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Mott Transition in the Asymmetric Hubbard Model at Half-filling: Equation of Motion Approach

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We investigate the Mott metal-insulator transition in the asymmetric Hubbard model, which may describe the ground states of fermionic atoms trapped in optical lattices. We use the dynamical mean-field theory and the equation of motion approach to calculate the density of states at the Fermi level and the double occupation for various values of the on-site interaction U and the hopping asymmetry r. The critical interaction is also obtained as a function of the hopping asymmetry. Our results are in good agreement with the ones obtained by using the dynamical mean field theory with the exact diagonalization and the quantum Monte Carlo techniques.

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I. INTRODUCTION

The metal-insulator transition (MIT) is a fundamental phenomenon in condensed matter physics. Numerous mechanism, including electron-phonon coupling, electron correlation, and disorder, have been proposed to explain that phenomenon. Among them, one is called the Mott transition, which can be attributed to a strong Coulomb interaction between electrons, resulting in an insulating state even in a system with a partially-filled band. Theoretical works on the Mott transition have mainly focused on the Hubbard model (HM) [1] and the Falikov - Kimball model (FKM) [2]. The asymmetric Hubbard model (AHM) is considered as a natural connection between the two above models. In the AHM, each spin species has a different hopping integral and a different value of the chemical potential. The Hamiltonian of the model is

$$H = \sum_{<i,j>,\sigma} t_\sigma (c^+_{i\sigma} c_{j\sigma} + hc) - \sum_{i,\sigma} \mu_\sigma n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where $c_{i\sigma}(c^+_{i\sigma})$ annihilates (creates) a fermion with spin σ at site i, $n_{i\sigma} = c^+_{i\sigma} c_{i\sigma}$, U is the on-site Coulomb interaction, t_σ is the nearest-neighbor hopping parameter and μ_σ is the chemical potential. The asymmetry parameter is defined as $r = t_\downarrow / t_\uparrow$ with two limits: $r = 0$ corresponding to the FKM and $r = 1$ to the HM. We should note that the AHM is also used for a description of two-component fermionic mixtures loaded in an optical lattice [3–5]. In this case, the index σ refers to the light and the heavy fermionic species, and $t_\uparrow \neq t_\downarrow$ implies fermionic mixtures having mass imbalance.

Dynamical mean field theory (DMFT) has proven to be a well-established and powerful method to investigate the physics of strongly correlated electrons on a lattice. In the DMFT, the original lattice model is mapped onto a effective Anderson model (SIAM) which describes a single correlated impurity embedded in an uncorrelated bath of conduction electrons. The problem is then to find an appropriate solver for the effective impurity model [6]. Recently, the Mott transition in the AHM has been intensively investigated within the DMFT with different standard numerical impurity solvers, such as the numerical renormalization group (NRG) [7], the Hirsch-Fye quantum Monte Carlo algorithm (HF-QMC) and the exact diagonalization method (ED) [8,9]. These numerical methods are seen to work well for the AHM, but each method has its limitations and all of them are computationally expensive, with their applications being strongly limited by available computer resources [10].

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In this paper, the dynamical mean-field theory and the equation of motion approach are used to investigate MIT of the AHM. The critical interaction is obtained analytically as a function of the hopping asymmetry. The density of states at the Fermi level and the double occupation for various values of the on-site interaction U and the hopping asymmetry r are also calculated. Our results are consistent with those ones obtained from the DMFT with the HF-QFC and the ED.

II. THEORETICAL FORMULATION

In the DMFT, the Hamiltonian model in Eq. (1) is mapped onto a self-consistent single impurity model and is given as

$$\begin{aligned} H_{imp} &= \sum_{k\sigma} \varepsilon_{k\sigma} c^+_{k\sigma} c_{k\sigma} + \sum_{k\sigma} (V_{k\sigma} c^+_{k\sigma} d_\sigma + V^*_{k\sigma} d^+_\sigma c_{k\sigma}) \\ &\quad - \sum_\sigma \mu_\sigma n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}, \end{aligned} \tag{2}$$

where d_σ and d^+_σ are the impurity operators with spin σ and $\varepsilon_{k\sigma}$ is the energy of conduction electrons hybridized with the impurity by $V_{k\sigma}$. The effective parameters $\varepsilon_{k\sigma}$ and $V_{k\sigma}$ enter the hybridization function as

$$\Delta_\sigma(\omega) = \sum_k \frac{V^2_{k\sigma}}{\omega - \varepsilon_{k\sigma}}. \tag{3}$$

