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Thermodynamics of the Generalized Spin-One-Half Falicov–Kimball Model in 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 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 and the spin-density-wave phase. The nonzero temperature studies showed that these phases persist also at finite temperatures. The same calculations that we performed for unsymmetric case showed that charge and spin ordering can be destroyed simultaneously or consecutively.

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1. Introduction

The Falicov–Kimball model (FKM) [1] 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 a description of the ground-states of rare-earth and transition-metal compounds, which has also motivated 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 different interaction terms to the FKM (e.g., a finite spin-dependent local interaction between localized f and itinerant d electrons and a finite local Coulomb interaction between f electrons) can lead to dramatic changes of the ground state and thermodynamic properties of the model [2–5]. The strong 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 the generalized FKM that includes both the spin dependent interaction between f and d electrons and the finite local repulsion between localized f electrons. The Hamiltonian of the model is

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

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 the localized f electrons. The third term is the above mentioned anisotropic, spin-dependent local interaction of the Ising type between the localized and itinerant electrons that reflects the Hund rule force. The fourth term is an on-site Coulomb interaction between f electrons with opposite spins. The last term stands for the localized f electrons whose sharp energy level is E_f. Since in this generalized version of the FKM the f-electron occupation number $n^{f}_{i\sigma}$ 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

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

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 (2) is the second-quantized version of the single--particle Hamiltonian h, so the investigation of the model (2) is reduced to the investigation of the spectrum of h for different configurations of f electrons.

2. Results and discussion

To examine effects of a finite spin dependent local interaction between localized f and itinerant d electrons and a finite local Coulomb interaction between f electrons on the ground-state and thermodynamic properties of the model (2) we have started with the symmetric case, where $H - \mu N$ remains unchanged under the particle–hole transformation (N is the total number of f and d electrons and μ is the chemical potential). This condition holds for all J if $\mu = U$, $U_{ff} = -2E_f$ and $N = 2L$. Using small-cluster exact diagonalization calculations and a well-controlled numerical method [6] we have found that for the scheduled conditions and above mentioned values of parameters only two types of f-electron configurations can be the ground states of the model, and namely, the charge-density-wave (CDW) phase (Fig. 1a), and the spin-density-wave (SDW) phase (Fig. 1b). The CDW phase which is the ground state below 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 U_{ff}.

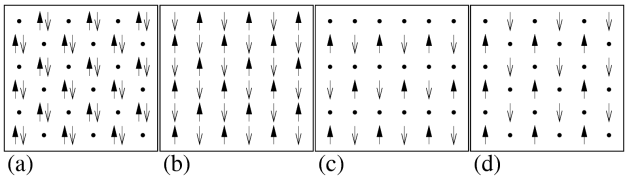

Fig. 1. The f-electron ground-state configurations: (a) CDW phase, (b) SDW phase, (c) phase stable for unsymmetric case $N = 2L$, $U = 2$, $J = 1$, $U_{ff} = 4$ and $E_f = 0$, (d) phase stable for unsymmetric case $N = 3L/2$, $U = 4$, $J = 0.8$, $U_{ff} = 8$ and $E_f = -2$.

The question, if or not the CDW and SDW phases persist up to finite temperatures motivated us to study the thermodynamic properties of the model. The grand canonical partition function of the model Hamiltonian (2) can be written directly in terms of eigenvalues ϵ_i^{σ} (of the matrix h), that depend on the f-electron configuration w:

$$\Xi = \sum_{\{w\}} \exp(-\beta((E_f - \mu)N_f + U_{ff} \sum_{i} w_{i\uparrow} w_{i\downarrow})) \times \prod_{i,\sigma} (1 + \exp(-\beta(\epsilon_i^{\sigma} - \mu))), \quad (3)$$

where $\beta = \frac{1}{\tau}$, $\tau = k_{\mathrm{B}}T/t$, μ is the chemical potential and the summation runs over all possible f-electron configurations. Thermodynamic quantities, as functions of temperature, have been calculated directly from the partition function by employing the standard statistical mechanics relations [7].

Though the condition of constant $\mu = U$ (the symmetric case) speeded up the numerical computations of thermodynamic properties significantly, we were able to perform the exact numerical study (over all possible f-electron configurations) only on small lattices up to $L = 10$ sites (for $L = 8$ and $L = 10$ the so-called "tilted" lattices [8] were used). 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, it was not necessary 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 have used the free energy

$$F(w) = (E_f - \mu)N_f + U_{ff} \sum_{i} w_{i\uparrow} w_{i\downarrow} - \frac{1}{\beta} \sum_{i,\sigma} \ln(1 + \exp(-\beta(\epsilon_i^{\sigma} - \mu))), \quad (4)$$

as the statistical weight in the Metropolis algorithm [9], allowed us to study the thermodynamic properties of the model on approximatively ten times larger lattices.

