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Superfluid-Insulator Phase Transitions of the Extended Bose-Hubbard Model

Xiao Qiang Su[1,*] and An Min Wang[2]

[1] *College of Physics and Information Engineering, Shanxi Normal University, Linfen, 041004, P.R. China*
[2] *Department of Modern Physics, University of Science and Technology of China, Hefei, 230026, P.R. China*

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In this paper, the extended Bose-Hubbard model with nearest neighbor interaction is discussed using the method of Green functions in the mean-field approximation. Starting from the two-sublattice approach developed by Hewson and ter Haar, we solve the equations of motion of the Green functions and obtain the energy-band structure. Then, by taking the limit of a vanishing energy gap in the energy-band structure, we find the superfluid-insulator phase boundaries for an integer filling density. Finally, the ground state phase boundaries of the one-dimension extended Bose-Hubbard model for $\rho = 1$ are presented, and the tricritical point is obtained.

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I. INTRODUCTION

In recent years, the study of quantum phase transitions in systems of interacting bosons is an exciting area, particularly in the topic of Bose condensed cold atoms trapped in optical-lattice potentials [1–6]. The advantages, such as the facility of experimental parameter control and the absence of disorder, make the cold atoms in optical lattices to be an ideal system for studying quantum phase transitions in strongly correlated systems. For example, Greiner *et al.* [3] have observed a superfluid-Mott-insulator transition for ^{87}Rb atoms, trapped in a three-dimensional optical-lattice potential, by changing the strength of the onsite potential. The Bose-Hubbard model is introduced as the starting point of the theoretical studies. By investigating the existence of a gap in the energy spectrum obtained with the Green function approach, Liang *et al.* [4] have obtained a phase transition condition.

The observation of a supersolid helium 4 phase [7, 8] has given stimulation to this area: in the extended Bose-Hubbard model with nearest neighbor interaction it is possible to exhibit a supersolid phase [9, 10]. Its Hamiltonian is

$$H = -t\sum_{\langle i,j\rangle}(a_i^\dagger a_j + \text{h.c.}) + \frac{U}{2}\sum_i n_i(n_i-1) + V\sum_{\langle i,j\rangle} n_i n_j \ , \tag{1}$$

where $a_i^\dagger(a_i)$ is the boson creation(annihilation) operator and $n_i = a_i^\dagger a_i$ is the particle number operator at site i; the bracket $\langle i,j\rangle$ means that i,j are nearest neighbor sites. The parameter t is the hopping parameter, and $U, V > 0$ are presented respectively for the onsite and nearest-neighbor repulsive interactions. The phase transitions of the one-dimensional

model have been studied by several numerical methods like quantum simulation [11], quantum Monte Carlo [12, 13], and the density-matrix renormalization group [14, 15]. The phase diagram of the model with a variational chemical potential μ was obtained by the methods of the Gutzwiller ansatz [9, 16, 17] and quantum Monte Carlo [13] too. In this paper, we investigate and obtain an analytic phase transition condition of the extended Bose-Hubbard model.

The extended Bose-Hubbard model with nearest neighbor interaction has a richer phase diagram than the usual Bose-Hubbard model, in the strong coupling region there are two insulator phases, the Mott insulator (MI) phase and the mass-density-wave insulator (MDW) [or charge-density-wave (CDW) if the bosons are charged] phase [11]. With an increase of the hopping t, a quantum phase transition occurs to the superfluid phase for both of the two insulator phases. In particular, the MDW phase comes through a spontaneous translational symmetry breaking [9] phase transition from the MI phase, so we introduce a two-sublattice approach [18, 19] which is suitable to the inhomogeneous MDW phase. Such an approach has also been applied to the system of the antiferromagnetic Heisenberg model [20]. In Sec. II we discuss the MI-MDW phase transition in the strong coupling region. In Sec. III we use the Green function method and mean-field approximation to get a closed equation of motion for the Green function. The two-sublattice approach [18, 19] is introduced in Sec. IV with four different kinds of Green functions. By solving the simultaneous equations for the Green functions we obtain the energy spectrum of the extended Bose-Hubbard model. Then in Sec. V we compare the energy spectrum with that of the usual Bose-Hubbard model with $V = 0$. By defining the energy gap and then taking it to vanish, we obtain the analytic phase boundaries where the insulator phases begin to exhibit a superfluid order. The ground-state phase diagram of one dimension is also presented.

