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Self-Consistent Approach for Mapping Interacting Systems in Continuous Space to Lattice Models *

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We propose a general variational principle for mapping the interacting systems in continuous space to lattice models. Based on the principle, we derive a set of self-consistent nonlinear equations for the Wannier functions (or, equivalently for the Bloch functions). These equations show that the Wannier functions can be strongly influenced by the interaction and be significantly different from their non-interacting counterparts. The approach is demonstrated with interacting bosons in an optical lattice, and illustrated quantitatively by a simple model of interacting bosons in a double well potential. It is shown that the so-determined lattice model parameters can be significantly different from their non-interacting values.

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Although the real condensed matter systems always live in the continuous space, it is not uncommon to use lattice models to describe them, for example, many systems can be well described by the Hubbard model.[1,2] Traditionally, the lattice model is often intuitively motivated, and the choice of Wannier functions[3] used in the mapping from the continuous space to the lattice is casual. This lack of rigor in choosing Wannier functions was noticed by Kohn and he proposed a variational approach to pick the "best" Wannier function. However, his approach relies on the choice of the trial localization function and the resultant Wannier functions can not be regarded as the best even in principle.[4]

This issue is becoming more urgent with the developments in ultra-cold atom systems. For the ultracold atom systems, the experiments have reached the high precision to clearly demonstrate the variation of effective lattice model parameters, such as the strength of the on-site repulsion with the number of atoms per site.[5,6] In the traditional electron systems, there have also been efforts to combine the first-principles density functional calculations with the strong-correlation techniques, and the latter is usually based on the lattice models.[7] These developments are calling for the more rigorous theoretical basis for properly mapping an interacting system from the continuous space to the lattice space. This issue has been the focus of many theoretical efforts.[7–15] However, the theory is still unsatisfactory because there exists no generally accepted criteria for what the best set of Wannier functions is.

In this Letter we propose a general variational principle for mapping an interacting system in continuous space to a lattice model: the choice of an incomplete set of Wannier functions minimizes the calculated ground state energy of the lattice model. Based on the principle, we derive a set of self-consistent nonlinear equations for the Wannier functions (or, equivalently, the corresponding Bloch functions), with the coefficients of the equations expressed in the correlation functions of the lattice model. As a result, these nonlinear equations have to be solved self-consistently with the lattice model. Even though the approach is general, we demonstrate it with interacting boson in an optical lattice, and eventually illustrated it quantitatively using a simple model of interacting bosons in a double well potential. It is shown that so-determined lattice model parameters can be significantly different from their non-interacting values.

To illustrate our approach, we consider the mapping of an interacting bosonic cold-atom system in the presence of the periodic potential to a single-band lattice model. The extensions to the fermionic systems and/or the multi-band lattice models are straightforward. The Hamiltonian in the continuous space can in general be written as

$$\hat{H} = \int d\boldsymbol{r}\, \hat{\psi}^{\dagger}(\boldsymbol{r})\Big[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\Big]\hat{\psi}(\boldsymbol{r}) + \frac{1}{2}\int d\boldsymbol{r}d\boldsymbol{r}'\Big[\hat{\psi}^{\dagger}(\boldsymbol{r})\hat{\psi}^{\dagger}(\boldsymbol{r}')U(|\boldsymbol{r}-\boldsymbol{r}'|)\hat{\psi}(\boldsymbol{r}')\hat{\psi}(\boldsymbol{r})\Big], \tag{1}$$

where m is the mass of the atom, $V(\boldsymbol{r})$ is a periodic potential and $U(|\boldsymbol{r}|)$ is the interaction between two atoms. Under the single-band approximation, the bosonic field operator $\psi(\boldsymbol{r})$ can be expanded as

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

where $W_j(\boldsymbol{r}) = W(\boldsymbol{r}-\boldsymbol{r}_j)$ is the Wannier function at site j and $\hat{a}_j$ is the associated annihilation operator.

