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Abstract. We derive the electronic phase diagram of the half-filled Anderson - Falicov-Kimball model with Gaussian distribution for impurities and box distribution for Coulomb disorder via dynamical mean field theory combined with typical medium theory. We show that the metal and the Mott insulator regions shrink as the strength of Coulomb disorder increases. The influence of the difference distributions (the box and the Gaussian) for impurities is also considered.

1. Introduction

The correlated and disordered lattice fermion systems have been at the forefront of condensed matter research for decades. In particular, Coulomb interaction prevailing in strongly correlated electron systems and disorder are two main sources leading to metal - insulator transitions (MITs). While the correlation induced MITs are called Mott- Hubbard transition, the coherent backscattering of non-interacting particles from randomly distributed impurities can cause Anderson localization [1, 2].

Since electronic interactions and disorders can both induce a MIT, one might expect their simultaneous presence to be even more effective in localizing electrons. However, this is not so simple. For, example, week disorder is able to weaken the effect of correlation and may turn an insulator into a bad metal. Furthermore, short-range interactions leads to transfer of spectral weight into the Hubbard subbands so that the critical disorder strength for Anderson MIT increases, implying a reduction of the effective disorder strength [3, 4]. Therefore, the interplay between disorder and interactions leads to subtle many-body effects, which pose fundamental challengers for theory and experiment not only in condensed matter physics but also in the field of ultracold atoms on optical lattice, which have proved to be versatile and flexible simulators.

The simplest model Hamiltonian of strongly correlated systems is the Falicov – Kimball model (FKM), which is a simplified of the Hubbard model (HM) where one of the spin species has zero hopping, so its motion is frozen. Similar to the HM, a Mott metal – insulator transition as a function of a local Coulomb interaction U was also found in the FKM at half filling [5]. The FKM is especially interesting because it is exactly solvable in infinite dimensions [6]. Besides, it contains important aspects of strongly correlation physics, such as the order-disorder transition in binary alloys [7], charge transport [8], and itinerant magnetism [9]. On the other hand, considering transport properties of free electrons on a lattice in presence of random on-site energies,

Anderson concluded that for disorder strengths bigger the critical one a particle, initially occupying any given lattice site, does not spread infinitely, but stays in a finite region around this site, i. e. , it gets localized [2]. The connection between Falicov-Kimball and Anderson models is the Anderson – Falicov – Kimball model (AFKM). Therefore, in comparison with the FKM, the AFKM is including a local potential, which disturbing the propagation of free fermions. This potential is a random quantity distributed to some specified probability distribution function (PDF). The often used different disorder distributions are the box, Gaussian, Lorentzian, and binary distributions. It is clear that the phase diagram of the AFKM is richer and more attracting than those of the FKM because of the appearance of the Anderson localization besides the Mott one. Moreover, in the AFKM one can study different realizations of the interplay of disorder and electron correlations.

In recent years, the dynamical mean field theory (DMFT) has been one of the most accepted method to capture the physics of the Mott - Hubbard MIT as well as strongly correlated systems. However, simply incorporating disorder effects into this approach through an arithmetic average of the local density of states (LDOS) does not yields Anderson localization. In contrast to the arithmetic average, the geometrical average gives a better approximation to the most probable value of the LDOS. Dobrosavljevic et al [10] developed the typical medium theory (TMT) to study disordered systems, where the typical density of states, approximated using the geometrical averaging over disorder configurations, is used instead of the arithmetically averaged LDOS. Within DMFT-TMT the ground state phase diagram for the AFKM at half – filling, where the local potentials are assumed to be independent and identically – distributed random variable with an uniform box distribution, has been obtained by Byczuk [11] and Gusmao [12]. Moreover, recently the AFKM with a Coulomb disorder, i. e., the interaction strengh between free and frozen fermions in each site is set randomly, is also considered by Carvalho et al [13]. They show that Coulomb disorder has a relevant role in the phase-transition behavior as the system is led towards the insulator regime.

Since a Gaussian distribution is more reasonable for real materials, in this paper we consider AFKM with Gaussian distribution for impurities and box distribution for Coulomb disorder by mean of DMFT-TMT. The role of Coulomb disorder as well as the influence of Gaussian distribution for impurities in the metal - insulator phase diagrams of the system are analysed.