II. STRONG COUPLING REGION

The Hamiltonian (1) can be divided into

$$H = H_1 + H_2, \tag{2}$$

where

$$H_1 = -t\sum_{\langle i,j\rangle}(a_i^\dagger a_j + \text{h.c.}), \quad H_2 = \frac{U}{2}\sum_i n_i(n_i-1) + V\sum_{\langle i,j\rangle} n_i n_j\,.$$

Based on the known studies, if U,V are very large compared with t, the ground state will be a MI phase for larger U and a MDW phase for larger V. For the one dimensional lattice, a MI-MDW phase transition takes place at $U = 2V$ [14]. With the integer filling density $\rho = g$ (where g is a nonnegative integer), the mean-field wave functions of the MI and MDW will be respectively

$$|\Psi\rangle = \begin{cases} \prod_i |g\rangle_i, & \text{(MI)} \\ \prod_i |0\rangle_{2i}\otimes|2g\rangle_{2i+1} \ \ (\text{or } \prod_i |2g\rangle_{2i}\otimes|0\rangle_{2i+1})\,, & \text{(MDW)} \end{cases}$$

where $|n\rangle_i$ denotes the Fock state with n particles at the site i; the contribution of the first term in Eq. (2) is

$$\langle\Psi|H_1|\Psi\rangle = 0\,.$$

For lattice number N, the energies of the two insulator phases are respectively

$$E = \langle\Psi|H|\Psi\rangle = \begin{cases} E_{\rm MI} = \dfrac{N(U+2V)}{2}g^2 - \dfrac{NUg}{2}\,, & \text{(MI)} \\ \\ E_{\rm MDW} = NUg^2 - \dfrac{NUg}{2}\,. & \text{(MDW)} \end{cases} \tag{3}$$

We can find $E_{\rm MI} < E_{\rm MDW}$ when $U > 2V$, $E_{\rm MI} > E_{\rm MDW}$ when $U < 2V$, and the energies of the two phases degenerate when $U = 2V$.

III. GREEN FUNCTION

The single-particle retarded Green function at zero temperature is defined by [4, 21] ($\hbar = 1$)

$$\langle\langle a_i(t); a_j^\dagger(t')\rangle\rangle = \begin{cases} -i\langle[a_i(t), a_j^\dagger(t')]\rangle, & (t > t') \\ \\ 0, & (t < t') \end{cases} \tag{4}$$

where $a_i(t)$, $a_j^\dagger(t')$ are the operators in the Heisenberg picture. The Green function $\langle\langle a_i(t); a_j^\dagger(t')\rangle\rangle$ depends only on the time difference $(t - t')$; the Fourier transformation reads

$$G_{ij}(\omega) \equiv \langle\langle a_i|a_j^\dagger\rangle\rangle_\omega = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dt\langle\langle a_i(t); a_j^\dagger(0)\rangle\rangle \exp[i(\omega + i\varepsilon)t], \qquad \varepsilon = 0^+\,. \tag{5}$$

From the Heisenberg equation, it follows that [4]

$$\omega G_{ij}(\omega) = \langle[a_i, a_j^\dagger]\rangle + \langle\langle[a_i, H] \mid a_j^\dagger\rangle\rangle_\omega\,, \tag{6}$$

where $\langle\ \ \rangle$ denotes the ground state expectation value. Substituting Eq. (1) into Eq. (6), we have

$$[a_i, H] = -t\sum_\delta a_{i+\delta} + Un_i a_i + V\sum_\delta n_{i+\delta}a_i\,, \tag{7}$$

the sum of δ means all the nearest neighbor sites of i. Again using Eq. (7), we obtain

$$\omega G_{ij}(\omega) = \delta_{ij} - t\sum_\delta G_{i+\delta,j} + \langle\langle\Omega_i a_i|a_j^\dagger\rangle\rangle_\omega\,. \tag{8}$$

