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Metal-insulator transitions in three-component Falicov-Kimball model within coherent potential approximation

Nguyen Thi Huong[1], **Le Duc Anh**[2] **and Hoang Anh Tuan**[3,†]

[1]*Thuy Loi University, 175 Tay Son, Dong Da, Hanoi, Vietnam*
[2]*Hanoi National University of Education, 136 Xuan Thuy, Cau Giay, Hanoi, Vietnam*
[3]*Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Ba Dinh, Hanoi 11108, Vietnam*

E-mail: †hatuan@iop.vast.vn

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Abstract. *We apply the coherent potential approximation to study the three-component Falicov-Kimball model, in which single-component and two-component fermionic particles are mixed in an optical lattice. In the model, the heavy single-component fermionic particles are localized while the light two-component fermionic particles can hop in the lattice. At half-filling, two transitions from an insulator via a metallic state to a Mott insulator are found with increasing the particle correlations. By contrast, at third-filling, only one transition from the metallic state to the Mott insulating phase is observed for strong repulsive interactions. Our results are consistent with those obtained by the dynamical mean field theory as well as by the slave boson mean field approach.*

Keywords: three–component Falicov–Kimball model; metal-insulator transition; coherent potential approximation.

Classification numbers: 71.27.+a; 71.30.+h.

1. Introduction

The metal-insulator transition (MIT) is one of the fundamental and fascinating problems of condensed matter physics, which has recently attracted a lot of attention [1]. It is well known established that the Mott-Hubbard MIT is caused by Coulomb correlations and the physics of

a Mott insulator is well described by the single band Hubbard and/or Falicov-Kimball models (FKM) [2].

The recently developed experiments with ultracold atoms in optical lattices have provided a new period for the MIT research. Indeed, the optical lattices allow one to control the atomic interactions and other relevant parameters as well as to introduce new parameters of the system. For example, binary mixtures of fermionic atoms with different masses (e.g., ^{6}Li,^{40}K) introduce the difference between the hopping parameter of two kinds of fermions. Moreover, some multicomponent correlation systems have been experimentally established [3], [4]. Theoretically, the MIT in three-component Hubbard models [5, 6] as well as in three-component Falicov-Kimball model were investigated [7], [8]. We note that the three-component Falicov-Kimball model in which one spices is two-component atoms with non-zero hopping amplitude and the other is a single-spin state atoms with zero hopping amplitude (i.e. completely localized) can be considered as a version of the three-component Hubbard model with extreme mass imbalance.

The MIT in the three-component FKM has been studied using various methods such as dynamical mean-field theory (DMFT) [7] and slave boson approach (SB) [8]. Different correlation-driven Mott transitions were found depending on the filling conditions and on-site Coulomb interactions. In particular, for a half-filled system, the re-entrant effect of Mott insulator is found with increasing the particle correlations. By contrast, at third-filling, only one transition from the metallic state to the Mott insulator is observed for strong local interactions.

It is known that the coherent potential approximation (CPA) has been used effectively for studying the Mott-Hubbard MIT in two-component strongly correlated electron systems such as the usual FKM [9], the Hubbard model [10] and the ionic Hubbard model [11]. The advantage of CPA compared with DMFT and SB is analytically simple. It can provide some analytic results and does not require much computer work. It is natural to ask whether the CPA is well suited for the study of three-component FKM. To answer this question, we revisit the MIT in the three-component FKM by using this method.

In Sec. 2 we present the three-component FKM and our CPA method. Numerical results are discussed in Sec. 3 and our conclusions are given in Sec. 4.

2. Model and formalism

We consider a three-component FKM, the Hamiltonian of which reads [7, 8]:

$$H = -t \sum_{\langle i,j\rangle,\sigma} \left[c^+_{i\sigma} c_{j\sigma} + h.c\right] - \mu \sum_{i,\sigma} c^+_{i\sigma} c_{i\sigma} + E_f \sum_{i,\sigma} f^+_i f_i + U_{cc} \sum_i c^+_{i\uparrow} c_{i\uparrow} c^+_{i\downarrow} c_{i\downarrow} + U_{cf} \sum_i f^+_i f_i c^+_{i\sigma} c_{i\sigma}, \quad (1)$$

where $c^+_{i\sigma}$ ($c_{i\sigma}$) creates (annihilates) a light fermion atom with spin σ ($\sigma \equiv \uparrow, \downarrow$) at lattice site i, and f^+_i (f_i) creates (annihilates) a localized fermion atom at lattice site i. t is the hopping amplitude between the nearest-neighbor light fermion atoms. μ is the chemical potential of the system. The energy level E_f can be considered as the chemical potential of the localized fermion atoms, which controls their filling in the system. U_{cc} is the on-site Coulomb interaction of the light fermion atoms, and U_{cf} is the on-site Coulomb interaction between the light and localized fermion atoms.

