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Two-component Fermions in Optical Lattice with Spatially Alternating Interactions

Anh-Tuan Hoang[1]*, Thi-Hai-Yen Nguyen[1], Thi-Thu-Trang Tran[2], and Duc-Anh Le[3]

[1]*Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Hanoi, Vietnam*
[2]*Ha Long University, Nam Khe, Uong Bi, Quang Ninh, Vietnam*
[3]*Faculty of Physics, Hanoi National University of Education, 136 Xuan Thuy, Hanoi, Vietnam*

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We investigate two-component mass-imbalanced fermions in an optical lattice with spatially modulated interactions by using two-site dynamical mean field theory. At half-filling and zero temperature, the phase diagram of the system is analytically obtained, in which the metallic region is reduced with increasing the mass imbalance. The ground-state properties of the fermionic system are discussed from the behaviors of both the spin-dependent quasi-particle weight at the Fermi level and the double occupancy for each sublattice as functions of the local interaction strengths for various values of the mass imbalance.

1. Introduction

In recent years, ultracold fermionic atoms in optical lattices have attracted a lot of attention. Noteworthy aspects of the cold atom systems include the variety of lattice types that can be created and the possibility of changing the strength and sign of atomic interactions by an external magnetic field as a result of Feshbach resonance.[1,2)] These tunable and controllable systems enable us to observe many fascinating phenomena such as a crossover from the BCS-type superfluid to the Bose–Einstein condensation in the attractive case using Li^6 atoms[3)] and a Mott insulating state in the repulsive case using K^{40} atoms.[4)] Furthermore, a mixture of fermionic atoms with different masses (e.g., Li^6, K^{40}), leading to a difference between the hopping parameters of the two kinds of fermions, has also been experimentally realized.[5,6)] Stimulated by these experiments, several theoretical studies on the Mott transition and low-temperature properties of fermionic mixtures with a mass imbalance in their optical lattices were carried out.[7–13)] It was found that at half-filling, the light species with a smaller bare mass is more affected by correlations than the heavy species and that the strength of the critical repulsion decreases monotonically as the mass imbalance grows.[9–13)] Recently, it has been reported that the strength of the atomic interaction can be spatially modulated in the Yb^{174} gas system.[14)] Therefore, it makes sense to theoretically investigate how the spatial modulation in the interactions affects the ground-state properties of the fermionic optical lattice system. In the mass-balanced case, it has been clarified that a single Mott transition occurs when two kinds of the interactions are increased.[15–17)]

In this paper, we study the Mott transition of a two-component mass-imbalanced fermionic system in an optical lattice with spatially modulated interactions by using two-site dynamical mean field theory (DMFT). At zero temperature, the critical interactions for the Mott transition at half-filling are analytically derived. The effect of both the mass imbalance and the spatial modulation in the interactions on the ground-state properties of the system is discussed from the behaviors of the spin-dependent quasi-particle weight and the double occupancy for each sublattice.

The paper is organized as follows. In Sect. 2 we present the model and our theoretical approach. The phase diagram, the quasi-particle weights, and the double occupancy are obtained and discussed in Sect. 3. A brief summary is given in Sect. 4.

2. Model and Theoretical Formulation

We study two-component mass-imbalanced fermions in an optical lattice with spatially modulated interactions described by the following asymmetric Hubbard model on a bipartite lattice made of two interpenetrating (A, B) sublattices arranged such that the neighbors of A sites are all B sites and vice versa:

$$\begin{aligned} H = &- \sum_{\langle ij\rangle,\sigma} t_\sigma (c^+_{i\sigma} c_{j\sigma} + \text{H.c.}) - \sum_{i\sigma} \mu_\sigma n_{i\sigma} \\ &+ \sum_{i\in A} U_A (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) \\ &+ \sum_{i\in B} U_B (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2), \end{aligned} \tag{1}$$

