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Numerical studies of the generalized spin-one-half Falicov-Kimball model in one and two dimensions

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The extrapolation of small-cluster exact-diagonalization calculations and the Monte-Carlo method is used to study the spin-one-half Falicov-Kimball model extended by the spin-dependent Coulomb interaction (J) between the localized f and itinerant d electrons as well as the on-site Coulomb interaction (U_{ff}) between the localized f electrons. It is shown that in the symmetric case, when the chemical potential μ equals to U (where U is the spin-independent on-site Coulomb interaction between the f and d electrons) the ground-state phase diagram of the model has an extremely simple structure that consists of only two phases, and namely, the charge-density-wave phase (with local f-electron pairs on one of two sublattices of a bipartite lattice) and the spin-densitywave phase. The nonzero temperature studies of the speci_c heat showed that these phases persist also at _nite temperatures. The critical temperature T_c for a transition from the low-temperature ordered phases to the high-temperature disordered one is calculated numerically for various values of J and U_{ff}.

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1. Introduction

Since its introduction in 1969 [1], the Falicov-Kimball model (FKM) has become an important model for a description of correlated fermions on lattices. The model was originally proposed to describe the metal-insulator transitions in the rare-earth and transition-metal compounds. Later it has been used in literature to study a great variety of many-body effects such as alloy formation, mixed valence and electronic ferroelectricity [2]. Recent theoretical studies of the FKM showed [3] that the model can yield the correct physics for description of the ground-states of rare-earth and transition metal-compounds, what has motivated also the study of thermodynamic properties of this model [4].

In its original version the FKM consists of particles localized on f orbitals which interact with a dispersive band of d orbitals through an on-site Coulomb interaction but various generalized versions of the FKM are being studied too. It was shown that including of different interaction terms to the FKM can lead to dramatic changes of the ground state and thermodynamic properties of the model [4-8]. Generalized versions of the FKM can describe a wide range of physical properties of the strongly correlated systems, that were not possible to explain by the original FKM.

In this paper we focus our attention on the spin one-half models with spin-dependent local interaction between localized f electrons and itinerant d electrons and models with local repulsive Coulomb interaction of finite magnitude between f electrons. Till now only a few analytical and numerical results have been obtained concerning the influence of these terms on ground-state as well as thermodynamic properties of the FKM [6-8].

For example the models with spin-dependent local interaction can describe the ferromagnetic ground state and various stable inhomogeneous charge and spin orderings observed in real materials [6,7]. It was shown analytically that in models with finite inter-orbital Coulomb interaction can arise an effective on-site attraction between the localized particles that can overcome a direct repulsion in the strong coupling limit [8]. This attraction leads to a chessboard-like pattern of localized f-pairs that can persist up to finite temperatures [8].

The essential influence of mentioned interactions on properties of the FKM and their ability to describe new famous phases was the main motivation for us to study the ground state and thermodynamic properties of generalized model that include both the spin dependent interaction and finite local repulsion of localized particles.
The Hamiltonian of the model is

$$H=\sum_{ij\sigma} t_{ij} d^{+}_{i\sigma} d_{j\sigma} + U \sum_{i\sigma\sigma'} n^{f}_{i\sigma} n^{d}_{i\sigma'} + E_f \sum_{i\sigma} n^{f}_{i\sigma} + J \sum_{i,\sigma} \left(n^{f}_{i-\sigma} - n^{f}_{i\sigma} \right) n^{d}_{i\sigma} + U_{ff} \sum_{i} n^{f}_{i\uparrow} n^{f}_{i\downarrow}, \quad (1)$$

where $n^{f}_{i\sigma}=f^{+}_{i\sigma}f_{i\sigma}$ ($n^{d}_{i\sigma}=d^{+}_{i\sigma}d_{i\sigma}$) is the f-electron (d-electron) occupation number and $f^{+}_{i\sigma}, f_{i\sigma}$ are the creation and annihilation operators for an electron of spin $\sigma=\uparrow,\downarrow$ in the local state at lattice site i and $d^{+}_{i\sigma}, d_{i\sigma}$ are the creation

and annihilation operators of the itinerant electrons in the *d*-band Wannier state at site *i*.