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The corresponding single-band lattice model reads

$$\hat{H}_{sb} = -\sum_{j_1 j_2} J_{j_1 j_2} \hat{a}^\dagger_{j_1} \hat{a}_{j_2} + \sum_{j_1 j_2}^{j_3 j_4} U_{j_1 j_4 j_2 j_3} \hat{a}^\dagger_{j_1} \hat{a}^\dagger_{j_2} \hat{a}_{j_3} \hat{a}_{j_4}. \tag{3}$$

The parameters are given by

$$J_{j_1 j_2} = -\int d\boldsymbol{r} W^*_{j_1}(\boldsymbol{r}) H_0 W_{j_2}(\boldsymbol{r}), \tag{4}$$

$$U_{j_1 j_4 j_2 j_3} = \frac{1}{2} \int d\boldsymbol{r} d\boldsymbol{r}' \Big[W^*_{j_1}(\boldsymbol{r}) W_{j_4}(\boldsymbol{r}) \times U(|\boldsymbol{r} - \boldsymbol{r}'|) W^*_{j_2}(\boldsymbol{r}') W_{j_3}(\boldsymbol{r}') \Big], \tag{5}$$

where $H_0 \equiv -\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})$.

Further approximations for $\hat{H}_{sb}$ are often needed. For instance, to obtain the well-known Bose-Hubbard model, one keeps only two terms, the nearest neighbor tunneling and the on-site interaction. Various exact or approximated many-body techniques, such as direct diagonalization, Gutzwiller projection,[16] density matrix renormalization group (DMRG),[17] time-evolving block decimation (TEBD),[18] or quantum Monte Carlo,[19] can be employed to solve the resulting simple lattice model. It is important to observe that the solution, no matter what approximations are employed to get it, can be considered as a trial wave-function of a functional of the Wannier functions.

The ground state $|G_t\rangle$ in the single-band approximation can be formally written as $|G_t\rangle = F(\hat{a}^\dagger_j)|\text{vaccum}\rangle$, where F is a certain function. The Wannier function in Eq. (2) is usually pre-determined. Here the Wannier function is not known *a priori*. We look for the Wannier functions that minimize the system's single-band ground state energy,

$$E_G = \langle G_t|\hat{H}|G_t\rangle = \langle G_t|\hat{H}_{sb}|G_t\rangle, \tag{6}$$

where $\hat{H}_{sb}$ is the usual single-band lattice Hamiltonian

We achieve the minimization of the ground state energy E_G by varying the Wannier function under the orthonormal constraints, $h_j = \int d\boldsymbol{r} W^*(\boldsymbol{r}) W(\boldsymbol{r} - \boldsymbol{r}_j) = \delta_{0,j}$. According to the Feynman–Hellman theorem, we have

$$\frac{\delta(E_G - \sum_j \mu_j h_j)}{\delta W^*(\boldsymbol{r})} = \langle G_t| \frac{\delta \hat{H}_{sb}}{\delta W^*(\boldsymbol{r})} |G_t\rangle - \sum_j \frac{\mu_j \delta h_j}{\delta W^*(\boldsymbol{r})} = 0, \tag{7}$$

where μ's are Lagrangian multipliers. After straightforward computation, we obtain a nonlinear equation for the Wannier functions

$$\sum_j \mu_j W(\boldsymbol{r} - \boldsymbol{r}_j) = \sum_{j_1, j_2} \langle \hat{a}^\dagger_{j_1} \hat{a}_{j_2} \rangle H_0 W(\boldsymbol{r} + \boldsymbol{r}_{j_1} - \boldsymbol{r}_{j_2}) + \sum_{j_1 j_2}^{j_3 j_4} \langle \hat{a}^\dagger_{j_1} \hat{a}^\dagger_{j_2} \hat{a}_{j_3} \hat{a}_{j_4} \rangle \int d\boldsymbol{r}' \Big[W^*(\boldsymbol{r}' + \boldsymbol{r}_{j_2} - \boldsymbol{r}_{j_1}) \times W(\boldsymbol{r}' + \boldsymbol{r}_{j_2} - \boldsymbol{r}_{j_4}) U(|\boldsymbol{r}' - \boldsymbol{r}|) \Big] W(\boldsymbol{r} + \boldsymbol{r}_{j_2} - \boldsymbol{r}_{j_3}). \tag{8}$$

