Effects of long range hopping in the Bose-Hubbard model

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We investigate the effects of an extended Bose-Hubbard model with a long range hopping term on the Mott insulator-superfluid quantum phase transition. We consider the effects of a power law decaying hopping term and show that the Mott phase is shrinked in the parameters’ space.

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I. INTRODUCTION

After the experimental realization of Bose-Einstein condensation in 1995 [1–3], the research in ultracold atomic physics has known great development. In particular, theoretical and experimental efforts have been done to study quantum phases of ultracold atomic bosons in optical lattices [4]. In this context, the pioneer experiment was performed by Greiner et al. in 2002 [5]. The authors confined a Bose-Einstein condensate with repulsive interactions at very low temperature in a three dimensional optical lattice and studied the interference pattern produced by the system as function of the lattice depth. A transition between a superfluid phase (each atom is spread out over the entire lattice and the interference pattern is peaked at reciprocal lattice wavevectors) and a Mott insulator phase (with a precise number of atoms in every well and a gaussian interference pattern peaked at zero-wavevector) is observed at some critical depth [6].

The many-body model which describes this phase transition is the Bose-Hubbard Hamiltonian

\[ \hat{H} = -J \sum_{\langle ij \rangle} \hat{b}_i^\dagger \hat{b}_j + U \sum_i \hat{n}_i (\hat{n}_i - 1) \]  

where \( J \) is the hopping energy, \( U \) is the interaction energy (both are assumed positive), \( \hat{b}_i \) and \( \hat{b}_i^\dagger \) are on-site bosonic annihilation and creation operators, \( \hat{n}_i = \hat{b}_i^\dagger \hat{b}_i \) and \( \langle ij \rangle \) means that \( i \) and \( j \) are nearest neighbors lattice sites. The effective parameters \( J \) and \( U \) can be obtained by microscopic quantities (mass and scattering length of atoms) and lattice parameters (spacing and depth) introducing Wannier functions, as shown in Refs. [4–6].

In recent years, many authors have extended the standard model to investigate new quantum phases, new transitions, and other properties with theoretical means and Quantum Monte Carlo simulations. In particular, some remarkable studies have considered exotic geometries, such as Bethe lattices, complex networks and more [7–9]. Some others have taken into account more complicated interaction terms, such as nearest and next nearest neighbors interactions, both for spinless and spin-1 bosons [10–12]. Even more recently, quantum phase transitions in disordered systems have been investigated [13, 14].

In the present work we will consider lattices with a simple geometry (hypercubic lattice in \( d \) dimensions) and ordered systems with only on-site interactions between atoms. Instead, we will take into account the possibility for an atom to tunnel from a site \( i \) to every other site \( j \) and study the effect of this generalization on the phase diagram.

II. LANDAU EFFECTIVE ACTION

Using a path integral approach, as discussed in Refs. [15–16], an effective action for the theory can be obtained after a Hubbard-Stratonovic decoupling of the hopping term. The relevant aspect for the present work is that this procedure can be set up in a more general frame, namely taking a more general hopping, such that our generalized Bose-Hubbard Hamiltonian reads

\[ \hat{H} = -\sum_{ij} J_{ij} \hat{b}_i^\dagger \hat{b}_j + U \sum_i \hat{n}_i (\hat{n}_i - 1) \]  

where the sum over \( i \) and \( j \) is not restricted to nearest neighbors.

Close to the superfluid-Mott phase transition, the order parameter \( \psi(\vec{r}, t) = (\hat{b}_i(t)) \) of the system corresponds to the expectation value of the bosonic annihilation operator \( \hat{b}_i \) at the imaginary time \( \tau \) and at the site \( i \) associated to the spatial position \( \vec{r} \) [15, 16]. After Fourier transforming this field and ignoring the effect of its fluctuations (\( \psi_{\vec{q}} = 0 \) for every momentum \( \vec{q} \neq 0 \)), one obtains...
the effective mean-field Landau action \[15\] [10].
\[
S[\psi_0^+, \psi_0] = S_0 + c_2 |\psi_0|^2 + c_4 |\psi_0|^4 \] (3)
where \(c_4 > 0\) and \(\psi_0\) is the order parameter. This action has only one global minimum \(\psi_0 = 0\) when \(c_2 > 0\), while develops infinite equivalent minima given by \(|\psi_0| = \sqrt{-c_2/2c_4}\) when \(c_2 < 0\). Since in the second case the \(U(1)\) symmetry of the action in Eq. (3) is spontaneously broken by the ground state, we interpret this as the superfluid phase, \(|\psi_0|^2\) being the superfluid density, and the other case as the Mott insulating phase. The critical behaviour occurs when \(c_2 = 0\), the coefficient \(c_2\) being
\[
c_2 = \beta N^d (J_0^{-1} - G_{loc}(0)) \] (4)
where \(N^d\) is the total number of lattice sites (\(N\) in each direction), \(\beta\) is the inverse temperature, \(J_0\) is the zero-momentum Fourier coefficient of the interaction matrix
\[
J_\vec{q} = \frac{1}{N} \sum_{ij \neq i,j} J_{ij} e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} \] (5)
and \(G_{loc}(0)\) is the local Green function at zero frequency
\[
G_{loc}(0) = \frac{\bar{n}}{\mu - U(\bar{n} - 1)} - \frac{\bar{n} + 1}{\mu - U \bar{n}} \] (6)
In Eq. (6) \(\mu\) is the chemical potential and \(\bar{n} = [\mu/U]\) is the first integer greater than \(\mu/U\) and represents the number of atoms in every site in the Mott phase (the lattice is not empty only when \(\mu > 0\)). For our purposes, the most important property of the local Green function is that \(G_{loc}(0) > 0\) for every \(\mu\).