Here we have defined a new operator

$$\Omega_i \equiv U n_i + V \sum_\delta n_{i+\delta} \,.$$

Note that $\langle\langle \Omega_i a_i | a_j^\dagger \rangle\rangle_\omega$ is the higher-order Green function; it satisfies the following equation

$$\omega \langle\langle \Omega_i a_i | a_j^\dagger \rangle\rangle_\omega = \langle [\Omega_i a_i, a_j^\dagger] \rangle + \langle\langle [\Omega_i a_i, H] | a_j^\dagger \rangle\rangle_\omega \,, \tag{9}$$

with

$$[\Omega_i a_i, H] = -t \underline{\Omega_i} \sum_\delta a_{i+\delta} + \underline{\Omega_i} \Omega_i a_i - U t \underline{\sigma_i} a_i - V t \sum_\delta \underline{\sigma_{i+\delta}} a_i \,, \tag{10}$$

where the operator σ_i is defined by $\sigma_i \equiv \sum_\delta (a_i^\dagger a_{i+\delta} - a_{i+\delta}^\dagger a_i)$. We use the mean-field approximation for the underlined operators, replacing the operators by their ground state expectation value, e.g., $\Omega_i \Omega_i a_i \to \langle \Omega_i \rangle \Omega_i a_i$ and $\sigma_i a_i \to \langle \sigma_i \rangle a_i$. Paying attention only to the insulator phases, we ignore the particle hopping of the insulator phases to assume that $\langle \sigma_i \rangle = 0$ for each site. We will find later (see Sec. V) when the insulator phases begin to exhibit a superfluid order. Here Eq. (10) is simplified as

$$[\Omega_i a_i, H] = -t \langle \Omega_i \rangle \sum_\delta a_{i+\delta} + \langle \Omega_i \rangle \Omega_i a_i \,. \tag{11}$$

Substituting Eq. (11) into Eq. (9) leads to

$$\langle\langle \Omega_i a_i | a_j^\dagger \rangle\rangle_\omega = \tag{12}$$
$$\frac{1}{\omega - \langle \Omega_i \rangle} \left[\left(2U \langle n_i \rangle + V \sum_\delta \langle n_{i+\delta} \rangle \right) \delta_{ij} + V \sum_\delta \langle a_{i+\delta}^\dagger a_i \rangle \delta_{i+\delta,j} - t \langle \Omega_i \rangle \sum_\delta G_{i+\delta,j}(\omega) \right] .$$

Substituting Eq. (12) into Eq. (8) yields

$$\omega G_{ij}(\omega) = \delta_{ij} \tag{13}$$
$$-t \sum_\delta G_{i+\delta,j} + \frac{\left(2U \langle n_i \rangle + V \sum_\delta \langle n_{i+\delta} \rangle\right) \delta_{ij} + V \sum_\delta \langle a_{i+\delta}^\dagger a_i \rangle \delta_{i+\delta,j} - t \langle \Omega_i \rangle \sum_\delta G_{i+\delta,j}(\omega)}{\omega - \langle \Omega_i \rangle} \,.$$

IV. SUBLATTICE APPROACH

For the existence of the MDW phase where empty and doubly occupied alternate, the properties for nearest neighbor sites may be different. We pay attention only to the lattices that can be divided into two equivalent interpenetrating sublattices A and B, so that all the nearest neighbors of A are on B and vice versa. According to which sublattice the particles live in, we introduce four kinds of Green functions:

$$G_{ij}^{AA}(\omega), \qquad G_{ij}^{AB}(\omega), \qquad G_{ij}^{BA}(\omega), \qquad G_{ij}^{BB}(\omega).$$

The superscripts mean which sublattice the i, j sites belong to, e.g., for $G_{ij}^{AB}(\omega)$, $i \in A$ and $j \in B$. Using the approach of Sec. III, we can obtain

$$\omega G_{ij}^{AA}(\omega) = \delta_{ij} - t\sum_{\delta} G_{i+\delta,j}^{BA} + \frac{(2U\langle n_i^A\rangle + V\sum_\delta \langle n_{i+\delta}^B\rangle)\delta_{ij} - t\langle\Omega_i^A\rangle\sum_\delta G_{i+\delta,j}^{BA}(\omega)}{\omega - \langle\Omega_i^A\rangle}, \quad (14)$$

$$\omega G_{ij}^{BA}(\omega) = -t\sum_{\delta} G_{i+\delta,j}^{AA} + \frac{V\sum_\delta \langle a_{i+\delta}^\dagger a_i^B\rangle\delta_{i+\delta,j} - t\langle\Omega_i^B\rangle\sum_\delta G_{i+\delta,j}^{AA}(\omega)}{\omega - \langle\Omega_i^B\rangle}. \quad (15)$$

