Self-consistent Single-band Approximation for Interacting Boson Systems

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Interacting many-body systems are notoriously hard to solve. One usual tactic is the single-band approximation, where the Wannier functions [1] for the lowest Bloch band are used to reduce the system to a lattice model, such as Hubbard model [2,3]. Traditionally, the Wannier functions used in the approximation are obtained either directly from the single-particle Bloch waves or with some variational approaches [4,5]. The interaction effect on the Wannier function is completely neglected in all these traditional methods. This neglect is at odds with the fact that the interaction evidently affects the shape of the Wannier functions.

Current strong interest in ultracold atoms in optical lattices has put this problem into spotlight [6]. A recent experiment with ultracold atoms clearly demonstrated that the on-site interaction, therefore, the Wannier functions, depends on the occupation number [7]. It has also been seen increased theoretical efforts to address this problem [8,9,10,11,12,13]. However, all the efforts have certain drawbacks from a general perspective. In the variational framework for transforming a periodic system into a lattice model self-consistently and can be generalized to systems where multiple bands are needed.

One can reformulate the nonlinear equation for Wannier functions in terms of Bloch functions, and obtain a set of nonlinear equations for Bloch functions. Simplified forms for these nonlinear equations are obtained for two special cases, the superfluid regime and deep in the Mott insulator regime. Our results are illustrated with a system of double-well potential, where some general properties of the nearest neighbor tunneling parameter $J$ and the on-site interaction $U$ are revealed.

Although our approach can be applied to other systems, e.g., fermionic systems, we here focus on the system of ultracold bosons in optical lattices [14,15]. For bosons of mass $m$, the Hamiltonian is

$$\hat{H} = \int dr \hat{\psi}^\dagger(r) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \hat{\psi}(r) + \frac{1}{2} \int dr dr' \left[ \hat{\psi}^\dagger(r) \hat{\psi}^\dagger(r') U(|r-r'|) \hat{\psi}(r) \hat{\psi}(r') \right], \quad (1)$$

where $v(r)$ is a periodic potential and $u(|r|)$ is the interaction between two atoms. If one is interested only in the low temperature properties of the system, one can use the single-band approximation and expand the bosonic field operator as

$$\hat{\psi}(r) = \sum_j \hat{a}_j W_j(r), \quad (2)$$

where $W_j(r) = W(r-r_j)$ is the Wannier function at site $j$ and $\hat{a}_j$ is the associated annihilation operator. In this case, the trial ground state $|G_\text{vacc}\rangle$ is given by $|G_\text{vacc}\rangle = F(\hat{a}_j^\dagger) |\text{vaccum}\rangle$, where the functional $F$ is to be determined. Usually, the Wannier function in Eq. (2) is pre-determined. Here the Wannier function is not known a priori except that it is expected to resemble the single-particle Wannier function. We look for the Wannier functions that minimize the system’s single-band ground

$$\min \langle G_\text{vacc}| G \right| G_\text{vacc}\rangle \left. \hat{F(^\dagger)} \right| G \right| G_\text{vacc}\rangle - \int \left. \hat{F} \right| G \right| G_\text{vacc}\rangle V(r) \left. \hat{F} \right| G \right| G_\text{vacc}\rangle dr \quad (3)$$

We address the interaction effect on Wannier function by re-examining the single-band approximation. We find that the interaction effect can be taken into account automatically once the single-band approximation is done self-consistently. The self-consistent single-band approximation is achieved by minimizing the ground state energy of the system by varying Wannier function. The minimization leads to a nonlinear equation for the Wannier function, which depends on the ground state of the system. Therefore, one has to solve the nonlinear equation self-consistently with the ground state of the resulted lattice model to find the interaction-dependent Wannier functions. Our results provide a general variational framework for transforming a periodic system into a lattice model self-consistently and can be generalized to systems where multiple bands are needed.
The parameters are given by
\[ H_{bh} = -\sum_{j_1,j_2} J_{j_1,j_2} \hat{a}_{j_1}^\dagger \hat{a}_{j_2} + \sum_{j_1,j_2} U_{j_1,j_2,j_3,j_4} \hat{a}_{j_1}^\dagger \hat{a}_{j_2}^\dagger \hat{a}_{j_3} \hat{a}_{j_4}. \]  