The first term of the model (1) is the kinetic energy corresponding to the quantum-mechanical hopping of the itinerant *d* electrons between sites *i* and *j*. These inter-site hopping transitions are described by the matrix elements t_{ij}, which are $-t$ if *i* and *j* are the nearest neighbors and zero otherwise (In the next all energies are measured in units of *t*). The second term represents the on-site Coulomb interaction between the *d*-band electrons and localized *f* electrons. The third term stands for the localized *f* electrons whose sharp energy level is E_f. The fourth term is the above mentioned anisotropic, spin-depended local interaction of the Ising type between the localized and itinerant electrons that reflects the Hund's rule force. The last term is an on-site Coulomb interaction between *f*-electrons with opposite spins. Thus from the major interaction terms [] that come into account for the interacting *d* and *f* electron subsystems only the Hubbard type interaction has been omitted. However, as we have shown in our previous paper the influence of this term can be neglected at least for intermediate and strong interactions *U* [7].

Since in this generalized version of the FKM the *f*-electron occupation number $n_{i\sigma}^{f}$ of each site *i* commutes with the Hamiltonian (1), it is a good quantum number, taking only two values: $w_{i\sigma}$=1 or 0, according to whether or not the site *i* is occupied by the localized *f* electron with spin σ. Thus the Hamiltonian (1) can be rewritten as

$$H=\sum_{ij\sigma} h_{ij\sigma} d_{i\sigma}^{+} d_{j\sigma} + U_{ff}\sum_{i} w_{i\uparrow} w_{i\downarrow} + E_f \sum_{i\sigma} w_{i\sigma} \qquad (2)$$

where $h_{ij\sigma}(w)=t_{ij}+(U(w_{i-\sigma}+w_{i\sigma})+J(w_{i-\sigma}-w_{i\sigma})\delta_{ij})$. Thus for a given *f*-electron configuration *w*, the Hamiltonian (1) is the second-quantized version of the single-particle Hamiltonian *h*, so the investigation of the model (1) is reduced to the investigation of the spectrum of *h* for different configurations of *f* electrons.

For further purposes it is suggestive to look at used lattices as consisting of two interpenetrating sublattices *A* and *B* and to define the sublattice magnetization

$$m_{A,(B)} = \frac{2}{L}\sum_{i\hat{I}A,(B)} \left(w_{i\text{-}} - w_{i^{-}}\right), \qquad (3)$$

(where *L* is the number of lattice sites) and the sublattice *f*-electron occupancy

$$n_{A,(B)} = \frac{2}{L}\sum_{i\hat{I}A,(B)} \left(w_{i\text{-}} + w_{i^{-}}\right), \qquad (4)$$

In the next study we concern our attention on the symmetric case of the model, where $H-\mu N$ (*N*- is the total number of *f* and *d* electrons) remains unchanged under particle-hole transformation. This condition holds for all *J* if $\mu=U$ and $U_{ff}=-2E_f$.

2. Ground state properties

As will be discussed latter the condition $\mu=U$ is satisfied for all temperatures just when the average number of all electrons in the system is equal to 2*L*. For this reason we have restricted our study of the ground state properties of the model (1) on the case $N=2L$. The ground state was studied in one and two dimensions in the weak, intermediate and strong-coupling limit of Coulomb interaction *U* (*U*=0.5,1,2,4,8) and for wide range of *J* and U_{ff} values ($0\le J\le 2U, 0\le U_{ff}\le 4U, E_f=-\frac{1}{2}U_{ff}$).

The total number of possible *f*-electron configurations for the model (1) is 4^L, thus only the clusters with $L\le 12$ have been accessible for the exact diagonalization studies. For $L>12$ we have used a well-controlled numerical method elaborated recently by one of the present authors [10].

Using these two methods we have found that for scheduled conditions and above mentioned values of parameters only two kinds of *f*-electron configurations can be the ground state of the model (1). The first is the charge-density-wave (CDW) phase, where one of the sublattices is fully occupied by *f* electrons (two *f* electrons per site) and the other is empty.

