Degenerate approach to the mean field Bose- Hubbard Hamiltonian

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A degenerate variant of mean field perturbation theory for the on-site Bose-Hubbard Hamiltonian is presented. We split the perturbation into two terms and perform exact diagonalization in the two-dimensional subspace corresponding to the degenerate states. The final relations for the second order ground state energy and first order wave function do not contain singularities at integer values of the chemical potentials. The resulting equation for the phase boundary between superfluid and Mott states coincides with the prediction based on the conventional mean field perturbation approach.

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The bosonic Hubbard model has been the subject of intense theoretical interest [1, 2]. It describes quantum phase transition between the superfluid and Mott phases of ultracold bosonic atoms in an optical lattice, first realized in experiment by Greiner et al. [3]. A qualitatively correct phase diagram of the model at zero temperature can be captured by a simple mean field theory [5, 6]. This theory predicts superfluid phase for non-integer fillings and a transition to an insulating Mott phase for integer fillings. This findings were confirmed with numerical calculations (quantum Monte Carlo simulation) [12, 14], variational approach [15] and more elaborate analytical methods, including strong-coupling perturbation theory [16], slave-boson theory [17, 18], effective action in strong-coupling limit [20], random phase approximation [21, 22], bosonic dynamical mean-field theory [24], and multisite mean-field theory [25].

In this paper, we present an alternative estimation of the zero-temperature ground state wave function \( |\psi_{gs}\rangle \) and energy \( E_{gs} \), which takes into account the degenerate character of the ground state of \( H_0 \) at integer values of the chemical potential. The resulting formulas for \( |\psi_{gs}\rangle \) and \( E_{gs} \) are free from singularities which otherwise are present at integer values of the chemical potentials in the conventional perturbative mean field approach [10].

In the framework of mean field approach the hopping term between cites \( i \) and \( j \) is decoupled as, \( b_i^\dagger b_j \approx (b_i^\dagger b_j^\dagger - b_i^\dagger b_j) \), and the Bose-Hubbard (BH) Hamiltonian is reduced to on-site Hamiltonian \( H = H_0 + H_t \),

\[
H_0 = -\mu n + \frac{U}{2} n(n-1),
\]

\[
H_t = -tv(\psi^\dagger b + \psi b^\dagger) + tv|\psi|^2,
\]

where \( U \) is a repulsive on-site boson-boson interaction, \( H_t \) is the mean field kinetic energy, \( t \) is the nearest-neighbor hopping amplitude, \( v \) is the number of nearest neighbors. The symbols \( b \) and \( b^\dagger \) denote destruction and creation operators for bosons at a lattice site, \( \psi = \langle b \rangle \) is the order parameter, \( n = b^\dagger b \) is the boson number operator. The chemical potential \( \mu \) controls the average number of bosons.

Further we shall use the dimensionless units \( \mu/U = \mu' \), \( tv/U = t' \), \( H/U = h \) and omit the primes. In these units \( h = h_0 + h_t + t|\psi|^2 \), where

\[
h_0 = -\mu n + \frac{1}{2} n(n-1), \quad h_t = -t(\psi^\dagger b + \psi b^\dagger)
\]

Eigenfunctions of \( h_0 \) are the number states \( |n\rangle \) and eigenvalues are \( \varepsilon_n = n^2/2 - (\mu +1/2), n = 0, 1, 2, \ldots \). The ground state of \( h_0 \), \( |\psi_{gs}^{(0)}\rangle = |n\rangle \), \( E_{gs}^{(0)} = \varepsilon_n \), corresponds to the number of bosons \( n \) if the chemical potential \( \mu \) is in the range \( n-1 < \mu < n \). At integer values, \( \mu = n \), the ground state is two-fold degenerate, \( \varepsilon_n = \varepsilon_{n+1}, |\psi_{gs}^{(0)}\rangle = \{ |n\rangle, |n+1\rangle \} \).