It is clear that the above equation depends on the solution of the single-band lattice model (3). Before solving Eq. (3), one can employ various approximations, for example, by choosing to keep only the nearest neighbor tunneling J and the on-site interaction U in the single-band Hamiltonian (3). Various many-body techniques[16–19] can be employed to solve the resulting simple lattice model. The solution, no matter what approximations are employed to get it, is still a valid trial wave-function of a functional of the Wannier functions. To implement the variational principle Eq. (6), it is essential to keep all terms in Eq. (8), even when the corresponding terms in Eq. (3) (e.g., off-site interaction) had been ignored in solving the lattice model. For instance, if the interaction terms are ignored when solving Eq. (3), Eq. (8) becomes the usual Hartree–Fock approximation. It is important to note that Wannier functions obtained in this way not only depend on the approximations applied to Eq. (3), but also depend on the many-body technique employed to solve the resulting lattice model. We call such an approach a self-consistent single-band approximation.

As an example, we consider the case of a deep Mott-insulator regime, where the ground state has the form $|n_0, n_0, \ldots, n_0\rangle$ with n_0 being the average number of particles per site. In this case, we have

$$\langle \hat{a}^\dagger_{j_1} \hat{a}_{j_2} \rangle = n_0 \delta_{j_1, j_2}, \tag{9}$$

$$\langle \hat{a}^\dagger_{j_1} \hat{a}^\dagger_{j_2} \hat{a}_{j_3} \hat{a}_{j_4} \rangle = n_0^2 \delta_{j_1, j_3} \delta_{j_2, j_4} + n_0^2 \delta_{j_1, j_4} \delta_{j_2, j_3} - (n_0^2 + n_0) \delta_{j_1, j_2} \delta_{j_2, j_3} \delta_{j_3, j_4}. \tag{10}$$

As a result, Eq. (8) is simplified and has the form for $U(|\boldsymbol{r}|) = g_0 \delta(\boldsymbol{r})$,

$$\frac{\mu_0}{N_0} W(\boldsymbol{r}) = H_0 W(\boldsymbol{r}) + g_0 n_0 \sum_{\boldsymbol{r}_j \neq 0} |W(\boldsymbol{r} - \boldsymbol{r}_j)|^2 W(\boldsymbol{r}) + g_0 (n_0 - 1) |W(\boldsymbol{r})|^2 W(\boldsymbol{r}). \tag{11}$$

When the off-site terms, which are often very small, are ignored, the above equation has the form of the familiar Gross–Pitaevskii equation.[20,21] Therefore, it is very clear that the Wannier function is greatly influenced by the interaction whenever $n_0 \geq 2$.

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

$$W(\boldsymbol{r} - \boldsymbol{r}_n) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_n} \Psi_{\boldsymbol{k}}(\boldsymbol{r}), \tag{12}$$

where $\Psi_{\boldsymbol{k}}$ is a Bloch function with Bloch wave number $\boldsymbol{k}$ and is normalized to one. In terms of Bloch

functions, the nonlinear equation (8) becomes a set of nonlinear equations

$$\tilde{\nu}_{\boldsymbol{k}}\,\Psi_{\boldsymbol{k}}(\boldsymbol{r}) = H_0\,\Psi_{\boldsymbol{k}}(\boldsymbol{r}) + \sum_{\langle \boldsymbol{k}_1\boldsymbol{k}\boldsymbol{k}_3\boldsymbol{k}_4\rangle} P_{\boldsymbol{k}_1\boldsymbol{k}\boldsymbol{k}_3\boldsymbol{k}_4} \int d\boldsymbol{r}' \cdot \Big[\Psi^*_{\boldsymbol{k}_1}(\boldsymbol{r}')\,\Psi_{\boldsymbol{k}_3}(\boldsymbol{r}')U(|\boldsymbol{r}'-\boldsymbol{r}|)\Big]\Psi_{\boldsymbol{k}_4}(\boldsymbol{r}), \tag{13}$$

