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Coherent potential approximation study of the Mott transition in optical lattice system with site-dependent interactions

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Abstract. We study the Mott transition in the half-filled Hubbard model with spatially alternating interactions by means of the coherent potential approximation. The phase boundary between metallic and insulating phases at zero temperature is derived and the nature of the Mott states is also considered. Our results are in good agreement with the ones recently obtained by the two-site dynamical mean-field theory.

1 Introduction

Ultracold atomic gases are versatile systems for probing fundamental condensed matter problems [1–5], as well as understanding atomic and molecular physics [6,7]. Particularly, ultracold fermionic atoms in optical lattice realize the Hubbard model which captures the essential physics of strongly correlated materials and contains extremely rich phenomena such as metallic and insulating phases, magnetic order and superconductivity. In addition, all the parameters of the Hubbard Hamiltonian (hopping, on-site Coulomb interaction, filling, lattice geometry and dimensionality) now can easily be controlled by varying the parameters of lasers being used [8].

The Mott metal-insulator transition (MIT) is a fundamental problem in condensed matter physics. It has been established that the Hubbard on-site Coulomb interaction between electrons can lead to a localization of the atoms in the lattice sites and drive the transition from a metallic to an insulating states. Most studies on the MIT focus on the lattice system with uniform interactions [9–11]. Recently, the spatial modulation of the interaction has been realized in ^{174}Yb gas system [12] and the MIT in half-filled Hubbard model with alternating interaction has been theoretically investigated by means of the two-site dynamical mean field theory (DMFT). It has been found that a single Mott transition occurs when two kinds of interaction are increased [13]. The nature of phase transition between metallic and Mott insulating phases has also been considered by using different impurity solvers in DMFT [14]. In this paper we employ the coherent potential approximation (CPA), which is a successful theory for a number of strongly correlated electron systems [15–19] to study the MIT in the half-filled model with site-dependent interactions. We derive an analytical expression for the phase boundary between metallic and insulating states in the phase diagram as well as support the main results obtained in reference [13].

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2 Model and formalism

We consider the following Hubbard model with alternating interactions on a bipartite lattice (sublattices A and B)

$$H = -t \sum_{\langle ij\rangle\sigma} [c^+_{i\sigma} c_{j\sigma} + \text{H.c.}] - \mu \sum_{i\sigma} n_{i\sigma} + \sum_{\alpha, i\in\alpha} U_\alpha \left(n_{i\uparrow} n_{i\downarrow} - \frac{1}{2} [n_{i\uparrow} + n_{i\downarrow}] \right), \quad (1)$$

where $c_{i\sigma}(c^+_{i\sigma})$ annihilates (creates) a fermion with spin σ at site i, $n_{i\sigma} = c^+_{i\sigma} c_{i\sigma}$ and $n_i = n_{i\uparrow} + n_{i\downarrow}$. U_α is the site-dependent onsite Coulomb interaction in the sublattice $\alpha(= A, B)$, t is the nearest neighbor hopping parameter. The chemical potential is chosen so that the average occupancy is 1 (half-filling).

In order to investigate the Hamiltonian (1), we firstly consider an alloy problem which is expressed by the following Hamiltonian:

$$H = \sum_{i\in A,\sigma} E_{A\sigma} n_{A\sigma} + \sum_{j\in B,\sigma} E_{B\sigma} n_{B\sigma} - t \sum_{i\in A, j\in B,\sigma} \left[c^+_{i\sigma} c_{j\sigma} + H.c. \right], \quad (2)$$

where

$$E_{\alpha\sigma} = \begin{cases} -\mu - \frac{U_\alpha}{2} & \text{with probability } 1 - n_{\alpha,\overline{\sigma}}, \\ -\mu + \frac{U_\alpha}{2} & \text{with probability } n_{\alpha,\overline{\sigma}}. \end{cases} \quad (3)$$

Here $\alpha = A, B$ and $n_{\alpha\sigma}$ is the average occupation with spin σ in the α-sublattice. As in reference [13] we focus in this paper on the paramagnetic case, for which $n_{A\uparrow} = n_{A\downarrow} = \frac{n_A}{2}$, $n_{B\uparrow} = n_{B\downarrow} = \frac{n_B}{2}$. Hereafter we will skip the spin index σ and choose the chemical potential μ so that the system is half-filled, i.e., $n_A + n_B = 2$.

