Interaction broadening of Wannier functions and $n > 1$ Mott transitions in atomic BEC

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Superfluid/Mott-insulator transitions of atomic BEC in optical lattices are investigated for the case of multi-atom occupation per site. By using Kohn's variational procedure, an orthogonal set of Wannier functions is obtained with account of mean field repulsion between the atoms in each well. The resulting parameters of hopping amplitude J and on-site interaction U are markedly different from those calculated from single-atom Wannier functions. Lattices of various dimensionality and different mean occupation are considered, and the critical lattice potentials are found to be considerably increased because of the interaction-broadening of the Wannier functions.

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Optical lattices have provided a paradigm playground for the study of many-body effects in Bose-Einstein condensates (BEC) [1, 2, 3]. Number squeezing is seen on ^{87}Rb atoms in a one-dimensional lattice of pancake-shaped wells [1], and superfluid/Mott-insulator transitions were also witnessed on such atoms in a three-dimensional optical lattice [2]. Such transitions were predicted by theoretical studies based on the Bose-Hubbard model [4] and by microscopic calculations of the model parameters for BEC in optical lattices [5, 6].

One unanswered question is whether it is possible to observe superfluid/Mott-insulator transitions for the mean occupation n larger or even much larger than unity. Such transitions are indeed predicted by the phenomenological Bose-Hubbard model. The experimental condition for n=2 seems to be straightforward, although one has to devise ways to distinguish from the n=1 transition. For $n = 3$ or larger, one must also struggle with three-atom collisional losses. In lower dimensional lattices with transverse potential wells bigger than the lattice wells, large occupation can be achieved without much collisional loss. In order to provide theoretical guidance to experimental observation of Mott transitions in such systems, it is imperative to obtain accurate critical values of the lattice potential for lattice occupations beyond unity. Previous calculations of the model parameters J and U are all based on Wannier functions for a single atom in an optical lattice. While this may be reasonable for the case of $n = 1$ (or small n with weak interactions), repulsive interaction between the atoms for $n > 1$ may cause the wave function in each well to expand in all directions, not only affecting the on-site interaction U [7] but also strongly enhancing tunneling J between neighboring wells.

In this Letter, we show how to formulate an orthogonal basis of Wannier functions with mean-field atomic interactions taken into account, and to calculate the critical potential V_c for various lattices of different dimensionality and mean occupation. For the cubic optical lattice with $n = 2$ or larger, our result for V_c is noticeably larger than that calculated without taking into account the mean field effect. This increase is more pronounced for the anisotropic cases with stronger lattice potentials in one or two directions. For the case of one-dimensional lattice of pancake-shaped wells [1] or two-dimensional lattice of tubes [3], our results show many multiples of increase over the critical values calculated from one-atom Wannier functions. This is in agreement with the experimental finding that much higher lattice potentials are needed to reach the transition point in such cases.

We will borrow Kohn's variational procedure developed many years ago for constructing electronic Wannier functions in crystals [8], making appropriate modifications to account for interactions between the BEC atoms. Taking the isotropic cubic lattice as an example, we describe our strategy as follows. We start with a trial wave function localized in each well, $g(\mathbf{r} - \mathbf{r}_i)$, where $\mathbf{r}_i$ labels the well positions. A Wannier function may be constructed according to Kohn's transformation:

$$W(\mathbf{r}) = \sum_i c_i g(\mathbf{r} - \mathbf{r}_i), \tag{1}$$

$$c_i = \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot\mathbf{r}_i}}{\sqrt{G(\mathbf{k})}},$$

where the integral is over the first Bulliouin zone and $G(\mathbf{k}) = \sum_i \int d\mathbf{r} g(\mathbf{r}) g(\mathbf{r} - \mathbf{r}_i) \cos(\mathbf{k} \cdot \mathbf{r}_i)$. One can show that such Wannier functions are normalized and are orthogonal to each other for different wells. Finally, we vary the trial function to minimize the on-site energy [9]:

$$f = nI + U_0 n(n-1)/2, \tag{2}$$

where the on-site single-atom energy I and the bare on-site repulsion U_0 are defined by

$$I = \int d\mathbf{r} W^*(\mathbf{r}) [-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})] W(\mathbf{r}),$$

$$U_0 = g \int d\mathbf{r} |W(\mathbf{r})|^4, \tag{3}$$

where $g = \frac{4\pi a_s \hbar^2}{m}$. We assume that the system lies approximately within the Hilbert space spanned by the variational Wannier functions in the sense that the boson

field operator may be expanded as $\psi(\mathbf{r}) = \sum_i b_i W(\mathbf{r}-\mathbf{r}_i)$, where b_i is the operator for destroying an atom in the Wannier state of site $\mathbf{r}_i$. Substituting this expansion into the many-body Hamiltonian of the atoms then leads to a problem of lattice bosons. Near the Mott phase, we may just keep nearest-neighbor hopping terms and work near the mean occupation n by expanding the on-site energy to second order in the deviation $n_i = b_i^\dagger b_i - n$, resulting in the standard Bose-Hubbard Hamiltonian

$$H = -J\sum_{\langle ij\rangle} b_i^\dagger b_j + \frac{U}{2}\sum_i n_i(n_i-1), \quad (4)$$

where the effective on-site repulsion U and the hopping amplitude J are defined by

$$U = \partial^2 f/\partial n^2,$$
$$J = \int d\mathbf{r} W^*(\mathbf{r})[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})]W(\mathbf{r}+\vec{\tau}), \quad (5)$$

with $\vec{\tau}$ being lattice vectors connecting nearest neighbor sites. We have also ignored the mean on-site energy, and omitted off-site interactions.

