Zoo of Quantum Phases and Excitations of Cold Bosonic Atoms in Optical Lattices

Ofir E. Alon,* Alexej I. Streltsov, and Lorenz S. Cederbaum

Theoretische Chemie, Physikalisch-Chemisches Institut, Universität Heidelberg, Im Neuenheimer Feld 229, D-69120 Heidelberg, Germany

(Received 22 December 2004; published 15 July 2005)

Quantum phases and phase transitions of weakly to strongly interacting bosonic atoms in deep to shallow optical lattices are described by a single multiorbital mean-field approach in real space. For weakly interacting bosons in one dimension, the critical value of the superfluid to Mott insulator (MI) transition found is in excellent agreement with many-body treatments of the Bose-Hubbard model. For strongly interacting bosons, (i) additional MI phases appear, for which two (or more) atoms residing in each site undergo a Tonks-Girardeau-like transition and localize, and (ii) on-site excitation becomes the excitation lowest in energy. Experimental implications are discussed.

DOI: 10.1103/PhysRevLett.95.030405 PACS numbers: 05.30.Jp, 03.75.Kk, 03.75.Lm, 32.80.Pj

Loading and manipulating cold bosonic atoms in optical lattices is a fascinating, rapidly growing branch of cold-atom physics; see, e.g., Refs. [1–3]. In a pioneering experiment, Greiner *et al.* [1] have demonstrated the quantum phase transition from the superfluid (SF) to Mott insulator (MI) phase of a cold gas of ^{87}Rb atoms trapped by a three-dimensional simple-cubic-type optical lattice. More recently, the SF to MI transition has been demonstrated in an effective one-dimensional (1D) optical lattice [2]. In the SF phase, which has no excitation gap, atoms are free to move throughout the lattice and are associated with a coherent state of matter. The MI phase amounts for commensurate filling of the optical lattice and has an excitation gap associated with moving an atom from one site to an occupied neighboring site. The SF to MI transition (in deep optical lattices) involves weakly interacting bosons and is well described by the Bose-Hubbard model [4–6] which assumes all bosons to occupy the lowest band of the lattice. Recently, the so-called Tonks-Girardeau gas, i.e., the strongly interacting regime, was realized in an optical lattice [3]. Generally, as the interaction between atoms increases—in deep as well as in shallow optical lattices—additional possibilities open up for the trapped cold atoms which can now occupy higher bands.

Our purpose in this Letter is to explore quantum phases and excitations of cold bosonic atoms in optical lattices not accounted for so far. We will present an approach which is able to treat weakly to strongly interacting bosons in the entire range of deep to shallow optical lattices. To peruse the above, we would like to describe cold bosonic atoms in optical lattices directly in real space, i.e., to provide their spatial wave function. Specifically, we will adopt our recently introduced multiorbital mean field [7,8] to cold bosonic atoms in optical lattices. As we shall see below, already for the standard case of weakly interacting atoms we found a promising and intriguing result concerning the critical value of the SF to MI transition in one dimension. Although our approach is mean field, it finds this value to be 3.855(7), in excellent agreement with density matrix renormalization group and other many-body calculations; see Ref. [9], and references therein.

Our starting point is the many-body Hamiltonian describing N bosons in an optical lattice, $\hat{H} = \Sigma_{i=1}^{N}[\hat{T}(\mathbf{r}_i) + V(\mathbf{r}_i)] + \Sigma_{i>j=1}^{N} U(\mathbf{r}_i - \mathbf{r}_j)$. Here, $\mathbf{r}_i$ is the coordinate of the ith particle, $\hat{T}(\mathbf{r}_i)$ and $V(\mathbf{r}_i)$ stand for the kinetic energy and optical lattice potential, respectively, and $U(\mathbf{r}_i - \mathbf{r}_j)$ describes the pairwise contact interaction between the ith and jth atoms.