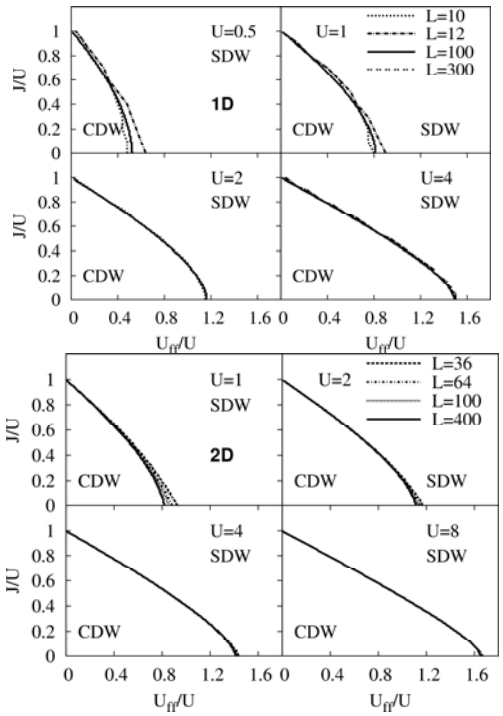

Fig. 1. Phase diagrams of the model (1) in the J/U-U_{ff}/U plane for different values of U in one (1D) and two (2D) dimensions. Different line types represents the boundary between the CDW and SDW phases for different cluster sizes.

The second is the spin-density-wave (SDW) phase, where all sites are occupied by one electron and for $J>0$ one of the sublattices is occupied by electrons with spin up and another by electrons with spin down. This means that for the CDW phase we have $m_A=m_B=0$, $n_{A,(B)}=0, n_{B,(A)}=2$ and for the SDW phase $m_{A,(B)}=-1, m_{B,(A)}=1$, $\nu_A=\nu_B=1$. The CDW phase which is the ground state bellow the critical values of U_{ff} and J is an example of local f-electron pairing that results from an effective on-site attraction between the localized electrons, produced by quantum mechanical effects which can overcome a direct Coulomb repulsion.

The fact that the ground-state of the model consists of only two phases was used to construct a phase diagrams in the J–U_{ff} plane for various U and lattices of several hundreds sites. These phase diagrams are shown in Fig.1, where the 1D represents the one dimensional case and 2D the two dimensional case. One can see that increasing U shifts the region of stability of the CDW phase to higher values of U_{ff}/U. Contrary to U the parameter J suppresses the CDW phase. The most interesting result is that the CDW phase can be the ground state of the model (1) even for $U_{ff}>U$ that represents the realistic situation of strongly correlated electrons systems described by model Hamiltonian (1).

The possibility of metal-insulator transition was studied too. The energy gap on the Fermi level is for the CDW phase equal to $2U$ and for the SDW phase $2J$. So there is a discontinuous metal-insulator transition (on U_{ff}) for $J=0$ and a discontinuous insulator-insulator transition for $J>0$.

3. Thermodynamics

The question if or not the CDW and SDW phases persist up to finite temperatures motivated our study of thermodynamic properties of the model (1). The grand canonical partition function of Hamiltonian (1) can be written directly as a function of eigenvalues ε_i^{σ} (of the operator h), that are dependent on the f electron configuration w.

$$\Xi=\sum_{\{\omega\}} e^{-\beta\left[(E_f-\mu)N_f+U_{ff}\sum_i \omega_{i\uparrow}\omega_{i\downarrow}\right]}\Pi(1+e^{-\beta(\varepsilon_i^{\sigma}-\mu)} \quad (5)$$

where $\beta=\frac{1}{\tau}$, $\tau=k_BT/t$, μ is the chemical potential and summation runs over all possible f electron configurations. Thermodynamic quantities as functions of temperature, have been expressed directly from the partition function by employing the standard statistical relations. For example the average number of all electrons in the system ($n=\frac{1}{L}\langle N^f+N^d\rangle$), the internal energy and the specific heat can be expressed as:

$$n=\tau\frac{\partial}{\partial\mu}\ln\Xi, \varepsilon=-\frac{1}{L}\frac{\partial}{\partial\beta}\Xi+\mu n, c_v=\frac{\partial\varepsilon}{\partial\tau}. \quad (6)$$

The first step in numerical calculations of the thermodynamic properties was to determine conditions under which the symmetric case condition ($\mu=U$ and $U_{ff}=-2E_f$) is satisfied for all temperatures. It is possible to show analytically that the chemical potential is constant when $n=2$ (analogically when we determine $\mu=U$ then $\langle N\rangle=2L$).

