Interaction Effects on Wannier Functions of a Bose-Einstein Condensate in an Optical Lattice and Implications for Bose-Hubbard Model

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We show that one can properly take into account of the interaction effects and construct a set of orthonormal Wannier functions for a Bose-Einstein condensate in an optical lattice. These interaction-dependent Wannier functions are used to compute the tunneling rate $J$ and the on-site repulsion $U$ in the Bose-Hubbard model. Both parameters are found to be substantially different from ones calculated with the single-particle Wannier functions. Our numerical results of $U$ are found in good agreement with the measured on-site energy in a recent experiment [Campbell et al. Science 314, 281 (2006)].

The system of a Bose-Einstein condensate (BEC) in an optical lattice has been one of the most exciting and studied systems in recent years. The system has enabled experimentalists to observe for the first time many interesting phenomena predicted a long time ago in condensed matter physics. The most spectacular example is the observation of the quantum phase transition from a superfluid to a Mott insulator in such a BEC. So far, these two parameters are usually computed with the single-particle Wannier function. Such treatment is good only in the low-filling regime. For higher fillings, due to stronger inter-atomic interactions, the shape of the Wannier function is expected to distinguish significantly from that of the single-particle Wannier function. As a result, $J$ and $U$ are interaction-dependent. In particular, $J$ is more sensitive since it depends on the tails of the Wannier function as seen in Eq. (2). This view is echoed in literature. For example, Bloch et al. pointed out, “For intermediate fillings, the Wannier functions entering both the effective hopping matrix element $J$ and on-site repulsion $U$ have to be adjusted to account for the mean-field interaction.” In a recent experiment by Campbell et al. [14], the one-site energy with the filling factors increasing from one to five was observed to have a 27% decrease.

To our best knowledge, there has been only one systematic theoretical attack on this important problem. This was carried out by Li et al. in Ref. [15], where the authors constructed a set of orthonormal interaction-dependent Wannier functions with Kohn’s variational approach [16]. This variational method has one intrinsic shortcoming: the chosen trial Wannier function may be quite different from the true Wannier function. In Ref.
Li et al. used Gaussian functions as the trial functions. However, as pointed out in Ref. \[15\], the Gaussian approximation is not good for calculating the tunneling parameter \(J\). This means that even the best Gaussian type Wannier functions obtained by variation in Ref. \[15\] are not good enough.

In this Letter we show that a set of Wannier functions can be constructed from the Bloch states of the Gross-Pitaevskii equation (GPE) for the periodic BEC system. These Wannier functions are proved to be orthonormal and are therefore suitable for the use of reducing the BEC system to the BHM. Moreover, these Wannier functions are interaction-dependent by construction; we call them nonlinear Wannier functions Eq. (4). With this, one can prove the orthonormality of the single-particle Wannier functions. That the interaction effects are properly taken into account in these nonlinear Wannier functions roots in the fact that the Bloch states used to construct them minimizes the system energy under the mean-field approximation. With these nonlinear Wannier functions, we find that both the tunneling rate \(J\) and the on-site repulsion \(U\) are substantially affected by the mean-field interaction. For simplicity, the construction and properties of the nonlinear Wannier functions are illustrated in detail for one-dimensional optical lattices, where the results for the BHM parameters \(J\) and \(U\) are presented for all dimensionality.

To define the nonlinear Wannier functions, we first introduce the mean-field Bloch states \(\psi_k(x)\) \[18, 19, 20\], which satisfy the following time-independent GPE \[21\]

\[
-\frac{\hbar^2 \nabla^2}{2m} \psi_k + V_{lat} \psi_k + g n_0 |\psi_k|^2 \psi_k = \mu(k) \psi_k ,
\]

where \(g = 4\pi \alpha_s / m\) and \(n_0\) is the average BEC density. The band index is omitted as we focus on the lowest Bloch band. The nonlinear Wannier functions are constructed from these Bloch states as follows

\[
w(r - r_i) = \frac{1}{|\Omega|} \int_\Omega \psi_k(r) e^{-i k \cdot r} d\boldsymbol{k} ,
\]