Close to the critical value of \( t \) the hopping term in the Hamiltonian (8) can be treated in perturbation theory. In the framework of non-degenerate perturbation theory corrections to the ground state wave function and energy are [10, 11]

\[
|\psi_{gs}\rangle = |\psi_{gs}^{(0)}\rangle + |\psi_{gs}^{(1)}\rangle = |n\rangle + \left[ \frac{(-t)\psi^\dagger \psi}{n-1-\mu} |n-1\rangle + \frac{(-t)\psi^\dagger \sqrt{n+1}}{\mu-n} |n+1\rangle \right],
\]

\[
E_{gs} = \varepsilon_n + t |\psi|^2 \left( 1 - t\chi_0(\mu, n) \right),
\]

\[
\chi_0(\mu, n) = \left[ \frac{n}{n-1-\mu} + \frac{n+1}{\mu-n} \right],
\]

where the value of the chemical potential is considered to be in the interval \( n-1 < \mu < n \).

The zero-temperature phase boundary between the Mott state, \( |\psi| = 0 \), and the superfluid state, \( |\psi| > 0 \), corresponds to the vanishing of the coefficient of the \( |\psi|^2 \)-term of the expansion of the energy functional \( E_{gs}(\psi) \), which gives the equation \( 1 = t\chi_0(\mu, n) \). The resulting line of critical values of \( t \) as a function of \( \mu \) is

\[
t(\mu, n) = \frac{(n-\mu)(\mu-n+1)}{1+\mu}
\]

Although expression for \( \chi_0(\mu, n) \), Eq. (6), is not defined close to the integer values of \( \mu \), the boundary equation (7) can be formally extended to include integer values \( \mu = n-1, n \).
The same boundary equation appears when one considers self-consistency equation for the order parameter, $\psi = \langle \psi_{gs} | \psi \rangle$. First order correction to the wave function enables to find the first term (linear in $\psi$) in the expansion $\langle \psi_{gs} | \psi \rangle = t \psi \chi_0 + \cdots$, where higher order terms in $\psi$ will come out if one takes into account next order corrections to the wave function. The critical boundary corresponds to the vanishing of the coefficient of the term linear in $\psi$, which amounts to $t = 0$, and we obtain the same boundary equation.

Expressions for $\langle \psi_{gs} | \psi \rangle$ and $E_{gs}$ are unsatisfactory for two reasons. First, they do not account for the degenerate character of the ground state at integer values of $\mu$. The corresponding Eqs. (4, 5) and (9) have singularities at $\mu = n - 1, n$. Second, the formal equation $\langle \psi_{gs} | \psi \rangle = \psi$, in fact, does not allow to find the value of order parameter $\psi$, it gives only the phase boundary $\psi = 0$.

The usual practice to handle the perturbation $h_t$ is numerical diagonalization of $h$ in the subspace spanned by the vectors $|n\rangle$, $n = 0, 1, \ldots, n_{\text{max}}$. This approach essentially equivalent to the formulation based on the Gutzwiller wave function $|\psi\rangle = \prod_i \sum_n f_n (|n\rangle_i$, see Refs. 2, 8, 20.

Below we show how to change the perturbation expansion to account for the degenerate case with integers values of $\mu$. This approach lets us identify the phase boundary of the insulating lobes with no divergence in resulting expressions. Though the resulting equation for the critical boundary will be the same as Eq. (7) this approach provides us information on the behavior of the order parameter in the superfluid phase.

The basic idea is to make first diagonalization of the perturbation in two dimensional subspace spanned by vectors $P^2 = \{|n\rangle, |n+1\rangle\}$. The value of $\mu$ is supposed to lie in the segment $[n, n+1]$. At integer $\mu = n$ this approach accounts for the degenerate level with $\varepsilon_n = \varepsilon_{n+1}$.