Though this condition (fixed μ and N) significantly speeded up the numerical computations of thermodynamic properties, we were able to perform the exact numerical study (over all possible f-electron configurations) only on small lattices (up to $L=12$). To overcome this limitation we have used the Monte-Carlo method. As the f-electron occupation number can be replaced by the classical variable w, we do not have to use the quantum Monte-Carlo algorithm and thus our calculations are not restricted to the high-temperature regime. The classical Monte-Carlo, where we used the free energy

$$F(w)=(E_f-\mu)N_f+U_{ff}\sum_i w_{i\uparrow}w_{i\downarrow}-\frac{1}{\beta}\sum_{i,\sigma}\ln(1+e^{-\beta(\varepsilon_i^{\sigma}-\mu)}), \quad (7)$$

as the statistical weight in the Metropolis algorithm, allowed us to study the thermodynamic properties of the model on approximatively ten times larger lattices.

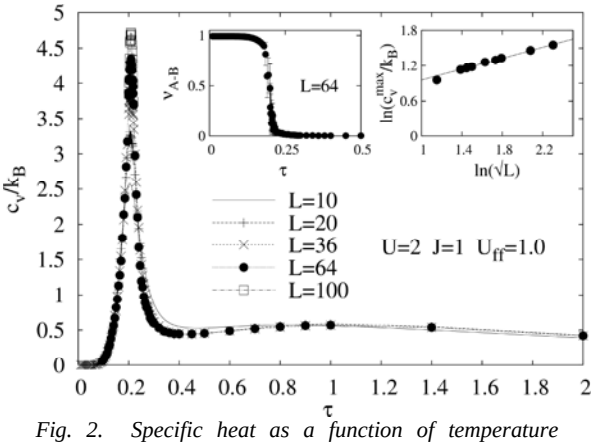

Fig. 2. Specific heat as a function of temperature $\tau=k_BT/t$ for $U=2, U_{ff}=1, J=1$ in two dimensions. The simple line represents the exact results for $L=10$, different symbols represent Monte-Carlo results for different lattices. Lines are only guides for eye. The left inset represents the temperature dependence of ν_{A-B}, The right inset represents a dependence of $\ln(c_v^{max}/k_B)$ on $\ln\sqrt{L}$ with a linear fit of a slope ~0.466.

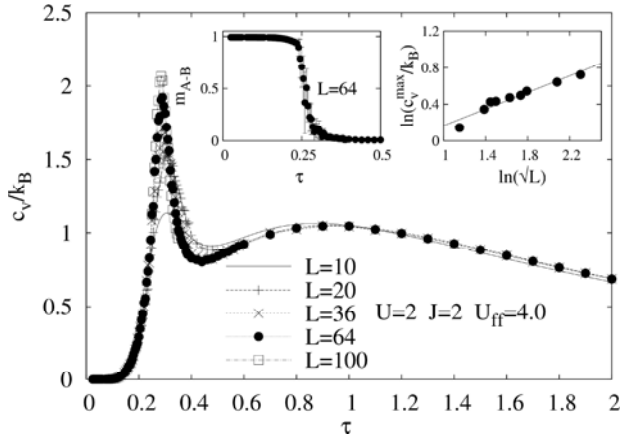

Fig. 3. Specific heat as a function of temperature $\tau=k_BT/t$ for $U=2, U_{ff}=4, J=2$ in two dimensions. The simple line represents the exact results for L=10, different symbols represent Monte-Carlo results for different lattices. Lines are only guides for eye. The left inset represents the temperature dependence of ν_{A-B}, The right inset represents a dependence of $ln(c_v^{max}/k_B)$ on $ln\sqrt{L}$ with a linear fit of a slope ~0.453.

The typical examples of the $c_v(\tau)$ dependence in two dimensions for U=2 and two different sets of U_{ff} and J values in that represent two different ground states (the CDW and SDW phase) are shown in Fig.2 and Fig.3. One can see that c_v as a function of τ shows the two-peak structure. There is a sharp low-temperature peak and a broad high temperature peak. The high-temperature peak is clearly of Schottky type, but the nature of the low temperature peak is not so evident. In the left insets of Fig.2 and Fig.3 we present the τ-dependence of parameters $\nu_{A-B}=\frac{1}{2}\langle|\nu_A-\nu_B|\rangle$ (CWD) and $m_{A-B}=\frac{1}{2}\langle|m_A-m_B|\rangle$ (SWD).

