Mott Insulator-Superfluid transition with cold atoms trapped in optical lattice

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We study the superfluid-Mott insulator quantum phase transition for ultracold atoms described by the Bose-Hubbard model. We first analyse the limiting regimes where only kinetic or interaction energies are present, corresponding to a superfluid (delocalized) or a Mott-insulator (localized) state, respectively. Using a variational wave-function, where the different sites are decorrelated, and imaginay time propagation we then interpolate between these two cases, and find the full phase diagram of the model by analysing the superfluid order parameter, and the average and variance of density of particles per site.

I. INTRODUCTION

A quantum phase transition, opposite to an ordinary thermal phase transition, is driven by quantum fluctuations [1]. For that reason it can take place in a system at a temperature of absolute zero where all thermal fluctuations are frozen out. That transition occurs when the microscopic quantum fluctuations, that arise as a consequence of the Heisenberg's uncertainty relation, can induce a macroscopic phase transition of a many body-system. The critical point is characterized by a radically change in the nature of the ground state of the system.

A paradigmatic example exhibiting the superfluid to Mott insulator phase transition is the Bose-Hubbard model, describing a system of bosonic particles with short-ranged repulsive interactions trapped in an external periodic lattice potential. The phase transition occurs since there are two non-commuting terms in the corresponding Hamiltonian. The competition of these two terms determines the exact nature of the ground state and the critical point of the quantum phase transition.

This model was first theoretically studied in the context of superfluid-to-insulator transitions in liquid helium [2]. Its implementation with ultracold atoms trapped in optical lattices was proposed in [3], and first experimentally observed in 2002 [4]. Ultracold atoms are systems prepared at very low temperatures for which the quantum mechanical properties become relevant. An optical lattice is an artificial crystal of light, resulting from the interference patterns of two or more counterpropagating laser beams. The wavelengths of the laser beams determine the spatial periodicity of the crystal [4, 6]. The bosons will be confined in the potential wells generated by this optical lattice. Due to their high degree of tunability and controllability these systems have been proposed as ideal quantum simulators of other more complex quantum systems, like high-temperature superconductors and other condensed-matter systems. Another great application of these systems is quantum computation and metrology.

Here we study the Bose-Hubbard model and the superfluid-Mott Insulator transition occurring in this system. The work is organized as follows. First, we analyse the Hamiltonian and the limiting cases where only one of the two non-commuting terms is present. Then, we consider the complete Hamiltonian and propose a variational wave function that interpolates between the limiting regimes. Using this variational ansatz we derive analytically and perturbatively the critical point between the two phases. Finally, using imaginary time propagation we obtain numerically the complete phase diagram by evaluating the superfluid order parameter and the local density fluctuations of the system.

II. THE MODEL

We study a system of ultracold bosonic atoms with repuslive short-range interactions that are trapped in a periodic potential. We consider the case where no additional external potential is present, and thus all sites are equivalent (homogeneous system) and assume the periodic potential is deep enough compared to the other parameters of the system (temperature and interaction-strength) so that the atoms can be described via the lowest energy band of the periodic potential. In this situation the physics are described by the Bose-Hubbard Hamiltonian, that takes the following expression:

$$\hat{H}_{\mathrm{BH}} = -t \sum_{\langle i,j \rangle} \left(b_i^\dagger b_j + b_j^\dagger b_i \right) + \frac{U}{2} \sum_{i=1}^{M} \hat{n}_i(\hat{n}_i - 1), \quad (1)$$

where $b_i^\dagger$ and b_i correspond to the bosonic creation and annihilation operators of atoms on the ith lattice site and $\hat{n}_i = b_i^\dagger\, b_i$ is the number operator that counts the number of bosons on the ith lattice site. The first sum extends over all possible pairs of first neighbours (each pair counted once) while the second sum is performed over all lattice sites. We have assumed periodic boundary conditions.

The first term of the Hamiltonian multiplied by the positive tunneling parameter t represents the kinetic and potential energy of a single boson in the presence of the lattice, and it is also known as hoping energy. This term annihilates a localized boson and creates it on a neighbouring site, and thus, it represents the capacity of the

bosons to go to adjacent sites by tunneling. The second term multiplied by the interaction parameter U, which will be positive in our case as we are considering repulsive interactions, is the many-body interaction. This term only operates on a single site at the same time, and represents the energy cost of having more than one repulsive particle at the same lattice site.