where $c_{i\sigma}$ ($c^+_{i\sigma}$) annihilates (creates) a fermion with spin σ ($= \uparrow, \downarrow$) at site i and $n_{i\sigma} = c^+_{i\sigma} c_{i\sigma}$. U_α is the site-dependent on-site interaction in sublattice α ($= A, B$), t_σ and μ_σ respectively denote the nearest neighbor hopping parameter and the chemical potential for the fermion with spin σ, where the effect of the mass imbalance is taken into account, keeping in mind that in the cold atom context, the "spin" degree of freedom can denote any two possible internal states. Note that in our Hamiltonian model in Eq. (1), half-filling (the number of fermions equals the number of lattice sites) is realized when $\mu_\sigma = 0$, and in this case the systems with (U_A, U_B), (U_B, U_A), $(-U_A, -U_B)$, and $(-U_B, -U_A)$ are identical because the Hamiltonian is invariant under the particle–hole transformations[18)] $c_{i\uparrow} \to \tilde{c}_{i\uparrow}$ and $c_{i\downarrow} \to (-1)^i \tilde{c}^+_{i\downarrow}$ with $(-1)^i = +1$ on the A-sublattice and $= -1$ on the B-sublattice.

To investigate the Hamiltonian model in Eq. (1) we use DMFT, which has resulted in many successes in understanding strongly correlated fermion systems.[19)] In DMFT, the original lattice model is mapped onto an effective single-impurity Anderson model embedded in an uncorrelated bath of fermions. The lattice Green function is then obtained via self-consistent conditions imposed on the impurity problem. When DMFT is applied to a system with a sublattice structure, the local lattice Green function is given as[20)]

$$G_{\alpha\sigma}(\omega) = \int_{-\infty}^{+\infty} \frac{\xi_{\bar{\alpha}\sigma}(\omega)\rho^0_\sigma(z)\,dz}{\xi_{A\sigma}(\omega)\xi_{B\sigma}(\omega) - z^2}, \tag{2}$$

where $\xi_{\alpha\sigma}(\omega) = \omega + \mu_\sigma - \Sigma_{\alpha\sigma}(\omega)$ with $\Sigma_{\alpha\sigma}(\omega)$ being the local self-energy for sublattice α and $\rho^0_\sigma(z)$ is the spin-

dependent noninteracting density of states. For the Bethe lattice with infinite coordination number

$$\rho_\sigma^0(z) = \frac{1}{2\pi t_\sigma^2}\sqrt{4t_\sigma^2 - z^2}, \tag{3}$$

the self-consistent condition is given by

$$\Delta_{\alpha\sigma}(\omega) = t_\sigma^2 G_{\bar{\alpha}\sigma}(\omega), \tag{4}$$

where $\Delta_{\alpha\sigma}(\omega) = \omega + \mu_\sigma - G^{-1}_{0\alpha\sigma}(\omega)$ is the hybridization function with $G_{0\alpha\sigma}(\omega)$ being the noninteracting Green function of the effective impurity model for sublattice α; $\bar{\alpha} = B, A$ if $\alpha = A, B$.

To proceed further, we make use of two-site DMFT, which is a simplified version of DMFT. This approach was proposed by Potthoff[21] and has successfully been applied to treating the Mott transition of fermionic mixtures with a mass imbalance, providing an almost correct critical interaction and qualitative electronic properties.[9,12] The extension of two-site DMFT to the asymmetric Hubbard model with spatially modulated interactions is straightforward. In the following, we consider the half-filling case and the calculation is performed at zero temperature.

In two-site DMFT, the hybridization function can be represented by a single pole function at $\omega = 0$,

$$\Delta_{\alpha\sigma}(\omega) = \frac{V_{\alpha\sigma}^2}{\omega}, \tag{5}$$

where $V_{\alpha\sigma}$ is the hybridization between the approximate bath and the impurity. Close to the critical interactions for the Mott transition when $V_{\alpha\sigma} \to 0$, we can approximate the quasi-particle weights to the second order in $V_{\alpha\sigma}$:

$$Z_{\alpha\sigma} = \frac{4(V_{\alpha\sigma} + 2V_{\alpha\bar{\sigma}})^2}{U_\alpha^2}. \tag{6}$$

Taking into account Eq. (5), the DMFT self-consistent condition in Eq. (4) can be rewritten as

$$V_{\alpha\sigma}^2 = Z_{\bar{\alpha}\sigma} t_\sigma^2. \tag{7}$$

Equations (6) and (7) lead to four linear equations for $V_{\alpha\sigma}$ ($\alpha = A, B$; $\sigma = \uparrow, \downarrow$):

$$V_{\alpha\sigma} = \frac{2t_\sigma}{|U_{\bar{\alpha}}|}(2V_{\bar{\alpha}\sigma} + V_{\bar{\alpha}\bar{\sigma}}). \tag{8}$$