The Green function corresponding to the Hamiltonian (2) has to be averaged over all possible configurations of the random potential which can be considered to be due to alloy constituents. As a second approximation we apply the CPA to the alloy problem. By using the semi-elliptic density of states (DOS) for non-interacting electrons, $\rho_0(\varepsilon) = \frac{2}{\pi W^2}\sqrt{W^2 - \varepsilon^2}$, where W is the half-width of the band to be set as the energy unit, the averaged local Green function for the A-sublattice G_A takes the form [17]

$$G_A = \frac{2}{W^2}\left[\omega - \sum\nolimits_B - \left[\left(\omega - \sum\nolimits_B\right)^2 - \frac{\omega - \sum_B}{\omega - \sum_A}W^2\right]^{\frac{1}{2}}\right], \quad (4)$$

where $\sum_\alpha$ is the self-energy for the α-sublattice. $G_B(\omega)$ is obtained by making the replacement $A \leftrightarrow B$. The CPA demands that the scattering matrix vanishes on average. This yields an expression for $\sum_\alpha$ of the form

$$\sum\nolimits_\alpha = \overline{E}_\alpha - \left(\mu + \frac{U_\alpha}{2} + \sum\nolimits_\alpha\right) G_\alpha(\omega) \left(\mu - \frac{U_\alpha}{2} + \sum\nolimits_\alpha\right) \quad (5)$$

where $\overline{E}_\alpha = -\mu + U_\alpha(n_\alpha - 1)/2$. Eliminating $\Sigma_\alpha(\omega)$ from (4) and (5) leads to a pair of equations for $G_A(\omega)$ and $G_B(\omega)$:

$$\frac{1}{16}G^2_{\bar{\alpha}}(\omega)G_\alpha(\omega) - \frac{1}{2}(\mu + \omega)G_{\bar{\alpha}}(\omega)G_\alpha(\omega) + \left[(\mu + \omega)^2 - \frac{U_\alpha^2}{4}\right]G_\alpha(\omega) + \frac{1}{4}G_{\bar{\alpha}}(\omega) - \mu - \omega - \frac{U_\alpha}{2}(n_\alpha - 1) = 0. \quad (6)$$

Equations (6) must now be solved with $n_A + n_B = 2$, where $n_\alpha = -2/\pi \int_{-\infty}^{0} \Im G_\alpha(\omega) d\omega$ (the chemical potential equals zero due to the electron-hole symmetry in the half-filled system). To study the MIT in the system with alternating interactions, we calculate the DOS for each sublattice $\rho_\alpha(\omega) = -\Im G_\alpha(\omega)/\pi$, DOS at the Fermi level $\rho_\alpha(0)$ and double occupancy $D_\alpha = \langle n_{\alpha\uparrow} n_{\alpha\downarrow}\rangle$. We have also checked a charge ordered solution of equation (6) and then constructed the phase diagram for the homogeneous phases at $T = 0$ K.

3 Results and discussions

We first consider limiting cases. Setting $U_A = U_B$ in equation (6) we reproduce the CPA equation for the Green function obtained by Velicky et al. in the usual Hubbard model [15]. The critical Coulomb repulsion for the Mott-Hubbard metal-insulator is found to be $U_c = W = 1$. In Figure 1 we show the DOS for each sublattice for $U_B = 0$ and for two values of U_A. It can be seen that in both cases the sharp quasiparticle peaks for B-sublattice appear in the vicinity of the Fermi level ($\omega = 0$), which implies that the system is metallic. Note that in the actual calculations we make $\rho_\alpha(\omega) = -\Im G_\alpha(\omega + i\eta)/\pi$ with $\eta = 0.001$. Figure 2 shows the DOS for each sublattice for fixed value $U_B/U_A = 2$ and for two values of U_A. When $U_A/W = -0.6$ the DOS for both sublattices at Fermi level is nonzero, which indicates that system is in a metallic state. In contrast, when $U_A/W = -1.5$ the DOS for both sublattices shows a gap around $\omega = 0$, indicating an insulating phase. From Figures 1 and 2 one can see that in all cases the DOS for each sublattice are symmetric ($\rho_\alpha(\omega) = \rho_\alpha(-\omega)$), which means that the solution of (6) is the homogeneous phase with $n_A = n_B = 1$. We have solved system of equations (6) numerically for a wide range of system parameters and then we may conclude that in contrast to the half-filled extended and the ionic Hubbard models [17,18,20,21], within the CPA there is no charge ordered solution with $n_A \neq n_B$ in the half-filled system with alternating interactions.

