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Pattern formation in the Falicov–Kimball model

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It is known that in the ground state of half-filled Falicov–Kimball model immobile particles form a checkerboard pattern. On the other hand, there is a wide range of model parameters, for which this model is expected to exhibit a phase separation. Using Monte Carlo simulations we demonstrate how the system reaches these states, as the temperature is lowered.

1 Introduction

The Falicov–Kimball model (FKM) [1] was introduced to explain a metal–insulator transition that occurs in transition metals and rare-earth compounds. Later, it was again considered to describe order in mixed valence systems and binary alloys. It has also been proposed as a model for crystalline formation [2]. From a theoretical point of view, it can be considered as a simplification of the Hubbard model [3], where one species of electrons has infinite mass and do not hop. In fact, the FKM is one of the simplest fermionic models, showing non-trivial many-body correlation effects. The model consists of two types of particles: itinerant conduction electrons and localized particles ("ions") that interact with electrons through an on–site Coulomb interactions. The Falicov–Kimball Hamiltonian is

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

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 massive particle. The ground state for fixed numbers of electrons and ions is defined by taking the ground state of the Hamiltonian with respect to the electrons for each ionic configuration and then minimizing the result with respect to the location of the ions. Similarly, at finite temperature one has to compute the electronic partition function for each ionic configuration and then average over these configurations. The averaging ("annealing") is responsible for the many–body effects in the FKM.

In this paper, we demonstrate how such an annealing can be realized within the framework of Monte Carlo (MC) simulations. It is organized in the following manner: in Sec. 2 we describe the details of the MC approach to the FKM. In Secs. 3 and 4 we present MC results for half–filled FKM and away from half-filling, respectively.

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2 Method of simulation

Our system contains classical (ions) as well as fermionic (electrons) degrees of freedom. The appropriate way to treat such a Hamiltonian is to define the grand canonical partition function as

$$\mathcal{Z} = \sum_{\mathcal{C}} \mathrm{Tr}_e \, \mathrm{e}^{-\beta\left(\mathcal{H}(\mathcal{C}) - \mu\hat{N}\right)}, \tag{2}$$

where $\mathcal{H}(\mathcal{C})$ is the Falicov–Kimball Hamiltonian (1) for a fixed ionic configuration $\mathcal{C}$, $\sum_{\mathcal{C}}$ indicates summation over ionic configurations, Tr_e denotes the trace over fermionic degrees of freedom, β is the inverse temperature, and $\hat{N}$ is the operator for the total number of electrons. For a given ionic configuration the Hamiltonian $\mathcal{H}(\mathcal{C})$ can be diagonalized numerically and the summation over fermion degrees of freedom gives the partition function in the following form

$$\mathcal{Z} = \sum_{\mathcal{C}} \prod_{n} \left(1 + \mathrm{e}^{-\beta(E_n(\mathcal{C}) - \mu)}\right), \tag{3}$$

where $E_n(\mathcal{C})$ is n-th eigenvalue of $\mathcal{H}(\mathcal{C})$. Introducing the electronic free energy

$$\mathcal{F}_e(\mathcal{C}) = -\frac{1}{\beta} \sum_{n} \log\left(1 + \mathrm{e}^{-\beta(E_n(\mathcal{C}) - \mu)}\right), \tag{4}$$

the partition function can be written in a form analogous to that used for a spin system,

$$\mathcal{Z} = \sum_{\mathcal{C}} \mathrm{e}^{-\beta\mathcal{F}_e(\mathcal{C})}. \tag{5}$$

Equation (5) indicates, that in the Metropolis algorithm we should use the electronic free energy rather than the internal we should use the electronic free energy rather than the internal energy.

Determining thermodynamic quantities the averages are calculated with the statistical weights

$$w(\mathcal{C}) = \frac{1}{\mathcal{Z}} \mathrm{e}^{-\beta\mathcal{F}_e(\mathcal{C})}, \tag{6}$$

of corresponding ionic configurations $\mathcal{C}$.

