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Peculiar Thermodynamic Properties of the Falicov-Kimball Model for small U Couplings

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We analyse a behaviour of the order parameter and specific heat of the Falicov-Kimball model (FKM) on the Bethe lattice using the Dynamical Mean Field Theory (DMFT) formalism, which provides the exact solution in the limit of large spatial dimensions. In the large U limit, the FKM maps onto the effective Ising model, with the order parameter of the Curie-Weiss form. However, in the small U limit the order parameter takes on unusual shape, with a sharp reduction near $T \approx T_c/2$. We focus our investigation on a crossover between these two limits, thus we perform our calculations for a set of intermediate and small values of U. We find the overall behaviour of the order parameter and specific heat as a function of temperature to be quite anomalous.

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Describing correlated electrons is fascinating, since it often turns out that the properties of these systems derived from calculations are difficult to predict or even surprising. Such situations occur even when we study the simplest models, such as e.g. the FKM [1], called also the simplified Hubbard model. Some time ago, P. van Dongen studied this model rigorously using the DMFT method and obtained a shocking result on the order parameter as a function of temperature [2]. In the limit of low local (on site) interaction value U, the order parameter d (the detailed definition is given in the next section) decreases abruptly at temperature about $T_c/2$ and assumes very small values in the interval between $T_c/2$ and T_c. On the other hand, for large U values the parameter d behaves in accordance with the Curie-Weiss law.

Since in his work van Dongen analyzed merely the boundary cases $U \to 0$ and $U \to \infty$, from his results it could not be deduced how the shape of function $d(T)$ evolves between these extreme cases. This problem was resolved to large extent by Chen et. al. in [3], where the function $d(T)$ was displayed for small U, down to $U = 0.005$, and it was demonstrated that the peculiar behaviour of $d(T)$ starts to emerge below $U \approx 0.5$.

But still, it was unclear whether this strange course of $d(T)$ was not related to the fact, that the system was investigated on the Bethe lattice and in the limit of large dimension. It turned out, however, that for small values of U also in the two-dimensional system, the dependence of $d(T)$ differs substantially from the Curie-Weiss curve. Indeed, Maśka and Czajka studied this model with the Monte Carlo method for $U = 0.01$, and obtained nearly linear decrease of the order parameter within a wide temperature range below T_c [4]. For that case they also observed an unusual behaviour of the specific heat C_v and susceptibility χ versus temperature, with plateaux of elevated C_v and χ values occuring before the characteristic for the phase transition λ-type peaks occur.

The results obtained in [2,3,4] inspired us to carry out a thorough analysis of the model focusing on small, but finite values of U. In particular, the aim of our studies here was to find out of how such an unusual behaviour of the order parameter impacts the specific heat behaviour. For this purpose, we examined rigorously the FKM on the Bethe lattice using the DMFT. Our research is an extension of the studies undertaken by Chen et. al. [3] and it consists in widening the range of investigated values of U down to $U = 0.0001$ and analyzing the specific heat evolution with a change of temperature. As far as we know, the results for the specific heat obtained using the DMFT for small U values have not been reported before. An important feature of our research is that the whole analysis is conducted exactly on the basis of analytical expressions, so that we can be sure that our results are free of uncontrolled approximations.

2. Model and method of calculation

We use the following Hamiltonian of the FKM [5]:

$$H = t \sum_{\langle m,n \rangle} d_m^+ d_n + U \sum_m w_m n_m^d \tag{1}$$

where $\langle m,n \rangle$ denotes the nearest neighbor lattice sites m and n, $d_m(d_m^+)$ is an annihilation(creation) operator of itinerant electrons, while n_m^d is their occupation number operator. The quantity w_m is equal to 1/2(-1/2) for the lattice site occupied by the ion A(B), therefore the Coulomb-type on-site interaction between itinerant electrons and the ions amounts to $U/2(-U/2)$. The hopping electron amplitude t we set equal to one, therefore we measure all energies in units of t.

