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Monte Carlo analysis of the half-filled Falicov–Kimball model

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Abstract

It is known that in the large-U limit the Falicov–Kimball (FK) model maps onto an effective Ising model. For small U, the situation is, however, not so clear. In the present paper we show Monte Carlo results, which indicate the presence of a first-order phase transition in the small-U FK model.

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The Falicov–Kimball (FK) model [1] assumes two kinds of particles in the lattice: classical (infinitely massive) "ions" and electrons that can hop between lattice sites. For simplicity, the particles are assumed to be spinless. The model Hamiltonian is given by

$$H = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + U \sum_i c_i^\dagger c_i w_i. \quad (1)$$

Here, $c_i^\dagger$ (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. Within the framework of a common interpretation of the Falicov–Kimball Hamiltonian (1), there are two species of particles: spinless itinerant electrons and classical, localized particles ("ions"), which interact on-site with the electrons. There are no direct interactions neither between the electrons nor between the ions. However, the electron–ion Coulomb interaction leads to an effective interaction between ions. As a result, for a given number of ions, the ground state energy depends on their distribution. At non-zero temperature, a partition function has to be calculated for each ionic configuration, and then one has to average over the configurations. However, since the number of ionic configurations increases very rapidly with the size of the system, such a procedure is possible in some cases only. One of them is called "restricted phase diagram" method [2], where only periodic configurations on an infinite lattice are taken into account. In order to include *all* possible configurations, one has to significantly restrict the size of the lattice. In the present paper we use the Monte

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Carlo (MC) method. Such an approach has several advantages. Since the frozen particles are classical ones, we do not have to use a quantum MC algorithm with the "fermionic sign" problem, and thus the calculations are not restricted to the high-temperature regime. Moreover, the size of the lattice, for which we are able to carry out simulations, is large enough to describe some properties of states with irregular structures. In the following we restrict our calculations to the half-filling case. It was proved by Kennedy and Lieb [3] that in this case at low enough temperature the FK model possesses a long-range order, i.e., the ions form a checkerboard pattern, the same as in the ground state. The aim of this paper is to investigate the nature of the phase transition to the ordered state.

In all simulations we have used the Metropolis algorithm. As 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

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

where $H(C)$ is the Hamiltonian (1) for a fixed ionic configuration C, $\sum_C$ 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 $H(C)$ can be diagonalized numerically and the summation over fermion degrees of freedom can be performed.

It is known that for large U, the FK model belongs to the same universality class as the Ising model and the order parameter is described by the Curie–Weiss law. Thus, the phase transition is of second order in this regime. On the other hand, it was shown in Ref. [4], that in infinite dimensions in the small-U limit, the order parameter has a strange non-BCS-like temperature dependence. Therefore, it is important to precisely determine the nature of the phase transition in this regime. We have used a method proposed by Challa et al. [5] to distinguish between first- and second-order phase transitions. Systems undergoing first-order phase transitions are accompanied by free energy barriers, which separate the free energy minima characterizing the coexisting phases. It results in discontinuities in the first derivatives of the free energy, e.g., the internal energy. This, in turn, leads to a δ-type singularity in the specific heat at the transition.

Within the framework of a Metropolis MC approach the internal energy E fluctuates with the probability distribution $P(E)$ usually given by a Gaussian. Its width is proportional to the specific heat. However, if the system is close to a first-order transition, the probability distribution $P(E)$ is a superposition of two Gaussians centered at different energies E_+ and E_-. Here, E_+ and E_- are the internal energies in the high- and low-temperature phases, respectively. The Gaussians are weighted by the Boltzmann factors of E_+ and E_-, and thus this splitting occurs in a vicinity of the transition temperature only. At higher temperatures $P(E)$ forms a single Gaussian centered at E_+, that evolves through the double-peak structure to a Gaussian centered at E_- as the temperature is lowered below T_c.

It can be shown that in the case of a system with both classical and fermionic degrees of freedom the Metropolis algorithm should use the electronic free energy instead of the internal energy to calculate the statistical weights of corresponding ionic configuration [6]. Fig. 1 shows the electronic

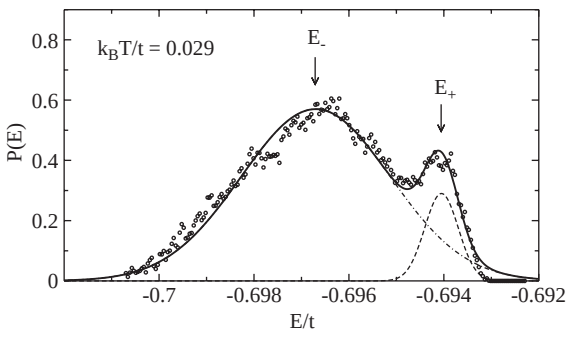

Fig. 1. Probability distribution of the electronic free energy at temperatures close to the critical temperature for $U/t = 0.5$. The thick solid lines represent a superposition of two Gaussians that fit the simulation results, whereas the dashed and dashed-dotted lines show the component Gaussians. The arrows indicate positions of the centers of the Gaussians representing low-temperature (E_-), and high-temperature (E_+) phases, respectively.

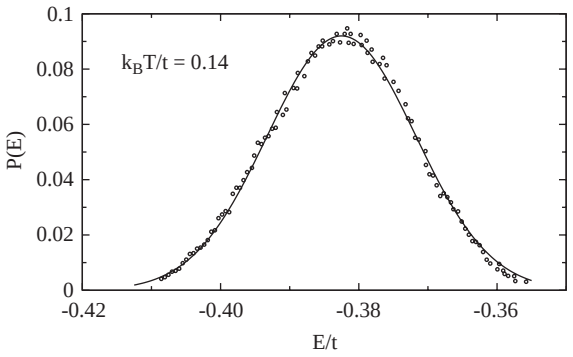

Fig. 2. Probability distribution of the electronic free energy at the phase transition for $U/t = 3$.

free energy distribution close to the phase transition for $U/t = 0.5$. Since the data has a double-peak structure, the phase transition is of the first order.

The magnitude of the splitting of the energy distribution close to T_c decreases with the increase in the interaction strength U and above a critical value U^* disappears. Fig. 2 presents the energy distribution at the phase transition for $U/t = 3$. One can notice the excellent agreement with the theoretical Gaussian curve, indicating an absence of any phase coexistence and the second-order character of the phase transition.

We have estimated the critical value $U^* \approx t$; however, extensive numerical studies are necessary in order to precisely determine U^*.

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