The impurity Green function is mapped onto the on-site Green function of the original lattice model in Eq. (1) by

$$G_\sigma(\omega) = G_{ii\sigma}(\omega) = \int_{-\infty}^{+\infty} \frac{\rho^0_\sigma(z) dz}{\omega - (z - \mu_\sigma) - \Sigma_\sigma(\omega)}, \tag{4}$$

where $\Sigma_\sigma(\omega)$ is the local self-energy. For the Bethe lattice with an infinite coordination number

$$\rho^0_\sigma(z) = \frac{1}{2\pi t^2_\sigma} \sqrt{4t^2_\sigma - z^2}, \tag{5}$$

and the self-consistent condition is given by

$$\Delta_\sigma(\omega) = t^2_\sigma G_\sigma(\omega), \tag{6}$$

$$G^{-1}_{0\sigma}(\omega) = \omega + \mu_\sigma - t^2_\sigma G_\sigma(\omega), \tag{7}$$

where $G_\sigma(\omega)$ is the local Green's function of the fermions with spin σ and $G_{0\sigma}$ are the bare Green's functions of the associated quantum impurity problem.

Decoupling the equations of motion at the second order yields the following approximation for the impurity Green function:

$$\begin{aligned} G_\sigma(\omega) =& \frac{1 - n_{\bar\sigma}}{\omega + \mu_\sigma - \Delta_\sigma + U\Pi_{1\sigma}(\omega)[\omega + \mu_\sigma - U - \Delta_\sigma - \Pi_{3\sigma}(\omega)]^{-1}} \\ &+ \frac{n_{\bar\sigma}}{\omega + \mu_\sigma - \Delta_\sigma - U - U\Pi_{2\sigma}(\omega)[\omega + \mu_\sigma - \Delta_\sigma - \Pi_{3\sigma}(\omega)]^{-1}}, \end{aligned} \tag{8}$$

in which the "self-energies" $\Pi_{i\sigma}$ read

$$\Pi_{i\sigma}(\omega) = \int_{-\infty}^{+\infty} dz\, \Gamma_{\bar\sigma}(z) \left(\frac{1}{\omega + \mu_\sigma - \mu_{\bar\sigma} - z} + \frac{1}{\omega + \mu_\sigma - \mu_{\bar\sigma} - U + z} \right) F_i(z), \tag{9}$$

where $F_1(z) = f(z)$, $F_2(z) = 1 - f(z)$, $F_3(z) = 1$, with $f(z) = \left(exp\left(\frac{z}{T}\right) + 1 \right)^{-1}$ being the Fermi distribution function; $\Gamma_\sigma(z) = -\frac{1}{\pi} Im\Delta_\sigma(z + i\eta)$ and $n_\sigma = \int dz\, f(z)\, \rho_\sigma(z)$. Equations (8)-(9), as far as we know, were first given in Ref. 11 and were employed to study the conductance through a quantum dot. Our study is restricted to the paramagnetic case at half-filling: $\mu_\uparrow = \mu_\downarrow = U/2$ and $n_\uparrow = n_\downarrow = 1/2$. Due to the particle-hole symmetry, getting

$$\Pi_{1\sigma}(\omega) = \Pi_{2\sigma}(\omega) = \frac{\Pi_{3\sigma}(\omega)}{2} = \Delta_{\bar\sigma}(\omega) \tag{10}$$

is simple. Inputting these conditions into Eq. (8), we obtain

$$\begin{aligned} G_\sigma(\omega) =& \frac{1}{2} \frac{1}{G^{-1}_{0\sigma}(\omega) + U\, \Delta_{\bar\sigma}(\omega)[G^{-1}_{0\sigma} - U - 2\Delta_{\bar\sigma}(\omega)]^{-1}} \\ &+ \frac{1}{2} \frac{1}{G^{-1}_{0\sigma}(\omega) - U - U\, \Delta_{\bar\sigma}(\omega)[G^{-1}_{0\sigma} - 2\Delta_{\bar\sigma}(\omega)]^{-1}}. \end{aligned} \tag{11}$$

Together with Eqs. (6) and (8), this leads to a pair of algebraic equations for $G_\sigma(\omega)$ ($\sigma = \uparrow, \downarrow$):

$$\begin{aligned} & t^4_\sigma G^3_\sigma + 2t^2_\sigma t^2_{\bar\sigma} G^2_\sigma G_{\bar\sigma} - 2\omega t^2_\sigma G^2_\sigma - 2\omega t^2_{\bar\sigma} G_\sigma G_{\bar\sigma} \\ &+ \left(\omega^2 - \frac{U^2}{4} + t^2_\sigma \right) G_\sigma + 2t^2_{\bar\sigma} G_{\bar\sigma} - \omega = 0. \end{aligned} \tag{12}$$

Equations (12) for $G_\uparrow(\omega), G_\downarrow(\omega)$ are exact in the limit $r = 0$ corresponding to the FKM [12] and are known as the (full) Hubbard III approximation of the HM in the limit $r = 1$ [13,14].