The ground state of the system has the checkerboard-type structure composed of two interpenetrating sublattices + and −, each of them is occupied only by one type of ion: the sublattice + by the ions A and the sublattice − by the ions B. Consequently, the density $\rho_A^+(\rho_B^-)$ of ions $A(B)$ on the sublattice $+(-)$ is equal to 1 ($\rho_A^+ = \rho_B^- = 1$),

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whereas the density $\rho_B^+(\rho_A^-)$ of ions $B(A)$ on the sublattice $+(-)$ is equal to 0 ($\rho_B^+ = \rho_A^- = 0$).

With an increase of temperature the densities ρ_A^+, ρ_B^- ($\rho_A^+ = \rho_B^-$) diminish below 1, while ρ_B^+, ρ_A^- ($\rho_B^+ = \rho_A^-$) increase above 0 and in the disordered phase all these densities are equal to 1/2. Therefore the quantity $d = \rho_A^+ - \rho_A^- = \rho_B^- - \rho_B^+$ is chosen to be the order parameter.

Our analysis of all physical properties is based on examination of the temperature dependant density of states (DOS) $\rho(U,T;\epsilon)$. Here the DOS is derived for the Bethe lattice in the limit of large dimensions using the exact formulas for the Green functions within the DMFT formalism [2].

The method is based on the following two exact analytical formulas for the Green functions $G^+(z)$ and $G^-(z)$, referring to the sublattice + and −, respectively:

$$G^+(z) = \frac{z + \frac{1}{2}Ud - G^-(z)}{[z + \frac{1}{2}U - G^-(z)][z - \frac{1}{2}U - G^-(z)]}$$
$$G^-(z) = \frac{z - \frac{1}{2}Ud - G^+(z)}{[z + \frac{1}{2}U - G^+(z)][z - \frac{1}{2}U - G^+(z)]}. \quad (2)$$

After finding selconsistent solutions of the equations (2) one gets the expressions for electron DOS $\rho^+(U,d;\epsilon)$ and $\rho^-(U,d;\epsilon)$, corresponding to the sublattice + and −, respectively:

$$\rho^+(U,d;E) = -\frac{1}{\pi}\mathrm{Im}G^+(U,d;\epsilon + \mathrm{i}0)$$
$$\rho^-(U,d;E) = -\frac{1}{\pi}\mathrm{Im}G^-(U,d;\epsilon + \mathrm{i}0) \quad (3)$$

and hence the total DOS

$$\rho(U,d;\epsilon) = \frac{\rho^+(U,d;\epsilon) + \rho^-(U,d;\epsilon)}{2}. \quad (4)$$

The functions $\rho^+(U,d;\epsilon)$ and $\rho^-(U,d;\epsilon)$ are not explicitly dependent on T, so their temperature dependence comes out from the temperature dependence of $d = d(U;T)$, only. Consequently, both the order parameter $d(U;T)$ and the DOS distributions $\rho^+(U,d;\epsilon)$ and $\rho^-(U,d;\epsilon)$ are determined selfconsistently from the following procedure. First, we determine the free energy $F(U,d,T)$ [5]:

$$F(U,d,T) = T\int_{-\infty}^{\infty} \mathrm{d}\epsilon\rho(U,d;\epsilon)\ln\frac{1}{1+\exp(-\epsilon/k_\mathrm{B}T)} - TS_{ions}, \quad (5)$$

where the ions entropy S_{ions} is given by

$$S_{ions} = -\frac{1+d}{2}\ln\frac{1+d}{2} - \frac{1-d}{2}\ln\frac{1-d}{2} \quad (6)$$

Then, from the minimization of $F(U,d,T)$ over d we find the order parameter $d(U;T)$ and subsequently $\rho^+(U,T;\epsilon)$ and $\rho^-(U,T;\epsilon)$. Next we determine the internal energy $E(U,T)$ using the formula:

$$E(U,T) = \int_{-\infty}^{\infty} \mathrm{d}\epsilon\rho(U,d(T);\epsilon)\frac{\epsilon}{1+\exp(\epsilon/k_\mathrm{B}T)}, \quad (7)$$

and the specific heat is calculated from the standard formula:

$$C_V = \frac{\mathrm{d}E(U,T)}{\mathrm{d}T} \quad (8)$$

3. Results

The dependence d vs T reported in [3] was obtained by summing over Matsubara frequencies and obeyed the range of $U \geqslant 0.005$. By contrast, we determined the function $d(T)$ for $U \geqslant 0.0001$ by minimizing the free energy (see Fig. 1). The temperature dependence of $d(T)$, that we got, is consistent with the previously reported results [2,3,4]. Furthermore, for small U our calculations confirm the square root character of the function $d(T)$ when it approaches T_c, as it was already noted in the limit $U \to 0$ by van Dongen [2] (see inset in Fig. 1).