For nearest neighbors hopping with \(J_{ij} = J\) and hypercubic lattices in \(d\) dimensions, writing \(\vec{q} = \sum_{k=1}^d 2\pi q_k \hat{e}_k / L\) (where \(q_k \in \mathbb{Z}\) and \(\hat{e}_k\) is the \(k\)-th element of the canonic base) one can perform the sums in Eq. (5) to find
\[
J_\vec{q} = 2J \sum_{k=1}^d \cos \left(\frac{2\pi a}{L} q_k\right) \] (7)
Hence the zero momentum term is \(J_0 = 2dJ\) and the coefficient \(c_2\) is
\[
c_2 = \frac{1}{2dJ} - G_{loc}(0) \] (8)

III. BOSE-HUBBARD MODEL WITH LONG RANGE HOPPING

The main purpose of this work is to extend the approach discussed in the previous section to a generalized Bose-Hubbard model in \(d\) dimensional hypercubic lattices with power law decaying hopping energy of the form
\[
J_{ij} = \frac{Ja^s}{|\vec{r}_i - \vec{r}_j|^s} \] (9)
where \(a\) is the lattice spacing and hence \(J\) is still the nearest neighbors hopping energy. The exponent \(s\) defines the hopping range: the larger \(s\), the smaller the probability of long range hopping. In the limit \(s \to \infty\) the hopping is \(J\) when \(i\) and \(j\) are nearest neighbors and 0 otherwise, which is the case studied in the previous section.

The zero momentum coefficient \(J_0\) can be found setting \(\vec{q} = 0\) in Eq. (4) and solving \(J_0 = (1/N) \sum_i \sum_{j \neq i} J_{ij}\). Taking periodic boundary conditions, every site of the lattice can be regarded as a bulk site, no surface effects have to be taken into account and then there is a perfect discrete translational invariance: this means that the sum \(\sum_{j \neq i} J_{ij}\) does not depend on \(i\). As a consequence, the sum over \(i\) can be performed and gives a factor \(N\), so that \(J_0 = \sum_{j \neq i} J_{0j}\).

Following the same procedure performed in Refs. [18, 19] for the Ising model, the remaining sum can be evaluated using the continuum approximation with the prescription \(a^d \sum_i \to \int d\vec{r}\). This is consistent for not too large values of \(s\), since in this way the integrand function doesn’t change abruptly from one site to his neighbors.

\[
J_0 = \frac{J}{a^{d-s}} \int d\vec{r} \frac{1}{r^s} \] (10)
The above integration is performed using polar coordinates \((d\vec{r} = r^{d-1} d\Omega dr)\), since the angular part can be integrated and gives the \(d\) dimensional solid angle
\[
\Omega_d = \frac{2\pi^{d/2}}{\Gamma(d/2)} \] (11)
where \(\Gamma(x)\) is the Euler Gamma function.

To compute the radial part we introduce upper and lower physical cutoffs. The most reasonable lower cutoff is the lattice spacing \(a\), while the upper one is the lattice size length \(Na\) [19].
\[
J_0 = \frac{J_0 \Gamma_d}{a^{d-s}} \int_a^{Na} r^{d-s-1} dr \] (12)
\[
= \begin{cases} 
\frac{J_0 \Omega_d}{a^{d-s}} (N^{d-s} - 1) & \text{if } s \neq d \\
J_0 \Omega_d \log N & \text{if } s = d
\end{cases}
\]
Taking the thermodynamic limit \(N \to \infty\) we can compute \(J_0^{-1}\) and finally write the coefficient \(c_2:\)
\[
c_2 = \begin{cases} 
-G_{loc}(0) & \text{if } s \leq d \\
\frac{d-s}{\Omega_d} - G_{loc}(0) & \text{if } s > d
\end{cases}
\] (13)