where the integration is over the first Brillouin zone and \(|\Omega|\) is its volume. This is exactly the same way how the single-particle Wannier function is constructed from Bloch states \[22, 23\]. Because of the nonlinear term in Eq. (4), one may doubt whether the Wannier functions constructed in such a way are orthonormal to each other and thus have any use. This doubt can be cast aside immediately by observing that the Bloch states defined in Eq. (4) are orthonormal to each other, i.e.,

\[
\int \psi_{k_1}^*(r) \psi_{k_2}(r) dr = \delta_{k_1 k_2} ,
\]

where the function is over the entire space. There was a concern in Ref. \[15\] that the definition in Eq. (5) would fail because of the existence of a loop structure in the mean-field Bloch band \(\mu(k)\) \[18, 19, 24\]. This concern is not justified because the BHM is a single-band approximation and it is a good description of the BEC system only when the band gap of the lattice potential is much larger than the interatomic interaction \[11\]. The loop structure in the Bloch band appears only for shallow optical lattices, where the BHM does not apply.

We now use the 1D case to illustrate some key points in the numerical computation of the nonlinear Wannier functions. The complete set of the Bloch functions \(\psi_k(x)\) in the lowest Bloch band can be obtained by solving Eq. (4) with the same method in Ref. \[25\]. Since an arbitrary phase can be added to each \(\psi_k(x)\), to obtain a proper Wannier function via Eq. (5), the numerical method must be designed to make sure that the resulted \(\psi_k(x)\) is analytic in \(k\). Usually, one also wants the Wannier function to be real and symmetric (or antisymmetric). To achieve this, one should pay attention to the values of \(w(0)\) and \(\psi_{\pi/d}(0)\) \[16\]. (i) If both \(w(0)\) and \(\psi_{\pi/d}(0)\) are nonzero, the phase of the Bloch function must be chosen such that \(\psi_k(0)\) is real. (ii) If both \(w(0)\) and \(\psi_{\pi/d}(0)\) vanish, the phase must be chosen such that \(\psi_k(0)\) is purely imaginary. (iii) If only one of \(w(0)\) and \(\psi_{\pi/d}(0)\) is zero, one can shift the origin in the \(x\) space by half of the lattice constant. With the new origin, one is then back to either case (i) or (ii). One can prove that (1) if \(w(0) \neq 0, w(-x) = w(x)\) and \(w'(x) = w(x)\), that is, the Wannier function \(w(x)\) is symmetric about \(x = 0\) and real; (2) if \(w(0) = 0, w(x)\) is antisymmetric about \(x = 0\) and real. Following Kohn’s strategy \[16\], one can also prove that no other choices of phases in \(\psi_k(x)\) can lead to nonlinear Wannier functions that are both real and symmetric (antisymmetric) about \(x = 0\).

![FIG. 1](image-url) (color online) 1D nonlinear Wannier functions \(w(x)\) for different mean-field interactions \(gn_0\). The insets show the decay of the local maximums of the 1D nonlinear Wannier function.

Our numerical results of the 1D nonlinear Wannier
functions are plotted in a semilog fashion in Fig. 1. As clearly shown, the decay of the the Wannier function remains exponential despite the nonlinearity. The effect of the nonlinearity (or interaction) is to make the decay slower and thus the Wannier function less localized. The single-particle Wannier function has been proven to decay exponentially by Kohn [24]. It was pointed out later [26] that this exponential decay is related to a well-known mathematical result that connects the behavior of a function near a branch point to the asymptotic decay of its Fourier transform [27,28]. Suppose that \( f_k(x) \) is a periodic function \( f_k(x) = f_{k+2\pi/d}(x) \) and has a leading behavior at the branch point \( k_0 = \pi/d + ih \) as \( f_k(x) = f_0(x) + \gamma (i(k - k_0))^{\gamma} \). Its Fourier transform is an exponential decay function, \( F(x) = \int dk f_k(x)e^{-ikx} = 2\gamma \sin \pi (1+\gamma) \Gamma(1+\gamma) e^{-hx} \). This means that the nonlinear Wannier functions, shown to decay exponentially in Fig. 1 may also have these analytical properties. The rigorous proof for this, however, is left for the future investigation. Also note that due to the power-law prefactor [28], the decay in Fig. 1 is not strictly exponential as indicated by the slight curving of the envelope of the peaks.

