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Stripes and phase separation in strongly correlated systems

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Using classical Monte Carlo approach we analyze two-dimensional Falicov–Kimball model away from half-filling. Both the weak and the strong interaction regimes are considered. We found that in the former case stripe configurations are the stable ones, whereas in the latter case the phase separation minimize the energy. We present also the spectral properties of the system.

1 Introduction

One of the problems in strongly correlated systems which is recently gaining attention is the possibility of nanoscale phase separation. Using recently developed version of the Monte Carlo approach [1] we demonstrate how phase separation occurs in the Falicov–Kimball model [2] away from half-filling. This method, based on the classical Metropolis algorithm [3], allows one to perform calculations for systems with both classical and fermionic degrees of freedom. So, it is suitable for the Falicov–Kimball model.

1.1 Falicov–Kimball model

The Falicov–Kimball model has been introduced in 1969 in order to describe the semiconductor-metal transition in SmB_6 [2]. Later, it has been used, e.g., to explain crystallization due to effective interactions mediated by conduction electrons [4, 5]. The Falicov–Kimball model can be obtained from one-band Hubbard model in the limit of infinitely massive spin-down electrons.

The Falicov–Kimball model describes mobile fermionic particles and localized classical ones. The only interaction explicitly included in the Hamiltonian is between these two kinds of particles. However, as the configuration of the classical particles minimizes the ground state energy at zero temperature or the free energy for finite temperatures, an effective interaction arises between the classical as well as between the mobile particles. This is why the Falicov–Kimball model can be regarded as a many-body model. The Hamiltonian in its simplest spinless form is given by

$$\mathcal{H} = -t\sum_{\langle ij\rangle} c_i^{\dagger}c_j + U\sum_i c_i^{\dagger}c_i w_i \,, \tag{1}$$

where $c_i^{\dagger}(c_i)$ creates (annihilates) a conduction electron at lattice site i and w_i is equal to 0 or 1, according to whether the site i is occupied or unoccupied by a localized particle. There are numerous interpretations of the localized particles: f-electrons, spin-down electrons, ions, impurities, nucleons.

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1.2 The method

It is known, that in half-filled Falicov–Kimball model at low temperature the localized particles form a chessboard pattern. On the other hand, away from half-filling the energy is minimized by forming other patterns, some of them with very large periods. Additionally, for strong enough interaction the mobile and localized particles segregate. Therefore, it is tempting to investigate the Falicov–Kimball model using some of cluster methods which are capable to describe the inhomogeneous system in the real space. In this paper we use the Monte Carlo method. However, since the Falicov–Kimball model describes classical as well as fermionic particles, the classical Monte Carlo method in its basic form cannot be used. On the other hand, since the mobile electrons do not interact directly, there is no need to use the Quantum Monte Carlo method. Therefore we have developed a modification of the classical Metropolis algorithm, that is able to tackle a system with both classical and quantum degrees of freedom. In this version of the algorithm in each Monte Carlo step the Hamiltonian (1) is numerically diagonalized for a given configuration of the localized particles $\{w_i\}$ giving energy spectrum. Then, the free energy is used to determine the statistical weights. Details of this approach are given in Ref. [1].

2 Results

References [1] is devoted to the half-filling case. In the present paper we analyze the Falicov–Kimball model away from half-illing. Namely, we perform simulations for the concentration of the mobile electrons (ρ_e) equal to the concentration of the localized electrons (ρ_i) and equal to 0.4 and 0.25. The simulations are carried out for a wide range of the strength of the interaction between the localized and mobile electrons ($1 \le U/t \le 10$) at different temperatures. The critical temperature of the phase transition between ordered and disordered phase is determined from the position of a peak in the specific heat. Figure 1 shows approximate phase diagrams. While there is a distinct border between the ordered and disordered phase, it is difficult to determine the border between regions with phase separation and with stripes. Moreover, the critical temperature has been obtained only at some values of U/t, indicated by points on the diagrams, whereas the lines connecting these points are guides for eyes.