As mentioned above, we are going to obtain a real space, wave function picture of the quantum state of cold atoms in the optical lattice. How are we going to achieve this? To this end, we attach an orbital to each of the N atoms. The simplest choice is the Gross-Pitaevskii approach, for which all bosons reside in the same orbital. There can be, however, many other situations for bosons [7]. Generally, we may take n_1 bosons to reside in one orbital, $\varphi_1(\mathbf{r})$, n_2 bosons to reside in a second orbital, $\varphi_2(\mathbf{r})$, and so on, distributing the N atoms among $n_{\mathrm{orb}} > 1$ orthogonal orbitals. At the other end of the Gross-Pitaevskii approach lies the situation where each boson in the optical lattice resides in a different orbital, i.e., $n_{\mathrm{orb}} = N$. More formally, the multiorbital mean-field wave function for N interacting bosons is the following single configuration wave function [7]:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \hat{S}\{\varphi_1(\mathbf{r}_1)\varphi_2(\mathbf{r}_2)\cdots\varphi_N(\mathbf{r}_N)\}, \quad (1)$$

where $\hat{S}$ is the symmetrization operator. Note that the Gross-Pitaevskii approach is a specific case of Eq. (1) where all orbitals are alike [7,8]. In order to find the ground state of the many-bosonic system with the ansatz (1), one has to minimize the energy $\langle\Psi|\hat{H}|\Psi\rangle$ with respect to Ψ [Eq. (1)]. This results in a set of n_{orb} coupled, nonlinear equations for the n_{orb} orbitals that have to be solved self-consistently. To fulfill the variational principle, we should search for the energy minimum of $\hat{H}$ with respect to (i) the shape of the self-consistent orbitals $\varphi_i(\mathbf{r})$, (ii) the occupation of each orbital, and (iii) the number n_{orb} of different

orbitals. The larger variational space of the multiorbital approach allows us to describe the underlining physics of various phenomena. Of course, more demanding many-body methods, such as diffusion Monte Carlo simulations [10], would also be valuable.

The multiorbital mean-field wave function (1) has been successfully employed and has led us to the prediction of macroscopic fragmentation of repulsive condensates in the ground and excited states; see Ref. [8]. In macroscopic fragmentation, a large number of atoms reside in a small number of orbitals. Specifically, two or three orbitals were considered in Ref. [8] within Eq. (1). What we have found out is that, when the number of orbitals is of the order of N (number of atoms), the multiorbital ansatz (1) is physically very relevant for various situations of atoms in optical lattices; see below. At the same time, we can now handle practically any number of atoms and sites in optical lattices. Specifically here, we employ more than 100 bosons/sites; i.e., the number of orbitals is $n_{\rm orb} > 100$. The numerical implementation employs the discrete variable representation method [11] and no assumptions are made *a priori* as to the shape of the $n_{\rm orb}$ orbitals which are obtained self-consistently.

In this work, we concentrate on 1D optical lattices, $V(x) = V_0 \sin^2(kx)$, where k is the wave vector. As usual, periodic boundary conditions are assumed. Thus we employ a supercell of a large number N_w of potential wells (unit cells). The strength of the interparticle interaction is expressed via the dimensionless parameter $\gamma = mg/\hbar^2 n$, where m is the mass of the atoms, n is the density, and g is related to the scattering length and the transverse harmonic confinement [12]. Optical potential depths, V_0, and energies will be expressed in terms of the recoil energy, $E_R = \hbar^2 k^2/2m$.

We begin our study with bosons in a deep optical lattice, $V_0 = 25E_R$, with commensurate filling of one atom per lattice site. This familiar SF to MI phase transition is to serve as a test tool for our multiorbital mean-field approach. The MI phase in this system will be denoted by MI(1). In practice, we minimized the energy of the Hamiltonian $\hat{H}$ with respect to the ansatz (1). For weakly interacting bosons we found that *all* bosons reside in one orbital, namely, that the Gross-Pitaevskii approach provides the lowest energy. This state, naturally, corresponds to the SF phase. For stronger interactions, the situation for the ground state changes completely: each and every atom occupies now a different self-consistent, orthogonal orbital. This, as we shall see below, is the MI(1) phase. In other words, we employ the ansatz (1) with $n_{\rm orb} = N$ equations to describe the MI(1) phase. In Fig. 1(a), we plot the energy per particle ε of the SF and MI(1) states as a function of the dimensionless parameter γ for $N_w = 102$ sites. The crossing of the energy curves indicates the critical value for which the phase transition from the SF to the MI(1) phase occurs. It is found to be $\gamma_c = 0.007777(3)$. We have numerical evidence that γ_c scales as $1/n_{\rm orb}$ with increasing