By comparing Eqs. (8) and (13) we can formally find the exponent \(s_0\) for which the two equations are equal
\[
s_0 = d + \frac{\pi^{d/2}}{d! (d/2)} \] (14)
Since the nearest neighbor hopping should be recovered in the limit \(s \to \infty\) (and not \(s \to s_0\)), we can use the value
FIG. 1: Boundary between the two phases (Mott phase inside the lobes and superfluid outside) in a two dimensional lattice, for some values of $s$. The lobes corresponding to $s = 2.3$ and $s = 2.6$ have been computed with the continuum approximation; the lobe at $s = 6$ has been computed with the discrete approximation of Eq. (16). Finally, the lobe at $s = \infty$ corresponds to nearest neighbors hopping. As $s$ moves from $\infty$ to $d$ the lobes are shrinked and eventually disappear for $s = d$.

$s_0$ as an upper limit for our approximation and expect it to give good results only for $s \ll s_0$.

The critical line at zero temperature in the parameters space $J/U, \mu/U$ is given by the condition $c_2 = 0$. When the range exponent $s$ is greater than the critical value $d$ (i.e. when the hopping is short-ranged), the phase diagram has the same shape as the one obtained with nearest-neighbors hopping, even if the phase boundary is shrinked depending on $s$. The lobes at $s = 2.3, s = 2.6$ in Fig. 1 have been computed within this approximation in $d = 2$.

When $s$ is below his critical value $d$ (i.e. when the hopping is long ranged), the thermodynamic limit is not well defined since the system would have infinite energy. However, if $N$ is finite but large, since $G_{loc}(0)$ is positive, $c_2 \approx -G_{loc}(0)$ is negative and the Mott-phase is almost unavailable for the system.

IV. EXACT SOLUTION IN ONE DIMENSIONAL LATTICE

If the dimensionality of the system is $d = 1$, the continuum approximation is not necessary since there is a simple exact solution. Taking $i = 0$ and $\vec{r}_j = aj$, $j \in \mathbb{Z}$, the sum we have to perform is $\sum_{j \neq 0} 1/|j|^s$. This sum diverges for $s \leq 1$ and converges to $2\zeta(s)$ (where $\zeta(s)$ is the Riemann zeta function) otherwise; so the coefficient $c_2$ is

$$c_2 = \begin{cases} -G_{loc}(0) & \text{if } s \leq 1 \\ \frac{1}{2\zeta(s)} - G_{loc}(0) & \text{if } s > 1 \end{cases}$$

(15)

In the limit $s \to 1^+$, since $\zeta(s) \approx (s - 1)^{-1}$, this result is in good agreement with the continuum approximation of Eq. (13). In the opposite limit $s \gg s_0$, where $s_0 = 2$ the approximation is expected to be unprecise. In Fig. 2 we present the continuum approximation error $\varepsilon(s) = 1 - J_0^{approx}/J_0^{true} = 1 - [(s - 1)\zeta(s)]^{-1}$ as function of $s$ to give a visual picture of what we have stated above.

It is remarkable that, as stated in Refs. 17 and 22, the mean field theory fails at describing the Mott-superfluid transition in $d = 1$. The exact mean field solution provided in this section does not predict the correct shape of the Mott lobes, but is a useful test for the accuracy of our approximation.

The exact solution of the one dimensional model suggests generalization for higher dimensional hypercubic...
lattices. For example, in a $d = 2$ square lattice, where $j$ is labeled by two integer indices $m, n$, we have to sum $(m^2 + n^2)^{-s/2}$ over the whole lattice excluding the origin. The contribution of all the sites lying on a straight line passing through the origin is proportional to $2\zeta(s)J$. The proportionality constant is the inverse distance between two sites on that line to the power of $s$, namely $(p^2 + q^2)^{-s/2}$, where $p$ and $q$ are the smallest coordinates of a point in that line. We can span one fourth of the lattice taking straight lines with slope only between 0 and 1 and notice that, by symmetry, every contribution is repeated 4 times, except the ones due to slope 0 and slope 1 lines, which are only repeated twice. The proportionality factor is 1 for the horizontal line and $2^{-s/2}$ for the bisector; while for all the other lines it is $(p^2 + q^2)^{-s/2}$ with $0 < q < p$ and $q$ coprime to $p$ (the sum over all values of $q$ respecting this condition is indicated as $\sum_q$).

