

Few-body study of the two-component Bose-Hubbard model

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Abstract: We consider a system of bosonic particles trapped in a one-dimensional optical lattice which we describe by the Bose-Hubbard model. The system properties, e.g. energy spectrum, are studied for different number of particles and interaction strengths. First, we consider the case of a single component, discussing in detail the non-interacting and strongly interacting regimes. Then we consider the case of two components, focusing on the particular case of impurities.

I. INTRODUCTION

The Bose Hubbard model is one of the simplest models that is able to capture the behaviour of interacting bosons in an optical lattice [1]. That is why it has been widely studied in the fields of cold atoms and quantum simulators [2]. This model shows several phenomena arising from the quantum many-body properties, such as the existence of a quantum phase transition between a Mott insulator and a superfluid phase [3].

In this work we use the one-dimensional (1D) Bose-Hubbard Hamiltonian (BHH) to describe a system of trapped interacting bosons in a periodic lattice. In order to study the model we have identified limiting cases where analytic predictions can easily be obtained, i.e. non-interacting and strongly interacting limits. Beyond this analytical study we have numerically obtained the spectrum for an arbitrary interaction strength by direct diagonalization of the Hamiltonian. In particular, we have studied the system with periodic boundary conditions and different species of atoms, number of particles, etc. The exact diagonalization task can be computationally hard when the size of the Hamiltonian matrix is very large. That is why we focus on the case of few sites and particles. Even so, obtaining the full energy spectrum allows for a deeper understanding of the model that other approximate methods, such as Tensor Networks, cannot provide.

We first present the theoretical framework of this model in Section II. Then, in Section III we sketch the main features of the Python program that we have developed. In Section IV we discuss the behaviour of the system under different interaction regimes, in this case for one single component. In Section V we bring our attention to some interesting results for the two-component case. Finally, in Section VI we provide a summary and the main conclusions of our work.

II. THEORETICAL FRAMEWORK OF THE MODEL

We consider a bosonic species trapped in a 1D optical lattice with contact-like pairwise interactions, described by a BHH. We assume the system to be well defined

when the lattice potential is deep enough and particles become localized in each potential well, which we refer to as sites [1, 4]. By relying on the lowest Bloch band the BHH is given by:

$$H_{BH} = -J \sum_{i=1}^M (\hat{a}_i^\dagger \hat{a}_{i+1} + h.c.) + \frac{U}{2} \sum_{i=1}^M \hat{n}_i (\hat{n}_i - 1). \quad (1)$$

Where \hat{a}_i is the annihilation operator for a boson at site i and \hat{n}_i is the corresponding number operator. The first term describes the hopping of one boson between nearest-neighbour sites with an strength J . The second term accounts for the total interaction energy of the system, where U is the interaction energy of a single pair. In the BHH (1) the number of particles is conserved, thus, in our analysis the number of particles in the system is taken to be fixed.

For a two-component system, the hopping term is considered to be equal for both species but now we will have two types of interactions: intra-species, proportional to U , and inter-species, proportional to U_{AB} . The resulting Hamiltonian is,

$$H_{BH} = -J \sum_{i=1}^M \sum_{\alpha=A,B} (\hat{a}_{i,\alpha}^\dagger \hat{a}_{i+1,\alpha} + h.c.) + \frac{U}{2} \sum_{i=1}^M \sum_{\alpha=A,B} \hat{n}_{i,\alpha} (\hat{n}_{i,\alpha} - 1) + U_{AB} \sum_{i=1}^M \hat{n}_{i,A} \hat{n}_{i,B}. \quad (2)$$

III. METHODOLOGY

We have created a Python program which provides the eigenvectors and eigenenergies of Eqs. (1) and (2). We can choose the value of the different parameters of the Hamiltonian, such as the number of particles, number of sites and the values of U and U_{AB} . The value of J is taken as the energy unit. Then, we express the Hamiltonian in a matrix form and diagonalize it to obtain its eigenvalues and eigenvectors. We always work with periodic boundary conditions, although the program works with open conditions as well.