For convenience, we will work from now on in the macrocanonical ensemble for which the atom number is not fixed, but only its average value through the chemical potential. Then the Hamiltonian reads:

$$\hat{H} = \hat{H}_{\mathrm{BH}} - \mu \sum_{i=1}^{M} \hat{n}_i. \tag{2}$$

In our final Hamiltonian Eq.(2) we have three independent parameters: t, U and μ. It is common to choose one of them and rescale the other magnitudes in units of this parameter. In our case we will work in units of U.

As previously mentioned, the kinetic and the interatomic potential term (now also including the chemical potential) do not commute with each other, as it does not exist a common basis that diagonalizes both terms simultaneously. The ground state of the Hamiltonian will be determined by the competition between these two terms, leading to a quantum phase transition that will be studied in the next sections.

Finally, let us briefly discuss on the implementation of the model with ultracold atoms optically trapped. An optical lattice can be generated by the constructive interference of two counter-propagating laser beams, yielding a periodic potential which for three dimensions can be written as $V_{\mathrm{lat}} = V_0 \left[\sin^2(k_0 x) + \sin^2(k_0 y) + \sin^2(k_0 z)\right]$, with $k_0 = 2\pi/\lambda$ and the lattice constant $d = \lambda/2$. The lattice depth V_0 is given by the laser intensity. For a deep lattice, the parameters t and U are given by [5]:

$$t \approx \frac{4}{\sqrt{\pi}} V_0^{3/4} e^{-2\sqrt{V_0}}, \qquad U \approx \sqrt{\frac{8}{\pi}} k_0 a_s V_0^{3/4}. \tag{3}$$

Here a_s is the scattering length which characterizes the short-range atomic interactions. Therefore, we observe that the tunneling parameter decreases with the optical depth V_0, while the interaction parameter increases with V_0 and also depends on the scattering length a_0 and k_0. Therefore, the ratio t/U is increased by decreasing the lattice depth V_0.

III. RESULTS

In the following, we will first analyze the ground state in the two limiting cases of vanishing tunneling ($t/U \to 0$) and no interaction between the particles ($U/t \to 0$). We will then propose a variational ansatz that continuously interpolates between these two cases and obtain the full phase diagram.

A. Mott insulator limiting regime

In the limit $t/U \to 0$ (in absence of the hoping term), occurring for very deep lattices, or equivalently, when the interactions dominate the Hamiltonian, we find the system in the Mott-insulator phase. In this case the Hamiltonian reads:

$$\hat{H}_{pot} = \frac{U}{2} \sum_{i=1}^{M} \hat{n}_i(\hat{n}_i - 1) - \mu \sum_{i=1}^{M} \hat{n}_i. \tag{4}$$

The interaction term accounts for the energy penalty of having $\hat{n}_i$ particles repulsively interacting on the same i-th lattice site. In addition, the chemical potential represents the energetic cost (if negative) or decrease in energy (if positive) when adding a particle to the system.

In this limit Eq.(4) is separable as a sum of local Hamiltonians per each lattice site, $\hat{H}_{\mathrm{pot}} = \sum_i \hat{h}_i$, with $\hat{h}_i = (U/2)\hat{n}_i(\hat{n}_i - 1) - \mu\hat{n}_i$. The eigenstates of this local Hamiltonian have a well defined number of particles n per lattice site. For the ground state, the exact value of n is determined by the balance between the U and μ terms. By imposing simultaneously that the energy per site with n particles $\epsilon_n = (U/2)(n(n-1) - \mu n)$ is smaller than the corresponding one for $n+1$ and $n-1$ particles, we arrive at the condition:

$$\varepsilon_n < \varepsilon_{n+1}, \varepsilon_{n-1} \Rightarrow n - 1 < \frac{\mu}{U} < n. \tag{5}$$

This inequality determines the range of μ/U for which the ground state is a Mott-insulator phase with n particles per site.