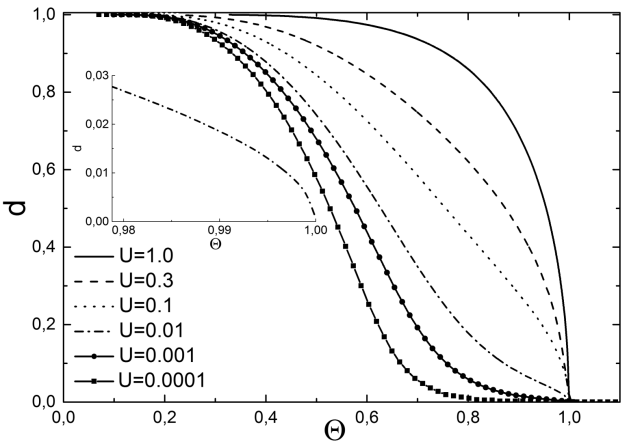

Fig. 1. Order parameter for the charge ordered phase of the Falicov-Kimball model vs the reduced temperature $\theta = T/T_c(U)$ for a set of small and intermediate U values. In the inset the function $d(\theta)$ close to $\theta = 1$ for $U = 0.01$ is displayed.

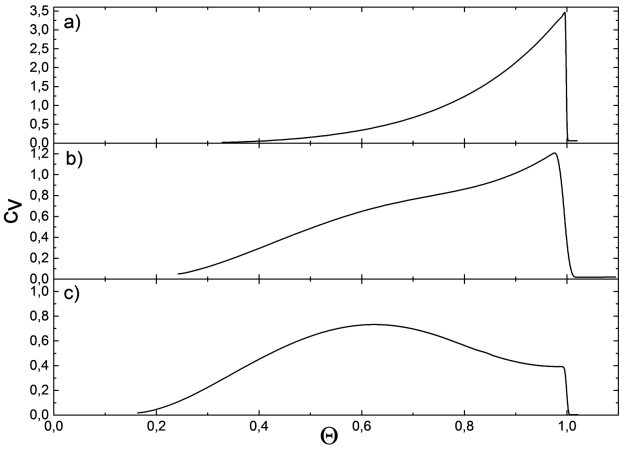

Fig. 2. Specific heat vs the reduced temperature for a set of intermediate U values: a) $U = 1.0$, b) $U = 0.3$, c) $U = 0.1$.

It turns out that atypical course of $d(T)$ implies also an unusual dependence of the specific heat C_v vs temperature. Indeed, as it can be seen in Figs. 2 and 3, the

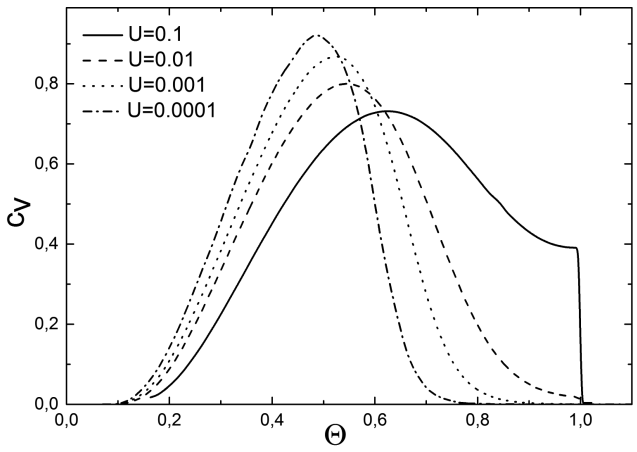

Fig. 3. Specific heat vs the reduced temperature for a set of small U values.