We apply the alloy analogy approach to the model. By viewing the system in terms of a disordered alloy where two-component fermion particles with spin σ can hop in the potential

of two-component fermion particles with spin $-\sigma$ and one-component localized particles. The many-body Hamiltonian (1) may be approximated by the one-particle Hamiltonian of the form

$$\tilde{H} = -t \sum_{\langle i,j\rangle,\sigma} \left[c_{i\sigma}^{+} c_{j\sigma} + c_{j\sigma}^{+} c_{i\sigma} \right] + E_f \sum_{i,\sigma} f_i^{+} f_i + \sum_{i,\sigma,\lambda} \varepsilon_{c\sigma}^{\lambda} c_{i\sigma}^{+} c_{i\sigma}, \tag{2}$$

where energy levels $\varepsilon_{c\sigma}^{\lambda}$ and configuration probabilities are given in Table 1. Here n_f is the filling of localized particles, $n_{c-\sigma}^{(0)}(n_{c-\sigma}^{(1)})$ is the filling of the light particles with spin $-\sigma$ in the lattice site that not occupied (occupied) by localized particles.
The Green function corresponding to the Hamiltonian (2) has to be averaged over all possible disorder configurations. The averaging cannot be performed exactly. To solve this problem, we use the CPA to replace the Hamiltonian (2) by an effective Hamiltonian with a self-energy $\Sigma_\sigma(\omega)$. Hamiltonian in the CPA takes the form

$$H_{CPA} = -t \sum_{\langle i,j\rangle,\sigma} \left[c_{i\sigma}^{+} c_{j\sigma} + c_{j\sigma}^{+} c_{i\sigma} \right] + E_f \sum_{i,\sigma} f_i^{+} f_i + \Sigma_\sigma(\omega) \sum_{i,\sigma} c_{i\sigma}^{+} c_{i\sigma}. \tag{3}$$

The lattice Green function for light fermion particles reads:

$$F_{c\sigma}(\omega) = \int \frac{\rho_0(x)}{\omega - x - \Sigma_\sigma(\omega)} dx. \tag{4}$$

where $\rho_0(x)$ is the bare density of states (DOS). Here for convenience we use a semicircular DOS $\rho_0(x)$, which corresponds to the Bethe lattice at infinite dimension [12]

$$\rho_0(x) = \frac{2}{\pi W^2} \sqrt{W^2 - x^2}, \tag{5}$$

where W is the half-width of the band and we will use it as the energy unit. The average Green function for two-component particles is calculated via the configuration probabilities $P_{c\sigma}^{\lambda}$ and the partial Green functions $G_{c\sigma}^{\lambda}(\omega)$

$$G_{c\sigma}(\omega) = \sum_{\lambda=1}^{4} P_{c\sigma}^{\lambda} G_{c\sigma}^{\lambda}(\omega). \tag{6}$$

Here $G_{c\sigma}^{\lambda}(\omega)$ is the Green's function for the configuration λ and is given by [13]

$$G_{c\sigma}^{\lambda}(\omega) = \frac{G_{c\sigma}(\omega)}{1 + \left(\Sigma_\sigma(\omega) - \varepsilon_{c\sigma}^{\lambda}\right) G_{c\sigma}(\omega)}. \tag{7}$$

The CPA demands that the average Green function in equation (6) must coincide with the lattice Green function in equation (4):

$$G_{c\sigma}(\omega) = F_{c\sigma}(\omega). \tag{8}$$

We take the filling of localized particles n_f as an input parameter, instead of the energy level E_f, then for a given total particle filling $n = \Sigma_\sigma n_{c\sigma} + n_f$, the chemical potential μ is obtained from the relation between the density of states (DOS) $\rho(\omega)$ and the light particle filling $n_{c\sigma}$ which read

$$\rho(\omega) = -\frac{1}{\pi} \mathrm{Im} G_{c\sigma}(\omega), \tag{9}$$

$$n_{c\sigma} = -\frac{1}{\pi}\int_{-\infty}^{0} \mathrm{Im}\left(G_{c\sigma}(\omega)\right) d\omega. \tag{10}$$