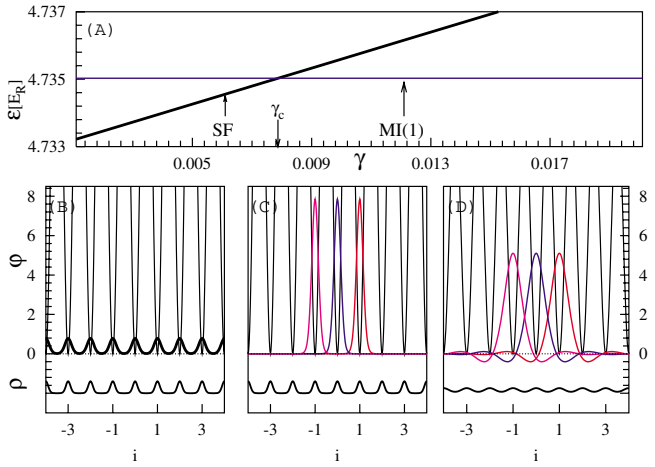

FIG. 1 (color online). Quantum phase transition from the SF to MI(1) phase and corresponding orbitals φ and densities ρ (shifted lower curves) for weakly interacting bosons in optical lattice with $V_0 = 25E_R$ and $N_w = 102$ sites. Orbitals and densities are normalized (on the segment of length 2π) and are plotted against the site index i. The optical lattice is illustrated for guidance by the background sinusoidal curve. (a) The phase transition is described by the intersection of the SF and MI(1) energy per particle curves, ε, which occurs at $\gamma_c = 0.007\,777(3)$. (b) Orbital and density of the SF phase for $\gamma = 0.007\,760\,02$. (c) Orbitals and density of the MI(1) phase for $\gamma = 0.007\,777\,31$, slightly above γ_c (shown are 3 adjacent orbitals). (d) Orbitals and density of the MI(1) phase for strongly interacting bosons in shallower optical lattice with $V_0 = E_R$ for $\gamma = 3.491$, slightly above the corresponding $\gamma_c = 3.4(9)$ (shown are 3 adjacent orbitals).

lattice sites, meaning that we can safely extrapolate γ_c to the thermodynamic limit. It is instructive to translate the value of γ_c to the "language" of the Bose-Hubbard model, i.e., express the corresponding U/J (on-site interaction divided by hopping) in terms of V_0/E_R and γ; see [6]. The resulting critical value corresponding to our γ_c is readily found to be $(U/J)_c = 3.855(7) = 2 \times 1.927(8)$. This value obtained with our multiorbital mean-field approach is in excellent agreement with density matrix renormalization group and other many-body calculations of the 1D Bose-Hubbard model; see Ref. [9], and references therein. The reason is that our multiorbital wave functions are very good approximations for the exact many-body wave functions of the SF and MI(1) phases when $\gamma \ll 1$ and $V_0 \gg E_R$. We remind in this context that the mean-field critical value of the 1D Bose-Hubbard model is $(U/J)_c \approx 2 \times 5.8$, which is rather off the many-body value; see [5], and references therein.