We introduce a projection operator $P$ onto the subspace $P^2$ and its orthogonal completion $P^\perp$.

$$P = |n\rangle\langle n| + |n+1\rangle\langle n+1|, \quad P^\perp = 1 - P \quad (8)$$

and rewrite the perturbation as $h_t = h_t^\perp + h_t''$, where

$$h_t^\perp = Ph_t P, \quad h_t'' = Ph_t P^\perp + P^\perp h_t P + P^\perp h_t P^\perp \quad (9)$$

The term $h_t''$ we include into $\tilde{h}_0 = h_0 + h_t'$ and the term $h_t''$ we shall treat as a new perturbation. Upon performing the exact diagonalization of $\tilde{h}_0$ in the two-dimensional subspace $P^2$ one obtains two new zero-order wave functions $|\psi_a^{(0)}\rangle$ (for lower level) and $|\psi_b^{(0)}\rangle$ (for upper level)

$$|\psi_{a,b}^{(0)}\rangle = C_1 |n\rangle + C_2 |n+1\rangle \quad (10)$$

where normalized coefficients are (the upper sign is for $|\psi_a^{(0)}\rangle$, the lower sign is for $|\psi_b^{(0)}\rangle$)

$$|C_1|^2 = \frac{1}{2} \left( 1 + \frac{\delta}{\Delta E} \right), \quad |C_2|^2 = \frac{1}{2} \left( 1 - \frac{\delta}{\Delta E} \right) \quad (11)$$

The corresponding energy levels are

$$E_a = \varepsilon_{n+1} - \frac{1}{2}(\Delta E - \delta), \quad E_b = \varepsilon_n + \frac{1}{2}(\Delta E - \delta), \quad (12)$$

with $\Delta E = \sqrt{\delta^2 + 4t^2 |\psi|^2 (n+1)}$ being splitting between the two states, and $\delta = \varepsilon_n - \varepsilon_{n+1} = \mu - n$, $0 \leq \delta < 1$ ($\mu \in [n, n+1]$). In the Mott phase $|\psi| = 0$, $\Delta E = \delta$, and $|\psi_a^{(0)}\rangle = |n+1\rangle, |\psi_b^{(0)}\rangle = |n\rangle$. At integer values of $\mu$ ($\delta = 0$) the splitting is proportional to the magnitude of the order parameter, $\Delta E = 2t |\psi| \sqrt{n+1}$. The value of $E_a$ gives the energy of the ground state of the Hamiltonian $\tilde{h}_0$.

According to the standard perturbation theory the first order correction to the ground state wave function is

$$|\psi^{(1)}_a\rangle = \sum_{k \neq n, n+1} \frac{(k|h''_a|\psi_b^{(0)})}{E_a - \varepsilon_k} |k\rangle$$

(13)

Of three terms of $h''_a$, Eq. (10), only term $P^\perp h_t P$ gives a contribution into matrix element $\langle k|h''_a|\psi_a^{(0)}\rangle$. As a result the perturbed wave function is

$$|\psi_a\rangle = |\psi_a^{(0)}\rangle + |\psi_a^{(1)}\rangle = C_1 |n\rangle + C_2 |n+1\rangle + C_3 \frac{(-t)\psi \sqrt{n+1}}{E_a - \varepsilon_{n+1}} |n+1\rangle + C_4 \frac{(t)\psi \sqrt{n+1}}{E_a - \varepsilon_{n+1}} |n\rangle \quad (14)$$

Comparing Eqs. (4) and (14) one can clearly see the advantage of this approach, namely the coefficients of the decomposition of $|\psi_a\rangle$ have regular behavior as functions of $\mu$.

Self-consistency equation for the order parameter, $\psi = \langle \psi_a | \psi \rangle$, can be reduced to

$$\psi = t \psi \frac{1}{\Delta E} \left[ (n+1) + n \frac{\Delta E - \delta}{2 + 3\delta + \Delta E} + (n+2) \frac{\Delta E + \delta}{2 - 3\delta + \Delta E} \right] \quad (15)$$

Close to the critical boundary, $|\psi|^2 \simeq 0$, Eq. (15) can be rewritten as an expansion in terms of $\psi$

$$\psi = \psi_0 \left[ \chi_0 (\mu, n+1) + a_2 |\psi|^2 + a_4 |\psi|^4 + \cdots \right] \quad (16)$$

Here the coefficients $a_i$ arise due to a formation of the ground state $|\psi_a^{(0)}\rangle$. In principle, one needs to account higher order corrections to the wave function $|\psi^{(0)}_a\rangle$ to find the proper coefficients $a_i$, but the qualitative behavior of $\psi$ near the critical boundary remains the same. Eq. (15) gives the same critical boundary, $t(\mu, n+1)$, as predicted by the standard perturbation approach, Eq. (7).