Table 1. Energy levels $\varepsilon_{c_\uparrow}^{\lambda}$ and configuration probabilities $P_{c_\uparrow}^{\lambda}$ for two-component fermion particles with spin up for the three–component Falicov–Kimball model. We focus on the paramagnetic case, for which $\varepsilon_{c\sigma}^{\lambda}, P_{c\sigma}^{\lambda}, n_{c\sigma}^{(0)}, n_{c\sigma}^{(1)}$ are spin-independent quantities.

Configurations λ	$c_\uparrow$	$c_\downarrow$	f	Energy levels $\varepsilon_{c_\uparrow}^{\lambda}$	Probabilities $P_{c_\uparrow}^{\lambda}$
1	1	0	0	$-\mu$	$(1-n_f)\left(1-n_{c_\downarrow}^{(0)}\right)$
2	1	1	0	$-\mu+U_{cc}$	$(1-n_f)\,n_{c_\downarrow}^{(0)}$
3	1	0	1	$-\mu+U_{cf}$	$n_f\left(1-n_{c_\downarrow}^{(1)}\right)$
4	1	1	1	$-\mu+U_{cc}+U_{cf}$	$n_f n_{c_\downarrow}^{(1)}$

3. Results and discussions

The self-consistent equation (8) does not have an exact solution but the self-energy and the Green function can be found by numerically solving with iteration. Beginning with a predictive self-energy $\Sigma_\sigma(\omega)$, the local Green function $F_{c\sigma}(\omega)$ and the average Green function $G_{c\sigma}(\omega)$ are obtained from equation (4) and equation (6), respectively. A new value of self-energy $\Sigma_\sigma(\omega)$ is determined as

$$\Sigma_\sigma(\omega) = \Sigma_\sigma(\omega) + \frac{1}{F_{c\sigma}(\omega)} - \frac{1}{G_{c\sigma}(\omega)}. \tag{11}$$

We iterate this procedure until convergence occurs. Actually, we add an analytic continuation $\omega \to \omega + i\delta$ when performing numerical calculations. Theoretically, δ is a small positive infinitesimal number. However, the value of δ should be in a range from 10^{-3} to 10^{-2} for iteration convergence to happen. If δ is smaller than 10^{-3}, the CPU has to undergo more computational time and the iterative process does not even converge.

In the following, we discuss results for $U_{cf} = 2.0$ at half-filling $n_{c\uparrow} = n_{c\downarrow} = n_f = 1/2$ in detail. Figure 1 shows the DOS of the light fermion particles and Fig. 2 presents the filling of light particle as a function of the chemical potential μ. In this paper, we choose the Fermi level as the origin of the energy axis. It is clear that for small values of U_{cc}, the DOS shows a gap at the Fermi level and thus the system is an insulator. This is shown in the example of the DOS in Fig. 1(a) and the plateau of the line in Fig. 2 at $n_{c\sigma} = 1/2$ for $U_{cc} = 0.5$. In this insulating phase, the on-site Coulomb interaction U_{cf} inhibits the double occupation of the heavy and light particles, therefore each lattice site is occupied by one particle. As U_{cc} is increased, the gap gradually closes and the DOS at the Fermi level becomes finite, indicating a transition to a metallic phase (Fig. 1(b) – 1(c)). Therefore, this is an inverse MIT. When U_{cc} increases, plateau $n_{c\sigma} = 1/2$ in the Fig. 2 disappears and simultaneously forming two plateaus at $n_{c\sigma} = 1/4$ and $n_{c\sigma} = 3/4$ correspond to the total filling n = 1 and n = 2. For larger U_{cc}, the light particle filling $n_{c\sigma}$ witnessed an additional