Thus, the many-body ground state for the homogeneous system can be written as product state

$$|\psi_{\mathrm{MI}}\rangle = \prod_{i}^{M} \frac{1}{\sqrt{n!}} (b_i^\dagger)^n |0\rangle, \tag{6}$$

where the product runs over the M sites of the lattice.

This state is an insulator, as particles are frozen at a fixed position, and the amount of energy required for creating an excitation is large and given by the interaction strength U. Finally, it is interesting to observe that the reduction of fluctuations in the atom number on each site leads to increased fluctuations in the phase. Thus in the state with a fixed atom number per site phase coherence is lost.

B. Superfluid limiting regime

In the limit $t/U \to \infty$, for which no interaction term is present, we find the system in a superfluid phase. In this case the Hamiltonian reads,

$$\hat{H}_{\mathrm{tun}} = -t \sum_{<i,j>} (b_i^\dagger b_j + b_j^\dagger b_i) \tag{7}$$

where the sum runs over all pairs of first neighbours. For simplicity, we will consider here the one-dimensional case with an even number M of lattice sites. An eigenstate for a single particle is a delocalized state over all lattice sites given by

$$|\psi^1_{\rm SF}\rangle_q = \frac{1}{\sqrt{M}}\sum_{j=1}^{M} e^{iqj}|j\rangle, \tag{8}$$

where q is the quasi-momentum of the particle. Its value can be calculated considering periodic boundary conditions. These conditions make the system invariant under a discrete translation of M lattice sites, for which the system returns to the same state. With these conditions we obtain $q = 2\pi n/M$, being $n = 0, \pm1, \cdots, \pm(M-1)/2, M/2$, so we can find M independent states.

By inserting Eq.(8) into the Hamiltonian Eq.(7) we find indeed that it is an eigenfunction of the tunneling term with energy,

$$\begin{aligned} H_{\rm tun}|\psi^1_{\rm SF}\rangle_q &= -t\frac{1}{\sqrt{M}}\sum_{j=1}^{M}\left[e^{iq(j+1)}|j\rangle + e^{iq(j-1)}|j\rangle\right] = \\ &= -2t\cos q|\psi^1_{\rm SF}\rangle_q. \end{aligned} \tag{9}$$

Hence, we obtain that the energy is $E^{1,q}_{SF} = -2t\cos q$, which takes a value between $-2t$ and $2t$ depending on q. As $t > 0$, the ground state (minimum value) corresponds to $q = 0$. The dispersion relation also tells us that for low values of t, in the deep lattice regime, the energy bands will be almost flat (and the states almost degenerate) while for a large value of t, they will be very broader.

We can now define new creation and annihilation operators in the delocalized basis

$$c^{(\dagger)}_q = \frac{1}{\sqrt{M}}\sum_{j=1}^{M} e^{iqj}b^{(\dagger)}_j \tag{10}$$

with $q = 2\pi n/M$ $(n = 0, \pm1, \cdots, \pm(M-1)/2, M/2)$. The Hamiltonian can then be rewritten as

$$\hat{H}_{\rm tun} = -2t\sum_q \cos q c^\dagger_q c_q \tag{11}$$

where the sum extends over all the possible quasi-momentum values.

Since we are dealing with non-interacting bosons, the many-body ground state is found by occupying with N particles the same single particle ground state previously found:

$$\begin{aligned} |\psi^N_{\rm SF}\rangle &= \frac{1}{\sqrt{N!}}(b^\dagger_{q=0})^N|0\rangle \\ &= \frac{1}{\sqrt{N!}}\left(\frac{1}{\sqrt{M}}\sum_{j=1}^{M} b^\dagger_j|0\rangle\right)^N. \end{aligned} \tag{12}$$