where $\langle \boldsymbol{k}_1\boldsymbol{k}\boldsymbol{k}_3\boldsymbol{k}_4\rangle$ stands for summation with the constraint $\boldsymbol{k}_1+\boldsymbol{k} = \boldsymbol{k}_3+\boldsymbol{k}_4+\boldsymbol{K}$, and $P_{\boldsymbol{k}_1\boldsymbol{k}\boldsymbol{k}_3\boldsymbol{k}_4} = \langle \hat{b}^\dagger_{\boldsymbol{k}_1}\hat{b}^\dagger_{\boldsymbol{k}}\hat{b}_{\boldsymbol{k}_3}\hat{b}_{\boldsymbol{k}_4}\rangle/\langle \hat{b}^\dagger_{\boldsymbol{k}}\hat{b}_{\boldsymbol{k}}\rangle$; $\hat{b}_{\boldsymbol{k}} = \frac{1}{\sqrt{N}}\sum_n \hat{a}_n e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_n}$, and $\tilde{\nu}_{\boldsymbol{k}} = (\frac{1}{N}\sum_n \mu_n e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_n})/\langle \hat{b}^\dagger_{\boldsymbol{k}}\hat{b}_{\boldsymbol{k}}\rangle$. $\boldsymbol{K}$ is a reciprocal lattice. In deriving Eq. (13), we have used the fact that the Bloch functions of different wave numbers $\boldsymbol{k}$ are orthogonal to each other automatically and, therefore, one can have an equation for each different Bloch wave number $\boldsymbol{k}$.

We now apply Eq. (13) in the superfluid regime, where the Bogoliubov mean-field theory can be applied.[22] For the simple interaction, $U(|\boldsymbol{r}|) = g_0\delta(\boldsymbol{r})$, the mean-field Hamiltonian is

$$\hat{H}_{bh} = \epsilon_0\mathcal{N}_0 + U_0\mathcal{N}_0^2 + \sum_{\boldsymbol{k}\neq 0}\Big[\epsilon_{\boldsymbol{k}} + 4\mathcal{N}_0U_{\boldsymbol{k}}\Big]\hat{b}^\dagger_{\boldsymbol{k}}\hat{b}_{\boldsymbol{k}} + \sum_{\boldsymbol{k}\neq 0}\mathcal{N}_0U_{\boldsymbol{k}}\Big(\hat{b}^\dagger_{\boldsymbol{k}}\hat{b}^\dagger_{-\boldsymbol{k}} + \hat{b}_{\boldsymbol{k}}\hat{b}_{-\boldsymbol{k}}\Big), \tag{14}$$

where $\mathcal{N}_0$ is the number of atoms in the state ψ_0, $\epsilon_{\boldsymbol{k}} = \int d\boldsymbol{r}\psi^*_{\boldsymbol{k}}H_0\psi_{\boldsymbol{k}}$, and $U_{\boldsymbol{k}} = (g_0/2)\int d\boldsymbol{r}|\psi_{\boldsymbol{k}}|^2|\psi_0|^2$. Following the standard procedure,[22] we find

$$P_{\boldsymbol{k}_1\boldsymbol{k}\boldsymbol{k}_3\boldsymbol{k}_4} = v^2_{k_1}(\delta_{\boldsymbol{k}_1,\boldsymbol{k}_4}\delta_{\boldsymbol{k},\boldsymbol{k}_3} + \delta_{\boldsymbol{k}_1,\boldsymbol{k}_3}\delta_{\boldsymbol{k},\boldsymbol{k}_4}) + \frac{u^*_k u_{k_3}v_{k_3}}{v_k}\delta_{-\boldsymbol{k}_1,\boldsymbol{k}}\delta_{-\boldsymbol{k}_3,\boldsymbol{k}_4} - 2\mathcal{N}_0\delta_{\boldsymbol{k}_1,0}\delta_{\boldsymbol{k},0}\delta_{\boldsymbol{k}_3,0}, \tag{15}$$

where $\mathcal{E}_{\boldsymbol{k}} = \sqrt{\eta^2_{\boldsymbol{k}} - 4\mathcal{N}_0^2U^2_{\boldsymbol{k}}}$; $u_0 = v_0 = \sqrt{\mathcal{N}_0}$, $u^2_{\boldsymbol{k}\neq 0} = 1 + v^2_{\boldsymbol{k}\neq 0}$; and $v^2_{\boldsymbol{k}\neq 0} = [\eta^2_{\boldsymbol{k}}/(\eta^2_{\boldsymbol{k}} - 4\mathcal{N}_0^2U^2_{\boldsymbol{k}}) - 1]/2$, with $\eta_{\boldsymbol{k}} = \epsilon^0_{\boldsymbol{k}} - \epsilon^0_0 + 4\mathcal{N}_0U_{\boldsymbol{k}} - 2\mathcal{N}_0U_0$. This leads to a set of simplified nonlinear equations for Bloch functions,