Within DMFT, the localization is associated with a vanishing quasi-particle weight or hybridization. A nonzero value of $V_{\alpha\sigma}$ is the signature of a metal, therefore the determinant of Eq. (8) must vanish when the Mott transition occurs, giving the following expression for the critical interactions:

$$|U_A U_B| = (t_\uparrow + t_\downarrow + \sqrt{t_\uparrow^2 + t_\downarrow^2 + 14 t_\uparrow t_\downarrow})^2. \tag{9}$$

Equation (9) is one of the main results of this paper. Setting $U_A = U_B$ in Eq. (9), we reproduce the result of the asymmetric Hubbard model with the homogeneous interaction,[9,12] keeping in mind that $D = t_\uparrow + t_\downarrow$; $\zeta = (t_\uparrow - t_\downarrow)/(t_\uparrow + t_\downarrow)$. On the other hand, when $t_\uparrow = t_\downarrow = D/2$, we have $|U_A U_B| = (3D)^2$ for the mass-balanced case.[15,16]

3. Results and Discussion

We consider the ground-state properties of the system at half-filling. In the mass-balanced case, it has been reported that at low temperatures the magnetically ordered state is stabilized in the repulsive model ($U_A, U_B > 0$) and the superfluid state is stabilized in the attractive model ($U_A, U_B < 0$).[16] Restricting our discussion to the paramagnetic sector with equal average numbers of each component in each sublattice (per site), $n_{\alpha\uparrow} = n_{\alpha\downarrow} = 1/2$, in the following we focus on the case where the signs of the interactions are different from each other ($U_A U_B < 0$). Note that although the paramagnetic solution of the system at half-filling is not the generic case, a study of the paramagnetic state can serve as a good starting point even in the regime where the model develops magnetic order. In addition, our paramagnetic solution will properly describe the system, at least, at finite temperatures above the Neel temperature. Owing to the particle–hole symmetry, as mentioned above, we may assume that $U_A > 0$, $U_B < 0$, and $U_A \le |U_B|$ or $0 < \gamma = U_A/|U_B| \le 1$. Under this condition, a nonmagnetic ground-state is expected and a Mott metal–insulator transition is possible when the interactions are switched on and gradually increased. Hereafter, we take $D = 2t_\uparrow = 1$ as the energy unit and $r = t_\downarrow/t_\uparrow$, a quantity which ranges from 0 (Falicov–Kimball limit) to 1 (balanced case), as the mass imbalance parameter.

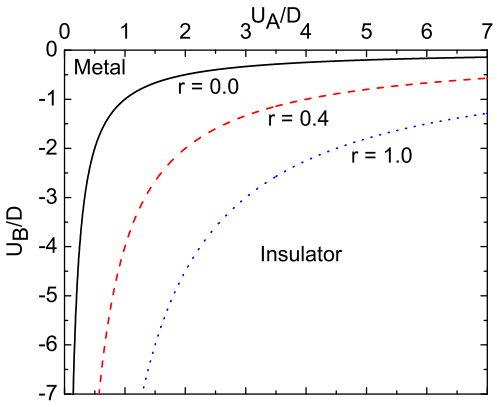

Fig. 1. (Color online) Ground-state phase diagram for the half-filled model as a function of the interactions U_A/D and U_B/D for $r = 1.0$, 0.4, and 0.0.

In Fig. 1 we present the phase diagram as a function of the interactions U_A and U_B for different values of the mass imbalance parameter r at zero temperature. For the mass-balanced system ($r = 1$), the two-site DMFT result Eq. (9) is in very good agreement with those obtained from DMFT with the numerical renormalization group (NRG) method.[16] When the mass imbalance increases (r decreases), the metallic region is reduced, because at fixed D or $t_\uparrow$, the larger the difference in the bare mass, the easier it is to localize the system.