Let us now derive the analytic expression of the critical value U_C of the Mott transition in the half-filled AHM. We denote $g_\uparrow(\omega) = t_\uparrow G_\uparrow(\omega)$, $\tilde{\omega} = \omega/t_\uparrow$, $\tilde{U} = U/t_\uparrow$, and $r = t_\downarrow/t_\uparrow$. Then from Eqs.(12), we obtain

$$g_\downarrow(\omega) = \frac{g_\uparrow^3(\omega) - 2\tilde{\omega}g_\uparrow^2(\omega) + \left(\tilde{\omega}^2 - \frac{\tilde{U}}{4} + 1\right) g_\uparrow(\omega) - \tilde{\omega}}{2r^2\left(\tilde{\omega}g_\uparrow(\omega) - g_\uparrow^2(\omega) - 1\right)}, \tag{13}$$

$$g_\uparrow(\omega) = \frac{r^4 g_\downarrow^3(\omega) - 2r^2\tilde{\omega}g_\downarrow^2(\omega) + \left(\tilde{\omega}^2 - \frac{\tilde{U}}{4} + r^2\right) g_\downarrow(\omega) - \tilde{\omega}}{2\left(\tilde{\omega}g_\downarrow(\omega) - r^2 g_\downarrow^2(\omega) - 1\right)}. \tag{14}$$

Due to the particle-hole symmetry $\rho_\sigma(\omega) = \rho_\sigma(-\omega)$ and the spectral theorem $G_\sigma(\omega) = \int dx \frac{\rho_\sigma(x)}{\omega - x}$, clearly that $g_\downarrow(0)$ and $g_\uparrow(0))$ are pure imaginary at the Fermi level $\omega = 0$. We denote $g_\downarrow(0) = i\alpha$ and $g_\uparrow(0) = i\beta$, with α and β being real; then, we insert them into Eqs. (13) and (14) to yield a pair of equations:

$$-2r^2\alpha(-\beta^2 + 1) = \beta\left(-\beta^2 + 1 - \frac{\tilde{U}}{4}\right), \tag{15}$$

$$-2\beta(-r^2\alpha^2 + 1) = \alpha\left(-r^4\alpha^2 + r^2 - \frac{\tilde{U}}{4}\right). \tag{16}$$

The metallic state ceases to exist when the density of states at the Fermi level $\rho_\sigma(0) \to 0$, *i.e.*, $\alpha \to 0$ and $\beta \to 0$ as $U \to U_C$. By excluding $lim_{U\to U_C}\frac{\alpha}{\beta}$ from this pair of equations, we finally have a biquadratic equation for $\tilde{U}_C$ with the solution

$$U_C = \left[2\left(t_\uparrow^2 + t_\downarrow^2 + \sqrt{t_\uparrow^4 + t_\downarrow^4 + 14t_\uparrow^2 t_\downarrow^2}\right)\right]^{\frac{1}{2}}. \tag{17}$$

The above expression for U_C was obtained in Ref. 15 by using the projecting technique on the basis of fermionic Hubbard operators. Here, we reproduce it in a simple manner, and we will discuss this result in the next section.

III. NUMERICAL RESULTS AND DISCUSSION

We numerically solve the self-consistent equations, Eqs. (6)-(11), to determine the selfenergy and the Green function. The algorithm is summarized as follows: Beginning with an initial selfenergy guess $\Sigma_\sigma(\omega)$, we obtain the local Green function $G_\sigma(\omega)$ from Eq. (4). Inputting the selfenergy and the local Green function calculated in the previous step into Eqs.(6), (7), and (11), we can calculate a new Green function $G_\sigma(\omega)$. Finally, a new selfenergy $\Sigma_\sigma(\omega)$ is determined by using the Dyson equation

$$\Sigma_\sigma(\omega) = G_{0\sigma}^{-1}(\omega) - G_\sigma^{-1}(\omega). \tag{18}$$

This procedure is iterated until convergence is reached. In actual numerical calculations, if the positive infinitesimal number η is too small, the convergence is never reached. Thus η must have a finite small value (should be in range from 10^{-3} to 10^{-2}) to make the iterations converge. After that, to get sharp pictures for the density of states, which is important to determine the critical value U_C for the metal-insulator transition, we use the spline extrapolation to reach the limit $\eta \to 0$.