Figure 2 presents examples of temperature dependence of configurations of mobile and localized particles in both weak and strong interaction regimes. Since the simulations are performed at finite temperature, the configurations change dynamically, so these pictures show only "snapshots", which are representative for given model parameters. At high temperature the localized electrons are distributed randomly over lattice sites, independently of the interaction potential. As the temperature is lowered,

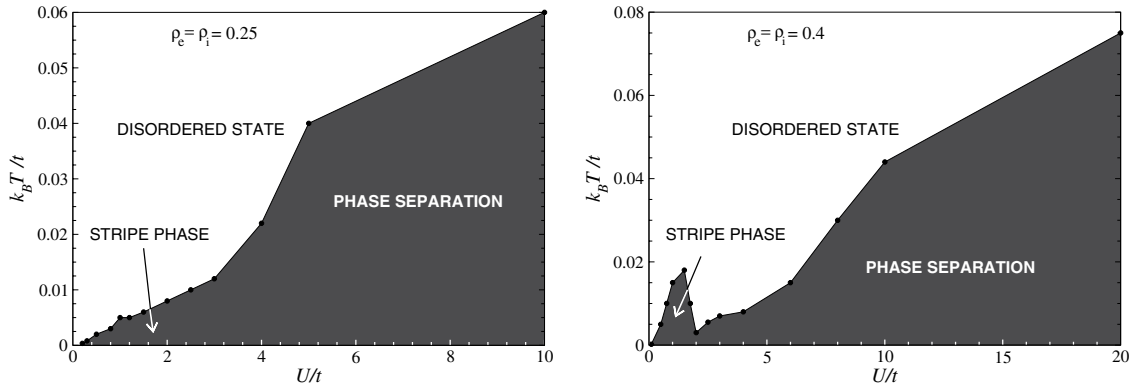

Fig. 1 Phase diagrams for the Falicov–Kimball model for two different electron concentrations: $\rho_d = \rho_f = 0.25$ (left panel) and $\rho_d = \rho_f = 0.4$ (right panel).