The parameters are given by
\[ J_{j_1,j_2} = -\int \mathcal{d}r W_j^*(r) H_0 W_{j_2}(r), \]
\[ U_{j_1,j_2,j_3,j_4} = \frac{1}{2} \int \mathcal{d}r \mathcal{d}r' \left[ W_j^*(r) W_{j_2}^*(r') \times U(|r - r'|) W_{j_2}(r) W_{j_4}(r') \right], \]

where \( H_0 = -\frac{\hbar^2}{2m} \nabla^2 + V(r). \) Usually further approximation is made so that only two terms, the nearest neighbor tunneling and the on-site interaction, are kept in the Bose-Hubbard model. For the purpose of deriving general formalism, this approximation is not needed so far.

We achieve the minimization of the ground state energy \( E_G \) by varying the Wannier function under the orthonormal constraints \( h_j = \int \mathcal{d}r W_j^*(r) W_j(r) = \delta_{0,j}. \) According to the Feynman-Hellman theorem, we have
\[
\delta (E_G - \sum_j \mu_j h_j) = \langle G_t | \frac{\delta H_{bh}}{\delta W_j^*(r)} G_t \rangle - \sum_j \frac{\mu_j h_j}{\delta W_j^*(r)} = 0,
\]

where \( \mu_j \) are Lagrangian multipliers. We obtain a nonlinear equation for the Wannier functions
\[
\sum_j \mu_j W(r - r_j) = \sum_{j_1,j_2} \langle \hat{a}_{j_1}^\dagger \hat{a}_{j_2} \rangle H_0 W(r + r_{j_1} - r_{j_2}) + \sum_{j_1,j_2} \langle \hat{a}_{j_1}^\dagger \hat{a}_{j_2} \hat{a}_{j_3} \hat{a}_{j_4} \rangle \int \mathcal{d}r' \left[ \frac{W^*(r') + W_{j_2}^*(r_2 - r_{j_1})}{W(r + r_{j_2} - r_{j_4})} \right] W(r + r_{j_2} - r_{j_4}).
\]

It is clear that the above equation depends on the ground state \( |G_t \rangle \) of the Bose-Hubbard model in Eq. (1), which can be found with many-body methods such as direct diagonalization, Gutzwiller projection, density matrix renormalization group (DMRG), or time-evolving block decimation (TEBD). At the same time, we need the Wannier functions to compute \( J \)'s and \( U \)'s for the Bose-Hubbard model. Therefore, the Bose-Hubbard model in Eq. (11) has to be solved self-consistently with the above nonlinear equation. We call this self-consistent single-band approximation. Due to the complexity of the equations, one can apply further approximations. For example, one can opt to completely ignore the interaction while solving Eq. (8). This is just what people have traditionally done with the single-band approximation. One can also choose to keep only the nearest neighbor tunneling \( J \) and the on-site interaction \( U \) in the Bose-Hubbard Hamiltonian (1). However, the off-site terms in the last summation in Eq. (8) can not be dropped simultaneously.

A periodic system can be described alternatively with Bloch functions. If we place the system in a box of \( N \) lattice sites, the Wannier functions are related to Bloch functions as
\[
W(r - r_n) = \frac{1}{\sqrt{N}} \sum_k \psi_k(r) e^{-i k \cdot r_n} \Psi_k(r),
\]