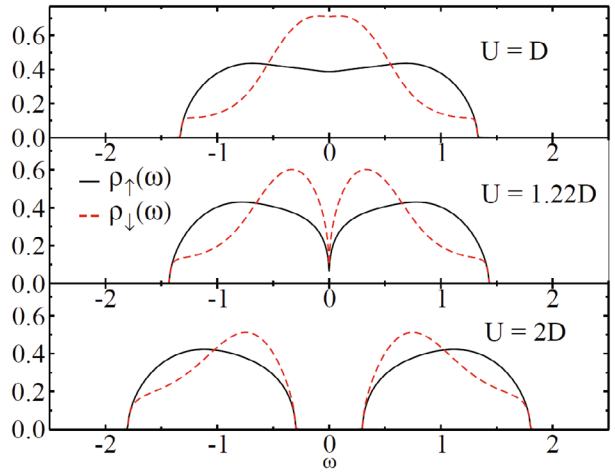

Fig. 1. (Color online) DOS for spin up and spin down for $r = 0.4$. Top panel: a metallic state for $U = D$; Middle panel: MIT occurs at $U = 1.22D$; Bottom panel: an insulator state for $U = 2D$ (the half bandwidth with spin up $D = 2t_\uparrow$).

We now turn to the numerical results. Hereafter, we take the half bandwidth with spin up $D = 2t_\uparrow$ as the energy unit, zero temperature and $\eta = 0.001$ in the numerical calculations. Figure 1 shows the density of states (DOS) for each spin species for three values of the on-site Coulomb interaction U and $r = 0.4$. Here, the symmetry of the DOS reflects particle-hole symmetry in the half-filled system. When $U = D$, the DOSs for both spin species at the Fermi level ($\omega = 0$) are nonzero, which indicates that system is in a metal state. In contrast, when $U = 2D$, the DOSs for both spin species show a gap around $\omega = 0$, indicating an insulating phase. The Mott transition in the system occurs at $U = 1.22D$.

Because the DOS at the Fermi level indicates the conduction properties of the system, we calculate this value and show it in Fig. 2. One can see that both $\rho_\sigma(0)$ simultaneously vanish in the strong coupling region. We note that because of the continuous nature of the transition, identifying the precise value of the critical interaction is difficult. In the case of $r = 0.4$, by using a simple spline extrapolation from the data for $U < 1.1D$, we ob-

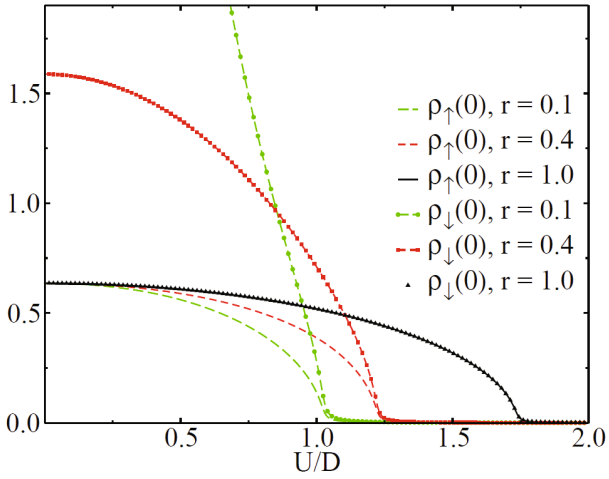

Fig. 2. (Color online) DOS at the Fermi level as a function of the on-site Coulomb repulsion for various values of r.

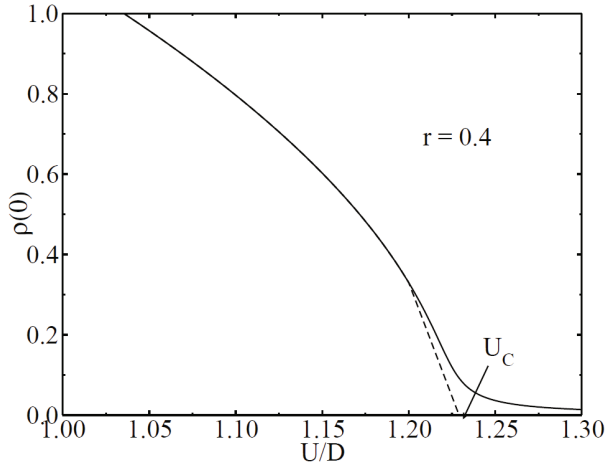

Fig. 3. Total DOS $\rho(0) = \rho_\uparrow(0)+\rho_\downarrow(0)$ at the Fermi level as a function of the on-site Coulomb repulsion for $r = 0.4$. The value of the critical interaction U_C obtained by extrapolating $U < 1.1D$ data is also indicated.