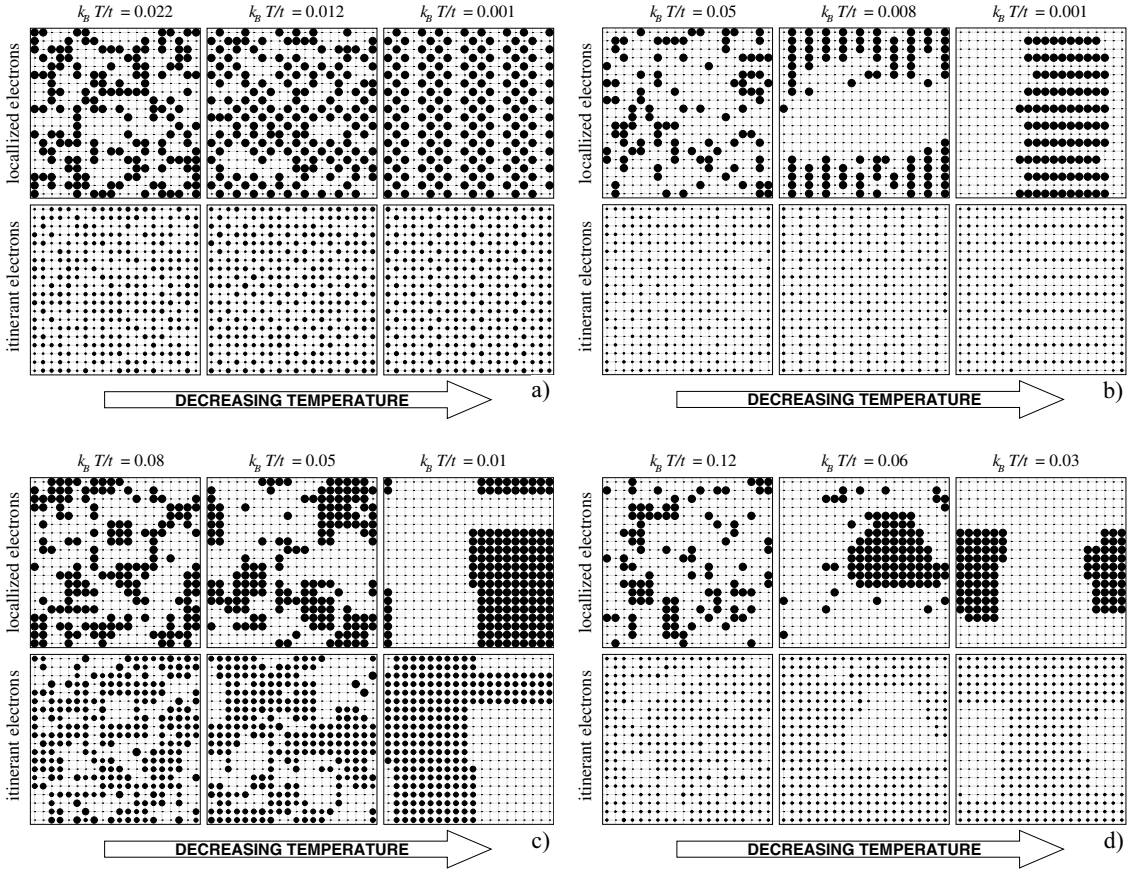

Fig. 2 Snapshots of configurations of mobile and localized electrons. The upper row in each panel shows f-electron configurations – black circles represent lattice sites occupied by localized particles. The lower rows show concentration of mobile electrons – diameters of the circles are proportional to the concentration of mobile electrons. Panels A to D display results for various concentrations and various interactions: a) $\rho_e = \rho_i = 0.4$, $U/t = 1$; b) $\rho_e = \rho_i = 0.25$, $U/t = 2$; c) $\rho_e = \rho_i = 0.4$, $U/t = 8$; d) $\rho_e = \rho_i = 0.25$, $U/t = 10$, where ρ_e is the concentration of mobile electrons, whereas ρ_i is the concentration of the localized ones.

they arrange themselves into various forms. This process is indicated by large arrows in Fig. 2. Configurations of the mobile electrons are determined by the competition between their kinetic energy and interaction with the localized electrons. Namely, when the interaction is weak-to-moderate, they occupy all lattice sites with the local density modulated by the presence of localized electrons (Fig. 2a and c). On the other hand, when the interaction is strong, they do not sit on sites occupied by massive electrons (Fig. 2b and d). However, since the concentration of mobile electrons is different from 0.5, even in the latter case the system does not undergo the Mott metal–insulator transition.

Figure 2 shows that for both densities ($\rho_e = \rho_i = 0.25$ and $\rho_e = \rho_i = 0.4$) at low enough temperature, the system separates itself into mobile-electron-rich and localized-electron-rich regions. Such a phase separation has been expected in the Falicov–Kimball model away from half-filling in the strong interaction regime [7]. In the weak-interaction regime the localized electrons form stripes. Configuration of electrons in these stripes (which can also be treated as a form of phase separation) strongly depends on the model parameters. These results fit with results obtained by means of e.g., *restricted phase diagram* method [6].

