Thermodynamics of the Falicov-Kimball model in the unsymmetric case

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Introduction

It was shown that the Falicov-Kimball model (FKM) [1] can yield the correct physics for a description of the ground-state as well as the thermodynamic properties of the rare-earth and transition-metal compounds (at least qualitatively). The Hamiltonian of the model can be written as a sum of three terms:

$$H = \sum_{i,j} t_{ij} d_i^+ d_j + U \sum_i f_i^+ f_i d_i^+ d_i + E_f \sum_i f_i^+ f_i, \qquad (1)$$

where f_i^+, f_i are the creation and annihilation operators for an electron in the localized state at lattice site i ($w_i = f_i^+ f_i$) with binding energy E_f and d_i^+, d_i are the creation and annihilation operators of the d electrons hopping between the nearest-neighbour sites with hopping probability $t_{ij} = -t$. The second term represents the on-site Coulomb interaction between the d and f electrons. Despite of a considerable amount of effort devoted to understanding the thermodynamic properties of the FKM, there are still **a lot of unsolved questions mostly related with the unsymmetric case**. We have decided to explore **the thermodynamics properties of the metallic phase**, which is important for the study of the metal-insulator transitions and lies far away from the symmetric point. For this purpose we introduced a simple **canonical form of the classical Monte Carlo** for the FKM, that can be used in the unsymmetric case.

Method

Partition function of the canonical ensemble $Z = Sp\, exp(-\beta H)$ for the FKM, where $\beta = 1/\tau$ and $\tau = k_B T/t$ can be rewritten as:

$$Z = \sum_{\{w^f\},\{w^\varepsilon\}} e^{-\beta(E_f N_f + \sum_i \varepsilon_i w_i^\varepsilon)} \qquad (2)$$

where ε_i are the eigenvalues of the matrix $h(w^f) = \mathbf{t} + U\mathbf{w}^f$ in the ascending order. The used notation $\{w^f\}$ means that the summation runs over all possible f-electron configurations and notation $\{w^\varepsilon\}$ means that the summation runs over all possible occupations of the single-particle energy levels ε_i. It is obvious that the Monte-Carlo procedure can be used to sample the configurations w^f, w^ε according to the weight $X = e^{-\beta(E_f N_f + \sum_i \varepsilon_i w_i^\varepsilon)}/Z$.

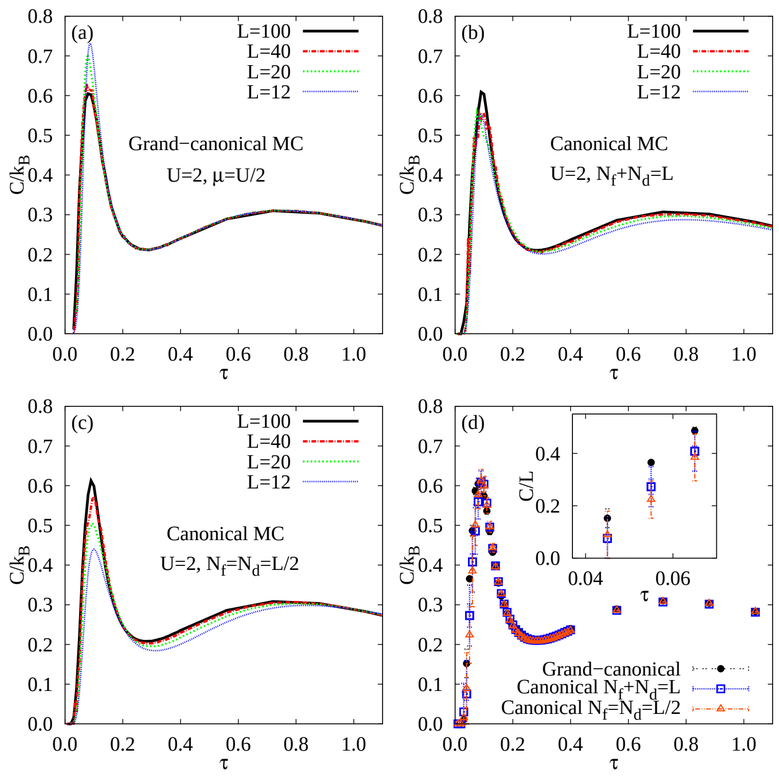


Fig. 1 Test of the method:(a)-(c) The specific heat of the FKM in the symmetric case for $U = 2$, $E_f = 0$, $D = 1$ and different lattice sizes computed by (a) GCM where $\mu = U/2$ [2, 3], (b) CMC where $N_f + N_d = L$ and (c) CMC where $N_f = N_d = L$. (d) Comparison of the specific heat computed with different methods for $L = 100$. The convergence of both canonical Monte Carlo cases is comfortable and the CMC is able to reproduce the results of the grand-canonical Monte Carlo.

Results and discussion

We have used the known results obtained for the one dimensional case ($D = 1$) [4, 5] as the starting point for our study and we also extended to the $D = 2$ case. The parameters U and E_f have been chosen so that the ground state of the model is phase separated and metallic [6] in all used cases. In following we use the parameters $U = 0.6$, $E_f = -1.44$ in $D = 1$ and $U = 2.0$, $E_f = -1.9$ in $D = 2$ as the typical representatives of the metallic region.