Nonlinear Wannier functions can be computed similarly for the 2D and 3D optical lattices. However, the computation time can become enormous in particular for the 2D case. Since our ultimate goal is to compute the two basic parameters \( J \) and \( U \) of the BHM from Eqs. (2) and (3), respectively, we can reduce the computation time significantly by not calculating out the Wannier function explicitly. For \( J \), one can combine Eq. (2) and Eq. (3) to express \( J \) in terms of the Bloch functions and then use this expression to compute \( J \) efficiently. For \( U \), one can reduce the computing time by utilizing a well-known fact that \( U \) is proportional to the difference between \( \mu(k = 0) \) and the system’s mean-field ground state energy.

Our numerical results for \( J \) and \( U \) are shown in Figs. 2 and 3 for different values of \( V_0 \) and \( gn_0 \). As clearly shown in the figures, the mean-field interactions \( gn_0 \) have pronounced effects on both the tunneling rate \( J \) and on-site repulsion \( U \). For a fixed lattice strength \( V_0 \), with the increase of \( gn_0 \), \( J \) increases while \( U \) decreases dramatically. This is expected as the Wannier function becomes less localized as \( gn_0 \) increases. Moreover, it is apparent from the figures, in higher dimensions, the interaction effects are much stronger. This highlights the need to take into account the interaction effect into \( J \) and \( U \) since most of the experiments are carried out with the 3D optical lattices. Since the optical lattices have the form \( V_{\text{lat}} = V_0E_R \sum_{j=1}^{D} \sin^2(q_{j}x_{j}) \), the different directions in our system are decoupled in the linear case \( gn_0 = 0 \). The dependence of the interaction effects on dimensionality shows that the interaction can strongly couple the motions along different directions.

Let us take a closer look at a BEC in a 3D optical lattice with \( V_0 = 10E_R \). At a low filling with \( gn_0 = 0.01E_R \), we have \( J/E_R = 0.019 \) and \( Ud/E_{R\sigma} = 22.4 \) (see Figs. 2 (b) and 3 (b)), which is consistent with the results calculated with the single-particle Wannier function in Ref. 29,30. However, at a higher filling with \( gn_0 = 2.0E_R \), \( J \) is approximately three times larger than the value calculated with the single-particle Wannier function. Meanwhile, the on-site energy \( Ud/E_{R\sigma} \) is significantly re-
duced to 6.6. This strong dependence of $J$ and $U$ on the $gn_0$ justifies the necessity of introducing the nonlinear Wannier functions. In this work, the parameters $gn_0$ in Figs. 2 and 3 relates to the filling factor $\langle n_i \rangle$, which is often used in the literature [2, 3], as $n_0 = \langle n_i \rangle / d^3$.

In a recent experiment by Campbell et al. [14], the on-site energy $U$ was measured for different filling factors with the two-photon Bragg spectroscopy [31]. They found that $U = 22$ Hz for the $\langle n_i \rangle = 5$ shell at $V_0 = 35 E_R$, a decrease of 27% from $U = 30$ Hz for $\langle n_i \rangle = 1 \sim 2$. Our numerical results are $U = 28.4$ Hz for $\langle n_i \rangle = 5$ and $U = 33.1 \sim 31.8$ Hz for $\langle n_i \rangle = 1 \sim 2$, in good agreement with the experiment. This shows that even though the nonlinear Wannier function is a mean-field concept, it somehow still captures much of the interaction effect in the Mott insulator regime. A possible method for the experimental study on the tunneling rate $J$ is to study the interference pattern produced by an expanding atomic cloud [30].