In the grand canonical ensemble, the total number of particles per site is not fixed, and only its average value $\bar{n}$ is determined from the chemical potential μ. The ground state with average particle per site $\bar{n}$ can be constructed as:

$$|\psi^{\rm MC}_{\rm SF}\rangle = ce^{\sqrt{M\bar{n}}b^\dagger_{q=0}}|0\rangle = c\prod_i^M e^{\sqrt{\bar{n}}b^\dagger_i}|0\rangle, \tag{13}$$

with normalization constant $c^2 = \exp(M\bar{n})$. This state is a product of coherent states at each lattice site, and every well has a Poissonian probability distribution to be filled with n particles [4], in other words, the variance is given by $\mathrm{Var}[\hat{\mathrm{n}}_\mathrm{i}] = \langle\hat{\mathrm{n}}_\mathrm{i}\rangle = \bar{\mathrm{n}}$. Unlike the Mott insulator phase, this wave function exhibits long-range phase coherence due to the fixed relative phase between sites (given by the quasi-momentum value $q = 0$). Furthermore, opposite to the Mott insulator phase, where on-site density fluctuations were completely suppressed, this limit is characterized by on-site density fluctuations and the particles are delocalized over the whole lattice.

C. The Gutzwiller Ansatz

In order to obtain the phase diagram when all terms are simultaneously present in the Hamiltonian Eq.(2), we propose a variational mean-field wave-function called the Gutzwiller (GW) ansatz:

$$\begin{aligned} |\psi_{\rm GW}\rangle &= \prod_{i=1}^{M}\left(f_0 + f_1 b^\dagger_i + f_2\frac{(b^\dagger_i)^2}{\sqrt{2}} + ... + f_n\frac{(b^\dagger_i)^n}{\sqrt{n!}}\right)|0\rangle \\ &= \prod_{i=1}^{M}\sum_{n=0}^{n_{max}} f^{(i)}_n|n\rangle_i, \end{aligned} \tag{14}$$

with normalization condition $\sum_i^{N_{\max}}|f_i|^2 = 1$. For an homogeneous system the amplitudes will be necessary the same for all sites, therefore, $f^{(i)}_n = f_n$.

With this variational state, we first have checked that the limiting cases studied previously are recovered and have found the specific values that the coefficients take. For the Mott-insulator limiting regime with n particles per well we find

$$f_j = \delta_{n,j}. \tag{15}$$

That is, only the coefficient of the GW-ansatz Eq.(14) that accompanies the operator which creates n particles in a well is different than 0 and equal to 1. For the superfluid regime, expressing the ground state in the second form from Eq. (13), we find the values for the coefficients of the GW to be

$$f_j = \frac{\sqrt{\bar{n}}^j}{\sqrt{j!}}. \tag{16}$$

We will now study the transition point and the full phase diagram using this variational ansatz. In order

to do this, we first have expressed the kinetic and the potential energy in terms of the coefficients, finding:

$$E_{kin} = -tz \left| (f_1 f_0^* + \sqrt{2} f_2 f_1^* + \cdots + \sqrt{n} f_n f_{n-1}^*) \right|^2 \quad (17)$$

where z is the number of first neighbours of a given lattice site (coordination number).

$$E_{pot} = -\mu |f_1|^2 + (-2\mu + U) |f_2|^2 + \cdots + \left(-n\mu + \frac{U}{2} n(n-1) \right) |f_n|^2 \quad (18)$$

Perturbative analysis.– We can do a perturbative analysis to find the critical point of the quantum phase transition. We consider a point close to the Mott insulator-superfluid transition, for which the GW ansatz consists mostly on the n-th component, plus a small contribution of the $n-1$ and $n+1$-th components, while all the remaining terms vanish:

$$f_n = \sqrt{1 - 2\alpha^2}, \qquad f_{n+1} = f_{n-1} = \alpha \quad (19)$$

with α being a small parameter that tends to zero if we approach the Mott insulator regime and takes a different value in the superfluid regime. If we fix $\mu = U(n - \frac{1}{2})$ (corresponding to the middle point of the insulating phase with n atoms, as we have find in Eq. (5)) the energy of the system up to the second order in α is given by:

$$E_{tot} = \left(-zt \left| \sqrt{n} + \sqrt{n+1} \right|^2 + U \right) \alpha^2, \quad (20)$$