In order to confirm the result obtained from Eq. (9), we also calculate the density of states (DOS) for each sublattice, $\rho_\alpha(\omega) = -\sum_\sigma \mathrm{Im}\, G_{\alpha\sigma}(\omega)/\pi$, and the DOS at the Fermi level $\rho_{\alpha\sigma}(0)$. Figure 2 shows the DOS for each sublattice of the system with $r = 0.4$, $U_B = -2U_A$, and for various values of U_A. It is seen that at half-filling, the DOS for each sublattice is symmetric [$\rho_\alpha(\omega) = \rho_\alpha(-\omega)$]. In a metallic state resonance peaks for both sublattices, which are a consequence of quasi-particle excitation, appear in the vicinity of the Fermi energy. Their widths become smaller with increasing strength of the local interactions, and at the critical values $U_\alpha/D = (U_\alpha/D)_c$, the quasi-particle peaks completely disappear.

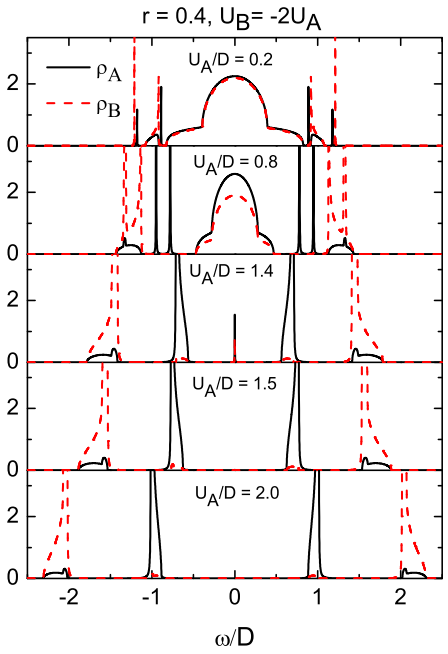

Fig. 2. (Color online) Density of states at $T = 0$ for the sublattice $A(B)$ for $r = 0.4$, $U_B = -2U_A$, and ratios $U_A/D = 0.2$, 0.8, 1.4, 1.5, and 2.0 (from top to bottom).

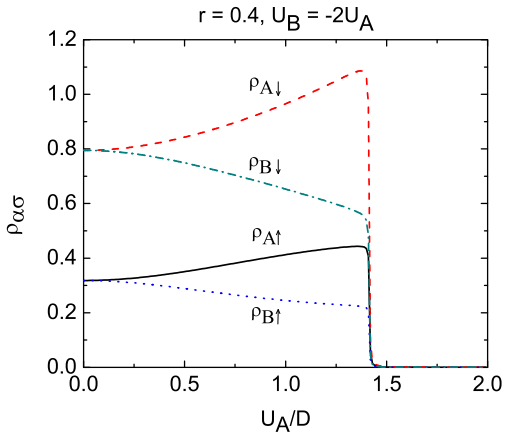

Fig. 3. (Color online) Density of states at the Fermi level $\rho_{\alpha\sigma}(0)$ as a function of U_A for the model with $r = 0.4$ and $U_B = -2U_A$.

Gap structure is formed around $\omega = 0$ in both sublattices. Its formation is connected with the vanishing of the quasi-particle weights and its value increases when the local interactions become larger. The transition from the metal to an insulating state resembles that found within DMFT applied to the usual paramagnetic Hubbard model, except here the insulating state is induced by the Mott and pairing transitions.[19] Figure 3 presents the DOS at the Fermi level for each component and sublattice for the same model parameters. Owing to the momentum independence of the self-energy within DMFT, Fermi liquid behavior at half-filling implies that $\rho_{\alpha\sigma}(0) = 1/(\pi D_\sigma)$ for $U_\alpha < (U_\alpha)_c$. However, as pointed out by Potthoff,[21] unlike full DMFT, two-site DMFT is not a conserving approach in the sense of Baym and Kadanoff,[22] and consequently a comparatively crude violation of the Fermi liquid relation occurs. Namely, we have $\rho_{A\sigma}(0) = \rho_{B\sigma}(0) = 1/(\pi D_\sigma)$ for $U_A = U_B = 0$, but these identities do not hold when the interactions are introduced. On the other hand, all quantities $\rho_{\alpha\sigma}(0)$ simultaneously vanish when U_α approaches $(U_\alpha)_c$. Therefore, we conclude that a single metal–insulator transition indeed occurs in the system with spatial modulated interactions. In addition, the metallic region above the phase boundary constructed in Fig. 1 is a Fermi liquid except at the Falicov–Kimball limit $r = 0$.