We can thus obtain the Bose-Hubbard parameters using the variational Wannier functions for a given lattice potential and mean occupation n. The critical condition for superfluid/Mott-insulator transition has been found approximately as

$$U/zJ = 2n + 1 + 2\sqrt{n(n+1)}, \quad (6)$$

where z is the number of the nearest neighbor sites [10]. By substituting our parameters into the critical condition, we can then map out the critical potential strength as a function of mean occupation.

In the following, we report our findings for a number of different lattices of current experimental interest: isotropic and anisotropic three-dimensional lattices, one-dimensional lattice of pancake wells, and two-dimensional lattice of tubes. Following standard practice, we will use the lattice period π/k, atomic mass m, and recoil energy $E_r = \hbar^2k^2/2m$ as the basic units of measure. In accordance with existing experiments, we choose in our calculations the ^{87}Rb $F = 2, m = 2$ state with $a_s = 5.8$ nm and the laser wavelength of 852 nm for the three- and two-dimensional lattices and 840 nm for the one-dimensional lattice. All numerical results are obtained using 21 lattice wells in each direction with periodic boundary condition, and convergence has been checked using 41 wells for some of the key results.

Isotropic cubic lattice: The lattice potential is of the form, $V(\mathbf{r}) = V_0(\sin^2(kx) + \sin^2(ky) + \sin^2(kz))$, where k is the wave number of the laser beams. We choose our trial function to be the product form $g(\mathbf{r}) = g(x)g(y)g(z)$, with $g(u) = (1+\alpha u^2)e^{-u^2/\sigma^2}$, where α and σ are variational parameters. Then the Wannier function must also be of product form $W(\mathbf{r}) = w(x)w(y)w(z)$, with the one-dimensional functions $w(u)$ and $g(u)$ related by the one-dimensional version of Kohn's transformation. All the three-dimensional integrals in eqs.(4)-(6) can then be reduced to one-dimensional ones, greatly simplifying the calculations.

Our calculations proceed as follows. For a given V_0 and n, we start with certain initial parameters α and σ to obtain a trial Wannier function through Kohn's transformation and calculate the on-site energy f. The procedure is repeated by varying the parameters until the on-site energy f is minimized. The resulting variational Wannier function will depend on both n and V_0. If only the on-site single-atom energy I is minimized, one obtains the single-atom Wannier function which only depends on V_0.

Once the Wannier function is determined, we can calculate the Bose-Hubbard parameters U and J. In Fig. 1(a), we depict the ratio U/zJ ($z = 6$) as a function of the mean occupation n for several values of the potential strength V_0. The decreasing trend can be understood from the fact that repulsive interaction increases with n, making the Wannier function broader, tunneling easier and the bare interaction U_0 smaller. The intersection with the line of critical condition (the up-going line obtained from eq.(6)) then yields the mean occupation for which these potentials are critical. For n=1,2,3 and 4, we find the critical potentials to be $V_c = 11.95, 14.32$, 16.25 and 18.15 respectively. For comparison, we make similar plots in Fig. 1(b) the results obtained from the single-atom Wannier function. The critical potentials become 11.85, 13.47, 14.61 and 15.43 for the first four mean occupations. For $n = 1$, the two results agree with each other within numerical uncertainty [11], and are also consistent with experimentally determined range for the critical potential [2]. For $n > 1$, the mean field repulsion makes the critical potential noticeably higher. It will be very interesting to observe this effect experimentally.

Anisotropic cubic lattices: Our procedure can also be applied to the case of an anisotropic lattice, in which the potential amplitude $V_\perp$ in one or two (transverse) directions is much stronger than the others. One may focus attention on the remaining two or one lattice directions in which hopping is allowed only. Following Ref. [5], we model the system as a lower dimensional problem with the reduced interaction parameter g_d obtained by multiplying g with the integral of $|\psi_\perp|^4$, where $\psi_\perp$ is the single-atom ground state wave function in a well of the transverse potential. In the harmonic approximation, the wave function can be found exactly, and the reduced interaction parameter is given by $g_1 = \frac{g\pi}{2}\sqrt{V_\perp}$ for the quasi-one-dimensional lattice and $g_2 = g\sqrt{\frac{\pi}{2}}\sqrt[4]{V_\perp}$ for the quasi-two-dimensional lattice. In our calculations to be discussed below, we take $V_\perp = 80E_r$.

