Superfluid–Mott-insulator transition of dipolar bosons in an optical lattice

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The superfluid–Mott-insulator phase transition of dipolar bosons in optical lattice is analyzed. By using the Bogoliubov approach and decoupling approximation, the energy spectrum and zero-temperature phase diagram of dipolar bosonic atoms in an optical lattice are obtained analytically. The results show that in these systems the superfluid–Mott-insulator phase transition can be induced by tuning the dipole-dipole interaction and the position of the phase boundary can be moved when the on-site interaction is varied. Corresponding to a large on-site interaction, the dipole-dipole interaction is attractive near the critical point of the superfluid–Mott-insulator phase transition.

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Introduction. The superfluid–Mott-insulator transition of ultracold bosons in optical lattices has been recently theoretically analyzed and experimentally demonstrated [1]. Based on the Bose-Hubbard model, understanding and determining the phase transition conditions for spinless and spinor bosons in an optical lattice have been obtained using the mean-field decoupling approximation, Green function method, etc. [2–8]. In the above systems, only on-site interactions are considered and the site-to-site interactions are neglected as they are typically two orders of magnitude smaller. But for systems of ultracold dipolar bosons confined in an optical lattice, the atomic dipole moments can be sufficiently large that the site-to-site interactions cannot be neglected. The dipole-dipole forces have long-range and anisotropy characteristics and may have great influence on the properties of ultracold bosons in optical lattices [9–16]. The sources of dipolar bosons include atoms or molecules with permanent magnetic or electric dipole moments or atoms with electric dipoles induced either by large dc electric fields or by optically admixing the permanent dipole moment of a low-lying Rydberg state with the atomic ground state in the presence of a moderate dc electric field. In Ref. [12], the superfluid–Mott-insulator transition has been studied in a two-dimensional optical lattice numerically. The results indicated that the dipole-dipole interaction has important influence on the quantum phase transition of dipolar bosons and additional quantum phases such as the supersolid, checkerboard phases, etc., can be induced. As the dipole-dipole interaction can be easily tuned by an external magnetic or electric field [17], systems of dipolar bosons will become an important area to investigate the properties of atomic quantum gases and are considered to be promising candidates for the implementation of fast and robust quantum-computing schemes [15].

In this paper, the properties of the superfluid–Mott-insulator transition of dipolar bosons in an optical lattice are analyzed by the Bogoliubov transformation and mean-field decoupling approximation scheme of Ref. [3]. Mean-field theory in a phase transition problem is an approximation based on treating the order parameter as a constant. It is a useful description if fluctuations are not important. It becomes an exact theory only when the range of interactions becomes infinite. It nevertheless makes quantitatively correct predictions (e.g., the phase diagram) about some aspects of phase transitions in high spatial dimensions and makes qualitatively correct predictions in physical dimensions. In low dimensions (e.g., one dimension), the application of a mean-field calculation could be questionable because of the possibly important role of fluctuations. If the fluctuations were incorporated, mean-field theory would also give some useful predictions but a definite proof of this requires further study [3]. Mean-field theory has the enormous advantage of being mathematically simple and it is almost invariably the first approach taken to predict phase diagrams and properties of new experimental systems. There are many formulations of mean-field theory and in this paper we will use the theory presented in Refs. [3,4] to discuss the Mott-insultor–superfluid phase transition of a dipolar Bose-Einstein condensate (BEC) in an optical lattice when the fluctuations are small. This theory has been adopted generally in problems of quantum phase transitions of spinorless and spinor BECs in an optical lattice [3,5–8]. The paper is organized as follows. In Sec. II, we introduce the Bose-Hubbard model for dipolar bosons in an optical lattice. Based on this model and using the above mean-field approximations, the relations of the phase transition condition, the energy spectrum, and the phase diagram with the dipole-dipole interaction are analyzed in Secs. III, IV, and V. Section VI is the summary.