In order to express the Hamiltonian in a matrix form we need a Fock state basis. Defining the Fock state basis

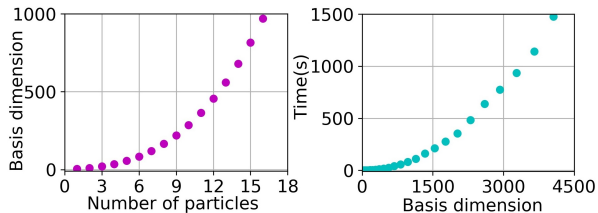


FIG. 1: Basis dimension (left) and time performance of the code (right) as a function of the number of particles and basis dimension, respectively. The computations have been performed on a intel I7 dual-core processor.

properly is crucial: it is formed by all the possible combinations of the particles in the sites, avoiding double-counting, since particles of the same species are indistinguishable. With N being the number of particles and M being the number of sites, the dimension of the basis is: $\#states = \binom{M+N-1}{N} = \frac{(M+N-1)!}{N!(M-1)!}$ [5].

For two different bosonic components the total Fock basis is given simply by the product of the Fock basis of each component separately $H = H_A \otimes H_B$. The notation we use for these states is $|n_{A,1}n_{B,1}, \dots, n_{A,i}n_{B,i}, \dots, n_{A,M}n_{B,M}\rangle$, being $n_{A(B),i}$ the number of $A(B)$ particles in site i and $N_{A(B)} = \sum_{i=1}^M n_{A(B),i}$.

It is important to optimize the time used in the generation of this basis, since its dimension grows exponentially with the number of particles and sites. After several tests, the most time-effective method was extracted from *combinations with replacement* provided by the Python library *itertools* [6], see Fig. 1.

To test the results, the outcome was compared to the values obtained with the density matrix renormalization group (DMRG) method [7] with certain number of particles and open boundary conditions. The results agreed with machine precision.

IV. SINGLE COMPONENT CASE

In this section, we consider the one-component system to discuss its main properties as we vary the parameters of the model. To guide the discussion it is useful to first describe two limiting cases where analytic results can be obtained. These are the non-interacting or the only-interacting cases, which correspond to neglecting the U or J terms in the BHH, respectively. This allows us to derive the ground state analytically for different number of particles.

A. Non-interacting case

With no interaction, the resulting ground state is a completely delocalized wavefunction throughout the lattice. This ground state can be constructed with the

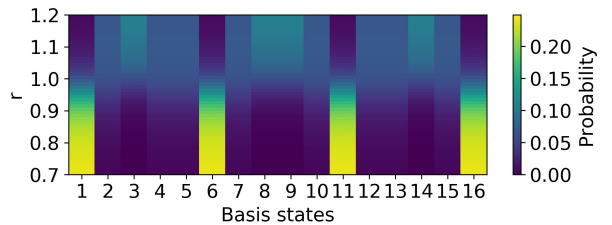


FIG. 2: Colormap of the probability for each Fock basis state in the ground state for $M = 4$ sites and $N_{A,B} = 1$ in terms of r . States 1,6,11 and 16 correspond to states where a pair AB is localized in a lattice site, such as $|AB, 0, 0, 0\rangle$. States 3,8,9 and 14 correspond to states such as $|A, 0, B, 0\rangle$. Note that all states have the same probability for $r = 1$.

single-particle state, which is a linear combination of all the Fock states. Since we consider all the particles to be in the same state: $|\phi_{SF}\rangle \propto \left(\sum_{i=1}^M \hat{a}_i^\dagger\right)^N |0\rangle$. This is known, for a many-body system, as a superfluid phase [3].