How do the corresponding wave functions (orbitals) look? In Fig. 1(b) we show the SF phase orbital, i.e., the corresponding Gross-Pitaevskii orbital. It, of course, extends throughout the optical lattice, representing a coherent state. In Fig. 1(c) a few adjacent orbitals describing the MI(1) phase are shown. We remind that these orbitals are obtained *self-consistently* as the solution of a coupled

system of $n_{\rm orb} = 102$ nonlinear equations, following ansatz (1). Namely, no preliminary assumptions are made regarding their shape. Because of the translational symmetry, a set of equivalent orbitals is obtained, each centered at one lattice site. It can be proved that, for vanishing interparticle interaction, these orbitals approach the lowest-band Wannier functions. This suggests a very appealing physical meaning to the ansatz (1). It describes the MI(1) phase with orbitals that can be interpreted as boson-dressed Wannier functions.

With a successful mean-field real-space description of the standard SF to MI transition, we set in to exploit more advantages of our method. The next system we considered is the SF to MI(1) phase transition in shallow optical lattices (here we took $V_0 = E_R$), i.e., for a system of strongly interacting bosons. For shallow optical lattices the MI(1) orbitals become more diffusive, as can be seen in Fig. 1(d), and extend beyond the next-nearest neighbor sites. Accordingly, the corresponding spatial density ρ becomes flatter—compare Figs. 1(c) and 1(d). Also, notice the negative values of the orbitals in the nearest neighbor wells which ensure their orthogonality. For $V_0 = E_R$, the intersection of the SF and MI(1) energy curves occurs at $\gamma_c = 3.4(9)$. It is instructive to find this mean-field value to agree very well with that found by Büchler *et al.* in the limit $V_0 \to 0$ by employing the sine-Gordon problem [6].

Aiming at exploring more physical situations in optical lattices, we considered another scenario of commensurate filling—with two atoms per lattice site. For weak interaction, the ground state is, of course, the SF phase where all bosons reside in a single orbital. As the interaction increases, a phase transition to the MI phase, which will be denoted here by MI(2), occurs. We obtained the MI(2) phase as the ground state of the system by ansatz (1). Technically, this is done by determining the $n_{\rm orb} = N/2$ self-consistent orbitals minimizing the energy with 2 bosons per orbital. As γ is further increased, it passes another critical value, and we find that the ground state of the system underwent a second, new phase transition [see Fig. 2(a)]. Now, there are still two atoms in each site but they reside in different orbitals, in contrast to the MI(2) phase where they reside in the same orbital. We denote this new MI phase by MI(1,1) (for obvious reasons). In real space, the two atoms in each site localize at the borders of the site, leading to minima in the spatial density.

Figures 2(b) and 2(c) present the wave functions (orbitals) of the standard and new MI phases, MI(2) and MI(1,1), respectively. The appearance of on-site minima in the corresponding spatial density is a clear fingerprint of the new MI phase, differentiating it from the standard MI(2) quantum phase. Experimentally, Bragg diffraction techniques should provide a direct tool to distinguish between the two MI phases. We have calculated the momentum distributions of the MI(2) and MI(1,1) phases and fount that, in comparison to MI(2), the momentum profile of MI(1,1) is lower and broader. Consequently, momentum distribution measurements should provide an additional