In order to quantitatively describe the ordered phase we have determined the density–density correlation function for the ions:

$$g_n = \frac{1}{4N} \sum_{i=1}^{N} \sum_{\tau_1, \tau_2 = \pm n} w(\boldsymbol{r}_i)\, w\left(\boldsymbol{r}_i + \tau_1\hat{\boldsymbol{x}} + \tau_2\hat{\boldsymbol{y}}\right), \tag{7}$$

where $w(\boldsymbol{r}_i) \equiv w_i$, $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{y}}$ denotes unitary vectors along the x and y directions, respectively (the lattice constant $a = 1$ has been assumed). Note that g_n describes correlations along the lattice axes. In a fully ordered (checkerboard) state it oscillates with a period equal to two lattice constants. It is convenient to define

$$G_n = (-1)^n \, 4\left(g_n - \rho_i^2\right), \tag{8}$$

where ρ_i is the concentration of ions. Such a function is equal to 1 for the checkerboard state and close to 0 (equal to 0 in the thermodynamic limit) for randomly distributed ions.

The specific heat was determined during each MC run in order to identify the critical temperature. It can be written in terms of the variance of the energy and this form is especially convenient for the MC calculations:

$$C_V = \frac{\partial\langle E\rangle}{\partial T} = \frac{1}{k_{\mathrm{B}}T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right). \tag{9}$$

Here, $\langle \ldots \rangle$ indicates an ensemble average, that is equivalent to averaging over the configurations selected by the Metropolis algorithm.

3 Falicov–Kimball model at half-filling

It is known that for the symmetric half filled case, when electron and ion concentrations are equal to one-half, the FKM on a bipartite lattice possesses long range order at low temperature [2]. In this state ions form a checkerboard pattern, that is destroyed as the temperature increases. It can be interpreted as a simple model of crystallization, where the system has a phase transition from ordered low temperature state to a disordered phase at high temperature.

In the following we report results obtained for 20×20 cluster with periodic boundary conditions. Finite size scaling indicates that such a size in most cases is sufficient to determine features of 2D FKM on an infinite lattice. More precisely, the width of the specific heat peak at the critical temperature changes a bit when the cluster size increases, however, the critical temperature itself remains almost unaffected.

There are two distinct regimes of half-filled FKM: one for small U and the other for large U. Large-U FKM can be mapped onto Ising model and therefore many of its characteristics are well known. The phase transition from disordered state to the checkerboard state is of second order. Figure 1 illustrates how the checkerboard pattern is formed as the temperature is lowered in the large-U regime.

From Fig. 1 one can see that in this regime temperature dependence of G_n for large n resembles the magnetization in the Ising model. On the other hand, G_n for small n describes short range correlations that survive above the critical temperature. A finite-size scaling is required, however, to precisely determine the correlation length and its temperature dependence.

The behavior of the FKM in the small-U regime is more unconventional. It was shown in Ref. [4] that for small U the charge density wave order parameter in infinite dimensions has an anomalous evolution as a function of temperature. In Fig. 2 we demonstrate that also in the case of two-dimensional lattice the CDW order behaves unusually. There is a wide temperature range in which the density–density correlations functions changes almost linearly with the temperature. Moreover, in contradistinction to the large–U limit, the correlation functions very weakly depend on the distance. There are also indications that the phase transition in this regime is of first order [5].

