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Monte Carlo study of the Falicov–Kimball model: implementation of the histogram method

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We show that the histogram method that is widely used in the Monte Carlo simulations for the Ising model, can also be implemented in the simulations carried out for the Falicov–Kimball model. We estimate the systematic errors arising from application of this method and discuss the regimes of model parameters, where these errors are minimal. We apply the histogram method for determining the transition temperature and demonstrate significant advantages over standard simulations.

1 Introduction Physics of strongly correlated electron systems has attracted a lot of interest over the last decades. It is commonly accepted that some of the most interesting phenomena in condensed matter physics are connected with electronic correlations. One believes that such correlations are crucial for understanding high temperature superconductivity (HTSC). In particular, they may lead to charge ordering and metal–insulator transition. The ability to confine ultracold Bose and Fermi gases gives another possibility to prepare and observe highly tunable and well controlled strongly correlated many body quantum systems. It allows one to validate theoretical models which have been used to describe such systems for decades.

The Hubbard model is frequently used as a starting point for studying the strongly correlated systems. This simple model has intensively been investigated for over forty years. It has originally been used for describing the metal–insulator transition. After discovery of HTSC, it was argued that this model captures the crucial physics of these materials. Despite the simplicity of the Hubbard model, only few rigorous results are known, mainly in one or infinite dimensional cases. The remaining results have been obtained with the help of various approximate methods. Some of them, based on exact diagonalization or quantum Monte Carlo (MC) simulations, were obtained for relatively small systems and suffer from the finite size effects.

The lack of exact solutions or even solutions obtained within controllable approximations encourages physicists to investigate even simpler models. One of them is the Falicov–Kimball model, proposed by Hubbard and Gutzwiller (for review see, e.g., [1,2]) as a simplification of the Hubbard model and further redeveloped by Falicov and Kimball to investigate phase transitions in rare earths and transition metals [3]. The model is a limiting case of the generalized, asymmetric Hubbard model. It describes a system consisting of two kinds of particles. One of them are itinerant fermions and the others – massive, immobile particles. The only interaction is between the fermions and the localized particles. The model is described by the following Hamiltonian:

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + U \sum_i \omega_i c_i^\dagger c_i, \qquad (1)$$

where t is hopping integral, $c_i^\dagger$ (c_i) are fermionic creation (annihilation) operators at site i, U is the on–site Coulomb interaction and ω_i is equal to 0 (1) if a massive particle is absent (present) at site i.

While the Falicov–Kimball model is simpler than the Hubbard one, it still cannot be solved in a general case. Fortunately, significantly larger number of rigorous results is known for the the Falicov–Kimball model than for the Hubbard model [4]. One of the most important theorem,

proved by Kennedy and Lieb [5], states that at low temperature there is a long range order for lattices of dimensionality grater then one for certain fillings and for all values of U. There exist also approximate results for the Falicov–Kimball model (see, e.g., Ref. [6]). Many important results have recently been obtained within dynamical mean–field theory (DMFT), which has some limitations.

It has recently been shown that the two dimensional Falicov–Kimball model can effectively be analyzed with the help of the classical MC method [8,9]. The method is general and it is possible to apply it for different geometries and for arbitrary fillings. The main obstacle is that this approach is very computer–time consuming. Then, the available CPU time strongly limits the accessible sizes of investigated systems.

In the present paper we demonstrate that similarly to the case of the Ising model the computational limitations can be relaxed by means of application of the histogram method [10]. The outline of the paper is as follows. Section 2 briefly describes a variation of the classical MC method which can be used to study systems with classical as well as quantum degrees of freedom. In section 3 we present the histogram method which, in section 4, is implemented to the MC simulation of the Falicov–Kimball model. Section 5 presents the numerical results. Finally, section 6 contains summary and conclusions.

2 Computational method In our simulations we use a modified Metropolis algorithm. As our system contains both fermions and classical particles, we use the grand canonical partition function in the following form

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

where $\mathcal{C}$ denotes configuration of the massive particles, β is the inverse temperature and $\hat{N}$ is the operator of total number of mobile fermions. For a given configuration $\mathcal{C}$ Hamiltonian $\mathcal{H}(\mathcal{C})$ can be diagonalized numerically and summation over fermionic degrees of freedom gives

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

where $E_n(\mathcal{C})$ is n–th eigenenergy of $\mathcal{H}(\mathcal{C})$. Introducing the free energy of the mobile particles

$$\mathcal{F}_e(\mathcal{C}) = -\frac{1}{\beta}\sum_n \ln\left\{1 + e^{-\beta[E_n(\mathcal{C})-\mu]}\right\} \tag{4}$$

the partition function can be written in a form analogous to that used for the Ising model:

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

Equation (5) indicates, that in order to carry out MC simulations for the Falicov–Kimball model, in the Metropolis algorithm we should use the electronic free energy instead of the internal energy. MC simulations allow us to estimate the partition function and thermodynamic functions such as the specific heat.