The paper is organized as follows. In the next Section 2, the AFKM with Coulomb disorder is introduced and solved within dynamical mean field theory - typical medium theory. In section 3, phase diagrams are presented and the interplay between the strength of both distribution are discussed. Finally, Section 4 contains our conclusions.

2. Model and formalism
We consider the Anderson - Falicov - Kimball model, as defined by the following Hamiltonian

$$H = -\sum_{<i,j>} t_{i,j} c_i^\dagger c_j + \sum_i \varepsilon_i c_i^\dagger c_i + \sum_i U_i f_i^\dagger f_i c_i^\dagger c_i - \mu \sum_i (c_i^\dagger c_i + f_i^\dagger f_i), \tag{1}$$

where $c_i^\dagger(c_i)$ and $f_i^\dagger(f_i)$ are fermionic creation (annihilation) operators for the mobile and immobile particles at a lattice site i. t_{ij} is a hopping amplitude for mobile particles between sites i and j, and U_i the local interaction strength between mobile and immobile particles occupying in the same site i; ε_i is the local impurity, μ the chemical potential. These two quantities are randomly distributed through the lattice, we assume a Gaussian distribution for

impurities $P(\varepsilon_i) = \sqrt{\frac{6}{\pi \Delta^2}} \exp\left(-6\varepsilon_i^2/\Delta\right)$ and a box distribution for local Coulomb interaction $\tilde{P}(U_i) = \theta(\delta/2 - |U_i - U|)/\delta$, where θ is the step function, $\Delta(\delta)$ measures the amount of Anderson (Coulomb) disorder, and U is the mean value of the Coulomb interaction strength. Here, we deal only with the repulsive interaction, $U_i \geq 0$, which leads to $U \geq \delta/2$. The mean particle number for the mobile and trapped fermions at the ith site are given by $n_i = < c_i^\dagger c_i >$ and $p_i = < f_i^\dagger f_i >$, respectively, and are independent from each other.

The AFKM is solved within the DMFT combined with the TMT. The equation of motion for Hamiltonian (1) are expressed by [14, 15]:

$$(\omega + \mu - \varepsilon_i)G_{ij}(\omega) - \sum_l t_{il}G_{lj}(\omega) = \delta_{ij} + U\Gamma_{ij}(\omega), \tag{2}$$

$$(\omega + \mu - \varepsilon_i - U_i)\Gamma_{ij}(\omega) - \sum_l t_{il}\Gamma_{lj}(\omega) = \delta_{ij}p_i, \tag{3}$$

where we used that a number of the immobile particles is conserved being zero or one, and here $f_i^\dagger f_i f_i^\dagger f_i = f_i^\dagger f_i$, $G_{ij}(\omega) = << c_i|c_j^\dagger >>_\omega$ and $\Gamma_{ij}(\omega) = << f_i f_i^\dagger c_i|c_j >>_\omega$ are the Green functions for the single and double particle states, and δ_{ij} is the Kronecker delta function. Here we assume the lattice to be homogeneous, that is $p_i = p$ with $p \in [0, 1]$.

By defining the site-dependent self-energy as

$$\Sigma_i(\omega) \equiv U_i \frac{\Gamma_{ij}}{G_{ij}(\omega)}, \tag{4}$$

we obtain a local (ε_i, U_i) Green function and the self - energy

$$G_{ii}(\omega) = \frac{1}{\omega + \mu - \varepsilon_i - \eta(\omega) - \Sigma_i(\omega)}, \tag{5}$$

$$\Sigma_i(\omega) = pU_i + \frac{p(1-p)U_i^2}{\omega + \mu - \varepsilon_i - (1-p)U_i - \eta(\omega)}. \tag{6}$$

where $\eta(\omega)$ is the hybridization function. Then the LDOS is given by

$$\rho(\omega, \varepsilon_i, U_i) = -\frac{1}{\pi}\text{Im}[G_{ii}(\omega)], \tag{7}$$

The averaged LDOS can be evaluated by using the arithmetic or geometric mean given by, respectively,

$$\rho_{arith}(\omega) = \int du \int d\varepsilon P(\varepsilon)\tilde{P}(u)\rho(\omega, \varepsilon, u), \tag{8}$$

$$\rho_{geom}(\omega) = \exp\left[\int du \int d\varepsilon P(\varepsilon)\tilde{P}(u)\log \rho(\omega, \varepsilon, u)\right]. \tag{9}$$

The lattice, i.e., translationally invariant, Green function is obtained by the Hilbert transform

$$G_{typ}(\omega) = \int d\omega' \frac{\rho_\alpha(\omega')}{\omega - \omega'}, \tag{10}$$

where the subscript α stands for either "geom" or "arith."

