuntion equals to zero. The density changes as U/J increases. When there is no interaction, the density has a peak in the middle of the lattice. As it increases, the bosons repel themselves and the density has several peaks.

This behaviour can also show the difference between SF and MI phases. As for $U/J \to 0$ the bosons are free to move around the lattice, but as $J/U \to 0$ they become localised with different distributions.

C. Variance

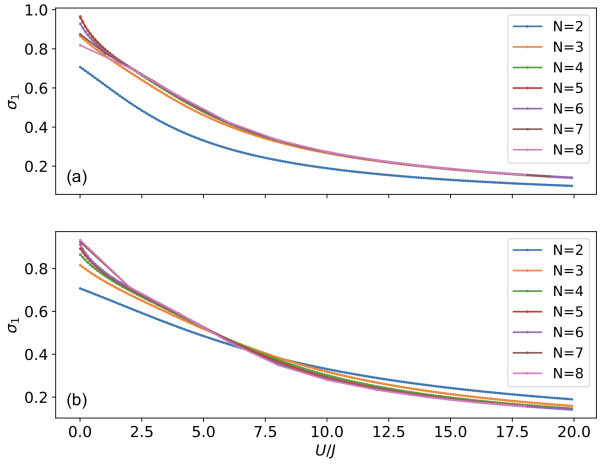

FIG. 6: Variance on the first site of the lattice for both OBC (a) and PBC (b) as a function of the rate between interaction and hopping strengths.

We study the fluctuations of the occupation number through its variance. In Fig.(6) it is demonstrated as the MI phase can be represented as a single Fock state, as the variance tends to zero (the bosons are localized). On the other hand, in the SF phase, many Fock states describe the wave function, as the variance is high (the bosons are spread all over the lattice).

D. Condensate fraction

As we can see in Fig.7, for any lattice size, when $U/J \to 0$, the system behaves as in a SF phase [9] as $f_c \to 1$. As the interaction grows the correlation lowers and tends to a finite value.

We observe an analogy to the Mermin-Wagner theorem in our 1D system, except for U/J = 0. Namely, that the condensate fraction decreases as we increase the system size.

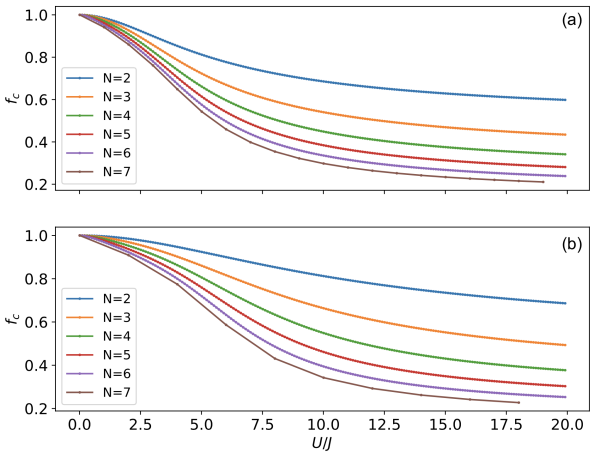

FIG. 7: Condensate fraction for both OBC (a) and PBC (b) as a function of the rate between interaction and hopping strengths.

V. CONCLUSIONS

We have studied the characterisation of the ground state of the Bose-Hubbard model for different system sizes and different values of rate between interaction and hopping strengths (U/J).

The choice of exact diagonalisation has given us access to the exact eigenstates and eigenvalues, and the different observables we computed. Thanks to this, we have differentiated both the MI and SF phases for the ground state of the Bose Hubbard model.

In this study from few to many-body systems we faced the difficulties of the size scaling of our systems and thus the computational cost. Exact diagonalisation is a rather simple method conceptually but it is never trivial in programming. The results obtained are the result of programming exact diagonalisation from scratch which has allowed us to have a better understanding of the physics and programming behind of this kind of simulations. Facing the limitation of working with a desktop computer, we could reach systems up to $N = M = 8$, with a dimension of $D = 6435$.

This motivates us to continue studying the Bose-Hubbard model or other many-body problems with other computational methods, which will require approximations or truncation, and will let us study bigger systems. Though, this results can always be bench-marked with exact diagonalisation.

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