that is, the energy is parabolic in α. This expression tells us that if the prefactor in front of the parameter α is positive, the energy will be minimized by $\alpha = 0$, which corresponds to the Mott-insulating transition with n atoms per well. Instead, as soon as the prefactor becomes negative, $\alpha = 0$ is now a maximum, and the Mott-insulating phase becomes unstable, indicating that we enter into the superfluid phase. This transition occurs when

$$U = zt \left| \sqrt{n} + \sqrt{n+1} \right|^2, \quad (21)$$

the point where the kinetic and the interaction energy have the same contribution to the total energy of the system. It reflects the competition of the two non-commuting terms in the Hamiltonian. If we have a higher value of U, the interatomic potential energy is dominant, so we will find the system in a Mott insulator phase, while for a smaller U the kinetic term will be the dominant and we will find the system in the superfluid phase. Therefore, it gives the critical point for the fixed value μ/U chosen.

For large value of n the critical value of t/U reduces to:

$$\lim_{n \to \infty} \frac{t}{U} \sim \frac{1}{4zn}. \quad (22)$$

This means that for an increasing n the transition will take place for smaller value of t, so the Mott insulator regime will occupy a smaller space in the phase diagram.

Numerical results.– Finally, we have numerically obtained the complete phase diagram using the imaginary time propagation method on the variational state given by Eq.(14) (see the Appendix for the description of the method and convergence). We have evaluated three different observables: the order parameter, the density and the variance of the number of particles per site.

The order parameter, which corresponds to the expected value of the boson anihilation operator for a site, is given in terms of the amplitudes of the GW ansatz by

$$\langle b \rangle = (1/M) \sum_{i=1}^{M} \langle \Psi(t) | b_i | \Psi(t) \rangle = f_0^* f_1 + \sqrt{2} f_1 f_2^* + ... + \sqrt{n} f_{n-1}^* f_n. \quad (23)$$

The density of the system, is obtained from the expectation value of the number operator at each site of the lattice:

$$\bar{n} \equiv (1/M) \sum_{i}^{M} \langle \Psi(t) | \hat{n}_i | \Psi(t) \rangle = = |f_0|^2 + |f_1|^2 + 2|f_2|^2 + ... + n|f_n|^2. \quad (24)$$

Finally, the variance of the number of particles per well is given by

$$\mathrm{Var}[\hat{n}_i] = \langle \hat{n}_i^2 \rangle - \langle \hat{n}_i \rangle^2 = \sum_{n=0}^{n_{max}} n^2 |f_n|^2 - \bar{n}^2. \quad (25)$$

From Eq. (15) and Eq. (16) we see that in the Mot insulator phase, the order parameter and the variance will be exactly zero and the density will take an integer value, contrary to the superfluid phase where the order parameter and the density can take arbitrary values and the variance of n will be equal to $\bar{n}$ due to the Poissonian probability distribution explained in Section III B.

The numerical results are shown in Figure 1. We can appreciate the Mott-insulator regime inside the dark blue lobes where the order parameter and the variance of the number of particles per site is exactly zero and in the case of the density has a constant and integer value. These lobes take the range given by (5), that is, the first lobe extends for the μ/U values where have $n_i = 1$ particles per well is favorable than have more or less, the second lobe for $n_i = 2$, etc. Moreover, we see reflected the analytical result given by Eq. (22) in the decreasing lobes width with $\bar{n}$. Outside the lobes the system is find in the superfluid regime where the order parameter is continuous, and increases its value with μ/U and ρ.

Outside the Mott-insulator lobes the system is found in the superfluid phase where the order parameter and the density are continous increasing their value with μ/U and t/U. For the variance of n_i, we find in the superfluid regime that there are separated regions where this observable is constant but not an integer. That is because in the superfluid phase the number of particles per site doesn't need to be an integer.