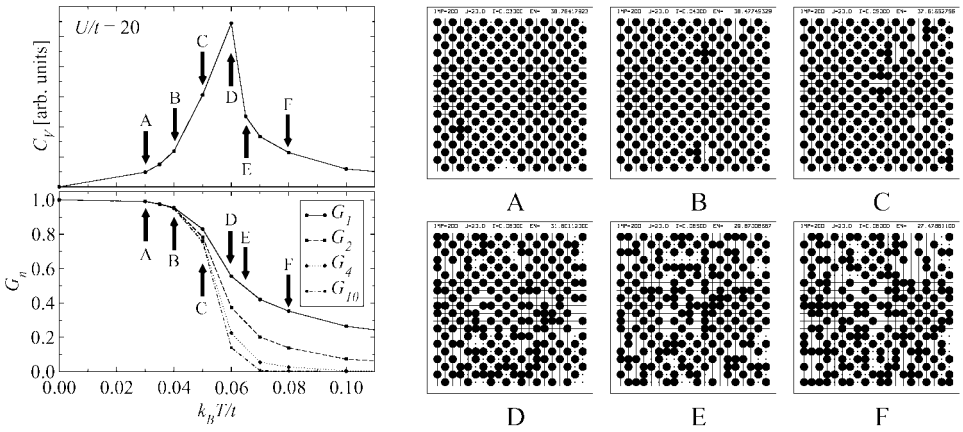

Fig. 1 Temperature dependence of the specific heat C_V and the correlation function G_n for $U/t = 20$ are presented in the left panel. The right panel show snapshots of ionic configurations at various temperatures. Individual configurations correspond to temperatures indicated by arrows in the left panel.

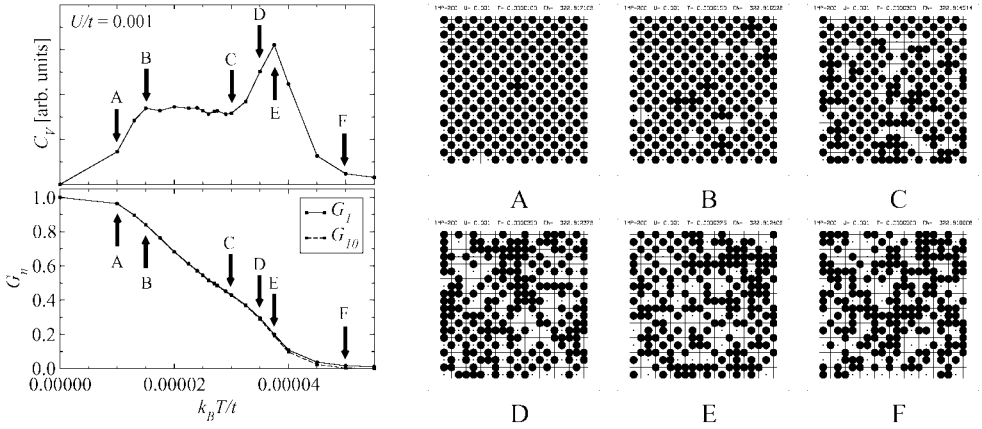

Fig. 2 Same as in Fig. 1, but in extremely small-U limit, $U/t = 0.001$.

4 Falicov–Kimball model away from half-filling

A long standing conjecture for the FKM was that, for sufficiently strong interactions, the localized and itinerant particles should segregate away from half-filling. This conjecture was proved in one dimension [6], in infinite dimension [7], and in any dimension in large U limit [8]. The presence of phase separation in two dimensions is suggested by approximate results as well [9]. In this section we demonstrate that also MC simulations for two dimensional FKM indicate phase separation, provided the interaction is strong enough. We have performed simulations for various values of the interaction strength, in a wide range of temperatures. Figure 3 qualitatively summarizes the results for $\rho_{\text{ions}} = \rho_{\text{electrons}} = 0.4$.

Apart from the case of $U/t = 1$, the ions evidently gather together forming ion-rich regions. Due to the strong electron–ion interaction the itinerant particles avoid these regions, forming separated electron-rich areas (not shown). Particularly interesting is the lowest row in Fig. 3. For $U/t = 1$ the phase separation also occurs, but there are no ion-rich regions in which all sites are occupied by the immobile particles. Instead, ions form in these regions checkerboard patterns, like in the ground state of half-filled FKM. The correlation function G_n, defined in Eq. (8), can be used to describe this behavior. Figure 4 shows this function at various temperatures.