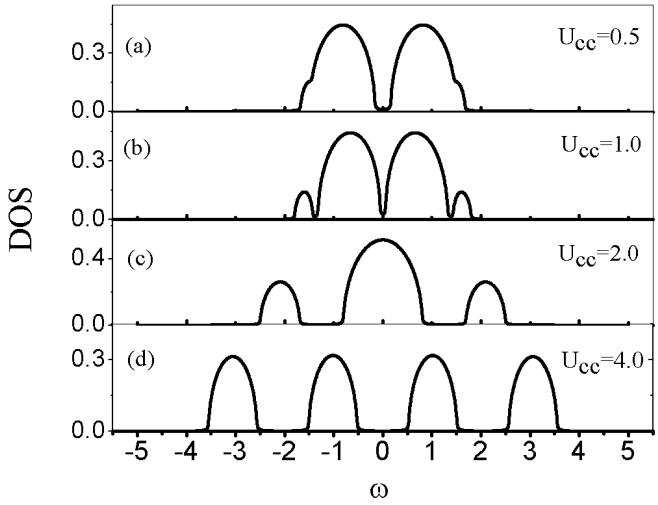

Fig. 1. Density of states of the light particles for various values of U_{cc} and $U_{cf} = 2.0$ at half-filling $n_{c\uparrow} = n_{c\downarrow} = n_f = 1/2$. Here as usual the Fermi level is chosen as the origin of the energy axis.

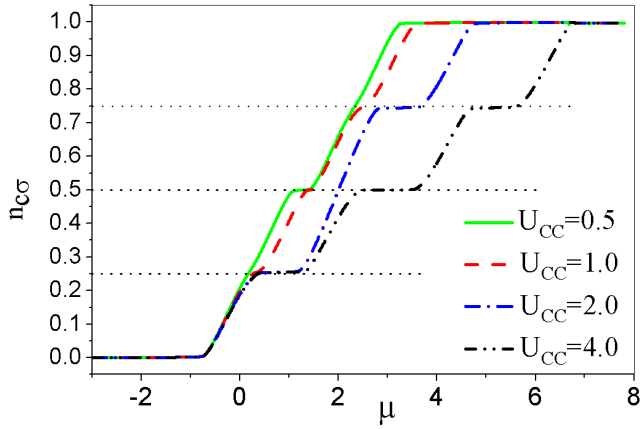

Fig. 2. (Color online) The filling of the light particle $n_{c\sigma}$ as a function of the chemical potential μ for various values of U_{cc} and $U_{cf} = 2.0$ at $n_f = 1/2$. The horizontal dotted lines indicate $n_{c\sigma} = 1/4$, $n_{c\sigma} = 1/2$ and $n_{c\sigma} = 3/4$.

plateau at $n_{c\sigma} = 1/2$ that indicates the system again in a insulator. This is shown in Fig. 1(d) for $U_{cc} = 4.0$ that the DOS has a gap at the Fermi level. However, different from the insulating phase at small values U_{cc}, in this case, each lattice site is occupied by one light two-component particle, and large on-site Coulomb interaction U_{cc} inhibits their double occupation. This is illustrated in Fig. 3 and Fig. 4, where the DOS of the light particles and their filling at $U_{cf} = 0.5$ are plotted, respectively.

Here, in contrast to $U_{cf} = 2.0$ case, for small values of U_{cc}, the system is in the metallic phase. However, for large values of U_{cc}, the correlation of light fermion particles drives the system from the metallic phase to the insulating one. The result shows that in this case MIT in the system does not depend on U_{cf} and the number of heavy fermion particles.

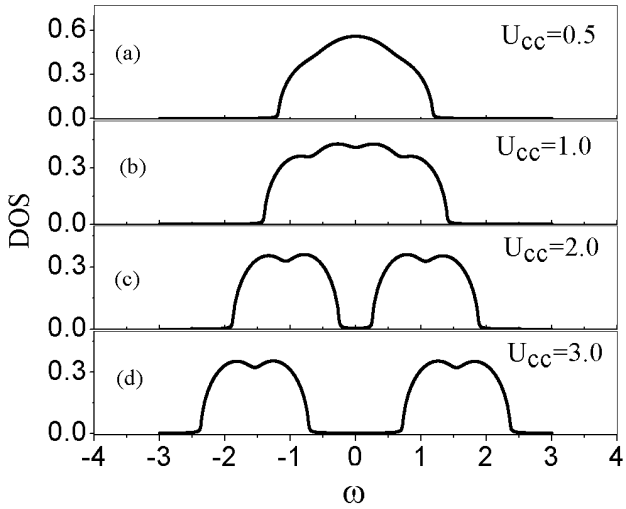

Fig. 3. Density of states of the light particles for various values of U_{cc} and $U_{cf} = 0.5$ at half-filling $n_{c\uparrow} = n_{c\downarrow} = n_f = 1/2$.