$$\tilde{\nu}_0\,\Psi_0 = H_0\,\Psi_0 + g_0\mathcal{N}_0|\,\Psi_0|^2\,\Psi_0 + 2g_0\sum_{\boldsymbol{k}\prime\neq 0}v^2_{\boldsymbol{k}\prime}|\,\Psi_{\boldsymbol{k}\prime}|^2\,\Psi_0 + g_0\sum_{\boldsymbol{k}\prime\neq 0}u_{\boldsymbol{k}\prime}v_{\boldsymbol{k}\prime}|\,\Psi_{\boldsymbol{k}\prime}|^2\,\Psi_0, \tag{16}$$

and for $\boldsymbol{k}\neq 0$

$$\tilde{\nu}_{\boldsymbol{k}}\,\Psi_{\boldsymbol{k}} = H_0\,\Psi_{\boldsymbol{k}} + g_0(2 + \frac{u_{\boldsymbol{k}}}{v_{\boldsymbol{k}}})\mathcal{N}_0|\,\Psi_0|^2\,\Psi_{\boldsymbol{k}} + g_0\sum_{\boldsymbol{k}'\neq 0}\Big[u_{\boldsymbol{k}'}v_{\boldsymbol{k}'}\frac{u_{\boldsymbol{k}}}{v_{\boldsymbol{k}}} + 2v^2_{\boldsymbol{k}'}\Big]|\,\Psi_{\boldsymbol{k}'}|^2\,\Psi_{\boldsymbol{k}}. \tag{17}$$

Since u_k and v_k themselves depend on $\psi_{\boldsymbol{k}}$, 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, $V(\boldsymbol{r}) = V(-\boldsymbol{r})$, so that $\psi_{-\boldsymbol{k}} = \psi^*_{\boldsymbol{k}}$. We have also ignored the scattering processes with nonzero $\boldsymbol{K}$.

Finally, we use a one-dimensional double-well potential under a 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:

$$W_l = \frac{\sqrt{2}}{2}(\Psi_0 + \Psi_1), \quad W_r = \frac{\sqrt{2}}{2}(\Psi_0 - \Psi_1), \tag{18}$$

where Ψ_0 and Ψ_1 are chosen such that they are both positive in the left well. These two Wannier functions satisfy the nonlinear equation (8). The corresponding lattice model is

$$\hat{H}_2 = \Big[-J + 2(N_0-1)U_3\Big](\hat{a}^\dagger_l\hat{a}_r + \hat{a}^\dagger_r\hat{a}_l) + U_2(\hat{a}^\dagger_r\hat{a}^\dagger_r\hat{a}_l\hat{a}_l + 4\hat{a}^\dagger_l\hat{a}_l\hat{a}^\dagger_r\hat{a}_r + \hat{a}^\dagger_l\hat{a}^\dagger_l\hat{a}_r\hat{a}_r) + U(\hat{a}^\dagger_l\hat{a}^\dagger_l\hat{a}_l\hat{a}_l + \hat{a}^\dagger_r\hat{a}^\dagger_r\hat{a}_r\hat{a}_r), \tag{19}$$

where $U_2 = U_{llrr}$, $U_3 = U_{lrrr}$, and $U = U_{llll}$.

We choose the double-well potential as a part of the one dimensional optical lattice created experimentally in Ref. [23]. Thus, the double well potential is given by $V(x) = V_0\sin^2(k_Lx)$, 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 $g_0 = (4\pi\hbar^2a_s/m)(m\omega_\perp/(2\pi\hbar)) = 2\hbar\omega_\perp a_s$, where a_s is the s-wave scattering length and $\omega_\perp$ the perpendicular confinement frequency. In our numerical calculations, the Hamiltonian in Eq. (19) is diagonalized directly and Eq. (8) is solved with the nonlinear equation solver in MATLAB. We use $c = \pi m g_0/(\hbar^2k_L)$ as the dimensionless interaction parameter.

The numerical results for the dependences 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. 1. J_0 and U_0 are the tunneling parameter and on-site interaction obtained with single-particle Wannier function.