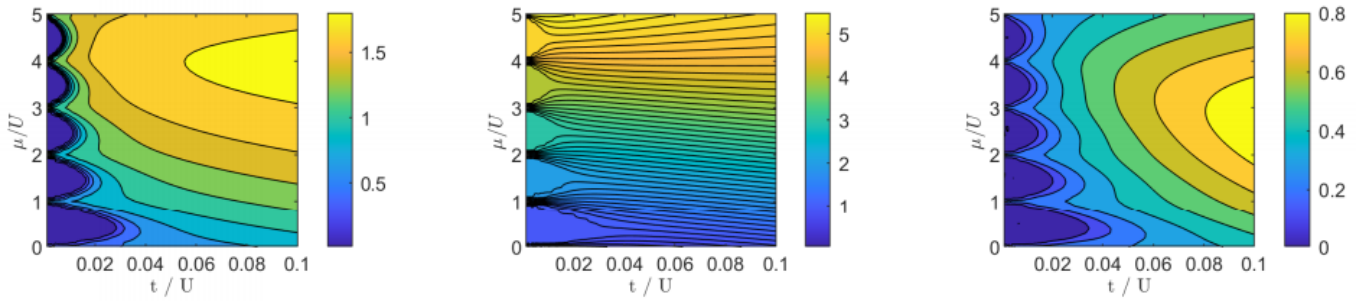

FIG. 1: Phase diagram of the Bose-Hubbard model. From left to right: order parameter, average density per site and variance of number of particles per site. We have considered a maximum number of particles per site $n_{i,max} = 6$ and coordination number $z = 6$ (cubic lattice). The dark lines represent constant values of the magnitudes plotted in the z-axis.

IV. CONCLUSIONS

We have studied the Bose-Hubbard model and the Superfluid-Mott insulator transition. We first analyse the ground state for the two non-commuting terms of the Hamiltonian independently. In the Mott insulator limiting regime the wave function is a Fock state in the localized basis, consisting of a product state with the same number of particles at each lattice site. The range of values of μ/U determining the Mott insulator lobes amplitude in the phase diagram is found by minimizing the energy of the system. For the superfluid phase we find a delocalized state over all the lattice sites, consisting of all particles in the same Bloch function with well definied quasimomentum $q = 0$ (assuming periodic boundary conditions). Observing the differences between the two regimes we conclude that phase coherence and local density are mutually exclusive and conjugated variables. That is, when one increases the other decreases, since they are related by the uncertainty principle.

In the second part we have considered a variational Gutzwiller ansatz for which the different sites are decorrelated. This allows us to interpolate between the two limiting regimes and find the ground state when the two non-commuting terms are simultaneously present in the Hamiltonian. After recovering the previously studied limiting regimes, we have performed a perturbative analysis to find the critical point of the phase transition for a fixed value of $\mu/U = n + 1/2$ (center of a Mott-insulator lobe). At this point the approximated interaction and kinetic energy become equal, indicating that as the value of n increases, the critical value of t/U decreases.

Finally, we have performed imaginary time propagation to find the variational ground state of the system for a continuous range of values of t/U and μ/U across the phase transition. We obtain the phase diagram in terms of the superfluid order parameter, the density and the variance of number of particles per site. All the previous studied features are reflected in the obtained phase diagram. For instance, we observe the Poissonian probably distribution in the superfluid regime, the constant density in the Mott insulator phase and the decreasing lobes with $\bar{n}$.

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APPENDIX

The imaginary time propagation method

To find the ground state of the many-body system modeled with the Bose-Hubbard Hamiltonian, we perform an imaginary time evolution starting with a random state, that has the form of the GW ansatz. Starting with a random state we make sure that the overlap with the ground state highly probably is different than zero and let the method converge to it.

Generally, the evolution in real space is given by the Schrödinger equation (in units of $\hbar$):

$$i\frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle \tag{26}$$

If we work in a proper basis, the hamiltonian can be writen as: $\hat{H} = \sum_n E_n|n\rangle\langle n|$, and we can also decompose the state in a lineal combination in this basis: $|\Psi\rangle = e^{-iE_0t}a_0|0\rangle + e^{-iE_1t}a_1|1\rangle + ... + e^{-iE_nt}a_n|n\rangle$, therefore, for a time-independent hamiltonian Eq. 26 is solved like:

$$|\Psi(t)\rangle = e^{-i\hat{H}t}|\Psi(t=0)\rangle = e^{-i\sum_n E_n|n\rangle\langle n|t}|\Psi(t=0)\rangle \tag{27}$$

Where the eigenvalues E_n will company the overlap of the generic state $|\Psi\rangle$ with the eigenstates $|n\rangle$.

