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.

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-insulator–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:

\[ H = \int d^3r \, \Psi^\dagger(r) \left( -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{opt}} \right) \Psi(r) + \int d^3r \int d^3r' \Psi^\dagger(r) \Psi^\dagger(r') V_{\text{int}} \Psi(r') \Psi(r), \]  

(1)

where \( \Psi^\dagger(r) \) and \( \Psi(r) \) are the boson field operators that annihilate and create a particle at the position \( r \). \( V_{\text{opt}} = V_0 \sin^2(2\pi r/\lambda) \) is the optical lattice potential, \( \lambda \) is the light wavelength, and \( V_{\text{int}} \) includes on-site and dipole-dipole interactions. In the case of polarized dipoles the interaction potential is
\[ V_{\text{int}} = \frac{d^2(1 - 3 \cos^2 \theta)}{(r - r')^3} + \frac{4 \pi \hbar^2 \alpha}{m} \delta(r - r') = V_{dd} + U_0 \delta(r - r'), \]

where the first term is the dipole-dipole interaction characterized by the dipole direction and the vector \( r - r' \), 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 \( \Psi(r) \) and \( \Psi^\dagger(r) \) can be expanded over Wannier functions \( w(r - r_n) \) of the lowest-energy band localized on the \( n \)th site:

\[ \Psi(r) = \sum_n C_n w(r - r_n), \quad \Psi^\dagger(r) = \sum_n C_n^\dagger w^\dagger(r - r_n). \]

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

\[ H = -J \sum_{i,j} (C_i^\dagger C_j + \text{H.c.}) + \frac{1}{2} \sum_i C_i^\dagger C_i C_i + \frac{1}{2} V \sum_{i,j} C_i^\dagger C_j C_i C_j, \]

where \( C_i^\dagger \) and \( C_i \) are the creation and annihilation operators of an atom at site \( i \), respectively. The parameter \( J = -\int w(r - r') \left[ (\hbar^2/2m) \nabla^2 + V_{\text{opt}}(r - r') \right] d^3r \) is the hopping term and \( V = \int [w(r - r')]^2 [V_{\text{dd}} + V_{\text{opt}}(r' - r)]^2 d^3r' \) is the short-range on-site interaction given by the \( s \)-wave scattering length \( a \) (here we assume that \( a > 0 \)).

The energy gap of the excitation spectrum is \( D = 1/\sqrt{N} \). The Hamiltonian (4) can be rewritten as (in the order of \( N_0 \))

\[ H = -2 \zeta J N_0 + \frac{1}{2} U_0 n_0 N_0 + \frac{1}{2} \zeta V n_0 N_0 + \sum_k \left[ \left( \frac{1}{2} U_0 n_0 \right) a_k^\dagger a_k + \frac{1}{2} V n_0 \zeta \cos(k a_0) \right] a_k^\dagger a_k + \left( \frac{1}{2} U_0 n_0 + \frac{1}{2} \zeta V n_0 \zeta \cos(k a_0) \right) a_k^\dagger a_k \]

\[ = A + \sum_k \left( B a_k^\dagger a_k + C a_k^\dagger a_k + D a_k^\dagger a_k \right), \]

where \( n_0 = N_0/N, \quad a_k^\dagger = -i \zeta \cos(k a_0), \quad \zeta = \sqrt{2} \zeta \cos(k a_0), \quad A = -\zeta J N_0 + \frac{1}{2} U_0 n_0 N_0 + \frac{1}{2} \zeta V n_0 N_0, \quad B = \frac{1}{2} U_0 n_0 + \frac{1}{2} \zeta V n_0 \zeta \cos(k a_0), \quad C = U_0 n_0 + \zeta V n_0 \zeta \cos(k a_0), \quad D = \frac{1}{2} U_0 n_0 + \frac{1}{2} \zeta V n_0 \zeta \cos(k a_0). \]

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

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

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

\[ H^\text{eff} = A + \sum_k E_k b_k^\dagger b_k, \]

where \( E_k = \sqrt{C^2 - 4B^2} \) is the energy spectrum of the quasiparticle. The energy gap of the excitation spectrum is \( \Delta_e \)
\[ E_k \sim (J_z U_d a^2 + J V^2 n_d a^2)^{1/2}. \]  
\[ \psi = \left( \frac{\partial E_k}{\partial k} \right)_{k \to 0} = (J_z U_d n_d a^2 + J V^2 n_d a^2)^{1/2}. \]  