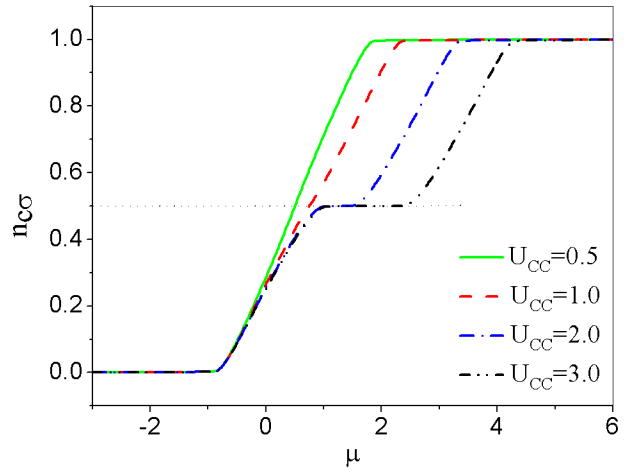

Fig. 4. (Color online) The filling of the light particles $n_{c\sigma}$ as a function of the chemical potential μ for various values of U_{cc} and $U_{cf} = 0.5$ at $n_f = 1/2$. The horizontal dotted line indicates $n_{c\sigma} = 1/2$.

Figure 5 shows the DOS of the light particles at the Fermi level as a function of U_{cc} for $U_{cf} = 2.0$. Here by using a simple extrapolation from the data for $1.0 < U_{cc} < 2.75$, we obtain $U_{cc}^{C1} \approx 0.92$ and $U_{cc}^{C2} \approx 2.85$, respectively.

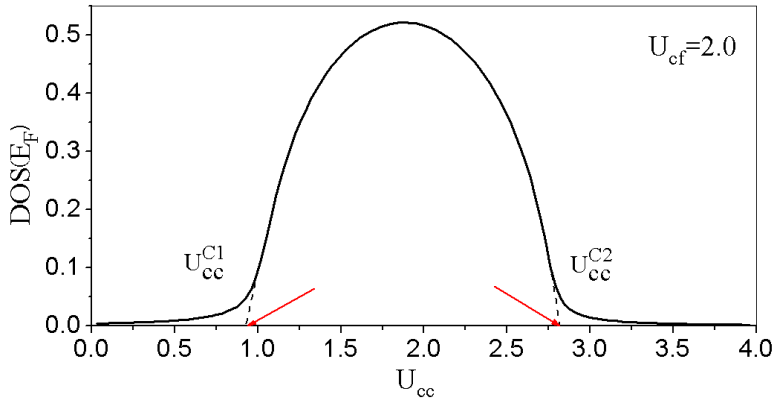

Fig. 5. (Color online) Density of states of the light particles at the Fermi level as a function of U_{cc}. The critical values obtained by extrapolating $1.0 < U_{cc} < 2.75$ data is also indicated ($U_{cf} = 2.0$, $n_{c\uparrow} = n_{c\downarrow} = n_f = 1/2$).

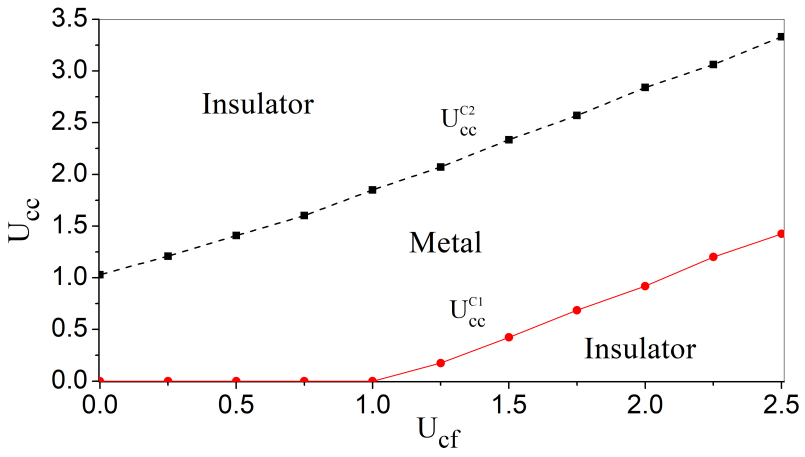

Fig. 6. (Color online) Phase diagram at half filling $n_{c\uparrow} = n_{c\downarrow} = n_f = 1/2$.