B. Strongly interacting case

When the interaction dominates over the tunneling we have two different behaviours. For attractive interaction the energy is minimized when all particles are localized together and the energy of the ground state is given by $E_{gs} = UN(N-1)/2$. For repulsive interaction the ground state is formed by those states that have the less number of pairs localized in the same site. An important parameter to consider in this case is the filling fraction $\nu = N/M$. In that case the energy of the ground state will be given by $E_{gs} = UM\nu_{\text{int}}(\nu_{\text{int}} - 1)/2 + RU\nu_{\text{int}}$, where R is the residue obtained from (N/M) and ν_{int} is the truncated integer value of ν . Therefore, the system prefers to have, if possible, the same number of particles localized in each site throughout the lattice to minimize the interaction energy. When the filling fraction is an integer the ground state can be written as: $|\phi_{MI}\rangle \propto \prod_{i=1}^M (\hat{a}_i^\dagger)^\nu |0\rangle$. This is known as Mott insulator phase [3].

V. BINARY MIXTURES

Now we turn our attention to the two component system, which is described by Eq. (2). The intra-species interaction U is considered to be repulsive and large, compared to the tunneling rate, we fix it at $U/J = 50$. We vary the inter-species interaction U_{AB} by changing the parameter $r = 1 + U_{AB}/U$. An r towards negative values means stronger attractive inter-species interaction and an r closer to positive values means stronger repulsive inter-species interaction, being $r = 1$ the threshold where $U_{AB} = 0$. Other values of interest are $r = 0$ and $r = 2$, since it is when $|U_{AB}| = U$.