Introducing the space Fourier transformation of the Green function $G_{\mathbf{k}}^{\lambda\lambda'}(\omega)$ defined [20] by

$$G_{\mathbf{k}}^{\lambda\lambda'}(\omega) = \frac{2}{N}\sum_{i,j}\exp[i\mathbf{k}\cdot(\mathbf{x}_i - \mathbf{x}_j)]G_{ij}^{\lambda\lambda'}(\omega), \qquad (\lambda = A, B) \quad (16)$$

and assuming that the average occupation number of particles in each site of the same sublattice are equal—i.e., $\langle n_i^\lambda\rangle = n^\lambda$, $\langle\Omega_i^\lambda\rangle = \Omega^\lambda$, and the $\langle a_{i+\delta}^\dagger a_i^B\rangle = \varphi_\delta^B$ are equal for each site i of sublattice B—we can write the equations of motion for the Green functions $G_k^{AA}(\omega)$ and $G_k^{BA}(\omega)$ for a simple cubic lattice as

$$\omega G_k^{AA}(\omega) = \frac{\omega - \Omega^A + 2Un^A + zVn^B}{\omega - \Omega^A} - \frac{z\omega t\cos(ka)}{\omega - \Omega^A}G_k^{BA}(\omega), \quad (17)$$

$$\omega G_k^{BA}(\omega) = \frac{V\sum_\delta \varphi_\delta^B e^{ik\delta a}}{\omega - \Omega^B} - \frac{z\omega t\cos(ka)}{\omega - \Omega^B}G_k^{AA}(\omega), \quad (18)$$

where z is the number of the nearest neighbors of each site and a is the lattice constant. It is easy to obtain the solutions of Eqs. (17) and (18) in the following form:

$$G_k^{AA}(\omega) = \frac{A_k^0}{\omega - E^0} + \frac{A_k^+}{\omega - E_k^+} + \frac{A_k^-}{\omega - E_k^-}, \quad (19)$$

$$G_k^{BA}(\omega) = \frac{B_k^0}{\omega - E^0} + \frac{B_k^+}{\omega - E_k^+} + \frac{B_k^-}{\omega - E_k^-}, \quad (20)$$

where E^0 and $E_k^\pm$ denote the poles of the Green functions, and

$$\begin{cases} A_k^0 = \dfrac{\Omega^A\Omega^B - (2Un^A + zVn^B)\Omega^B - ztV\cos(ka)\sum_\delta \varphi_\delta^B e^{ik\delta a}}{E_k^- E_k^+}, \\ A_k^+ = \dfrac{[E_k^+ - \Omega^A + (2Un^A + zVn^B)](E_k^+ - \Omega^B) - ztV\cos(ka)\sum_\delta \varphi_\delta^B e^{ik\delta a}}{E_k^+(E_k^+ - E_k^-)}, \\ A_k^- = \dfrac{[E_k^- - \Omega^A + (2Un^A + zVn^B)](E_k^- - \Omega^B) - ztV\cos(ka)\sum_\delta \varphi_\delta^B e^{ik\delta a}}{E_k^-(E_k^- - E_k^+)}, \end{cases}$$

$$\begin{cases} B_k^0 = \dfrac{\Omega^A[zt\cos(ka) - V\sum_\delta \varphi_\delta^B e^{ik\delta a}] - (2Un^A + zVn^B)zt\cos(ka)}{E_k^- E_k^+}, \\ B_k^+ = \dfrac{(E_k^+ - \Omega^A)[zt\cos(ka) - V\sum_\delta \varphi_\delta^B e^{ik\delta a}] - (2Un^A + zVn^B)zt\cos(ka)}{E_k^+(E_k^+ - E_k^-)}, \\ B_k^- = \dfrac{(E_k^- - \Omega^A)[zt\cos(ka) - V\sum_\delta \varphi_\delta^B e^{ik\delta a}] - (2Un^A + zVn^B)zt\cos(ka)}{E_k^-(E_k^- - E_k^+)}. \end{cases}$$

Specially, for $k = \pm\pi/2a$ we have $A_k^- = 0$ and $B_k^+ = 0$. It is seen that the excitation spectrum possesses a band structure (see Fig. 1) such as

$$\begin{cases} E^0 = 0, \\ E_k^\pm = \dfrac{(\Omega^A + \Omega^B) \pm \sqrt{(\Omega^A - \Omega^B)^2 + 4z^2t^2\cos^2(ka)}}{2}. \end{cases} \tag{21}$$

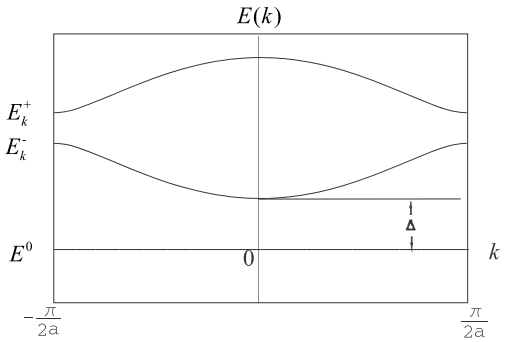

FIG. 1: The band structure of the energy spectrum and the energy gap. The k runs over the first Brillouin zone.