These numerical results have confirmed our intuitive understanding that the Wannier function is broadened as the interaction strength c increases. This is evidently illustrated by the decrease of U/U_0 with the increase of c shown in the right column of Fig. 1. Although the broadening of the Wannier function always leads to the decrease of U/U_0, it does not always lead to the increase of J/J_0 as one would intuitively expect. This is demonstrated such that J/J_0 generally decreases as c increases in the right column. This is also supported by the fact that J/J_0 can decrease with U/U_0 as v increase in Figs. 1(a2) and 1(a3). This rich behavior of J/J_0 is due to the fact that J depends not only on the size of the Wannier function tail but also on the detailed oscillatory structure of the tail. Nevertheless, one can still have some intuitive understanding of the behavior of J/J_0. For the right column, one can roughly understand the

decrease of J/J_0 with increasing c as the result of the effective reduction of band width, which becomes narrower as the increased interaction enhances the band-energy at the $k = 0$ state more quickly than $k = \pi$ state.

We also notice that J/J_0 and U/U_0 does not vary much with c when there is only one particle per well on average. As shown in Figs. 1(a1) and 1(b1), the change of J/J_0 and U/U_0 caused by the interaction is less than 1%. However, the change becomes significant when there is more than one particle per well. This is evident in the lower four panels of Fig. 1.

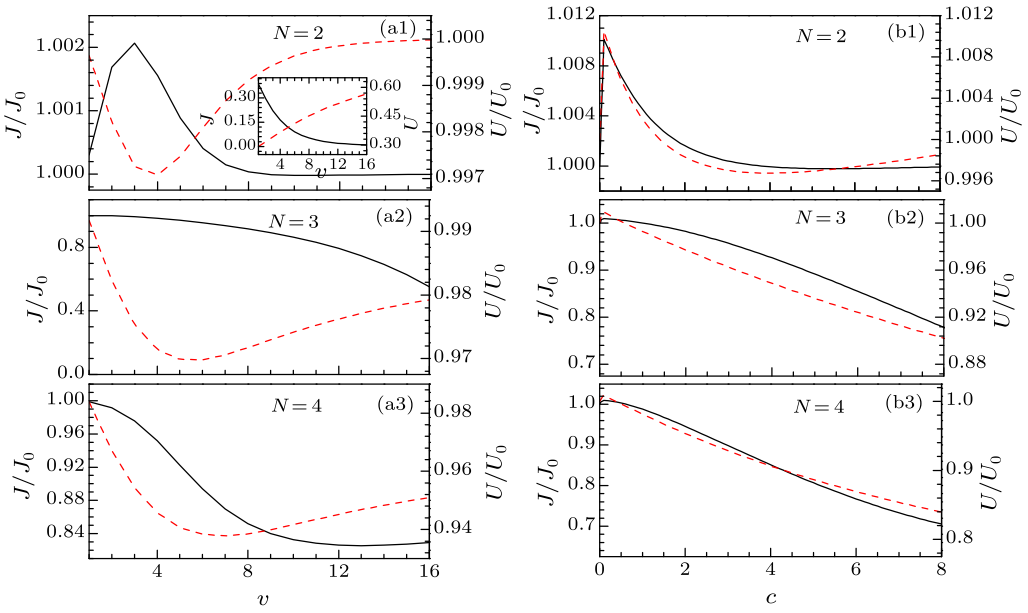

Fig. 1. The tunneling parameter J and the on-site interaction U as functions of the double-well depth and the interaction strength. For (a1, a2, a3), $c = 2.5$; for (b1, b2, b3), $v = 5.0$. The left vertical axis is for the solid line while the right one is for the dashed line. The results for $c < 0.1$ are not accurate due to the numerical difficulties caused by the intrinsic structure problem in the system. The energy unit is the recoil energy $E_r = \hbar^2 k_L^2/2m$. The inset in (a1) shows how J and U change with v.

We expect that the behaviors of J/J_0 and U/U_0 revealed in Fig. 1 are not limited to the double-well systems, and should hold generally for ultracold bosons in optical lattices. This is to be confirmed by future work.

Currently in typical experiments, ultracold atoms are also trapped by a harmonic potential.[20,21] Consequently, the wells are not identical to each other. Also a random potential can be added to make the wells non-identical.[24] 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

$$W_j(x) = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{i\frac{2kj\pi}{N}} \psi_k, \quad j = 0, 1, \ldots, N-1, \tag{20}$$

where ψ_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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