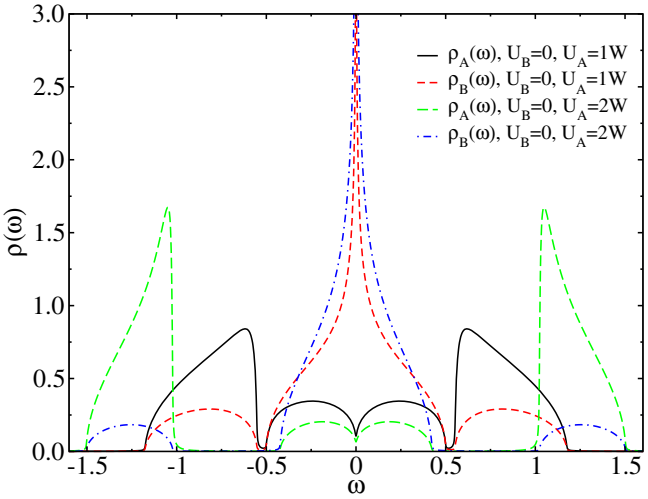

Fig. 1. The DOS for the sublattice $A(B)$ for $U_B = 0$ and two values of U_A. In both cases the system is in the metallic state. Energy scale: $W = 1$.

We turn now to analyze system of equations (6) for the homogeneous phase with $n_A = n_B = 1$. It is easy to show that in this case, (6) is reduced to a biquadratic equation for $G_\alpha(0)$ and the condition for the yielding a positive DOS in the Fermi level is $|U_A U_B| < W^2$. As a result, the phase boundary between the metallic and insulating phases in the system with alternating interactions at half-filling is given as

$$U_A U_B = \pm W^2. \quad (7)$$

Expression (7) is our main result. In the case of the usual Hubbard model $U_A = U_B$, we have well-known result: $U_c = W$ for the Bethe lattice. Furthermore, we find from

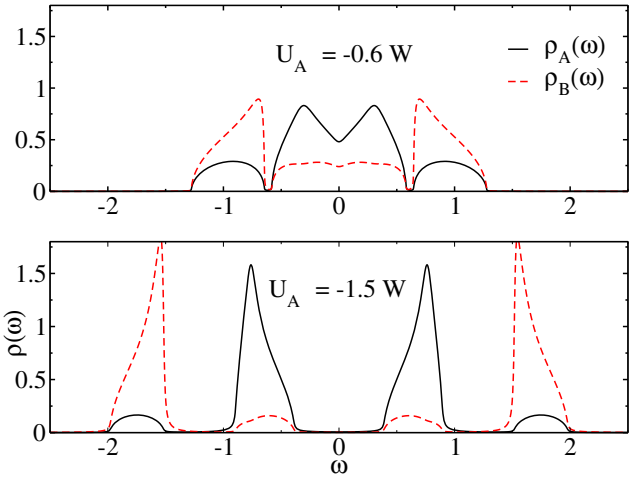

Fig. 2. The DOS for the sublattice $A(B)$ for $U_B/U_A = 2$. Upper (lower) panel shows the results for the metallic state with $U_A = -0.6$ W (the insulating state with $U_A = -1.5$ W).

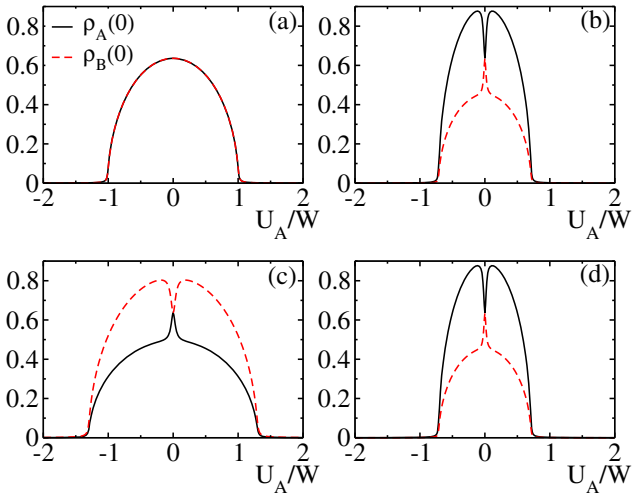

Fig. 3. The DOS at Fermi energy $\rho_\alpha(0)$ as a function of U_A for different fixed values of $U_B/U_A = 1.0$ (a), 2.0 (b), -0.6 (c), and -2.0 (d). In the CPA the phase transition is clearly continuous.