where \( \psi_k \) is a Bloch function with Bloch wave number \( k \) and is normalized to one. For Bloch functions, the nonlinear equation (8) becomes
\[
\sum \nu_k \psi_k(r) = \sum_k \langle \hat{b}_k^\dagger \hat{b}_k \rangle H_0 \psi_k + \sum_{k \neq k_1} \langle \hat{b}_k^\dagger \hat{b}_k \hat{b}_k^\dagger \hat{b}_k \rangle 
\times \int \mathcal{d}r' \left[ \psi_k(r') \psi_k(r') U(|r' - r|) \right] \psi_k(r),
\]

where \( \nu_k = \frac{1}{N} \sum \mu_n \psi_n e^{-i k \cdot r_n} \), and \( \mu_n \) is a reciprocal lattice. While we can not split Eq. (8) into a set of equations for Wannier functions at different sites, we are allowed to split the above equation for different Bloch wave numbers \( k \) and obtain
\[
\tilde{\nu}_n \psi_n(r) = H_0 \psi_n(r) + \sum_{k \neq k_1} P_{k,k_1,k_1,k_4} \int \mathcal{d}r' \left[ \psi_k(r') \times U(|r' - r|) \right] \psi_k(r),
\]

where \( P_{k,k_1,k_1,k_4} = \langle \hat{b}_k^\dagger \hat{b}_k^\dagger \hat{b}_k^\dagger \hat{b}_k \rangle \tilde{\nu}_k = \nu_k / \langle \hat{b}_k^\dagger \hat{b}_k \rangle. \) In the following discussion, for simplicity, we shall use dilute atomic gases, where \( u(|r|) = g_0 \delta(r), \) to discuss two special cases.

We consider first the superfluid regime. With the Bogoliubov mean-field theory, we have
\[
\hat{H}_{bh} = \epsilon_0 N_0 + U_0 N_0^2 + \sum_{k \neq 0} \left[ \epsilon_k + 4 N_0 U_0 k \right] \hat{b}_k^\dagger \hat{b}_k 
\times \sum_{k \neq 0} N_0 U_k \left( \hat{b}_k^\dagger \hat{b}_k + \hat{b}_k^\dagger \hat{b}_k \right),
\]

where \( N_0 \) is the number of atoms in the state \( \psi_0, \) \( \epsilon_k = \int \mathcal{d}r \psi_k^* H_0 \psi_k, \) and \( U_k = (g_0/2) \int \mathcal{d}r |\psi_k|^2 |\psi_0|^2. \) Following
the standard procedure\cite{19}, we find that
\begin{equation}
\hat{P}_{k_i,k_k,k_3} = v_k^2 \delta_{k_i,k_k,k_3} + \delta_{k_i,k_k,k_3} \delta_{k_3,k_4,k_5} + \delta_{k_k,k_3,k_4} - 2 \delta_{k_i,0} \delta_{k_3,0} N_0, \tag{13}
\end{equation}
where \( u_0 = v_0 = \sqrt{N_0} \), \( v_k^2 \neq 0 \) is \( [(\epsilon_k + 4N_0 U_{jk})/\delta_k - 1]/2 \), and \( v_k^2 = 1 + v_k^2 \neq 0 \). \( \epsilon_k = \sqrt{(\epsilon_k + 4N_0 U_{jk})^2 - 4N_0 U_{jk}^2} \). This leads to a set of simplified nonlinear equations for Bloch functions
\begin{equation}
\tilde{\chi}_0 \Psi_0 = H_0 \Psi_0 + g_0 N_0 |\Psi_0|^2 \Psi_0 + g_0 \sum_{k \neq 0} v_k^2 |\Psi_k|^2 \Psi_0, \tag{14}
\end{equation}
and for \( k \neq 0 \)
\begin{equation}
\tilde{\chi}_k \Psi_k = H_0 \Psi_k + 2g_0 N_0 |\Psi_0|^2 \Psi_k + g_0 \sum_{k' \neq 0} \left[ u_{kk'} \chi_{kk'} + 2 v_{kk'} \right] |\Psi_k|^2 \Psi_k. \tag{15}
\end{equation}
Since \( u_k \) and \( v_k \) themselves depend on \( \psi_k \), the above two equations have to be solved self-consistently. Note that in the above derivation we have assumed that the lattice potential is symmetric, \( V(r) = V(-r) \), so that \( \tilde{\chi}_k = \psi_k^* \). We have also ignored the scattering processes with non-zero \( \mathbf{K} \).