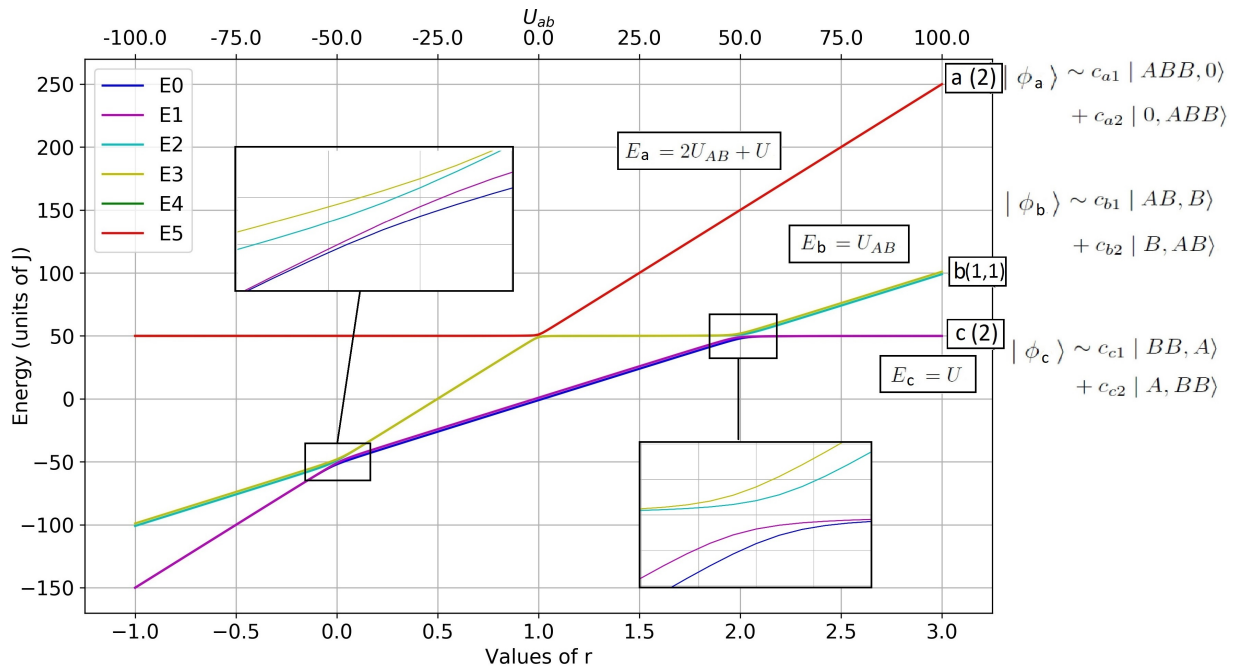


FIG. 3: Energy spectrum for $M = 2$ sites and $N_A = 1$, $N_B = 4$. We can see the structural change in the ground state for the critical values $r = 0$ and $r = 2$, where in the zoomed areas we can identify as an avoided crossing. The general structure of the spectrum is organized in three asymptotic behaviours labeled as a , b and c . The degeneracy for each of those asymptotic behaviours is also presented: (2) corresponds to double-degenerated and (1, 1) corresponds to two asymptotic energy levels that are non-degenerated. The combination of Fock states with higher probability for each of the asymptotic energy states is also presented outside the figure.

A. Pair formation

In this section we consider the case where a pair is formed. To do so we study the probability density of the Fock basis states for $N_A = 1$ and $N_B = 1$ in $M = 4$ sites depending on r . The discussion is illustrated in Fig. 2, where we see that the ground state for $r < 1$ is a combination of the four possible states (labelled as 1, 6, 11, and 16 in the figure axis) where the AB pair is localized in site 1, 2, 3 and 4. Interestingly, this structure continuously breaks when $r \sim 1$, where all Fock states have the same probability and thus we have a completely delocalized wavefunction. Note that $r = 1$ corresponds to $U_{AB} = 0$, therefore we can describe the ground state as two separate single-particle problems in $M = 4$ sites. Finally, for increasing $r > 1$ there is a continuous change to other formations with states of localized separated particles.

B. Impurity case study

Let us now consider the case in which the number of atoms in one species is much larger than the number of atoms in the other one, which is taken as an impurity. We study the configuration of $N_B = M$ ($\nu_B = 1$) and a single A particle, $N_A = 1$ in $M = 2$ sites. We noticed that for weak $|U_{AB}|$ interaction, when the inter-species interaction $U/J = 50$ dominates in the system we can interpret

the results as a frozen Mott insulator of B -particles and a single-particle problem for the A -particle.

In the following subsections we discuss three relevant features, the energy spectrum, the evolution of the first gap and the structure of the ground state in the Fock basis.

1. Energy spectrum

The energy spectrum is depicted in Fig. 3 as a function of r . The behaviour of the ground state shows two clear changes for $r = 0$ and $r = 2$. The shape of the energy spectrum is dominated by the interaction terms and it has different bands which are separated in two doubly-degenerated ones (a and c in Fig. 3) and two non-degenerated bands with the same asymptotic behaviour (b in Fig.3).

At first glance it could seem the lines experience a crossing, but if we take a closer look we can recognize an avoided crossing between a and b and b and c . Therefore both the ground state and the first excited state experience a continuous change, since every asymptotic behaviour gathers two energy levels.

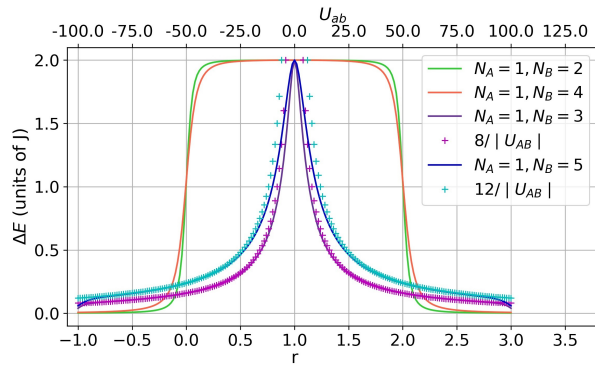


FIG. 4: Gap between the ground state and the first excited state for different combinations of number of particles in $M = 2$ sites. We see clear differences for integer/non-integer filling fraction of B particles. The $+$ symbols correspond to the analytical prediction from the perturbation theory described in Section V C.