If we now replace t by an imaginary time, the state will evolve like:

$$|\Psi(\tau)\rangle = e^{-\sum_n E_n|n\rangle\langle n|\tau}|\Psi(\tau=0)\rangle \tag{28}$$

Observe, that now the exponential is real and negative, so first of all, the norm of the state is losed. Secondly, for a long time $\Psi(\tau)$ will tend to zero. Nevertheless, the bigger term of the sum will be the corresponding to the ground state because it has the minimum energy, so the bigger exponential. Therefore, at the end, all the excited states will tend to zero more rapidly than the ground state, so we will be able to recognise it and consequently determine the phase where the system is found.

An equivalent formulation of the Schrödinger equation is obtained by minimizing the action of the system, given by $S = \int dt\mathcal{L}$. The Lagrangian of the system in the quantum state $|\Psi\rangle$ is given by [8]:

$$\mathcal{L} = \frac{\langle\Psi|\dot{\Psi}\rangle - \langle\dot{\Psi}|\Psi\rangle}{2i} - \langle\Psi|\hat{H}|\Psi\rangle \tag{29}$$

Where $|\dot{\Psi}\rangle$ is the time derivative of the wave function. Putting on $|\Psi\rangle$ the variational mean field function, GW ansatz,

$$\langle\dot{\Psi}|\Psi\rangle = \sum_i^M \sum_{n=0}^{n_{max}} \dot{f}_n^* f_n \tag{30}$$

and the quantum Lagrangian reads:

$$\begin{aligned}\mathcal{L} = &-\frac{i}{2}\sum_i^M \sum_n^{n_{max}} (\dot{f}_n^* f_n - \dot{f}_n f_n^*) - \\ &- tz\sum_i^M |f_0^* + f_1 + \sqrt{2}f_1^* f_2 + \sqrt{3}f_2^* f_3 + .. + f_{n-1}^* f_n| - \\ &- \mu|f_1|^2 + (U-2\mu)|f_2|^2 + ... + \\ &+ (\frac{U}{2}n(n-1) - \mu n)|f_n|^2\end{aligned} \tag{31}$$

We can minimize the action with respect the variational parameters f_n or f_n^*. Choosing the complex one we obtain for each site i:

$$i\frac{d}{dt}f_n = -tz(\sqrt{n}f_{n-1}\varphi + \sqrt{n+1}f_{n+1}\varphi^*) + [\frac{U}{2}n(n-1) - \mu n)]f_n \tag{32}$$

In units of $\hbar$. Where $z\varphi = \sum_{<j>_i}\varphi_j$ is an effective field that in each site i depends on the nearest neighbours, in our case takes an easy expression due to the system is homogeneous, therefore,

$$\varphi = \sum_n^{n_{max}} = f_n^* f_{n+1}\sqrt{n+1} \tag{33}$$

The equations described in 32 are of mean-field type, because they are written for a single site i and the "field" φ_i represent the influence of neighboring sites on the site i, and have to be determined self-consistently. We can write these equations for all the amplitudes in a matrix form like:

$$i\frac{d}{dt}\vec{f} = \mathcal{M}\vec{f} \tag{34}$$

Where $\vec{f}$ is a vector containing all the parameters f_0, f_1, ..., f_n. and the matrix M reads,

$$\mathcal{M} = \begin{pmatrix} 0 & -tz\varphi^* & 0 & \cdots & \cdots & 0 \\ -tz\varphi & -\mu & -tz\sqrt{2}\varphi^* & 0 & \cdots & 0 \\ 0 & -tz\sqrt{2}\varphi & U-2\mu & -tz\sqrt{3}\varphi^* & \cdots & 0 \\ \vdots & 0 & \ddots & \ddots & \ddots & \vdots \end{pmatrix} \tag{35}$$