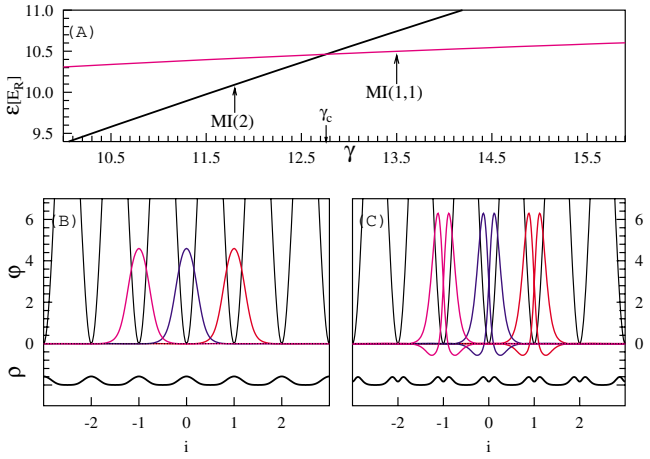

FIG. 2 (color online). Quantum phase transition from the MI(2) to MI(1,1) phase and corresponding orbitals φ and densities ρ (shifted lower curves) for weakly interacting bosons in optical lattice with $V_0 = 25E_R$ and $N_w = 51$ sites. Orbitals and densities are normalized (on the segment of length 2π) and are plotted against the site index i. The optical lattice is illustrated for guidance by the background sinusoidal curve. (a) The phase transition is described by the intersection of the MI(2) and MI(1,1) energy per particle curves, ε, which occurs at $\gamma_c = 12.7(6)$. (b) Orbitals and density of the MI(2) phase for $\gamma = 12.7418$ (shown are 3 adjacent orbitals). (c) Orbitals and density of the MI(1,1) phase for $\gamma = 12.7609$, slightly above γ_c (shown are 6 adjacent orbitals). Notice the on-site minima in the density of the MI(1,1) phase in comparison to the standard MI(2) phase.

tool to differentiate between MI(2) and MI(1,1). The transition of MI(2) to the quantum phase MI(1,1) when the interaction is increased can be interpreted as an on-site transition to the Tonks-Girardeau regime of the MI(2) phase. The results obtained so far are straightforwardly extended to more MI phases with more atoms per site. For instance, the MI phase with three atoms per lattice site, which we denote by MI(3), would eventually end up as the new MI phase, MI(1,1,1), where all three atoms reside in different orbitals, and two on-site minima now appear in the spatial density.

So far, we successfully applied the ansatz (1) to the ground state of atoms in optical lattices. This has been obtained by solving a coupled system of $n_{\rm orb}$ nonlinear equations for the orbitals. It is natural to ask whether the ansatz (1) can also provide physical information on self-consistent excited states. We remind in this respect that ansatz (1) boils down to the Gross-Pitaevskii approach if all orbitals are alike [7,8]. The self-consistent excited states of the latter—solitons and vortices—are well known and have been observed for condensates; see, e.g., Ref. [13], and references therein. In optical lattices, the self-consistent excited states are the nonlinear Bloch bands, the lowest of which is quadratic in k and has zero gap [14]. By definition, in the self-consistent excited states of the Gross-Pitaevskii approach, all bosons reside in the same higher-energy orbital. In contrast, the flexibility of putting

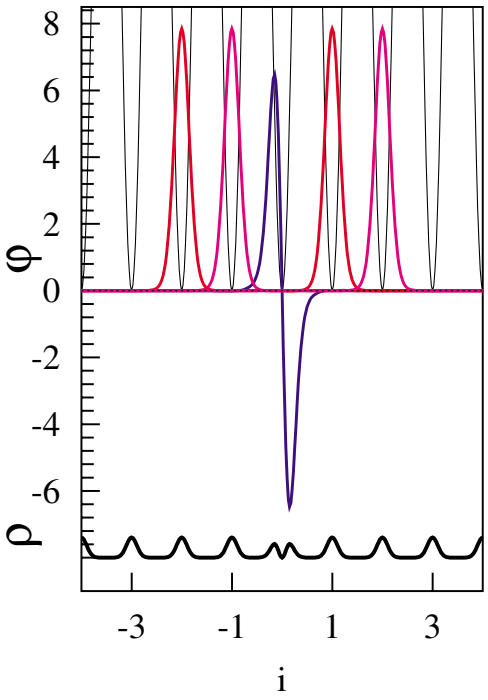

FIG. 3 (color online). On-site self-consistent excited state of the MI(1) phase in optical lattice with $V_0 = 25E_R$ and $N_w = 102$ sites for strongly interacting bosons, $\gamma = 76.64$. Orbitals and density (shifted lower curve) are normalized (on the segment of length 2π) and are plotted against the site index i. The optical lattice is illustrated for guidance by the background sinusoidal curve. Shown are the excitation site and 4 adjacent orbitals. For the present γ, this is the excitation lowest in energy, accommodating the energy gap of the MI(1) phase calculated here to be $0.90\sqrt{4V_0E_R}$.

atoms in different orbitals suggests that Eq. (1) can also be employed to describe many self-consistent excited states.