2. First energy gap

The gap between the ground state and the first excited state $\Delta E = E_1 - E_0$ is shown in Fig. 4. We expect it to close around the values of $r = 0$ and 2 where we see the avoided crossings in Fig. 3, since the energy asymptotic lines a and c are degenerated (no gap) and b is not. When the inter-species interaction is weak $|U_{AB}| \ll U$ the gap corresponds to that of a single-particle delocalized in the lattice. The single-particle energy spectrum for 2 sites is $E_i/J = -1, 1$ and the gap is $\Delta E/J = 2$. In this situation the B -particles are frozen as a Mott insulator and do not play a role in the energy gap and we are left with a single A particle in two sites. When this Mott insulator configuration breaks, the gap is reduced until it closes.

3. Fock state structure

The probability for each Fock state in the ground state is shown in Fig. 5. The structural change in the ground state is clear. Since this change is due to an avoided crossing, it has to be continuous, as we can see in Fig. 5, where we observe a smooth change. For values of the inter-species interaction $|U_{AB}| \ll U$ the state of minimum energy is the one formed by the B -Mott insulator and the free A particle. Close to those limits we will have a mix between that state and the corresponding states for attractive ($U_{AB} < -U$) and repulsive ($U_{AB} > U$) interactions. For strong $|U_{AB}|$ the particles become frozen and the ground state becomes degenerated.

To broaden the picture it can be helpful to recognize the states that correspond to the asymptotic behaviors shown in Fig. 3 as a combination of the Fock states. In both energy levels within a line, the states that conform it only differ by a relative phase, and therefore correspond to two orthogonal combinations of the same Fock

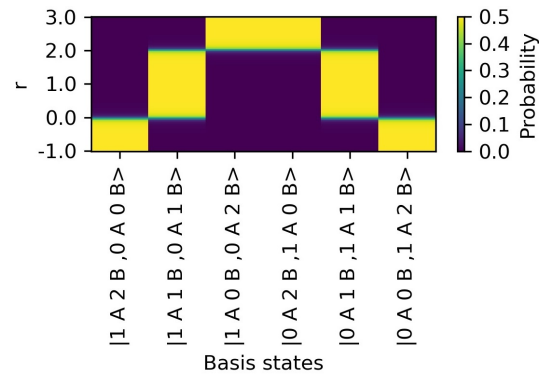


FIG. 5: Colormap of the probability for each state of the Fock basis in the ground state in different values of r for $M = 2$ sites. The number of particles are $N_A = 1$ and $N_B = 4$. We can see two clear structural changes for $r = 0$ and $r = 2$.

state vectors. As mentioned above, when approaching the critical values for the parameter $r = 0$ and $r = 2$, these states become a mixture of the asymptotic energy states.

C. Non-integer filling fraction ν_B

Now we focus on the case of an extra B -particle $N_B = M + 1$ and an impurity $N_A = 1$ in two sites $M = 2$. We consider two limiting situations (in absence of tunneling):

1. for $U_{AB} < 0$ we can describe the system as one pair of AB particles moving in a B -Mott Insulator.
2. for $U_{AB} > 0$, the configuration would be two different particles moving in the B -Mott insulator.

The attractive and repulsive cases are notably different, but in this case both can be treated within the same approach. For $J \ll U, U_{AB}$, i.e. the interaction dominating over the hopping, we can treat the latter as a perturbation. We can apply degenerate perturbation theory to find an effective Hamiltonian, which will lead us to characterize the behaviour of the gap presented in Fig. 4.

For attractive inter-species interaction U_{AB} the process consists in the following: We assume two B particles to be frozen in a Mott Insulator and consider an effective theory of pairs AB . Therefore we focus in the following states:

$$|L\rangle \equiv |ABB, B\rangle, |R\rangle \equiv |B, ABB\rangle,$$

which are degenerated if we only consider the interaction terms.