By carrying out a similar procedure for many different values of U_{cf}, we obtain the phase diagram of the system at half-filling plotted in Fig. 6. It is obvious that in the region $U_{cf} < 1.0$, there is one MIT in which the particle correlations drive the system from the metallic phase to the insulating phase. By contrast, in the region $U_{cf} \geq 1.0$, there are two MITs. While at the first transition $\left(U_{cc}^{C1}\right)$, particle correlations drive the system from the insulating phase to the metallic phase, at the second transition $\left(U_{cc}^{C2}\right)$, particle correlations drive the system from the metallic phase to the Mott insulating phase.

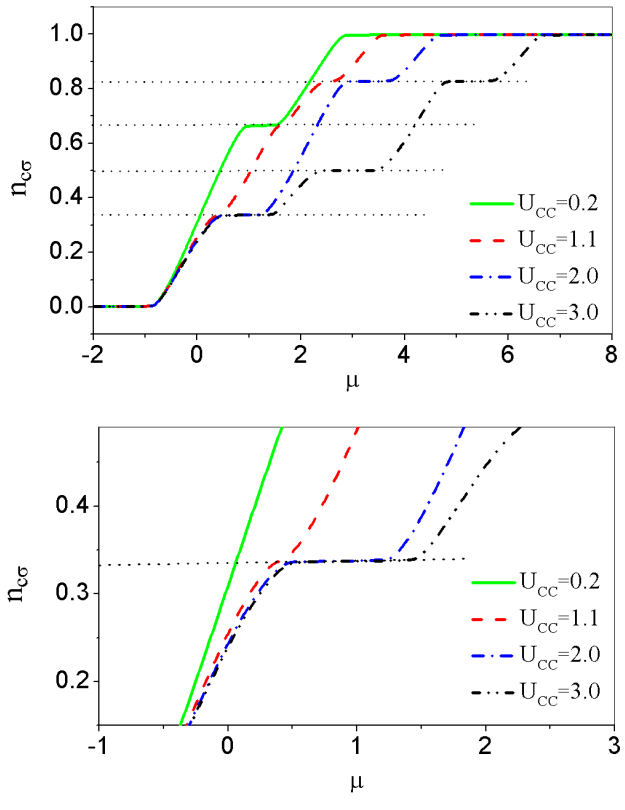

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Fig. 7. (Color online) Top panel: the filling of the light particles $n_{c\sigma}$ as a function of the chemical potential μ for various values of U_{cc} and $U_{cf} = 2.0$ at $n_f = 1/3$. The horizontal dotted lines indicate $n_{c\sigma} = 1/3$, $n_{c\sigma} = 1/2$, $n_{c\sigma} = 2/3$ and $n_{c\sigma} = 5/6$. Bottom panel: the filling of the light particle $n_{c\sigma}$ as a function of the chemical potential μ for various values of U_{cc} and $U_{cf} = 2.0$ focus the MIT at $n_{c\sigma} = 1/3$. The horizontal dotted lines indicate $n_{c\sigma} = 1/3$.

Next, we consider the MIT at third filling $n_{c\sigma} = n_f = 1/3$. Note that the two-third filling case $n_{c\sigma} = n_f = 1/3$ can be considered as a particle-hole symmetry of the third filling one [7]. We have checked the result of [7] that for $U_{cf} < U_{cf}^C \approx 1$ the MIT does not occur in the system at the third filling. Figure 7 presents the filling of the light particles $n_{c\sigma}$ as a function of the chemical potential μ at $n_f = 1/3$ for various values of U_{cc} and $U_{cf} = 2.0$. One can see that the plateaus appear at different values of $n_{c\sigma}$: $n_{c\sigma} = 1/3; 1/2; 2/3$ and 5/6. It means that the MIT can occur at different values of $n_{c\sigma}$, where $n_{c\sigma} + n_f = 1$ and $n_f = a/b$ with a, b being integer $(a < b)$. In contrast to the half-filling case, in the third filling the system is in metallic phase for small values of U_{cc}. When U_{cc} increases, the correlation of the light particles drives the system from the metallic phase to the insulating one as shown in Fig. 8 for various values of U_{cc} and fixed $U_{cf} = 2.0$ at $n_{c\uparrow} = n_{c\downarrow} = n_f = 1/3$. In numerical calculations, the chemical potential μ and the energy level of localized particles E_f are adjusted to maintain $n_f = 1/3$.