To discuss how the mass imbalance and the spatially modulation in the interactions affect the stability of the normal metallic state, we compute the quasi-particle weights at the Fermi level for both fermion species in both sublattices:

$$Z_{\alpha\sigma} = \left(1 - \frac{d\,\mathrm{Re}\,\Sigma_{\alpha\sigma}(0)}{d\omega}\right)^{-1} = \frac{1}{1 + \dfrac{U_\alpha^2}{4(V_{\alpha\sigma} + 2V_{\alpha\bar{\sigma}})^2}}. \quad (10)$$

The obtained results are shown in Figs. 4(a)–4(d). In Fig. 4(a) we plot the quasi-particle weight for the model with $\gamma = 1.0$ $(U_B = -U_A)$ for two different mass imbalances, $r = 0.4$ and 0.8. In both cases, we find that $Z_{A\sigma} = Z_{B\sigma}$, i.e., the quasi-particle weight is independent of the sign of the interaction, as already suggested by Eq. (10). However, the introduction of the mass imbalance leads to different behavior of the quasi-particle weight, namely, $Z_{\alpha\uparrow} < Z_{\alpha\downarrow}$ for both cases, i.e., the light fermions are more renormalized than the heavy ones (the effective mass renormalization factor is $m^* \sim 1/Z$). This is consistent with the results of the asymmetric Hubbard model with homogeneous interactions.[9,12] We refer to Dao et al.[9] for a detailed discussion of this interesting effect in the model with homogeneous interactions. In the Fermi system with repulsive and attractive interactions at half-filling, the explanation is analogous to the one above: when the system is at (or close to) half-filling and the correlation is strong, we essentially have one fermion on each A-sublattice site, whereas empty and doubly occupied states are equally realized in the B-sublattice (see Fig. 5 later). Moreover, it should be kept in mind that the mean number of each component in each sublattice is the same, $n_{\alpha\uparrow} = n_{\alpha\downarrow} = 1/2$. Under these particle number conditions and owing to the minimum total potential energy principle, it can be verified that we can not only move fermions of the same species, but we are forced to move the heavy fermions as soon as we move the light ones and vice versa. To illustrate this, consider four sites of a bipartite square lattice: site A_1 with an up-spin (light fermion), site A_2 with a down-spin (heavy fermion), a doubly occupied site B_1, and an empty site B_2. Immediately after moving the light fermion from A_1 to B_2, we must move the light one from B_1 to A_1 in order to conserve the number of light fermions in each sublattice. Simultaneously, we must also move the heavy fermion from A_2 to B_2 owing to the minimum total potential energy principle [hoppings between the sites of the same sublattice are forbidden, see Eq. (1)], then the heavy one from B_1 to A_2 owing to the conservation of the number of heavy fermions in each sublattice. As a result, when two species with different bare masses (or hopping parameters) are mixed and the filling is half, the interactions tend to balance their renormalized hoppings $Z_{\alpha\sigma}t_\sigma$, and one finds that $Z_{\alpha\uparrow} < Z_{\alpha\downarrow}$ for $t_\downarrow < t_\uparrow$ with $\alpha \in \{A, B\}$, in contrast to the case of two bands in a solid. Figure 4(b) shows the result for a fixed $\gamma = 1/2$ $(U_B = -2U_A)$ and $r = 0.4$. As one might