The resulting Eq. (15) enables not only to identify the critical boundary but also gives the information about the behavior of order parameter in the superfluid phase.
Namely, one can recover the dependence of the order parameter on parameters \((\mu, t)\), \(|\psi|^2 = f(\mu, t)\). This dependence is shown in Fig. 1. Mott insulating lobes (thick lines) coincide with the prediction of standard perturbation approach, Eq. (7). Thin lines outside the insulating lobes correspond to a few contours of \(|\psi| = \text{const}\) inside the superfluid phase. The contour plot is discontinuous at points corresponding to the integer values of \(\mu\). This can be expected from our restriction of the Hamiltonian \(h_n\) to the two-dimensional subspace \(P_n^2\). By going from \(P_n^2\) to another \(P_{n+1}^2\) matrix elements of the restricted perturbation \(h'_n\) jump to new values. This artificial feature can be circumvented if to use the bigger vector space of number states \(|n\rangle\), \(n = 0, 1, \cdots, n_{\text{max}}\). Then it will be equivalent to the approach of Refs. [8, 26].

Another way to obtain the position of the phase boundary on the plane \((\mu, t)\) is to consider a correction to the ground state energy. It is a sum of three terms, \(\Delta E_{gs} = t|\psi|^2 + (E_a - \varepsilon_{n+1}) + \Delta E_{gs}^{(2)},\) originating from: (i) the mean-field treatment of the hopping term, (ii) a correction due to the formation of the state \(|\psi^{(0)}\rangle\), \(E_a - \varepsilon_{n+1} \simeq -t^2|\psi|^2(n+1)/\delta\), and (iii) the second order correction due to the perturbation \(h'_n\),

\[
\Delta E_{gs}^{(2)} = t^2|\psi|^2 \left[ \frac{|C_1|^2 n}{E_a - \varepsilon_{n-1}} + \frac{|C_2|^2(n + 2)}{E_a - \varepsilon_{n+2}} \right] = \\
\quad = -t^2|\psi|^2 \left[ \frac{(\Delta E - \delta)n}{2 + 3\delta + \Delta E} + \frac{(\Delta E + \delta)(n + 2)}{2 - 3\delta + \Delta E} \right] 
\]

(17)

Gathering all three terms one obtains that the correction to the ground state energy is \(\Delta E_{gs} = t|\psi|^2(1 - \chi_a),\) where

\[
\chi_a = \frac{n + 1}{\delta} + \frac{1}{\Delta E} \left[ \frac{(\Delta E - \delta)n}{2 + 3\delta + \Delta E} + \frac{(\Delta E + \delta)(n + 2)}{2 - 3\delta + \Delta E} \right] 
\]

(18)

At the phase boundary, \(\Delta E = \delta\), \(\chi_a = \chi(\mu, n + 1)\) and one recovers the resulting equation for the boundary, which is equivalent to Eq. (7).

In summary, we presented an alternative way to estimate perturbation corrections to the ground state wave function of the mean field BH Hamiltonian [4]. This approach has an advantage that the corrections to \(|\psi_{gs}\rangle\) and \(E_{gs}\) do not have singularities at integer values of the chemical potential. The main improvement over previous related approaches is also the possibility to describe the \(|\psi\rangle\) in the superfluid phase. However, the restriction of the perturbation onto the two-dimensional subspace \(P_n^2\) introduces the discontinuity in the behavior of order parameter \(|\psi\rangle\) at integer values of \(\mu\) in the superfluid phase.

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