In the present paper we restrict our considerations to a special case of half-filling both for fermions and massive particles.

3 The histogram method One of the most important limitations of the MC method originates from the time that is needed to obtain the numerical data. In order to overcome this severe problem one should use the obtained results as efficiently as possible. It can be achieved with the help of the histogram method. This method was introduced by Ferrenberg and Swendsen in Ref. [10] and later generalized and extended. The main idea behind this approach comes from the observation, that configurations sampled in the MC simulations are independent of some of model parameters. Therefore, once we obtain a set of configurations we may reweight probabilities of their occurrence and calculate the partition function for some other parameters. For the sake of completeness we briefly recall the implementation of the histogram method to the Ising model. Following the discussion of Ref. [10] we consider the Ising model with the Hamiltonian

$$-\beta H = K\sum_{\langle i,j\rangle}\sigma_i\sigma_j = KS.$$

In the simulations carried out for some particular dimensionless coupling constant K, the probability distribution of S is given by:

$$P_K(S) = \frac{1}{Z(K)}N(S)\exp(KS), \tag{6}$$

where $N(S)$ is the number of spin configurations corresponding to S and $Z(K)$ is the canonical partition function. The reweighted distribution corresponding to some other value of the coupling constant K' is given by

$$P_{K'}(S) = \frac{P_{(K)}(S)\exp[(K'-K)S]}{\sum_S P_{(K)}(S)\exp(K'-K)S}. \tag{7}$$

The simple histogram method has widely been used in the MC simulations. The main disadvantage of the method is that extrapolation from one parameter K to another K' may be carried out only in a limited range of the coupling constant. This limitation may be overcome by using modified versions of the algorithm, e.g., the broad histogram method or the flat histogram method. Generally, storing of the histogram may be difficult for systems with large number of free parameters. Moreover, estimation of errors introduced by this method is a difficult problem, as it is discussed in Ref. [11].

4 The implementation In our implementation of the histogram method we use the inverse temperature instead

of dimensionless coupling constant ($K \to \beta$) and the free energy $\mathcal{F}_e(\mathcal{C})$ as a point in the phase space [$S \to \mathcal{F}_e(\mathcal{C})$]. Then, equation (6) takes the form:

$$P_T(\mathcal{C}) = \frac{1}{\mathcal{Z}(T)} N\left[\mathcal{F}_e(\mathcal{C})\right] e^{-\beta \mathcal{F}_e(\mathcal{C})}. \quad (8)$$

The main obstacle for implementation of the histogram method to the Falicov–Kimball model arises from the fact that the free energy, given by equation (4), depends on temperature. Therefore, reweighting of probabilities of states [see Eq. (7)] should be considered as an approximation. Nevertheless, we show that in many cases the temperature dependence of the free energy may be neglected. The free energy of the mobile fermions (4) can be written in the form

$$\mathcal{F}_e(\mathcal{C}) = \sum_n -\frac{E_n - \mu}{a(n)} \ln\left[1 + e^{-a(n)}\right] \equiv \sum_n X_n, \quad (9)$$

where $a(n) = (E_n - \mu)/k_B T$. One can see that

$$\lim_{a(n)\to\infty} X_n = 0, \quad (10)$$

$$\lim_{a(n)\to-\infty} X_n = E_n - \mu, \quad (11)$$

$$\frac{\partial X_n}{\partial T} \leq 0. \quad (12)$$

The well known properties of the Falicov–Kimball model lead to some important conclusions on the temperature dependence of X_n. First, for the case of half-filling and for arbitrary U there is a phase transition at the temperature T_c. The value of $k_B T_c$ depends on U, however, in all the cases it is lower than $t/5$. Below T_c there is a gap in the energy spectrum of the order of U. Therefore, for temperatures lower than T_c one can estimate that $|a(n)| > 5U/2t$. Then, the neglected temperature dependence of $\mathcal{F}_e(\mathcal{C})$ leads to systematic errors, which do not exceed a few percents, provided $U > t$. This error can be estimated upon investigating the function $\ln(1 + e^{-a})/a$.

Similar argumentation allows one to estimate the systematic errors also in the large–U limit. It is well known that for $U > 8t$ there is a gap in the fermionic energy spectrum of the width $\Delta \geq U/t - 8$. It holds true at arbitrary temperature. Therefore, for $k_B T$ much lower than Δ, $|a(n)|$ become large and the temperature dependence of the free energy can be safely neglected. For moderate and weak interactions (that is $U/t < 8$) the energy gap vanishes at T_c. However, application of the histogram methods still provides accurate results, as will be demonstrated in the following section.