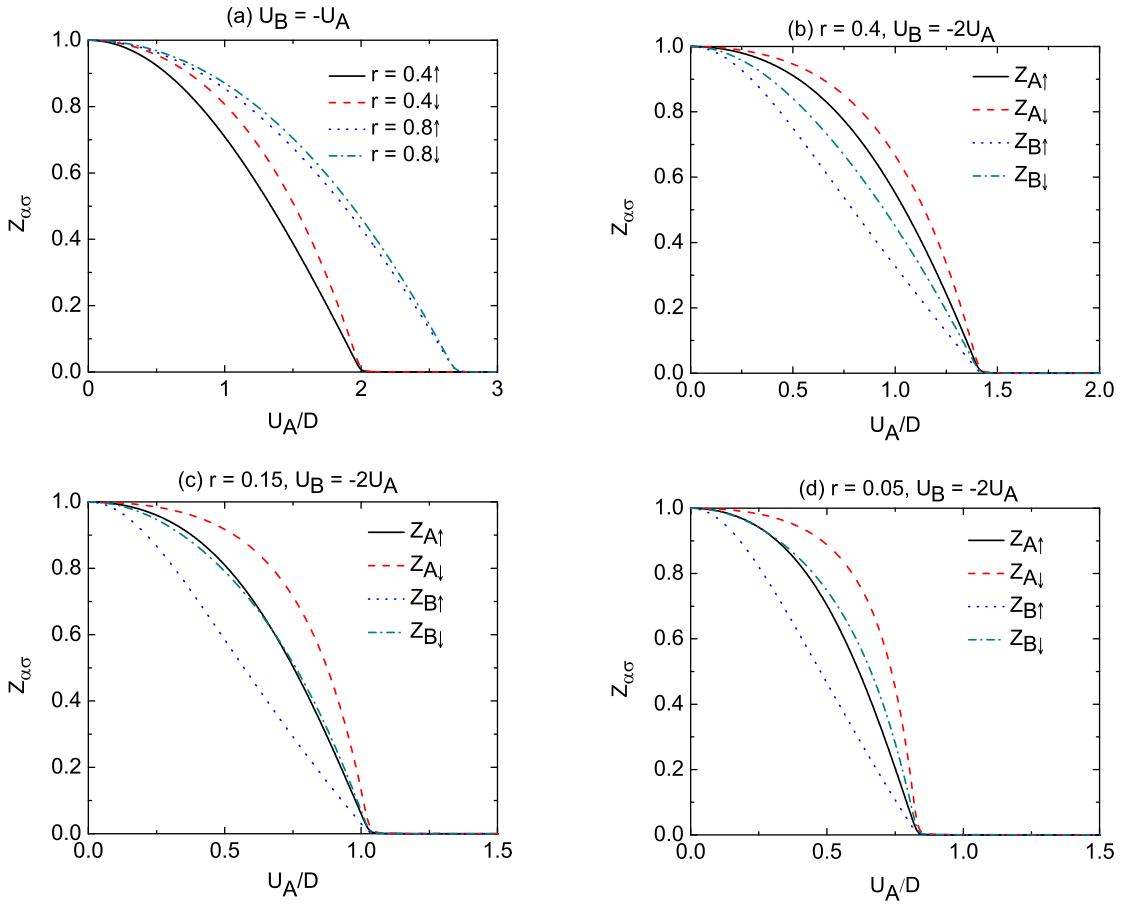

Fig. 4. (Color online) Quasi-particle $Z_{\alpha\sigma}$ at the Fermi level for the model as a function of U_A/D with $U_B = -U_A$ and $r = 0.4, 0.8$ (a), $U_B = -2U_A$ and $r = 0.4$ (b), $U_B = -2U_A$ and $r = 0.15$ (c), $U_B = -2U_A$ and $r = 0.05$ (d).

expect, stronger renormalization appears in the sublattice with a larger local interaction, so we have $Z_{B\sigma} < Z_{A\sigma}$. On the other hand, as mentioned above, we find that $Z_{\alpha\uparrow} < Z_{\alpha\downarrow}$ for each sublattice. Consequently, $Z_{B\uparrow} = \min\{Z_{\alpha\sigma}\}$ and $Z_{A\downarrow} = \max\{Z_{\alpha\sigma}\}$ for $0 < \gamma, r < 1$, as shown in Figs. 4(b)–4(d). We turn now to compare $Z_{A\uparrow}$ and $Z_{B\downarrow}$. For a fixed $\gamma = 1/2$, it is possible that $Z_{B\downarrow} < Z_{A\uparrow}$ for $r = 0.4$, as presented in Fig. 4(b). However, with increasing mass imbalance, at $r = 0.15$ we have the opposite result $Z_{A\uparrow} < Z_{B\downarrow}$ for larger values of U_A [see Fig. 4(c)]. Increasing the mass imbalance further, at $r = 0.05$ we find that $Z_{A\uparrow} < Z_{B\downarrow}$ for almost every value of $U_A < (U_A)_c$, as shown in Fig. 4(d). In addition, for $\gamma = 1/2$ the strength of the critical interaction $(U_A)_c$ decreases as the mass imbalance grows: $(U_A/D)_c \approx 1.41$ for $r = 0.4$ and $(U_A/D)_c \approx 0.83$ for $r = 0.05$. Therefore, we may claim that both the mass imbalance and the spatial modulation in the interactions affect the stability of the normal metallic state, but their effects are different. Nevertheless, the quasi-particle weights at the Fermi level for the two fermion species in both sublattices vanish simultaneously at the critical point. As a result, for fixed D and r, a single Mott transition occurs when two kinds of interactions with different signs are switched on and gradually increased, as plotted in Fig. 1. Furthermore, as in the balanced case obtained from two-site DMFT[15] and from DMFT by the NRG method,[16] the metal–insulator transition at zero temperature in the mass-imbalanced system is clearly continuous.