The Bose-Hubbard model for dipolar bosons in optical lattices. We consider a dilute gas of bosons in an optical lattice with the following Hamiltonian:

$$H = \int d\mathbf{r}\, \Psi^{\dagger}(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{opt}}\right)\Psi(\mathbf{r}) + \int d\mathbf{r}\, d\mathbf{r}'\, \Psi^{\dagger}(\mathbf{r})\Psi^{\dagger}(\mathbf{r}')V_{\mathrm{int}}\Psi(\mathbf{r}')\Psi(\mathbf{r}), \quad (1)$$

where $\Psi^{\dagger}(\mathbf{r})$ and $\Psi(\mathbf{r})$ are the boson field operators that annihilate and create a particle at the position $\mathbf{r}, V_{\mathrm{opt}} = V_0 \sin^2(2\pi z/\lambda)$ is the optical lattice potential, λ is the light wavelength, and V_{int} includes on-site and dipole-dipole interactions. In the case of polarized dipoles the interaction potential is

$$V_{\rm int} = \frac{d^2(1-3\cos^2\theta)}{(\mathbf{r}-\mathbf{r}')^3} + \frac{4\pi\hbar^2 a}{m}\delta(\mathbf{r}-\mathbf{r}') = V_{dd} + U_0\delta(\mathbf{r}-\mathbf{r}'), \tag{2}$$

where the first term is the dipole-dipole interaction characterized by the dipole d and the angle θ between the dipole direction and the vector $\mathbf{r}-\mathbf{r}'$, and the second term is the short-range interaction given by the s-wave scattering length a [12].

If we assume that the atoms are cooled to within the lowest Bloch band of the periodic potential, the boson field operator of $\Psi(\mathbf{r})$ and $\Psi^\dagger(\mathbf{r})$ can be expanded over Wannier functions $w(\mathbf{r}-\mathbf{r}_n)$ of the lowest-energy band localized on the ith site:

$$\Psi(\mathbf{r}) = \sum_n C_n w(\mathbf{r}-\mathbf{r}_n), \quad \Psi^\dagger(\mathbf{r}) = \sum_n C_n^\dagger w^*(\mathbf{r}-\mathbf{r}_n). \tag{3}$$

If we consider only nearest-neighbor sites of n, Eq. (1) can be expressed as

$$H = -J\sum_{i,j}\left(C_i^\dagger C_j + \text{H.c.}\right) + \frac{1}{2}U\sum_i C_i^\dagger C_i^\dagger C_i C_i + \frac{1}{2}V\sum_{i,j} C_i^\dagger C_j^\dagger C_i C_j, \tag{4}$$

where $C_i^\dagger$ and C_i are the creation and annihilation operators of an atom at site i, respectively. The parameter $J=-\int w^*(\mathbf{r}-\mathbf{r}_i)[-(\hbar^2/2m)\nabla^2+V_{\rm opt}]w(\mathbf{r}-\mathbf{r}_j)d\mathbf{r}$ is the hopping term and $U=(4\pi\hbar^2 a)/m\int|w(\mathbf{r}-\mathbf{r}_i)|^4 d\mathbf{r}$ is the short-range on-site interaction given by the s-wave scattering length a (here we assume that $a>0$). $V=\int|w(\mathbf{r}-\mathbf{r}_i)|^2 V_{dd}|w(\mathbf{r}'-\mathbf{r}_j)|^2 d\mathbf{r}\, d\mathbf{r}'$ is the dipole-dipole interaction.