In contrast to the superfluid regime, deep in the Mott-insulator regime, we have
\begin{align}
\langle \hat{a}^\dagger_{j_1} \hat{a}_{j_2} \rangle &= n_0 \delta_{j_1,j_2}, \tag{16} \\
\langle \hat{a}^\dagger_{j_1} \hat{a}^\dagger_{j_2} \hat{a}_{j_3} \hat{a}_{j_4} \rangle &= n_0^2 \delta_{j_1,j_2} \delta_{j_3,j_4} + n_0^2 \delta_{j_1,j_3} \delta_{j_2,j_4} + n_0^2 \delta_{j_1,j_4} \delta_{j_2,j_3} \\
&\quad - (n_0^2 + n_0^2) \delta_{j_1,j_2} \delta_{j_3,j_4}. \tag{17}
\end{align}
where \( n_0 \) is the averaged number of bosons per site. In this case, Eq.(3) is simplified and has the form
\begin{equation}
\frac{\hbar \omega}{N_0} W(r) = H_0 W(r) + g_0 n_0 \sum_{r_j \neq 0} |W(r - r_j)|^2 W(r) + g_0 (n_0 - 1) |W(r)|^2 W(r). \tag{18}
\end{equation}
The off-site terms on the right hand side is usually very small and can be ignored. With this in mind, we immediately have one observations. With one atom per site, i.e., \( n_0 = 1 \), the Wannier function is approximated by the single-particle ground state wave function of each individual well of the lattice; there is no interaction effect on the Wannier function.

We now use one dimensional double-well potential with periodic boundary condition to illustrate our theory. The two Wannier functions for the left well and the right well are related to the ground state and the first excited state for the double-well potential as follows
\begin{equation}
W_l = \frac{\sqrt{2}}{2} (\Psi_0 + \Psi_1), \quad W_r = \frac{\sqrt{2}}{2} (\Psi_0 - \Psi_1), \tag{19}
\end{equation}
where \( \Psi_0 \) and \( \Psi_1 \) are chosen so that they are both positive in the left well. These two Wannier functions satisfy the nonlinear equation\textsuperscript{[5]}. The corresponding Bose-Hubbard model is
\begin{equation}
\hat{H}_2 = \left[ - J + 2(N_0 - 1)U_0 \left( \hat{a}^\dagger \hat{a}^\dagger \hat{a}^\dagger \hat{a} \right) + U_2 (\hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a}^\dagger \hat{a}^\dagger \hat{a}^\dagger \hat{a}) + \right]
+ U_3 (\hat{a}^\dagger \hat{a}^\dagger \hat{a}^\dagger \hat{a}^\dagger \hat{a}^\dagger \hat{a}^\dagger \hat{a}) + \left(2 \frac{\hbar^2 k_L^2}{m} \right), \tag{20}
\end{equation}
where \( U_2 = U_{lrr}, U_3 = U_{lrr'}, U_3 = U_{lrr}, U_3 = U_{llr} \). We choose the double-well potential as a part of the on dimensional optical lattice created experimentally in Ref.\textsuperscript{[20]}. So, the double well potential is given by \( V(x) = V_0 \sin^2 (k_L x) \), where \( k_L \) is the wave number of the laser that creates the potential. Due to the lateral confinement, the interaction strength \( g_0 \) is given by \( g_0 = (4\pi \hbar^2 a_s/m)(\omega_{\perp}/(2\hbar)) = 2\hbar \omega_{\perp} a_s \), where \( a_s \) is the s-wave scattering length and \( \omega_{\perp} \) the perpendicular confinement frequency. We consider the case of \( n_0 = 1(N_0 = 2) \). In our numerical calculations, the Hamiltonian in Eq.(20) is diagonalized directly and Eq.(5) is solved with the nonlinear equation solver in MATLAB. And we use \( c = \pi mg_0/(\hbar^2 k_L^2) \) as the dimensionless interaction parameter.