Parameters ν_{A-B} a m_{A-B} change rapidly from 1 to 0, near the temperature where the maximum of c_v ($c_v^{max}(L)$) appears. This suggests that the maximum of c_v is related to breaking of the charge and spin ordering. The kind of phase transition can be estimated from the finite size scaling of c_v^{max}. In the right insets of Fig.2 and Fig.3 we present the dependences $ln(c_v^{max}/k_B)$ on $ln(\sqrt{L})$ with plotted linear fits. The $ln(c_v^{max}/k_B)$ dependence for the CDW ground state (Fig.2) is in very good agreement with the linear fit with a slope ~0.466, and the same dependence for SDW ground state phase (Fig.3) is in very good agreement with the linear fit with a slope ~0.453. This indicates an Ising-like phase transition for both cases what means that the CDW phase as well as the SDW phase persist up to finite temperatures.

The corresponding critical temperatures for both above mentioned phase transitions are displayed in Fig.4.

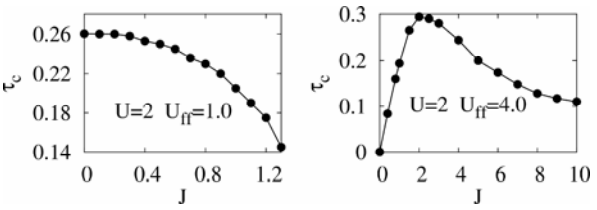

Fig. 4. Dependence of the critical temperature for the Ising-like phase transition on spin-dependent interaction J for $U=2$ and $U_{ff}=1,4$.

These critical temperatures have been extrapolated from the location of the c_v^{max} and by using the standard Binder cumulant method [13], each other with good agreement. As Binder cumulant we have chosen

$$B_{CDW}=1-\frac{\langle\nu_{A-B}^4\rangle}{3\langle\nu_{A-B}^2\rangle^2}, B_{SDW}=1-\frac{\langle m_{A-B}^4\rangle}{3\langle m_{A-B}^2\rangle^2}. \quad (8)$$

In the CDW area the maximum value of the critical temperature is for J=0 and with increasing J the critical temperature decreases. The reason for such behavior is that the spin-dependent interaction J suppresses the stability of CDW phase. More complicated is the behavior of critical temperature in the SDW area, where for J=0 the ground state is 2^L degenerated, so no finite temperature transition was observed for any U_{ff}. The critical temperature increases rapidly with increasing J and reaches its maximum at J~U then gradually decreases. Quantitatively the J-dependence of the critical temperature in the SDW phase resembles the U-dependence of the critical temperature of the conventional spinless FKM in te CDW phase, but τ_c values in the SDW phase are approximatively two times larger than ones of the spinless FKM [14].

4. Conclusion

In summary, the extrapolation of small-cluster exact-diagonalization calculations and the Monte-Carlo method were used to study the spin-one-half Falicov-Kimball

model extended by the spin-dependent Coulomb interaction between the localized *f* and itinerant *d* electrons as well as the on-site Coulomb interaction between the localized *f* electrons. It was shown that in the symmetric case, when the chemical potential μ equals to *U* the ground-state phase diagram of the model has an extremely simple structure that consists of only two phases, and namely, the charge-density-wave phase (with local *f*-electron pairs on one of two sublattices of a bipartite lattice) and the spin-density-wave phase. One of the most important results is that the charge-density-wave phase can be the ground state of the model (1) even for $U_{ff}>U$ that represents the realistic situation of strongly correlated electrons system described by model Hamiltonian (1).

The nonzero temperature studies of the specific heat showed that both these phases persist also at finite temperatures. The critical temperature for a transition from the low-temperature ordered phases to the high-temperature disordered phase was extrapolated from numerical calculations for various values of *J* and U_{ff}. It was found that in CDW area the maximum value of critical temperature is for $J=0$ and in the area SDW for $J\sim U$.

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