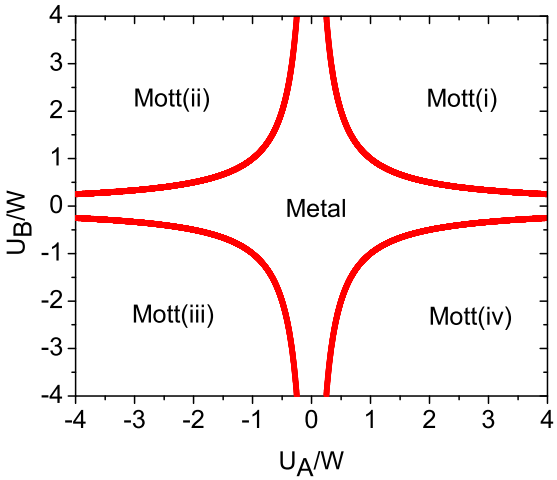

Fig. 4. The phase diagram of the half-filled Hubbard model with spatially-modulated interactions at zero temperature.

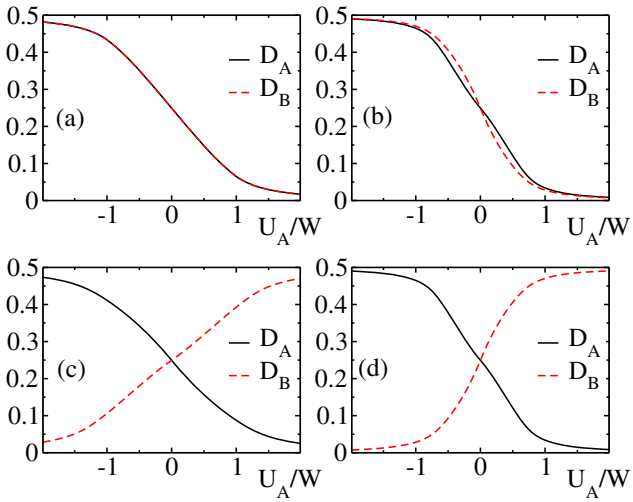

Fig. 5. The double occupancy D_α as a function of U_A for different fixed values of $U_B/U_A = 1.0$ (a), 2.0 (b), -0.6 (c), and -2.0 (d).

the biquadratic equation for $G_\alpha(0)$ that

$$|U_\alpha|\rho_\alpha(0) = \frac{2}{\pi W^2}\sqrt{W^2|U_A U_B| - (U_A U_B)^2}, \qquad (8)$$

under the condition of a positive square root for $|U_A U_B| < W^2$. Therefore, both $\rho_A(0)$ and $\rho_B(0)$ simultaneously vanish in the strong coupling region $|U_A U_B| \geq W^2$. The DOS at Fermi level for each sublattice $\rho_\alpha(0)$ as a function of U_A for different values of U_A/U_B are shown in Figure 3. One can see that exclusive of the vicinity of $U_A = U_B = 0$, $\rho_\alpha(0)$ is larger in the sublattice with a smaller local interaction. As in DMFT with the NRG method [14], in the CPA the phase transition at zero temperature is clearly continuous. The ground state phase diagram is shown in Figure 4. The shapes of our metallic and four Mott states regions are similar to the ones obtained in [13]. Next, to clarify these Mott states we calculate the double occupancy $D_\alpha = \langle n_{\alpha\uparrow} n_{\alpha\downarrow}\rangle$. The numerical results are plotted in Figure 5. It can be seen that the double occupancy in each sublattice approaches zero when the local repulsive interaction is large, and this quantity approaches half as the local attractive interaction increases. Consequently, in Mott states regions (i) and (iii) where the signs of interactions are the same ($U_A U_B > W^2$), the singly occupied states as well as the empty or doubly occupied states are realized simultaneously at each sublattice, as shown in Figures 5a and 5b. In contrast, in Mott states regions (ii) and (iv) where the signs of interactions are different from each other ($U_A U_B < -W^2$), the Mott and pairing transitions occur simultaneously in the corresponding sublattices, as shown in Figures 5c and 5d. The same results were obtained in [13] within the two-site DMFT, and here we confirm these by using the CPA. However, in contrast to [13], the calculated D_α does not vanish at the transition. This is to be expected, because virtual hopping in the insulator produces a very small but nonzero double occupancy, as was noted in reference [22].

4 Conclusions

We have studied the MIT in the half-filled Hubbard model with spatially alternating interactions by means of the coherent potential approximation. Within this approximation in combination with the semi-elliptical model DOS we show that the charge ordering phase does not exist in the system and we derive the phase boundary between metallic and insulating phases at zero temperature. We calculate the double occupancy and clarify the Mott states, as well as find continuous phase transition between the metallic and insulating phases. Comparing our results with the ones obtained by DMFT [13,23], we believe that the CPA is able to catch the essential physics at low temperature and gives a correct qualitative picture of the MIT in the system with spatially alternating interactions. In this paper we restrict ourselves to consider only the paramagnetic sector. At low temperature one may expect the stability of magnetically ordered or/and superfluid states. We leave this problem for further studies.

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