In the following, we would like to employ ansatz (1) to understand the nature of the gap in the MI phase of strongly interacting atoms in optical lattices. For this, we recall that for weakly interacting bosons in the MI(1) phase the lowest-in-energy excitation is obtained by moving one boson from its site to a neighboring site; see, e.g., Refs. [1,5]. But what happens when the interaction between bosons increases, entering even deeper into the MI regime? In that case, the energy of this excited state increases substantially due to the on-site interaction between the two bosons. We therefore employed ansatz (1) and searched for the low-lying self-consistent excited states of the system. We found many such states, where, e.g., two atoms reside in a single delocalized orbital, or where two atoms in the same site occupy different orbitals localized at the borders of this site [similarly to Fig. 2(c)]. For sufficiently strong interaction, the excitation lowest in energy does not accommodate two bosons in the same site or orbital. Rather, it emerges as an on-site excitation; see Fig. 3. It is instructive to compare the energy of the self-consistent on-site excitation with the excitation gap of a single well in the harmonic approximation given by $\sqrt{4V_0E_R}$ [5]. For the parameters used here, $\gamma = 76.64$, $V_0 = 25E_R$, and $N_w = 102$, we find this value to be $0.90\sqrt{4V_0E_R}$, slightly lower than the bare-well gap. The difference comes from the strong repulsion between atoms, which lowers the gap in comparison to the interaction-free problem.

In conclusion, weakly to strongly interacting cold bosonic atoms in deep to shallow optical lattices have been described by a multiorbital mean-field approach in real space, giving the wave function of cold atoms in the lattice. With it, we described quantum phases and phase transitions of cold bosonic atoms in 1D optical lattices not accounted for so far. As the interparticle interaction is increased, on-site excitation becomes the excitation lowest in energy. The employment of self-consistent mean-field orbitals has been shown to provide an accurate value of the SF to MI transition in one dimension. The findings demonstrate the wide potential of our multiorbital ansatz for cold bosonic atoms and motivate concrete studies in higher dimensions. Finally, the predictions obtained are within reach of (effective) interaction strengths presently employed in experiments, where values up to $\gamma = 200$ have been realized [3]. In addition, if needed, Feshbach-resonance techniques can be employed to further increase scattering lengths.

We thank Jörg Schmiedmayer and Markus Oberthaler for discussions.

*Electronic address: ofir@tc.pci.uni-heidelberg.de

[1] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature (London) **415**, 39 (2002).
[2] T. Stöferle, H. Moritz, C. Schori, M. Köhl, and T. Esslinger, Phys. Rev. Lett. **92**, 130403 (2004).
[3] B. Paredes, A. Widera, V. Murg, O. Mandel, S. Fölling, I. Cirac, G. V. Shlyapnikov, T. W. Hänsch, and I. Bloch, Nature (London) **429**, 277 (2004).
[4] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B **40**, 546 (1989).
[5] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).
[6] H. P. Büchler, G. Blatter, and W. Zwerger, Phys. Rev. Lett. **90**, 130401 (2003).
[7] L. S. Cederbaum and A. I. Streltsov, Phys. Lett. A **318**, 564 (2003).
[8] L. S. Cederbaum and A. I. Streltsov, Phys. Rev. A **70**, 023610 (2004); A. I. Streltsov, L. S. Cederbaum, and N. Moiseyev, *ibid.* **70**, 053607 (2004).
[9] S. Rapsch, U. Schollwöck, and W. Zwerger, Europhys. Lett. **46**, 559 (1999).
[10] J. L. DuBois and H. R. Glyde, Phys. Rev. A **68**, 033602 (2003).
[11] Z. Bačić and J. C. Light, J. Chem. Phys. **85**, 4594 (1986).
[12] M. Olshanii, Phys. Rev. Lett. **81**, 938 (1998).
[13] A. J. Leggett, Rev. Mod. Phys. **73**, 307 (2001).
[14] M. Krämer, C. Menotti, L. Pitaevskii, and S. Stringari, Eur. Phys. J. D **27**, 247 (2003).