One-dimensional case

In Fig. 2 a typical example of the specific heat in $D = 1$ is plotted. Contrary to previous results we have observed in $D = 1$ two maxima, the broad hight temperature maximum of Schottky type and a **sharp low temperature maximum** which take a place near $\tau = 0.0035$ (Fig. 2) and which was **not observed before** [5]. Also the charge susceptibility shows a sharp maximum near the $\tau = 0.0035$, and then it rapidly decreases with decreasing temperature to the zero. Therefore we can conclude that the low temperature maximum is related to the temperature induced electron fluctuations between the f and d subsystem.

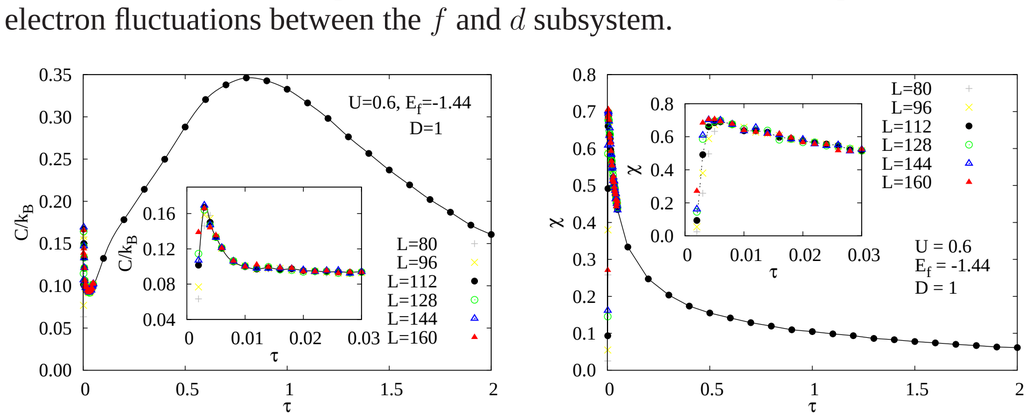
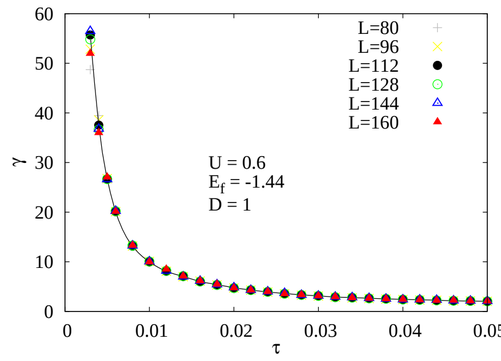


Fig. 2 The specific heat $C = \beta^2\left(\langle E^2\rangle - \langle E\rangle^2\right)/L$ and the dependence of the charge susceptibility $\chi = \beta^2\left(\langle N_f^2\rangle - \langle N_f\rangle^2\right)/L$ of the FKM for $U = 0.6$, $E_f = -1.44$ and various lattice sizes in $D = 1$. The insets are the details of the low temperature peaks.

The rapid increase of the specific heat coefficient $\gamma = C/\tau$ at low temperatures, indicates the presence of the quasiparticles with large effective masses and there is no sign of the Fermi liquid like behaviour.



The temperature dependence of the specific heat coefficient $\gamma = C/\tau$, of the FKM for $U = 0.6$, $E_f = -1.44$ and various lattice sizes in $D = 1$.

Two-dimensional case

The thermodynamics properties in two dimensions significantly differ from the one dimensional case. The results suggest that the low temperature maximum in the specific head of the two-dimensional case will not survive in the thermodynamic limit (Fig. 3). Therefore there is no order-disorder transition in the metallic region at finite temperatures in $D = 2$. The specific heat coefficient γ for $\tau > 0.01$ increase with the decreasing temperature. Similarly as in $D = 1$ this indicates the presence of the quasiparticles with large effective masses.

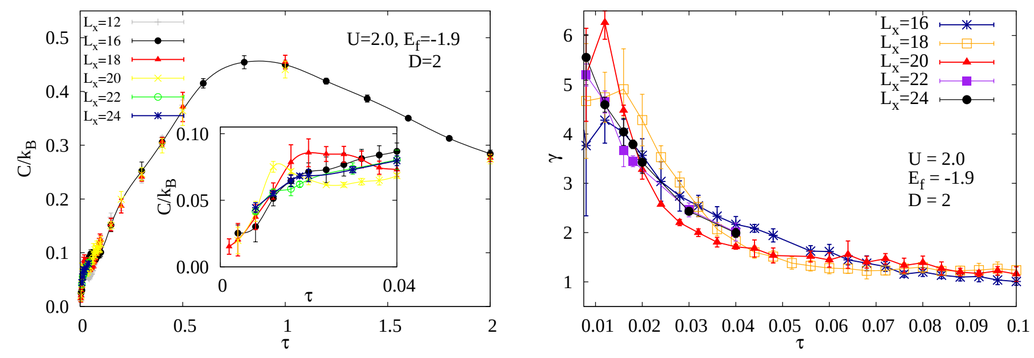


Fig. 3 The specific heat and the specific heat coefficient of the FKM for $U = 2.0$, $E_f = -1.9$ and various lattice sizes in $D = 2$. Here L_x means the linear size ($L = L_x \times L_x$)

Acknowledgments

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