Bogoliubov transformation. The energy spectrum of boson atoms in the optical lattice can be obtained by the Bogoliubov method. We first transform the Hamiltonian to the momentum space by introducing creation and annihilation operators $a_k^\dagger$ and a_k, respectively, such that

$$C_i = \frac{1}{\sqrt{N_s}}\sum_k a_k \exp(-i\mathbf{k}\cdot\mathbf{r}_i),$$

$$C_i^\dagger = \frac{1}{\sqrt{N_s}}\sum_k a_k^\dagger \exp(i\mathbf{k}\cdot\mathbf{r}_i), \tag{5}$$

where N_s is the number of lattices site and $\mathbf{r}_i$ is the coordinate of site i. The wave vector $\mathbf{k}$ runs only over the first Brillouin zone. The prefactor $1/\sqrt{N_s}$ ensures that the total number of particles obeys $N=\Sigma_i C_i^\dagger C_i=\Sigma_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$ which can be readily obtained by the relation $\Sigma_i \exp[-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i]=N_s\delta_{\mathbf{k},\mathbf{k}'}$. Using Eq. (5), the Hamiltonian, (4) can be converted into

$$H = -J\sum_k\sum_\delta a_k^\dagger a_k \exp(i\mathbf{k}\cdot\boldsymbol{\delta}) + \sum_{kk'k''k'''}\left(\frac{U_0}{2N_s}a_k^\dagger a_{k'}^\dagger a_{k''}a_{k'''}\delta_{\mathbf{k}+\mathbf{k}',\mathbf{k}''+\mathbf{k}'''} + \frac{V}{2N_s}\sum_\delta a_k^\dagger a_{k'}^\dagger a_{k''}a_{k'''}\delta_{\mathbf{k}+\mathbf{k}',\mathbf{k}''+\mathbf{k}'''}\exp[i(\mathbf{k}'-\mathbf{k}'')\cdot\boldsymbol{\delta}]\right). \tag{6}$$

For approximation, we consider only the nearest-neighbor interactions (which are denoted by δ) for the hopping and dipole-dipole interaction terms. Since the number of atoms condensed in the zero-momentum state is much larger than 1, we have $a_0 a_0^\dagger \approx a_0^\dagger a_0+1\approx N_0 \gg 1$, where N_0 is the total number of condensed atoms. Thus, we can replace the operators a_0 and $a_0^\dagger$ with a "c" number $\sqrt{N_0}$. The Hamiltonian (6) can be rewritten as (in the order of N_0)

$$\begin{aligned} H &= -2zJN_0 + \frac{1}{2}U_0 n_0 N_0 + \frac{1}{2}zVn_0N_0 + \sum_k{}'\Bigg[\left(\frac{1}{2}U_0 n_0 + \frac{1}{2}Vn_0 z\cos(ka)\right)a_k a_{-k} + [U_0 n_0 + \varepsilon_k + Vn_0 z\cos(ka)]a_k^\dagger a_k + \left(\frac{1}{2}U_0 n_0 + \frac{1}{2}Vn_0 z\cos(ka)\right)a_k^\dagger a_k^\dagger\Bigg] \\ &= A + \sum_k{}'\left(Ba_k a_{-k} + Ca_k^\dagger a_k + Da_k^\dagger a_k^\dagger\right), \end{aligned} \tag{7}$$

where $n_0=N_0/N_s, \epsilon_k=-zt\cos(ka)$, z is the number of nearest-neighbor sites for the optical lattice, and Σ_k' denotes the sum with exclusion of the term of $k=0$,

$$A = -zJN_0 + \frac{1}{2}U_0 n_0 N_0 + \frac{1}{2}zVn_0 N_0,$$

$$B = \frac{1}{2}U_0 n_0 + \frac{1}{2}Vn_0 z\cos(ka),$$

$$C = U_0 n_0 + \epsilon_k + zVn_0\cos(ka),$$

$$D = \frac{1}{2}U_0 n_0 + \frac{1}{2}Vn_0 z\cos(ka). \tag{8}$$

The effective Hamiltonian (7) can be diagonalized by the following Bogoliubov transformation:

$$b_k = u_k a_k + v_k a_{-k}^\dagger, \quad b_{-k} = u_k a_{-k} + v_k a_k^\dagger,$$

$$b_{-k}^\dagger = u_k a_{-k}^\dagger + v_k a_k, \quad b_k^\dagger = u_k a_k^\dagger + v_k a_{-k}. \tag{9}$$