We finally clarify the nature of the Mott state by calculating the double occupancy $d_\alpha = \langle n_{\alpha\uparrow} n_{\alpha\downarrow} \rangle$, a quantity

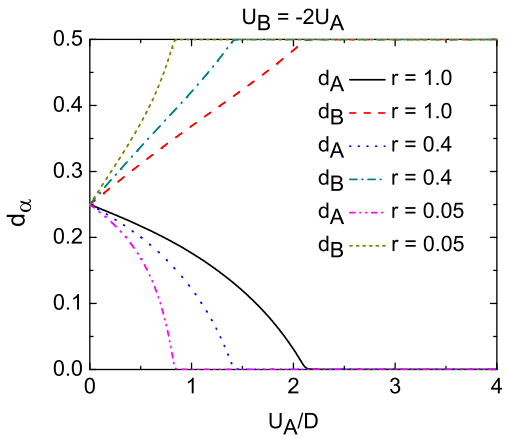

Fig. 5. (Color online) Double occupancy $d_A(d_B)$ for the $A(B)$ sublattice in the system with $U_B = -2U_A$ as a function of the interaction U_A/D for $r = 1.0$, 0.4, and 0.05.

that can be used as a thermometer in cold atom systems on optical lattices.[23] The numerical results for $U_B = -2U_A$ ($\gamma = 1/2$) and for $r = 1.0$, 0.4, and 0.05 are shown in Fig. 5. For a fixed r, in the non-interacting case ($U_A = U_B = 0$) the double occupancy for each sublattice is a quarter. When the interactions are introduced and gradually increased, the double occupancy for sublattice A decreases and vanishes at the critical point $(U_A)_c$, while the quantity for sublattice B increases and equals half at the critical point $(U_B)_c = -2(U_A)_c$. Hence, we can conclude that when the

repulsive and attractive interactions alternate in the system, the Mott insulating state is stabilized in the strong coupling region, where the singly occupied states are realized in the sublattice with the repulsive interaction, while the empty or doubly occupied states are equally realized in the other sublattice. Again, these behaviors happen under the conditions $n_{\alpha\uparrow} = n_{\alpha\downarrow} = 1/2$ and the findings are consistent with the results of the mass-balanced case.[15,16] In addition, by introducing mass imbalance into the system, at smaller values of r, the double occupancy for sublattice A (sublattice B) rapidly decreases (increases) owing to the reduced values of the critical interaction.

4. Conclusions

We have studied two-component fermionic mixtures with mass imbalance in an optical lattice with spatially modulated interactions. At half-filling and zero temperature, when the repulsive and attractive interactions alternate in the system, the phase boundary between a metal and a Mott insulator is analytically derived. Our result successfully recovers the limiting mass-balanced case ($r = 1$) as well as the homogeneous interaction case ($U_A = U_B$). By calculating the spin-dependent quasi-particle weights at the Fermi level for each sublattice as functions of the local interaction strength for various values of the hopping asymmetry, we clarify how the mass imbalance and spatial modulation of the interactions affect the stability of the normal metallic state. In particular, we show that for a large mass imbalance the light fermions are more renomalized than the heavy ones, even if they are in sublattice with a smaller local interaction, and for a fixed ratio $\gamma = U_A/|U_B|$ the strength of the critical interactions decreases with increasing mass imbalance. It is also found that in the strong coupling region of a two-component fermionic system with repulsive and attractive interactions, the Mott and pairing transitions occur simultaneously in the corresponding sublattices and the phase transitions at zero temperature are continuous.

In this paper we have restricted our study to the nonmagnetic phase. Possible instabilities toward other ordered states, such as a magnetically ordered state and a superfluid, are yet to be considered. These will be dealt with in the future.

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*hatuan@iop.vast.ac.vn

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