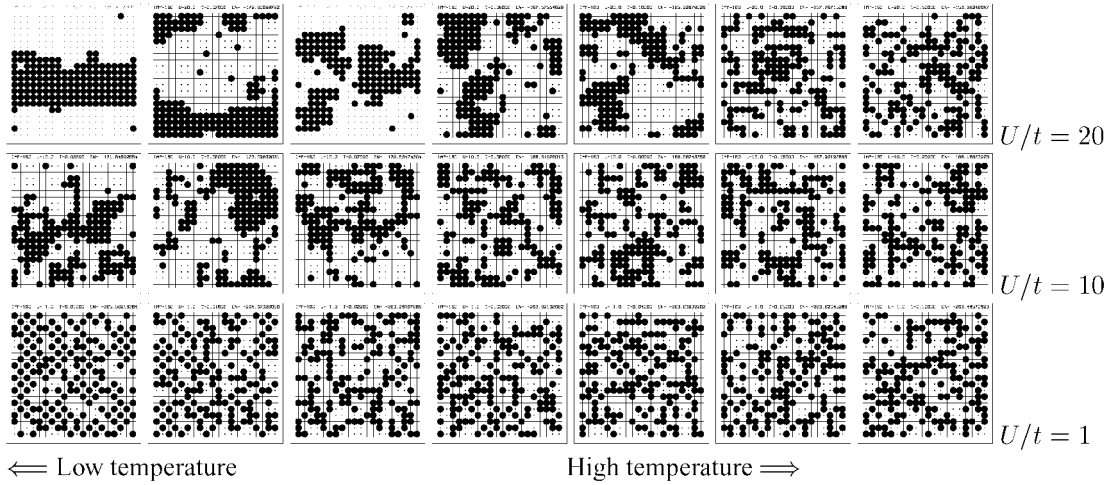

Fig. 3 Ionic configurations characteristic of the FKM at various temperatures for $U/t = 1, 10$ and 20. The configurations correspond to temperature ranges: $k_{\text{B}}T/t = 0.06 \ldots 0.5$ for $U/t = 20$, $k_{\text{B}}T/t = 0.055 \ldots 0.2$ for $U/t = 10$, and $k_{\text{B}}T/t = 0.01 \ldots 0.1$ for $U/t = 1$.

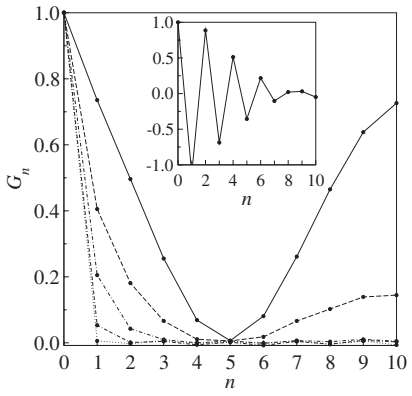

Fig. 4 Distance dependence of the corelation function G_n for $U/t = 1$ determined at temperatures $k_B T/t = 0.01$ (solid line), 0.018, 0.03, 0.1, 1 (dotted line). The inset shows the same function, but in phase separated state $U/t = 20$ and $k_B T/t = 0.06$. The corresponding ionic configuration is presented in the leftmost panel of the uppermost row in Fig. 3.

In 20×20 cluster with periodic boundary conditions the maximum effective distance between different sites is 10 lattice constants and therefore the presented results are restricted to $n \leq 10$. The solid line ($k_B T/t = 0.01$) represents a system in the low temperature phase, the other curves correspond to temperatures above T_c. The decrease of the correlation function with increasing distance is connected with finite sizes of the checkerboard regions. The increase of this function at low temperature for distance larger then 5 lattice constants indicates that ions in one checkerboard region are correlated with ions in another one. The concentration of ions is equal to 0.4 and on average every fifth position in the checkerboard pattern is then unoccupied. This is the reason for the minimum of G_n at $n = 5$. For other ion concentrations the average size of the ordered regions would be different and the minimum of G_n would take place for sites at different distance.

In both the large-U and small-U regimes there are singularities in the specific heat, indicating the presence of phase transitions to the low temperature states. Their shapes are similar to that presented in Figs. 1 and 2.

The critical value of the interaction, above which a standard phase separation in 2D FKM occurs remains as an open issue. This value should depend on both the electronic and ionic concentrations. If such a segregation of checkerboard regions occurs also in a regime of low concentration of ions, it can be regarded as a model for antiferromagnetic stripes formation in cuprates and nickelates.

Another question that should be addressed concerns the low temperature phase for small and very small U. This regime is, however, difficult to be approached within the framework of the MC method.

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