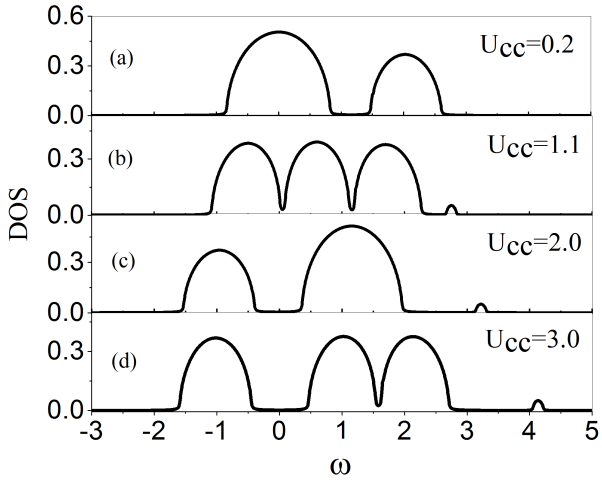

Fig. 8. Density of states of the light particles for various values of U_{cc} and $U_{cf} = 2.0$ at third filling $n_{c\uparrow} = n_{c\downarrow} = n_f = 1/3$.

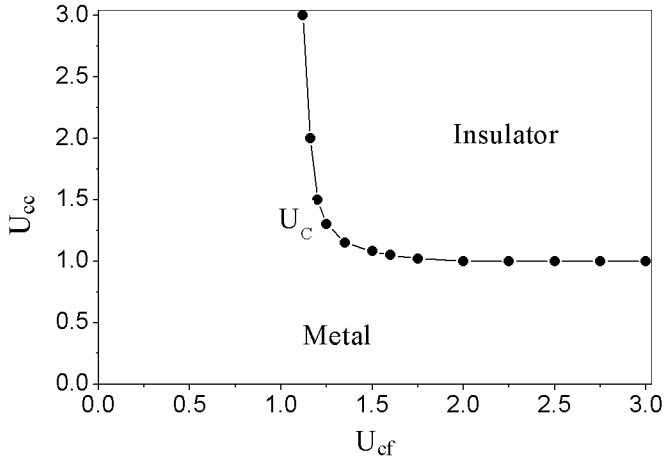

Fig. 9. Phase diagram for third filling $n_{c\uparrow} = n_{c\downarrow} = n_f = 1/3$.

Figure 9 depicts the phase diagram for the third-filling case. As it can be seen, in the region $U_{cf} < 1.0$, the system is in a metallic phase with any values of U_{cc}. When $U_{cf} > 1.0$, there is a transition from a metal to an insulator driven by the local repulsion U_{cc} between the light particles. In addition, the critical values U_C at the MIT point rapidly increase as U_{cf} approaches the value 1.0, while it slowly decreases as U_{cf} increases.

4. Conclusions

We have revisited the MIT in the three-component FKM by using the CPA. Within this method the MIT at half-filling and third-filling have been studied in detail. At half-filling, with

increasing U_{cc} there is a transition from the metallic phase to the insulator one when the values of U_{cf} are small. By contrast, when U_{cf} are large, the on-site Coulomb interaction of the light particles drives system from the insulating phase via the metallic to the insulating phase. It is interesting to note that this re-entrant effect of insulating phase was also observed in the MIT of the ionic Hubbard model at half-filling [11, 14]. At third-filling, the system is in the metallic phase for weak repulsive interaction U_{cf} and the MIT from the metallic phase to the Mott insulating one occurs when both U_{cc} and U_{cf} are large enough. Our CPA results are in good agreement with those obtained by the more sophisticated DMFT [7] and SB approach [8].

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Conflict of interest

The authors declare that they have no competing financial interests.

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