We emphasize here that our calculation of the two basic parameters of the BHM has been done with the mean-field theory. Further improvement of the theoretical framework is also needed to include the effects of quantum fluctuations [32].

To conclude, we have demonstrated a way to construct a set of orthonormal Wannier functions by properly incorporating interaction effect for a BEC in an optical lattice. Although these nonlinear Wannier functions are less localized than the single-particle Wannier functions due to the repulsive interaction, they retain many of the analytical properties of the single-particle Wannier functions. For example, our numerical results show that they decay exponentially. We have used these Wannier functions to compute the tunneling rate $J$ and the on-site interaction $U$ in the Bose-Hubbard model. The computed $U$ are found in good agreement with experimental results.

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[1] I. Bloch, Nat. Phys. 1, 23 (2005).
[2] O. Morsch and M. Oberthaler, Rev. Mod. Phys. 78, 179 (2006).
[3] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008).
[4] V. I. Yukalov, Laser Phys. 19, 1 (2009).
[5] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature (London) 415, 39 (2002).
[6] T. Stöferle, H. Moritz, C. Schori, M. Köhl, and T. Esslinger, Phys. Rev. Lett. 92, 130403 (2004); M. Köhl, H. Moritz, T. Stöferle, C. Schori, and T. Esslinger, J. Low. Temp. Phys. 138, 635 (2005).
[7] K. Xu, Y. Liu, D. E. Miller, J. K. Chin, W. Setiawan, and W. Ketterle, Phys. Rev. Lett. 98, 080804 (2007).
[8] I. B. Spielman, W. D. Phillips, and J. V. Porto, Phys. Rev. Lett. 100, 120402 (2008).
[9] I. B. Spielman, W. D. Phillips, and J. V. Porto, Phys. Rev. Lett. 100, 120402 (2008).
[10] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B 40, 546 (1989).
[11] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. 81, 3108 (1998).
[12] D. van Oosten, P. van der Straten, and H. T. C. Stoof, Phys. Rev. A 63, 053601 (2001).
[13] W. Zwerger, J. Opt. B: Quantum Semiclassical Opt. 5, 9 (2003).
[14] G. K. Campbell et al., Science 313, 649 (2006).
[15] J. B. Li, Y. Yu, A. Dudarev, and Q. Niu, New. J. Phys. 8, 154 (2006).
[16] W. Kohn, Phys. Rev. B 7, 4388 (1973).
[17] M. Krämer, C. Menotti, L. Pitaevskii, and S. Stringari, Eur. Phys. J. D 27, 247 (2003).
[18] Biao Wu and Qian Niu, Phys. Rev. A 64, 061603(R) (2001); Biao Wu and Qian Niu, New J. Phys. 5, 104 (2003).
[19] D. Diakonov, L. M. Jensen, C. J. Pethick, and H. Smith, Phys. Rev. A 66, 013604 (2002); M. Machholm, C. J. Pethick, and H. Smith, ibid. 67, 053613 (2003).
[20] J. C. Bronski, L. D. Carr, B. Deconinck, and J. N. Kutz, Phys. Rev. Lett. 86, 1402 (2001).
[21] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 71, 463 (1999).
[22] W. Kohn, Phys. Rev. 115, 809 (1959).
[23] N. W. Ashcroft and N. D. Mermin, Solid State Physics, (Saunders, Philadelphia, 1976).
[24] B. T. Seaman, L. D. Carr, and M. J. Holland, Phys. Rev. A 72, 033602 (2005).
[25] Z. X. Liang, X. Dong, Z. D. Zhang, and Biao Wu, Phys. Rev. A 78, 023622 (2008).
[26] J. des Cloiseaux, Phys. Rev. 135 A685 (1964).
[27] F. W. J. Olver, Asymptotic and Special Functions (A. K. Peters, Wellesley, MA, 1997).
[28] L. X. He and D. Vanderbilt, Phys. Rev. Lett. 86, 5341 (2001).
[29] K. Xu, Doctoral Thesis (Massachusetts Institute of Technology), Page 122.