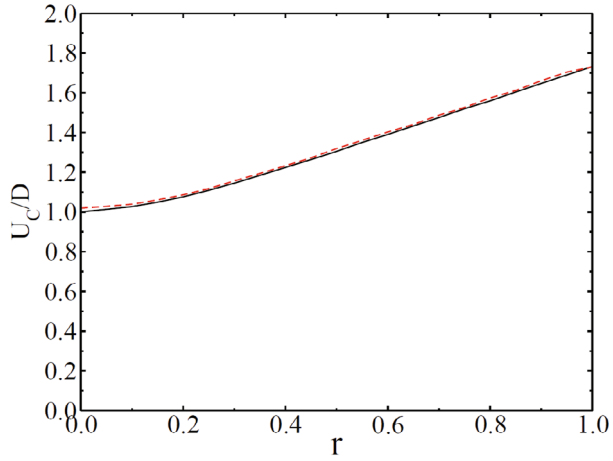

Fig. 4. (Color online) Critical interaction as a function of r. The dashed line corresponds to numerical results, and the solid line corresponds to the results obtained by using the analytic expression in Eq. (17).

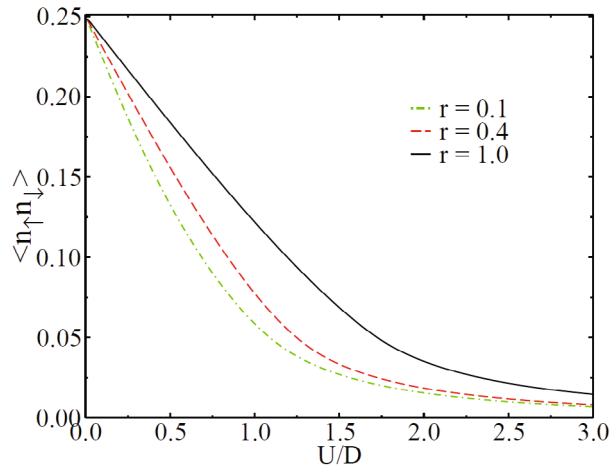

Fig. 5. (Color online) Double occupation $< n_\uparrow n_\downarrow >$ as a function of U for different fixed values of r.

tain $U_C/D \approx 1.22$, which is shown in Fig. 3. Repeating this with many different values of r, we get the critical interaction as a function of r, which is presented in Fig. 4 and is almost identical with the analytic result of Eq.(17) over the whole r range. The calculated result for U_c is exact in the limit $r = 0$ for the Falikov-Kimball model ($U_C/D = 1$) [12]. For $r = 1$, the equation of motion approach presented here is known as the Hubbard III approximation, and it displays a Mott transition at $U_C/D = \sqrt{3}$ for the Bethe lattice [14].

Next, in order to establish a link between the behavior of the model and the physical observable accessible in cold atom systems on optical lattices, we calculate the double occupation $< n_\uparrow n_\downarrow >$. The numerical results are plotted in Fig. 5 for various values of U and r. As in Ref. [8], in the noninteracting case ($U = 0$), the double occupation is 0.25, and it quickly decreases when U increases. A metal is characterized by a linear decrease in the double occupation with increasing interaction U while in the insulating region, at a larger value of the interaction, the double occupation remains small and weakly depends on U. As one might expect, at smaller values of r, the double occupation more rapidly decreases, and the value of the critical interaction is reduced.

IV. CONCLUSIONS

In summary, we have used the equation of motion approach as an impurity solver for the DMFT to investigate the MIT in the AHM at half-filling. The technique has been implemented directly on the real-frequency axis, which turns out to be computationally efficient. In ad-

dition, it allows an explicit expression for the critical interaction in the system to be obtained as an increasing function of the hopping asymmetry. We also numerically computed the DOS at the Fermi level and the double occupation that may permit the experimental identification of this remarkable physical behavior. The main results have been compared with the results obtained by using the exact diagonalization and the quantum Monte Carlo techniques and were found to be in good agreement. This work demonstrates that the equation of motion approach is a simple, but reliable, impurity solver for studying the MIT in the AHM. With a suitable decoupling scheme, this approach can also be applied to the AHM with charge and spin orders. This is left to a future work.

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