The Wannier functions found numerically are plotted in Fig.\textsuperscript{1} As expected, the Wannier function becomes more and more localized as the depth of the well increases. It is worthwhile to note that the Wannier functions for shallow wells (e.g., \( v = 3.0 \)) have nodes, which shows that nodeless ground state does not necessarily imply a nodeless Wannier function.

The numerical results for the dependence of \( J \) and \( U \) on the well depth and interaction strength are shown in terms of the ratios \( J/J_0 \) and \( U/U_0 \) in Fig.\textsuperscript{2}. \( J_0 \) and \( U_0 \) are the tunneling parameter and on-site interaction obtained with single-particle Wannier function. Certain interesting behaviors of \( J/J_0 \) and \( U/U_0 \) are revealed. For a fixed interaction strength, both \( J/J_0 \) and \( U/U_0 \) approach
one as the lattice gets stronger. If the lattice strength is fixed and the interaction strength changes, $J/J_0$ and $U/U_0$ reach their respective extremum values at a critical interaction strength.

We argue that the behaviors of $J/J_0$ and $U/U_0$ revealed in Fig. 2 is not limited to the double-well systems, and should hold generally for ultracold bosons in optical lattices. As already discussed, deep in the Mott insulator regime, the solution of Eq. (13) is single-particle Wannier function for $n_0 = 1$. This implies that both of the ratios $J/J_0$ and $U/U_0$ should approach one as the optical lattice gets stronger with fixed interaction strength. This is exactly what is seen in Fig. 2 (a,c). If one fixes the lattice strength and increases the repulsive interaction, then one has single-particle Wannier function at both the beginning ($c = 0$) and the end ($c \gg 1$) of this change. This indicates that $J/J_0$ should reach its maximum point and $U/U_0$ arrive at its minimum point during this process as shown in Fig. 2 (b,d). If one simulates the superfluid-Mott insulator transition with the self-consistent single band approximation proposed here, the behaviors of $J/J_0$ and $U/U_0$ in Fig. 2 (b,d) can be used to determine the transition point between superfluid and Mott insulator.

Note that the interaction effect on $J$ and $U$ is much smaller compared to the mean-field results in Ref. [14]. This is likely due to the finite size of our example system, where the Wannier function is confined and can not extend to infinity. More extensive numerical studies are needed to clarify this. If future numerical computation indeed indicates that the interaction effect on $J$ and $U$ is as large as indicated in the mean-field results [10], then the behaviors of $U/U_0$ in Fig. 2 (c,d) may be used as an experimental means to detect the superfluid-Mott insulator transition as $U$ can now be measured experimentally [1] and the interaction can be adjusted with the Feshbach resonance [21].

Currently in typical experiments, ultracold atoms are also trapped by a harmonic potential [14, 15]. Consequently, the wells are not identical to each other. Also a random potential can be added to make the wells non-identical. Nevertheless, single-band approximation can still be applied as long as the difference between the site energies is smaller than the energy gaps between the ground state and the first excited state in the wells. For simplicity, we consider a one dimensional potential of $N$ wells, which are not identical. In this case, the Wannier functions for the lowest “band” can be defined as

$$W_j(x) = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} \epsilon^{\frac{2\pi i j}{N}} \psi_k , \quad j = 0, 1, \cdots, N-1 , \quad (21)$$

where $\psi_k$’s are the lowest $N$ eigenstates. Our variational approach can be easily adopted to this case with just one modification. Since the Wannier functions at different sites have different shapes, the constraint is now $h_{n,m} = \int dx W_n^*(x) W_m(x) = \delta_{n,m}$. As a result, one obtains a set of nonlinear equations for the Wannier functions. Since everything is straightforward, we shall not write out the equations here.

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