We consider the Bethe lattice with infinite connectivity, $\rho_0(\varepsilon) = 4\sqrt{1 - 4(\varepsilon/W)^2}/(\pi W)$, for which the self-consistent condition is given by $\eta(\omega) = W^2 G(\omega)/16$. In addition, we study the

band is half - filled, i.e., $n_i = n = 1/2$ and $p = 1/2$. The chemical potential was set to $\mu = U/2$ in order to fix the band center at $\omega = 0$.

To proceed further, we note that in the half-filled band case, the ground state properties can be determined by the averaged LDOS at the Fermi level ($\omega = 0$): $\rho_{geom}(0) > 0$ denotes a metallic phase; $\rho_{arith}(0) = 0$ indicates a Mott insulator phase (hard gap); and $\rho_{geom}(0) = 0$, $\rho_{arith}(0) > 0$ denote a Anderson insulator phase (gapless). In addition, the Green function at the Fermi level is purely imaginary, $G(0) = -i\pi\rho_\alpha(0)$ and on the metallic side the LDOS is arbitrarily small in the vicinity of the MIT region. Therefore, the transition points on the phase diagram can be found by linearizing the DMFT equations [11, 13]. The equations which determine the MIT for both arithmetic and geometric means, respectively, take the form

$$4\Delta\delta = \int\limits_0^\infty \sqrt{\frac{6}{\pi}} \left[\frac{U/2 - \delta/4}{(U/2 - \delta/4)^2 - \varepsilon^2} - \frac{U/2 + \delta/4}{(U/2 + \delta/4)^2 - \varepsilon^2} \right] \exp\left(-\frac{6\varepsilon^2}{\Delta^2}\right) d\varepsilon, \qquad (11)$$

$$1 = \frac{1}{16} \exp\left[\frac{4}{\Delta\delta} \sqrt{\frac{6}{\pi}} \int\limits_0^{+\infty} f(\delta, U, \varepsilon) \exp\left(-\frac{6\varepsilon^2}{\Delta^2}\right) d\varepsilon \right], \qquad (12)$$

where

$$f(\delta, U, \varepsilon) = t\ln[t^2 + \varepsilon^2] - 2t\ln|t^2 - \varepsilon^2| + 2t + 2\varepsilon \left(\arctan\frac{t}{\varepsilon} + \ln\left|\frac{t - \varepsilon}{t + \varepsilon}\right| \right)\Bigg|_{t_1}^{t_2}, \qquad (13)$$

with $t_1 = \frac{U}{2} - \frac{\delta}{4}$, $t_2 = \frac{U}{2} + \frac{\delta}{4}$.

For each value of δ, equations (11) - (13), which determine the $U - \Delta$ phase diagram of the half - filled Anderson-Falicov-Kimball model with Coulomb disorder, are our main result.

3. Numerical results and discussion

Through this work we set the bandwidth W as the unit of the energy. Firstly, we calculate the case without Coulomb disorder ($\delta = 0$). The $U - \Delta$ phase diagram of AFKM with the Gaussian impurity disorder distribution is shown in Fig. 1 (dash gray lines) as well as well as in Fig. 2 (top-left part). As in the case of the box impurity disorder distribution [11], we find that the metallic phase is identified for small value of U and Δ, the Mott insulator appears when we increases U, and the Anderson insulator naturally overcomes for large Δ. This is clearly seen in Fig. 1 where we compare the phase diagrams evaluated at the band center with and without Coulomb disorder. In the case without Coulomb disorder ($\delta = 0$), there are three different inter-action regimes can be identified regarding the metallic and Mott phase boundaries (noted in the U - axis in Fig. 1): weak ($0 < U < 0.5$), intermediate ($0.50 < U < 1.0$), and strong ($U \geq 1.0$). When $\delta \neq 0$, these regimes still hold but for different critical values, with the intermediate one shrinking as δ increases. Here, we just deal with a repulsive interaction, $U_i \geq 0$, which leads to $U \geq \delta/2$, i. e., we consider only the right hand of the vertical dotted lines in Fig. 1. Therefore, in Fig. 1 we show that the major effect of including Coulomb disorder is the narrowing of the metal and the Mott insulator regions as the strength of Coulomb disorder increases.