To find the matrix form for the effective Hamiltonian $H_{\text{eff}} = H_{\text{int}} + H_J$ we apply perturbation theory [8]:

$$\langle \alpha | H_{\text{eff}} | \beta \rangle = \langle \alpha | H_U | \beta \rangle - \sum_{\gamma} \frac{\langle \alpha | H_J | \gamma \rangle \langle \gamma | H_J | \beta \rangle}{E_{\gamma}^{(0)} - E_{\alpha}^{(0)}}$$

where $\alpha, \beta = L, R$. Therefore: $E_\alpha^{(0)} = E_\beta^{(0)} = 2U_{AB} + U$. Note that $\langle R | H_U | L \rangle = \langle L | H_U | R \rangle = 0$. By applying the hopping term to these states we can find the excited states:

$$|\gamma_0\rangle = |AB, BB\rangle, |\gamma_1\rangle = |BB, AB\rangle$$

. Given $E_\gamma^{(0)} = U_{AB} + U$ we obtain $E_\gamma^{(0)} - E_\alpha^{(0)} = -U_{AB}$. Proceeding to compute the expected value for each state we find the effective Hamiltonian in matrix form,

$$H_{\text{eff}} = \begin{pmatrix} 2U_{AB} + U + \frac{5J^2}{U_{AB}} & \frac{4J^2}{U_{AB}} \\ \frac{4J^2}{U_{AB}} & 2U_{AB} + U + \frac{5J^2}{U_{AB}} \end{pmatrix} \quad (3)$$

The energy eigenvalues are (taking into account $U_{AB} < 0$ for attractive interaction): $E_0 = -2|U_{AB}| + U - 5J^2/|U_{AB}| - 4J^2/|U_{AB}|$ and $E_1 = -2|U_{AB}| + U - 5J^2/|U_{AB}| + 4J^2/|U_{AB}|$. The energy gap that we obtain is $\Delta E = 8J^2/|U_{AB}|$ (4).

It is interesting to note that for the repulsive part the states we focus on, $|L_r\rangle$ and $|R_r\rangle$, correspond to the $|\gamma_0\rangle$ and $|\gamma_1\rangle$ states, which describe a frozen Mott insulator of B particles and two particles A and B that repulse each other. This results in the same behaviour of the gap and simplifies this characterization, but it does not happen for different number of sites.

Finally, if we add two more B -particles, we observe the behaviour is similar, see Fig. 4. Therefore, we treat the case with the same approach, but considering a Mott insulator of BB pairs, filling $\nu_B = 2$. For the attractive case we find $\Delta E = 12J^2/|U_{AB}|$ (5). The repulsive case again follows the same idea as before.

These analytical formulas, Eqs. (4) and (5), agree well with the exact diagonalization results, see Fig. 3. In fact, we noted that this behaviour still holds when we add two extra B -particles. Nevertheless we expect this treatment to fail when the system becomes larger, since we rely on a perturbative approach.

For slightly larger systems, we recognize the same behaviour for the integer filling fraction of B -particles. In the system with the extra B -particle the approach for attractive interaction holds, but the behaviour for repulsive

interaction is different, since the balance of interactions will lead to other preferred configurations.

VI. CONCLUSIONS

In this work we have studied the physics of a few ultracold bosons trapped in an optical potential modelled by the BBH for one and two bosonic species. We have employed a methodology based on exact diagonalization of the Hamiltonian matrix, being able to obtain detailed results which allowed a thorough characterization of the system behaviours under different conditions. These results can be summarized as follows.

For the one component case we have understood the structures preferred for the ground state with large U/J , finding analytical solutions that agree with the numerical results. It is important to notice the importance of the role of the filling fraction ν for repulsive interactions.

For the two component case we have studied the behaviour for different inter-species interactions. We have described first the existence of a pair formation in a system with two particles of different species. Finally we have focused on studying the system with one impurity, being able to describe the energy spectrum behaviour and characterizing the gap between the ground state and the first excited state. This characterization differed greatly for integer and non-integer filling fractions of B -particles. We have described the latter by an effective theory and we have obtained results that match the results of the simulation.

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