We substitute Eq. (9) into the effective Hamiltonian (7) and when the nondiagonal elements equal zero, we can get

$$H^{\rm eff} = A + \sum_k{}' E_k b_k^\dagger b_k, \tag{10}$$

where $E_k=\sqrt{C^2-4B^2}$ is the energy spectrum of the quasiparticle. The energy gap of the excitation spectrum is Δ_g

$=A/N_0=-zJ+U_0n_0/2+zVn_0/2$. We can see that when $\Delta_g>0$, a gap exists, implying the Mott-insulator phase, and when $\Delta_g=0$, the gap disappears, implying the superfluid phase. Comparing with the nondipolar systems of BECs in an optical lattice, the condition for the superfluid–Mott-insulator phase transition in systems of dipolar bosons in an optical lattice is determined by three parameters, the hopping term J, the on-site interaction term U_0, and the dipole-dipole interaction term V. The dispersion relation as $k\to 0$ is

$$E_k \sim (JzU_0n_0a^2 + JVz^2n_0a^2)^{1/2}k. \tag{11}$$

From Eq. (11), we can see that the relation of the excitation spectrum E_k with k is linear. This explicitly indicates superfluidity, in agreement with the Bogoliubov superfluid theory for weakly interacting bosons in the absence of a periodic potential. The persistent velocity of the superfluid or quasiparticle can be found as

$$v_s = \left(\frac{\partial E_k}{\partial k}\right)_{k\to 0} = (JzU_0n_0a^2 + JVz^2n_0a^2)^{1/2}. \tag{12}$$

From Eq. (12), we can also see that the velocity of the superfluid in a system of dipolar bosons in an optical lattice can be controlled by V in addition to J and U_0.

The decoupling approximation with dipole-dipole interaction. To find more information about the phase transition of dipolar bosons in an optical lattice, we now determine the analytic relation of the phase diagram with dipole-dipole interactions using the decoupling approximation method in Ref. [3]. We introduce the superfluid order parameter $\psi=\sqrt{n_i}=\langle C_i^\dagger\rangle=\langle C_i\rangle$, where n_i is the expectation value of the number of particles on site i. This value we often take to be real. In the mean-field approximation and assuming that the average occupation number of Bose atoms condensed in the ground state in each site of the optical lattice is the same, we can get the effective Hamiltonian on the site i,

$$H^{\text{eff}} = \frac{1}{2}\overline{U}_0\hat{n}(\hat{n}-1) + \frac{1}{2}z\overline{V}\hat{n}\hat{n} - \overline{\mu}\hat{n} - \psi(C^\dagger + C) + \psi^2, \tag{13}$$

where μ is the chemical potential $\overline{U}_0=U_0/zJ$, $\overline{\mu}=\mu/zJ$, $\overline{V}=V/zJ$, and $\hat{n}_i=C_i^\dagger C_i$ is the number operator. In the above equation, we consider only the nearest-neighbor interactions for the dipole-dipole interaction and the subscript i is neglected for convenience. The effective Hamiltonian (13) can be diagonal with respect to the site i. The phase diagram can be analytically determined using second-order perturbation theory. H^{eff} can be divided into two parts as

$$H_0 = \frac{1}{2}\overline{U}_0\hat{n}(\hat{n}-1) - \overline{\mu}\hat{n} + \frac{1}{2}z\overline{V}\hat{n}^2 + \psi^2,$$

$$H_1 = -(C^\dagger + C). \tag{14}$$

In an occupation number basis the odd powers of the expansion of the energy in ψ will always be zero. If we denote the unperturbed energy of the state with exactly n particles by $E_n^{(0)}$, we find that the unperturbed ground-state energy is given by $E_g^{(0)}$. Comparing $E_n^{(0)}$ and $E_{n+1}^{(0)}$, we find that $E_g^{(0)}=0$ if $\overline{\mu}<0$ and $E_g^{(0)}=\frac{1}{2}\overline{U}g(g-1)-\overline{\mu}g+\frac{1}{2}z\overline{V}g^2$ if $\overline{U}_0(g-1)+\frac{1}{2}\overline{V}z(1-g)<\overline{\mu}<\overline{U}_0g+\frac{1}{2}\overline{V}z(1+g)$. The second-order correction to the energy is calculated by the following expression:

$$E_g^{(2)} = \psi^2\sum_{n\neq g}\frac{|\langle g|H_1|n\rangle|^2}{E_g^{(0)}-E_n^{(0)}} = \psi^2\sum_{n\neq g}\frac{\langle g|H_1|n\rangle\langle n|H_1|g\rangle}{E_g^{(0)}-E_n^{(0)}}, \tag{15}$$

where $n=g$ particles are in the ground state. Since the interaction V couples only to states with one more or one less atom than in the ground state, we find

$$\langle g|H_1|n\rangle = -\langle g|(C^\dagger + C)|n\rangle = \begin{cases}\sqrt{g+1}, & n=g+1,\\ \sqrt{g}, & n=g-1.\end{cases} \tag{16}$$

Combining Eqs. (14)–(16), we get

$$E_g^{(2)} = \left(\frac{(g+1)}{\overline{\mu}-\overline{U}_0g-\frac{1}{2}\overline{V}z-\overline{V}gz} + \frac{g}{\overline{U}_0g-\overline{\mu}-\overline{U}_0-\frac{1}{2}\overline{V}z+\overline{V}gz}\right). \tag{17}$$

So, $E_g(\psi)=a_0(g,\overline{U}_0,\overline{V},\overline{\mu})+a_2(g,\overline{U}_0,\overline{V},\overline{\mu})\psi^2+\cdots$, where

$$a_0(g,U_0,V,\mu) = \frac{1}{2}\overline{U}_0g(g-1) - \overline{\mu}g + \frac{1}{2}z\overline{V}g^2,$$

$$a_2(g,U_0,V,\mu) = 1 + \left(\frac{(g+1)}{\overline{\mu}-\overline{U}_0g-\frac{1}{2}\overline{V}z-\overline{V}gz} + \frac{g}{\overline{U}_0g-\overline{\mu}-\overline{U}_0-\frac{1}{2}\overline{V}z+\overline{V}gz}\right). \tag{18}$$

The phase diagram with dipole-dipole interaction. According to the Landau procedure for second-order phase transitions, the boundary between the superfluid and the insulator phases can be determined by $a_2(g,U_0,V,\mu)=0$. The result is

$$\overline{\mu}_\pm = \frac{1}{2}F \pm \frac{1}{2}\sqrt{F^2+4G}, \tag{19}$$

where the subscripts $\pm$ denote the upper and lower halves of the Mott-insulating regions of phase space and

$$F = B + D - 1, \quad G = g(D-B) + D - BD,$$

$$B = \overline{U}_0g + \frac{1}{2}\overline{V}z + \overline{V}gz, \quad D = \overline{U}_0g - \overline{U}_0 - \frac{1}{2}\overline{V}z + \overline{V}gz. \tag{20}$$

The phase boundaries can be obtained from Eq. (9). In contrast to the phase diagram of a one-species BEC which is drawn in $\overline{U}_0$-μ space (see, e.g., Fig. 2 in Ref. [3]), we draw the phase diagram of dipolar bosons in the optical lattice in $\overline{V}$-μ space. Figure 1(a) shows a plot of Eq. (19) for $g=1$, 2, 3 with $\overline{U}_0=9$, where "SF" indicates the superfluid phase and "MI" indicates the Mott-insulator phase. The critical value of $\overline{V}_c$ is determined by equating μ_+ and μ_-,