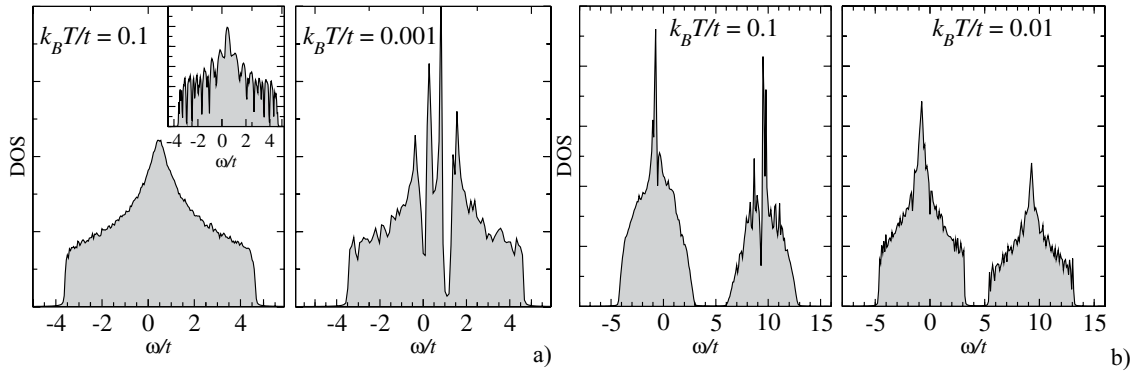

Fig. 3 Density of states of the itinerant electrons for $\rho_d = \rho_f = 0.4$ in the weak [a) $U = t$] and strong [b) $U = 10t$] interaction regime. The inset in the left panel shows results obtained without the use of the ABC method.

The properties of the mobile electrons can be analyzed using their density of states (DOS). The DOS can be determined from the standard formula

$$\rho(\omega) = -\frac{1}{\pi}\mathrm{Im}\sum_{\boldsymbol{k}} G(\boldsymbol{k}, \omega + i0^+)\,, \tag{2}$$

where the localized-electron-configuration-averaged electronic Green function $G(\boldsymbol{k},\omega)$, is given by

$$\sum_{\boldsymbol{R}_i}\sum_{\boldsymbol{R}_j} \exp\{i(\boldsymbol{k}\cdot\boldsymbol{R}_i - \boldsymbol{k}'\cdot\boldsymbol{R}_j)\}\,\langle \mathcal{G}(\boldsymbol{R}_i,\boldsymbol{R}_j,z)\rangle = G(\boldsymbol{k},z)\,\delta(\boldsymbol{k}-\boldsymbol{k}')\,. \tag{3}$$

Here, $\mathcal{G}(\boldsymbol{R}_i,\boldsymbol{R}_j,z) = \{[z - \mathcal{H}(\mathcal{C})]^{-1}\}_{ij}$ is the real-space Green function for a given configuration of the localized electrons $\mathcal{C}$ and $\langle\ldots\rangle$ indicates averaging over configurations accepted in the Metropolis algorithm. For long enough Monte Carlo run $\langle\mathcal{G}(\boldsymbol{R}_i,\boldsymbol{R}_j,z)\rangle$ is translational invariant, so $G(\boldsymbol{k},\omega)$ depends only on one momentum vector $\boldsymbol{k}$. In order to minimize the finite size effects we have applied a method known as *averaging over boundary conditions* (ABC) [8]. Within the framework of this method each time the hopping term in the Hamiltonian makes a particular electron jump out of the cluster, it is mapped back into the cluster with different phase of its wave function. In the momentum space such a change of the phase corresponds to a shift of the point in the Brillouin zone. The whole reciprocal space can be swept, when the phase is allowed to vary continuously. Physical quantities, e.g., the DOS, calculated for a given phase shift are then averaged over the value of the shift. This method can be very easily adopted to Monte Carlo simulations for the FK model. In each Monte Carlo step a random phase shift is added to the hopping term in the Hamiltonian (1), and therefore the averaging over localized electron configurations in Eq. (3) is accompanied by an averaging over the phase shift. In this way, in contrast to e.g., the exact diagonalization study, no additional computational effort is needed to perform averaging over boundary conditions.

Figure 3 shows the DOS determined for various particle density and various interaction strength using the ABC method. At high temperature the localized particles are randomly distributed over the whole cluster. When the interaction is weak (Fig. 3a), their averaged influence on the itinerant electrons vanishes. Therefore, in this regime the DOS is the same as for a free electron gas on a square lattice. As the temperature is lowered, some features occur in the DOS, but the interaction is too small to open a gap. On the other hand, if the interaction is much larger than the bandwidth (Fig. 3b), the band is splitted into two subbands independently of the temperature. However, since the system is away from half-filling, the Fermi level lies inside the conduction band and despite the presence of the gap the system is metallic at arbitrary temperature.

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