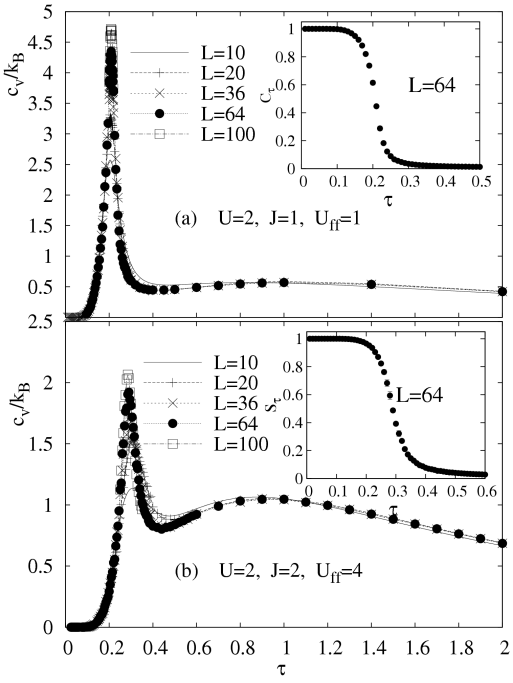

Fig. 2. Specific heat as a function of temperature $\tau = k_{\mathrm{B}}T/t$, for the CDW phase (a) and the SDW (b) phase. The insets represent temperature dependences of C_τ and S_τ defined in the text.

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 that represent two different ground states (the CDW phase and the SDW phase) are shown in Fig. 2. One can see that c_v curves as functions of τ show the two-peak structure. There is a sharp low-temperature peak and a broad high temperature peak in both cases. The high-temperature peaks are clearly of the Schottky type (there is a finite gap at the Fermi energy in the single-particle spectrum of $h(w)$ for both the CDW phase and the SDW phase). In the insets of Fig. 2 we present τ-dependences of averages over generated ionic configurations of the f-electron structure factors

$$X^{\pm}(\boldsymbol{Q}) = \frac{1}{L}\sum_{j,k}^{L}[\exp\left(\mathrm{i}\boldsymbol{Q}\left(\boldsymbol{R}_j - \boldsymbol{R}_k\right)\right) \times \left(w_{j\uparrow} \pm w_{j\downarrow}\right)\left(w_{k\uparrow} \pm w_{k\downarrow}\right)]. \quad (5)$$

The structure factors $C_\tau = \langle X^+(\pi,\pi)\rangle/L$ and $S_\tau = \langle X^-(\pi,\pi)\rangle/L$ change rapidly from 1 to ≈ 0, near the temperature where the maximum of c_v appears. This suggests that the maximum of c_v is related to the breaking of the charge and spin ordering in localized subsystem.

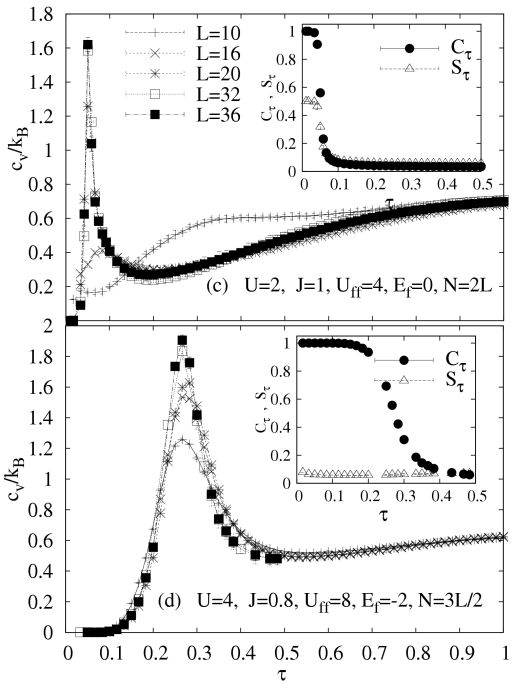

Fig. 3. Specific heat as a function of temperature $\tau = k_B T/t$, for the phase (c) and the phase (d) (Fig. 1). The insets represent temperature dependence of C_τ and S_τ defined in the text.

Unfortunately, the special type of charge and spin ordering that realizes at the symmetric case does not allow us to study another important problem, and namely, how realizes the transition from the low-temperature ordered phase to the high-temperature disordered phase for both spin and charge ordering. There are two possible scenarios: the spin and charge ordering can be destroyed simultaneously at the same critical temperature τ, or consecutively at two different temperatures. To examine this problem we have investigated the extended FKM in the unsymmetric case. In particular, we have considered two cases with ground-state configurations depicted in Fig. 1c and Fig. 1d. One can see that both configurations have such a form that breaking of one type of ordering, for example the spin ordering, need not be accompanied by breaking of the charge ordering. The numerical results obtained for model parameters corresponding to (c) and (d) phases at $\tau = 0$ are shown in Fig. 3. The temperature dependences of the specific heat and the charge/spin structure factors (for (c) phase: $C_\tau = 4\langle|X^+(0,\pi) - X^+(\pi,0)|\rangle/L$, $S_\tau = 4\langle|X^-(\frac{\pi}{2},\pi) - X^-(\pi,\frac{\pi}{2})|\rangle/L$, for (d) phase: $C_\tau = 4\langle X^+(\pi,\pi)\rangle/L$, $S_\tau = 2\langle|X^-(0,\pi) + X^-(\pi,0)|\rangle/L$) show that the system behaves fully differently for (c) phase and (d) phase. In the first case both the charge and spin ordering disappear simultaneously at the same critical temperature τ, while in the second case the spin and charge ordering disappear at temperatures that differ significantly. Indeed, we have found that already temperature of the order 0.01 destroys fully the spin ordering for (d) phase, while the charge ordering persists up to $\tau_c \approx 0.25$ which is in a good agreement with results of Lemanski [10] obtained for infinite U_{ff} and fixed n_f.

Acknowledgments

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