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 \( \psi = \sqrt{n_{C_i} - (C_i)^\dagger} \), 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 \( i \),

\[ H_{\text{eff}} = \frac{1}{2} \hat{U}_0 \hat{n} (\hat{n} - 1) + \frac{1}{2} \hat{V} \hat{n} \hat{n} - \hat{\mu} \hat{n} - \phi (C_i^+ + C_i) + \psi^2, \]  

where \( \mu \) is the chemical potential \( \tilde{U}_0 = U_0 / J, \tilde{\mu} = \mu / J, \tilde{V} = V / J \), and \( \hat{n} = C_i^\dagger C_i \) 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. \( H_{\text{eff}} \) can be divided into two parts as

\[ H_0 = \frac{1}{2} \hat{U}_0 \hat{n} (\hat{n} - 1) - \hat{\mu} \hat{n} + \frac{1}{2} \hat{V} \hat{n}^2 + \psi^2, \quad H_1 = - (C_i^+ + C_i). \]  

In an occupation number basis the odd powers of the expansion of the energy in \( \psi \) 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 \( E_n^{(0)} + \psi^2 \), we find that \( E_g^{(0)} = 0 \) if \( \tilde{\mu} < 0 \) and \( E_g^{(0)} = \frac{1}{2} \tilde{U}_0 g (g - 1) - \frac{1}{2} \tilde{V} g^2 \) if \( \tilde{U}_0 g (g - 1) + \frac{1}{2} \tilde{V} (1 - g) < \tilde{\mu} < \tilde{U}_0 g + \frac{1}{2} \tilde{V} (1 + g) \). The second-order correction to the energy is calculated by the following expression:

\[ E_g^{(2)} = \psi^2 \sum_{n \neq g} \frac{\langle [n|H_g|n]\rangle^2}{E_n^{(0)} - E_n^{(0)} - E_g^{(0)} - E_n^{(0)}}, \]  

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

\[ \langle [n|H_g|n]\rangle = \langle (C_i^+ + C_i)|n\rangle = \begin{cases} (g + 1), & n = g + 1, \\ (g - 1), & n = g - 1. \end{cases} \]  

Combining Eqs. (14)–(16), we get

\[ E_g^{(2)} = \frac{(g + 1)}{\tilde{U}_0 g - \frac{1}{2} \tilde{V} g - \tilde{V} g^z} + \frac{g}{\tilde{U}_0 g - \tilde{\mu} - \tilde{U}_0 - \frac{1}{2} \tilde{V} g + \tilde{V} g^z}. \]  

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

\[ a_0(g, U_0, V, \mu) = \frac{1}{2} \tilde{U}_0 g (g - 1) - \tilde{\mu} g + \frac{1}{2} \tilde{V} g^2, \quad a_2(g, U_0, V, \mu) = \frac{(g + 1)}{\tilde{U}_0 g - \frac{1}{2} \tilde{V} g - \tilde{V} g^z} + \frac{g}{\tilde{U}_0 g - \tilde{\mu} - \tilde{U}_0 - \frac{1}{2} \tilde{V} g + \tilde{V} g^z}. \]  

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

\[ \tilde{\mu} \pm = \frac{1}{2} F \mp \frac{1}{2} \tilde{F}^2 + 4G, \]  

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

\[ F = B + D - 1, \quad G = g(D - B) - D - BD, \quad B = \tilde{U}_0 g + \frac{1}{2} \tilde{V} g + \tilde{V} g^z, \quad D = \tilde{U}_0 g - \tilde{U}_0 - \frac{1}{2} \tilde{V} g + \tilde{V} g^z. \]  

The phase boundaries can be obtained from Eq. (9). In contrast to the phase diagram of a one-species BEC which is drawn in \( \tilde{U}_0 - \mu \) space (see, e.g., Fig. 2 in Ref. [3]), we draw the phase diagram of dipolar bosons in the optical lattice in \( V - \mu \) space. Figure 1(a) shows a plot of Eq. (19) for \( g = 1, 2, 3 \) with \( \tilde{U}_0 = 9 \), where “SF” indicates the superfluid phase and “MI” indicates the Mott-insulator phase. The critical value of \( \tilde{V}_c \) is determined by equating \( \mu_+ \) and \( \mu_- \).
A large on-site interaction shows that the dipole-dipole interaction is attractive for negative with increasing on-site interaction. This phenomenon shows that the critical value $V_c$ of the dipole-dipole interaction $V = V_c$ for an example interaction between atoms. We use the tunability of the magnetic dipoles are polarized along the $z$ 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 $\varphi = 54.7^\circ$, 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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**References**