5 Results In order to demonstrate advantages of using the histogram method we compare the temperature dependence of the specific heat for the Falicov-Kimball model determined by means of the histogram method and determined directly from Monte Carlo simulations. In the former case we need to carry out simulations at only one temperature, whereas in the later one we have to do it at several temperatures. The most interesting regime is close to the phase transition, where MC simulations suffer from the *critical slow down* and a lot of CPU time is needed to determine precisely the critical temperature. Therefore, this is the regime, where application of the histogram method gives significant advantages over the standard simulations. In Fig. 1 we show the specific heat for temperatures close to the transition temperature for a 20×20 system with $U = 4t$ and periodic boundary conditions. From MC simulations at a series of temperatures (dashed line) we can estimate, that the critical temperature is approximately $k_B T_c \simeq 0.14t$. The histograms used to determine the specific heat have been generated from simulations carried out at temperature $k_B T_s = 0.15t$.

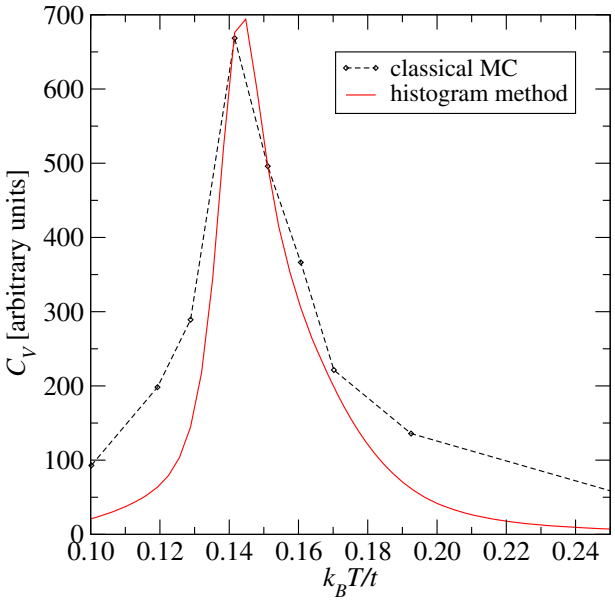

Figure 1 Comparison of the specific heat calculated directly from MC simulations at different temperatures and with the help of the histogram method with histograms generated at temperature close to the phase transition ($k_B T_s/t = 0.15$). The simulations were carried out on a 20×20 cluster for $U = 4t$.

Unfortunately, in order to obtain accurate value of the critical temperature the histograms have to be generated at temperatures not far from the phase transition, i.e., in a regime where the autocorrelation time is very long and the MC simulations run slowly. Moreover, before we start generating the histograms we have to know, at least approximately, what is the expected critical temperature. On the other hand, it is known that if the histograms are generated far from the critical temperature, the resulting peak in the specific heat is shifted from its correct position towards the temperature, at which the histograms are generated. This feature is illustrated in Fig. 2, where the specific heat was determined from histograms generated at temperatures $k_B T_s = 0.25t,\ 0.19t,\ 0.16t$ and $0.14t$.

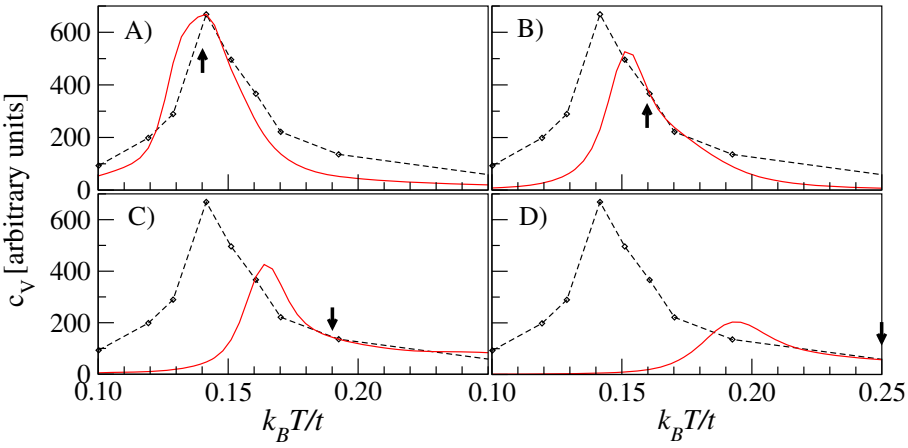

Figure 2 The same as in Fig. 1 but for histograms generated at different temperatures k_BT_s (indicated by the arrows): A – $0.14t$, B – $0.16t$, C – $0.19t$ and D – $0.25t$.