Where the rows are for the same n and the columns for the variational parameters f_n. As we could deduce from Eq. (32) the $\mathcal{M}$ matrix is tridiagonal. Also, notice that the $\mathcal{M}$ matrix depend on the parameters through φ, so the evolve in time of $\vec{f}$ involves the evolve in time of $\mathcal{M}$. It is a self-consistent method, so, we have to discretize time in steps Δt and for each step find $\vec{f}$ with the last $\mathcal{M}$ matrix and then actualize with the new $\vec{f}$ the $\mathcal{M}$ matrix. It is, integrating Eq. 34:

$$\vec{f}(t_{s+1}) = e^{-i\mathcal{M}[\vec{f}(t_s),\mu,U,t]\Delta t}\vec{f}(t_s) \tag{36}$$

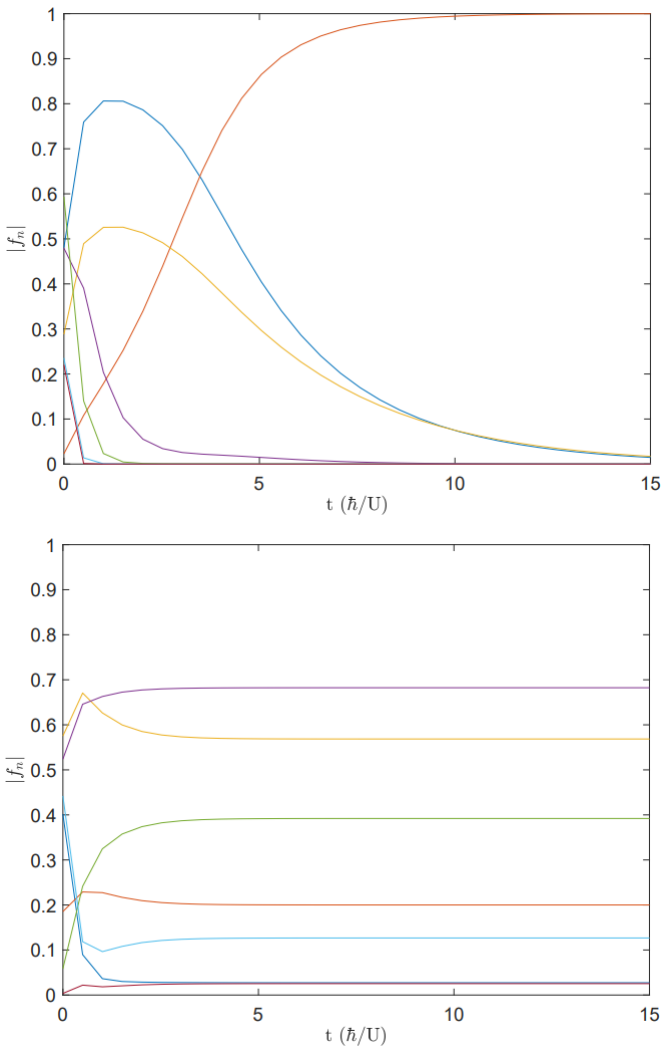

FIG. 2: Dynamic evolution of the GW Ansatz amplitudes for n_{max}=6 with the imaginary time method. Above for the Mott insulator phase, (t/U, μ/U)=(0.01, 0.5) and under for the superfluid phase, (t/U, μ/U)=(0.07, 2).

Obtaining the dependence on time of the amplitudes. Then, if we change the variable for the time for an imaginary one, -$i\tau$ instead of t, the amplitudes evolve like:

$$\vec{f}(\tau_{s+1}) = e^{-\mathcal{M}[\vec{f}(\tau_s),\mu,U,t]\Delta\tau}\vec{f}(\tau_s) \tag{37}$$

Remembering that the norm is losed, we will have to renormalize in each step of time and as we have said, for a large τ we will obtain the amplitudes corresponding to the ground state.

Method convergence

In 2 we can observe how the amplitudes in the two phases converge to the values calculated in Eqs 15 and 16 respectively. In the Mott insulator phase all coefficients go to zero except the one f_1 because for (t/U, μ/U)=(0.01, 0.5) we are in the first lobe of the phase diagram that corresponds to have one particle per site. In the superfluid phase all coefficients take a different value than zero as expected.

With this figure we conclude that the method converges to the correct values of the amplitudes and it is faster in the superfluid regime than for the Mott-insulator regime.