V. PHASE TRANSITION

Comparing with the usual Bose-Hubbard model with $V = 0$ [4], the up-energy-band ($E_k^{(2)}$ in Ref. [3]) is divided into two bands: E_k^+ and E_k^-, and the low-energy-band ($E^{(1)}$ in Ref. [3]) still remains. The two bands E_k^+ and E_k^- are joined at $k = \pm\pi/2a$ for the MI phase, and disjoined for the MDW phase by a split: $(E_k^+ - E_k^-)|_{k=\pm\pi/2a} = |\Omega^A - \Omega^B|$. Obviously, the energy band split arises from the inhomogeneity in the onsite particle density. A similar energy spectrum for the MDW phase with a half-integer filling density $\rho = \frac{1}{2}$ has been obtained [16]. The energy gap can be defined by (see Fig. 1)

$$\Delta = E_k^-|_{k=0} - E^0 = \frac{(\Omega^A + \Omega^B) - \sqrt{(\Omega^A - \Omega^B)^2 + 4z^2t^2}}{2}. \tag{22}$$

The existence of the gap implies an insulator phase; with increasing t the gap width Δ decreases and finally disappears, indicating the appearance of the superfluid order [4]. For the integer filling density $\rho = g$, we have

$$\begin{cases} n^A = n^B = g, \\ \\ \Omega^A = \Omega^B = Ug + zVg. \end{cases} \qquad \text{(MI)} \tag{23}$$

$$\begin{cases} n^A = 2g, \quad n^B = 0, \\ \\ \Omega^A = 2Ug, \quad \Omega^B = 2zVg. \end{cases} \qquad \text{(MDW)} \tag{24}$$

Substituting Eq. (23) and Eq. (24) into Eq. (22) and using the condition of the superfluid-insulator phase transition $\Delta = 0$, we obtain

$$\begin{cases} (U + zV)g = 2t, & \text{(MI} - \text{SF)} \\ \\ zUVg^2 = t^2. & \text{(MDW} - \text{SF)} \end{cases} \tag{25}$$

Recalling the discussion in Sec. II, we can obtain the ground state phase diagram (see Fig. 2) of the one dimensional extended Bose-Hubbard model for $g = 1$. The phase boundaries of MI-SF and MDW-SF are respectively $U + 2V = 2$ and $2UV = 1$ (rescaling by $t = 1$), and the MI-MDW phase transition occurs at $U = 2V$. The tricritical point is at $(U, V) = (1, 0.5)$.

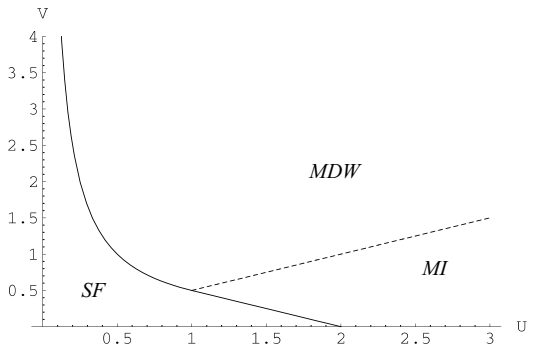

FIG. 2: The ground state phase diagram of the one-dimensional extended Bose-Hubbard model for $g = 1$.

VI. CONCLUSION

We used the two-sublattice Green function method and the mean-field approximation together to calculate the energy spectrum of the extended Bose-Hubbard model, and compared the results with the usual Bose-Hubbard model with $V = 0$, the up-energy-band is divided into two bands and the low-energy-band still remains. By redefining the energy gap we obtained the phase boundaries between the insulator phases and the superfluid phase, MI-SF and MDW-SF. For the coexistence of inhomogeneous density wave order and superfluid order in the supersolid phase, it is possible to use for judgment the appearance of a supersolid phase that is expected to have synchronously an energy band split and an energy band overlap in the energy spectrum.

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* Electronic address: suxq@mail.ustc.edu.cn

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