All the considerations lead to the exact equation

$$J_0 = 4\zeta(s)J \left[ 1 + 2^{-s/2} + 2\sum_{p=2}^{\infty} \sum_{q \text{ coprime to } p} (p^2 + q^2)^{-s/2} \right]$$ (16)

The main idea is to use Eq. (16) as an approximation for high $s$ by cutting off the sum at some point. This provides a good approximation for $s \gg s_0$ (when the system is intrinsically discrete) and as we expect, in the limit $s \to \infty$, $J_0 \to 4J$, which is the result for nearest neighbors hopping. A picture of the scheme proposed above is provided in Fig. 2. In Fig. 4 we have computed the lobe at $s = 6$ using this approximation.

V. LONG RANGE HOPPING WITH A SCREENING TERM

In some contexts a more physical form of the interaction matrix is

$$J_{ij} = \frac{J a^s}{|\vec{r}_i - \vec{r}_j|^s} e^{-|\vec{r}_i - \vec{r}_j|^2/4l^2}$$ (17)

where $l$ is a characteristic length of the Wannier function which decreases when increasing the lattice depth. In this context a dimensionless control parameter

$$\eta = \frac{a}{2l}$$ (18)

can be defined: in the limit $\eta \to 0$ we recover the previous case.

If $J_{ij}$ doesn’t change abruptly from one site to his neighbors ($s \ll s_0$, $\eta \ll 1$), we can apply the continuum approximation and use integrals instead of sums. The radial part of the integration can be performed with the substitution $t = \sqrt{2}/4l^2$, introducing the same cutoffs and using the upper incomplete Euler Gamma function

$$\Gamma(s, x) = \int_{x}^{\infty} t^{s-1} e^{-t} dt.

J_0 = \frac{J\Omega_d}{2\eta^{d-s}} \left[ \Gamma \left( \frac{d-s}{2}, \eta^2 \right) - \Gamma \left( \frac{d-s}{2}, N^2 \eta^2 \right) \right]$$ (19)

FIG. 3: Amplitude of the first Mott lobe ($J_0/U$) as a function of the exponent $s$ in a two dimensional lattice with $N = 100$ at different values of $\eta$.

For a fixed value of $N$, since for $\eta \to 0$ the function $\Gamma(z, \eta^2) - \Gamma(z, N^2 \eta^2) \approx \eta^2 (N^{2z} - 1)/z$ when $z \neq 0$, while $\Gamma(0, \eta^2) - \Gamma(0, N^2 \eta^2) \approx 2 \log N$, in this limit we get Eq. (12) as expected.

The thermodynamic limit is realized taking $\eta$ small but fixed and $N \to \infty$ in Eq. (19). Considering that $\lim_{x \to \infty} \Gamma(z, x) = 0$, we conclude that in the thermodynamic limit $J_0$ is always finite and positive. The corresponding coefficient $c_2$ is

$$c_2 = \frac{2\eta^{d-s}}{J\Omega_d \Gamma \left( \frac{d-s}{2}, \eta^2 \right)} - G_{\text{loc}}(0)$$ (20)

This fact has remarkable consequences in the phase diagram of Fig. 4 because the Mott phase is now available for the system for every $s$, even in the thermodynamic limit: the exponential attenuation factor significantly screens the hopping, lowering the effective range.

VI. CONCLUSIONS

In this work we have presented the main results of the standard Bose-Hubbard theory with hopping between nearest neighbors, and then we have extended the model considering tunneling from one site to every other, with hopping energy decreasing with the distance as a power law. We have studied the extended model using two approximations: a continuum approximation (substitution of sums with integrals) for $s \ll s_0$ and a discrete approximation for $s \gg s_0$, inspired by the exact solution to the one dimensional problem. In both cases we have assumed perfect discrete translational invariance along the directions of the basis vectors by taking periodic boundary conditions. We have checked the consistency of these approximations, and we have deduced the most important result in the thermodynamic limit: when the range exponent $s$ is lower than the lattice dimension $d$ the Mott phase does not exist; instead, above this critical value...
\( s = d \) the phase transition occurs but the Mott phase is shrunk in the parameters space. However, if the system is finite, the phase transition occurs even when \( s < d \), but the Mott phase is extremely shrunk in parameters' space. Finally, we have considered a more general and physically motivated hopping energy, taking into account a screening exponential term with a control parameter \( \eta \) and applying the continuum approximation, valid for small \( s \) and small \( \eta \). The screening term weakens the long range hopping and makes the phase transition possible for every \( s \), even in the thermodynamic limit, which in this case is obtained taking \( N \to \infty \) at fixed \( \eta \). Moreover, increasing \( \eta \) leads to an expansion of the Mott phase in the parameters’ space.

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