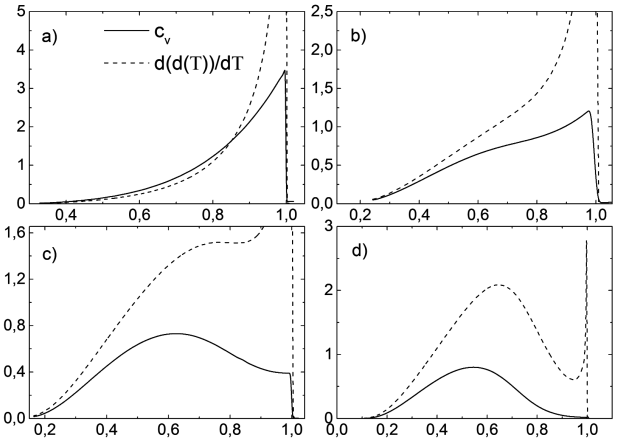

Fig. 4. Specific heat C_v and the derivative of the order parameter $d(\theta)$ over θ ($\mathrm{d}(d(\theta))/d\theta$) vs the reduced temperature θ for a) $U = 1.0$, b) $U = 0.3$, c) $U = 0.1$ and d) $U = 0.01$.

function $C_v(T)$ changes its shape from *the lambda-type* for $U = 1$, assuming two maxima in the intermediate range of $0.1\langle U\langle 0.3$, and finally reaching only one maximum around $T = T_c/2$ when $U\langle 0.01$.

Looking for a relationship between $d(T)$ and $C_v(T)$ we have determined the derivative $d(T)$ over T and observed some similarities of the waveforms of $C_v(T)$ and $\mathrm{d}(d(T))/\mathrm{d}T$ as functions of temperature, what is illustrated in Fig. 4.

Indeed, the substantial drop in the specific heat occurs at the transition point, when the derivative $\mathrm{d}(d(T))/\mathrm{d}T$ tends to infinity. And for small U's the maximum of $C_v(T)$ occurs somewhat above $T = T_c/2$, when there is a clear decrease in the order parameter, although the maxima of C_v and $\mathrm{d}(d(T))/\mathrm{d}T$ are sligthly displaced.

The similarities of forms of the functions $C_v(T)$ and $\mathrm{d}(d(T))/\mathrm{d}T$ can be explained as follows. Since the dependence of $\rho(U, d(T); \epsilon)$ vs T comes entirely from $d(T)$, calculation of $\mathrm{d}\rho(U, d(T); \epsilon)/\mathrm{d}T$ requires the external derivative $\mathrm{d}(\rho(U, d(T)); \epsilon)/\mathrm{d}(d(T))$ to be multiplied by the internal derivative $\mathrm{d}(d(T))/\mathrm{d}T$. Applying this reasoning to the formulae (7) and (8), gives insight how $C_v(T)$ and $\mathrm{d}(d(T))/\mathrm{d}T$ are related with each other.

4. Conclusions

Our rigorous results based on the minimization procedure of the free energy confirm the anomalous behaviour of the order parameter $d(T)$ of the FKM for small U values obtained earlier within the method of summation over Matsubara frequencies [3].The method we used allowed us to investigate the system with a minimum U value of 50 times less than in case of work [3] ($U_{min} = 0.0001$ in our case vs. $U_{min} = 0.005$ in [3]) and enabled us to confirm a square-roor singularity of $d(T)$ near T_c obtained in the limit of $U \to 0$ [2].

We also determined an evolution of the shape of $C_v(T)$ with U and we have found the relationship between the course of $C_v(T)$ and $d(T)$. In all examined cases the phase transition point is indicated by an abrupt drop of $C_v(T)$, but the value of C_v just before this drop diminishes with lowering of U. Consequently, we observe an interesting evolution of the shape of $C_v(T)$ curve from the λ-type for $U\rangle 0.5$, through the curves possessing two maxima for $0.1\langle U\langle 0.5$, to the curve with only one maximum near $T \approx T_c/2$ for $U\langle 0.1$.

When U tends to 0, then the maximum of C_v occurring close to $T_c/2$ becomes more steeper and the C_v curve starts to resemble the λ shape, but with its steepest descent corresponding not to the phase transition point T_c, but to the steepest descent of the order parameter $d(T)$ near $T_c/2$. There still remains an open question about the reason for this strange behavior of the order parameter $d(T)$ for small U, we intend to investigate this issue in our future studies.

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