We note that all the critical curves presented in Fig. 1 were obtained directly from equations (11) - (13), however, it can verified that the numerical results obtained by solving the self - consistent equations of DMFT absolutely matches with those from the linearised DMFT.

In Fig. 2 we compare our result with those obtained in [13], where the AFKM with box distribution for the local impurities $P(\varepsilon_i) = \Theta(\Delta/2 - |\varepsilon_i|)/\Delta$ and box distribution for Coulomb
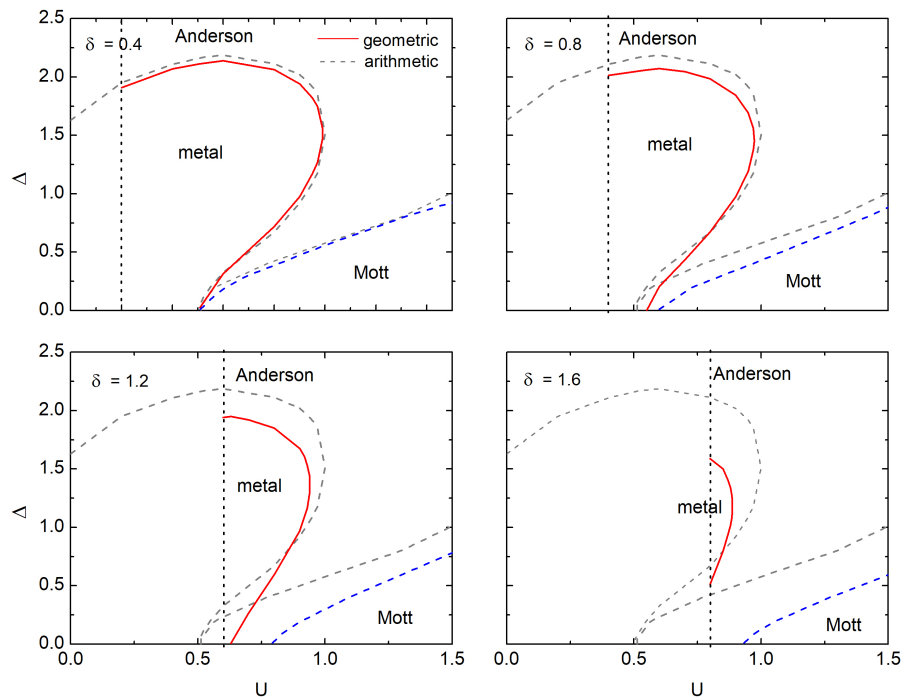
Figure 1. Phase diagrams of the AFKM for different Coulomb disorder strengths (solid red (dash blue) lines for geometric (arithmetic) mean) compared with the $\delta = 0$ case (dash gray lines). The vertical dotted line splits the regions for which $U < \delta/2$ (left side; not considered) and $U \geq \delta/2$ (right side). W sets the energy unit.