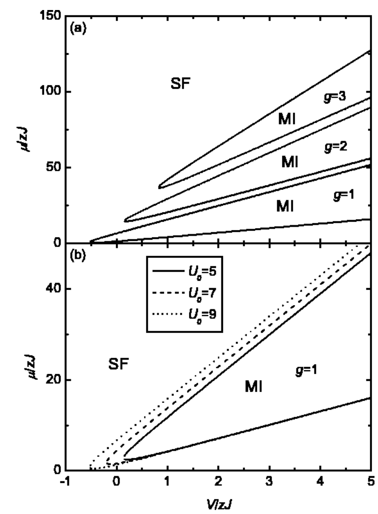

FIG. 1. Phase diagram of dipolar Bose-Hubbard model in an optical lattice with (a) $U_0=9$ and (b) different on-site energies U_0. The vertical axis shows the dimensionless chemical potential $\mu/zJ=\overline{\mu}$ and the horizontal axis shows the dimensionless dipole-dipole interaction $V/zJ=\overline{V}$. "SF" and "MF" mean "superfluid phase" and "Mott-insulator phase", respectively.

$$\overline{V}_c = \frac{1}{z}\left(1 + 2g - \overline{U}_0 + 2\sqrt{g + g^2}\right). \tag{21}$$

Figure 1(b) shows a plot of Eq. (19) for $g=1$ with $\overline{U}_0=9$, 7, 5. We can see that the critical value $\overline{V}_c$ varies from positive to negative with increasing on-site interaction. This phenomenon shows that the dipole-dipole interaction is attractive for a large on-site interaction (corresponding to a large *s*-wave scattering length) near the superfluid–Mott-insulator phase transition critical point.

The beauty of the dipolar interaction lies in the fact that it is a directional interaction in contrast to the usual *s*-wave interaction between atoms. We use the tunability of the magnetic dipolar interaction for an example [17]. In a time-dependent external magnetic field $\mathbf{B}(t)=B\{\cos\varphi\hat{\mathbf{z}} +\sin\varphi[\cos(\Omega t)\hat{\mathbf{x}}+\sin(\Omega t)\hat{\mathbf{y}}]\}$, which is a combination of a static magnetic field B_z directed along the $\mathbf{z}$ direction and a fast rotating field B_ρ in the radial plane, the frequency is chosen such that the atoms are not significantly moving during the time Ω^{-1}, while the magnetic moments will adiabatically follow the external field $\mathbf{B}(t)$. In this limit, the average of the magnetic dipole-dipole interaction in a cylindrically symmetric interatomic potential and in the period $2\pi/\Omega$ is

$$\langle U_{dd}(r,\theta,\phi)\rangle = -\frac{\mu_0 m^2}{4\pi}\left(\frac{3\cos^2\theta - 1}{r^3}\right)\left(\frac{3\cos^2\varphi - 1}{2}\right). \tag{22}$$

From Eq. (22), we can see that the angle φ between the dipole orientation and the $\mathbf{z}$ axis determines the strength of the sign of the dipole-dipole interaction. For $\varphi=0$, the magnetic dipoles are polarized along the $\mathbf{z}$ direction and the dipole-dipole interaction is positive. For $\varphi=\pi/2$, the sign of the dipole-dipole interaction is inverted and the absolute value is only one-half of that in the polarized case. For $\varphi=54.7°$, the dipolar interaction averages to zero. Around the magic angle, there exists a stable phase diagram area in which we can observe the phase transition we suggest in our paper.

Conclusion. Based on the Bose-Hubbard model, the superfluid–Mott-insulator phase transition for systems of dipolar bosons in an optical lattice has been studied. Using the Bogoliubov transformation and decoupling approximation scheme, the condition for the phase transition between the superfluid phase and Mott insulator, the energy and the velocity of the quasiparticles in the superfluid phase, and the phase diagram relation to the dipole-dipole interaction have been obtained analytically. The results show that the superfluid–Mott-insulator phase transition of dipolar bosons in an optical lattice can be tuned by the dipole-dipole interaction as well as the interatomic repulsion and the hopping term. So dipolar boson systems in an optical lattice give us an additional tool to study the quantum phase transition.

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