This feature can be adopted to determine the critical temperature in an iterative way: first, we generate histograms at a given temperature, possibly far from the phase transition and determine the temperature at which the specific heat takes on the maximal value. This temperature can be off the actual critical temperature. Nevertheless, it is much closer to it than the temperature at which the histograms were generated and in the next step we generate another set of histograms at this very temperature. Then, once more we determine the specific heat and generate a new set of histograms at temperature indicated by the new position of the peak. This procedure quickly converges and after few iterations it ends up with the correct critical temperature. The convergence can be inferred from Fig. 2. It is important to note, that at a final stage of the iterative method, temperature dependence of the free energy of the mobile particles does not affect the resulting transition temperature.

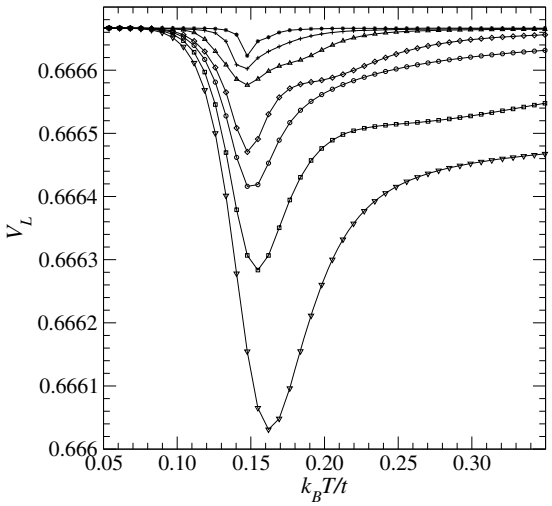

Figure 3 Binder cumulants calculated for systems of different size: 6×6 (the lowest line), 8×8, 10×10, 12×12, 16×16, 20×20, and 30×30 (the uppermost line).

Of course, the specific heat accurately determined from this iterative procedure still suffers from finite size effects and in order to obtain reliable results one has to carry out a finite size scaling. It can be done with the help of Binder cumulants [12, 13] and, also at this stage, the histogram method can be applied to reduce the time of simulations. The cumulant for a system of size L is defined as

$$V_L = 1 - \frac{\langle \mathcal{F}_e^4 \rangle_L}{3\langle \mathcal{F}_e^2 \rangle_L^2}, \tag{13}$$

and takes a minimum value at the effective transition temperature. Figure 3 shows the cumulants calculated for various system sizes from 6×6 to 30×30. In all these cases histograms were generated at only one temperature $k_BT_s = 0.15t$. The extrapolation to $L \to \infty$ is presented in Fig. 4.

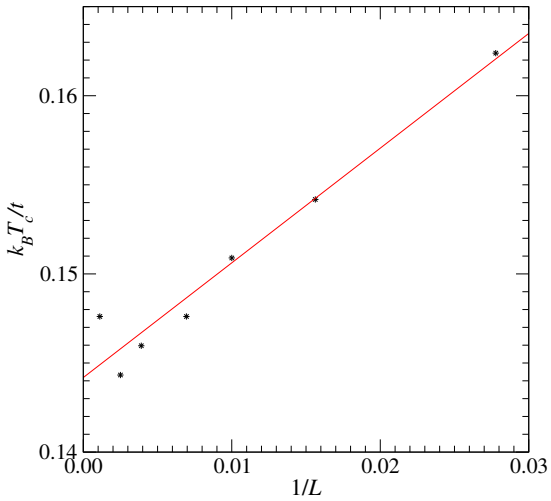

Figure 4 Finite size scaling for the critical temperature. The point for $L = 900$ (30×30 system) is off the fitting line due to a relatively small number of generated configurations, what, in turn, results from the fact that the simulation for such a large system is slow.

6 Conclusions We have shown that the histogram method, commonly used in MC simulations for the Ising model, can be implement in simulations carried out for the Falicov-Kimball model. The systematic error originating from unconventional temperature dependence of the statistical weights is small for simulations carried out below the transition temperature in the large-U limit. Moreover, these errors do not influence the transition temperature, provided T_c is determined from iterative application of the histogram method. Thermodynamic functions, obtained from reweighted states are in a good agreement with those obtained in traditional MC simulation. It is important to emphasize that time needed to obtain numerical results is at least one order of magnitude shorter than in the case of traditional simulations. Such significant speed up allows one to analyze the model in much wider range of parameters or for much larger clusters. It remains an open question, whether the histogram method is applicable to the Falicov–Kimball model in the weak interaction limit. This problem needs a separate study and will be reported elsewhere.

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