interaction strength $\tilde{P}(U_i) = \theta(\delta/2 - |U_i - U|)/\delta$ is considered. In order to be able to compare the box and Gaussian distributions, we choose their variances equal. There is not a big difference between the two phase diagrams when $\delta = 0$: for both disorder distributions one finds a metallic core for small and intermediate strengths of both the disorder and the interaction. Also the re-entrance behavior as a function of Δ for intermediate U is similarly predicted for both disorder distributions. However, on a quantitative level the results differ each other. We find that for small values of U the critical disorder strength in the system with the Gaussian distribution is larger than those in the system with the box distribution. For example, in the non-interacting system the critical disorder ($\Delta_c(U = 0) \approx 1.63$) for the Gaussian distribution larger than those ($\Delta_c(U = 0) \approx 1.36$) for the box distribution. Furthermore, for the Gaussian disorder distribution the intermediate regime ($0.50 < U < 1.0$) is narrowing than those of the box distribution ($0.50 < U < 1.36$). In addition, the border between the Mott and the Anderson insulators for the system with the Gaussian distribution is located lower than those with the box distribution in the (U, Δ) plane. The similar results have been found in Anderson-Hubbard model with the Gaussian and the box disorder distributions [16]. As commented there the higher disorders associated with the exponential nature of the Gaussian distribution may be responsible for quantitative differences between them. When $\delta \neq 0$, the similar pictures still hold but for different critical values, with the intermediate one shrinking as δ increases and for $\delta \geq 1.2$ the border between the Mott and the Anderson insulators for the system almost does not depend
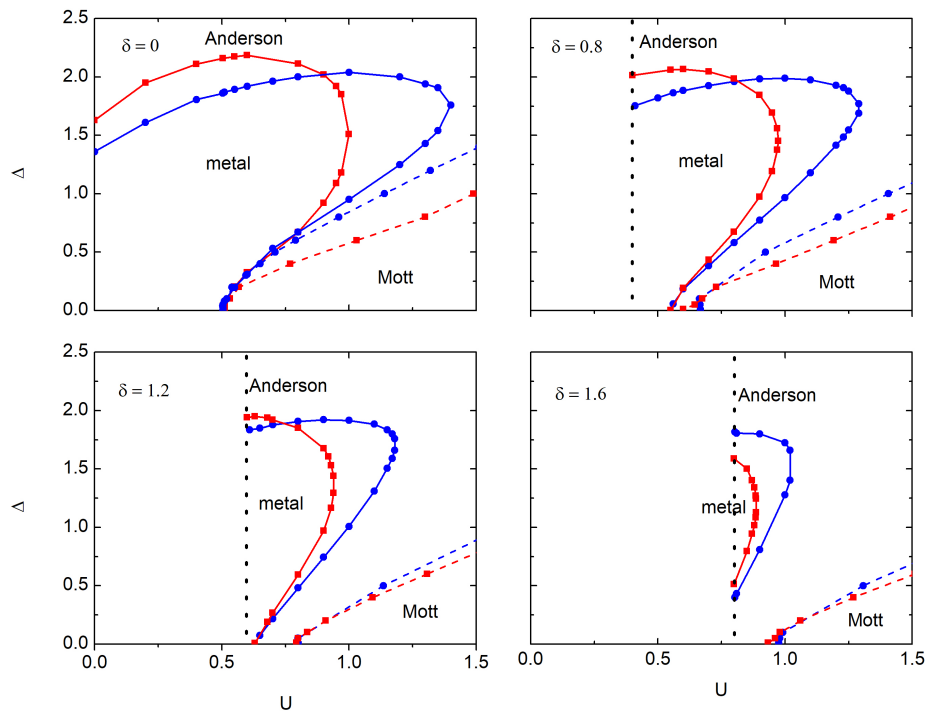
Figure 2. Phase diagrams of the AFKM with the Gaussian impurity disorder distribution and the box Coulomb disorder distribution (our result, red lines with squares) compared to those with the box impurity distribution and the box Coulomb disorder distribution in Ref. [13] (blue lines with dots).

to the impurity distribution that we chose.

4. Conclusions

In summary, in this paper the nonmagnetic ground state phase diagram for the Anderson-Falicov-Kimball model with Gaussian distribution for impurities and box distribution for Coulomb disorder at half-filling are obtained within the typical-medium theory using the equation of motion as an impurity solver. For a fixed local Coulomb disorder the explicit equations determining the boundary between the correlated metal, Mott insulator, and Anderson localization phases are derived. We show that the metallic and Mott insulator regimes shrink as the local Coulomb disordered strengths increases. In addition, the critical values associated with the MIT change as the intensity of Coulomb disorder is tuned. We also show that within DMFT-TMT the phase diagrams of the AFKM with the box and the Gaussian distribution for impurities are qualitatively similar.

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