To find the Wannier functions for the lower dimensional lattices, we use these reduced interaction parameters in our procedure, replacing all the three-dimensional integrals in Eqs.(1), (3) and (6) by lower dimensional ones. The critical lattice potential V_c calculated using such variational Wannier functions

is depicted in Fig. 2(a) and (b) for the one- and two-dimensional cases respectively. For comparison, we also include results calculated using the one-atom Wannier function. The increase of critical potential due to mean-field repulsion on the Wannier functions is somewhat bigger in the lower dimensional cases.

One- and two-dimensional lattices: BECs in one-dimensional lattice of pancake-shaped wells and two-dimensional lattice of tube-shaped wells have been studied in experiments [1, 3]. Because of the large transverse dimensions of such wells, many atoms can be held in a well without suffering too much three-atom collisional loss, opening the possibility of studying superfluid/Mott-insulator transition for relatively large n [7, 12]. In a theoretical investigation, Oosten et al [7] considered the interaction effect by using a transverse wave function in the Thomas-Fermi approximation without modifying the single-atom Wannier function in the lattice direction(s). Here we extend their work by considering the interaction effect on the Wannier functions as well.

We begin by writing the Wannier function in the form, $W(\mathbf{r}) = w(\mathbf{r}_L)\phi(\mathbf{r}_\perp)$, where ϕ is the wave function for the transverse direction(s), and w is the Wannier function in the lattice direction(s), both to be determined variationally by minimizing the on-site energy. The part of the on-site energy involving ϕ is just the n-particle Gross-Pitaevskii energy in the transverse potential and with the interaction parameter g modified into g_d by multiplying the integral of $|w(\mathbf{r}_L)|^4$. In the Thomas-Fermi approximation, this 'transverse energy' is given by $f_\perp = \frac{2n-1}{3}\sqrt{nm\omega_\perp^2 g_1/\pi}$ for the 1d case and $f_\perp = \frac{5n-2}{10}(9m\omega_\perp^2 n^2 g_2^2)^{1/3}$ for the 2d case. The total on-site energy is the sum of this 'transverse energy' and n times of the single-atom energy of the lattice Wannier function:

$$f = f_\perp + n\int d\mathbf{r}_L w^*(\mathbf{r}_L)[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}_L)]w(\mathbf{r}_L). \quad (7)$$

Our lattice Wannier function, obtained by the procedure of Kohn's transformation and minimization of the on-site energy, will be affected by the interaction because the 'transverse energy' depends on it through the reduced interaction parameter g_d. After $w(\mathbf{r}_L)$ is determined variationally, the Bose-Hubbard parameters J and U can be calculated immediately. In Fig. 3(a) and (b) we show the critical potential V_c for the case of one-dimensional lattice with transverse trap frequency $\omega_\perp/2\pi = 19$ s^{-1} and 120 s^{-1}, respectively.

For comparison, we also show the corresponding results obtained using the single-atom Wannier function of the lattice and the Thomas-Fermi transverse wave function. It is clear that V_c is raised dramatically due to the broadening of the Wannier function. In the experiment of Ref. [1], the magnetic trap potential is 19 s^{-1}. The transverse trap frequency is enhanced to 120 s^{-1} if the optical confining potential with $V_0 = 50E_r$ is turned on, and the mean occupation number is $n \sim 50$. Evidence from Bragg interference pattern shows that the critical value of the lattice potential should be somewhat larger than $44E_r$. This observation is contradictory to the prediction based on the single-atom Wannier function, but is consistent with our result based on the variational Wannier function.

In the case of two-dimensional lattice, our results for the critical lattice potential are shown in Fig. 3(c) for $\omega_\perp/2\pi = 24$ s^{-1} which is used in [3]. We predict $V_c \sim 33E_r$ for $n \sim 100$, while the single-atom Wannier function yields $V_c \sim 27E_r$. The largest lattice potential used in the experiment was 12 E_r, so further experiment is needed to verify the theoretical predictions.

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FIGURE CAPTIONS

Fig. 1 The ratio U/zJ versus mean occupation n calculated from (a) the variational and (b) single-atom Wannier functions. For each given lattice potential V_0, intersection with the up-going line, the critical condition according to eq. (6), yields the mean occupation number for which the given V_0 is critical.

Fig. 2 The critical lattice potential V_c calculated from the variational and single-atom Wannier functions for anisotropic cubic lattices: (a) quasi-1-dimensional, (b) quasi-2-dimensional. The lines are guide to eyes.

Fig. 3 The critical lattice potential V_c v.s. mean occupation n calculated from the variational and single-atom Wannier functions for: (a) the one-dimensional lattice with $\omega_\perp = 2\pi \times 19\ \mathrm{s}^{-1}$, (b) with $\omega_\perp = 2\pi \times 120\ \mathrm{s}^{-1}$, and (c) two-dimensional lattice with $\omega_\perp = 2\pi \times 24\ \mathrm{s}^{-1}$. The lines are guide to eyes.


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