Thermodynamics of the three-dimensional Falicov-Kimball model

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Introduction

The Hamiltonian of the Falicov-Kimball model (FKM) [1] 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 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. **Most of the results obtained for the FKM have been calculated for the limiting cases of $D = 1$, $D = 2$ and $D = \infty$ (where D is the dimension of the system) and it is not clear if these results hold also in the realistic case ($D = 3$).** In this paper we consider only the symmetric point of the model ($\mu = U/2$, $E_f = 0$). The Classical Metropolis algorithm [2, 3], is used for the investigation of thermodynamics of the FKM. Where the so called electronic free energy

$$F(w) = (E_f - \mu) N_f - \frac{1}{\beta} \sum_i \ln(1 + e^{-\beta(\epsilon_i - \mu)}), \qquad (2)$$

is used as the statistical weight in the algorithm. The simulations started mostly at high temperatures with random configuration. Data were generated typically with 10^5 MC steps per site after discarding at least 3×10^4 initial MC steps per site.

Critical temperatures

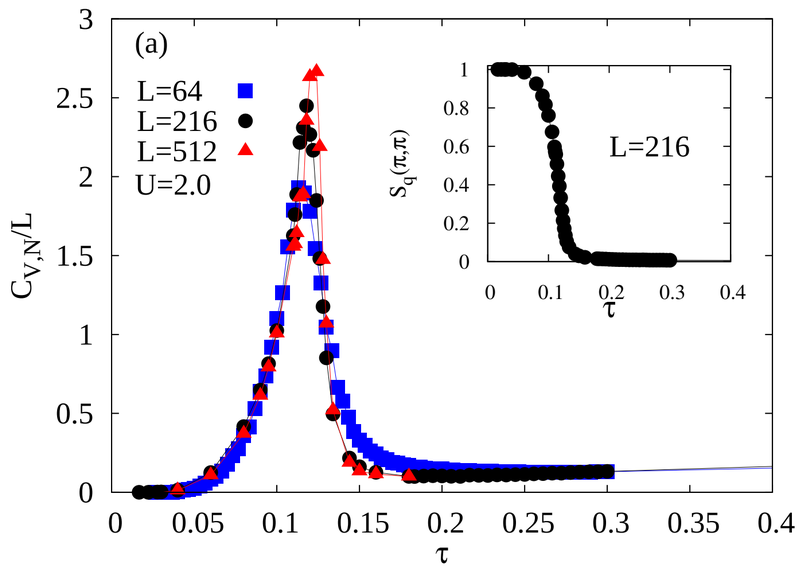
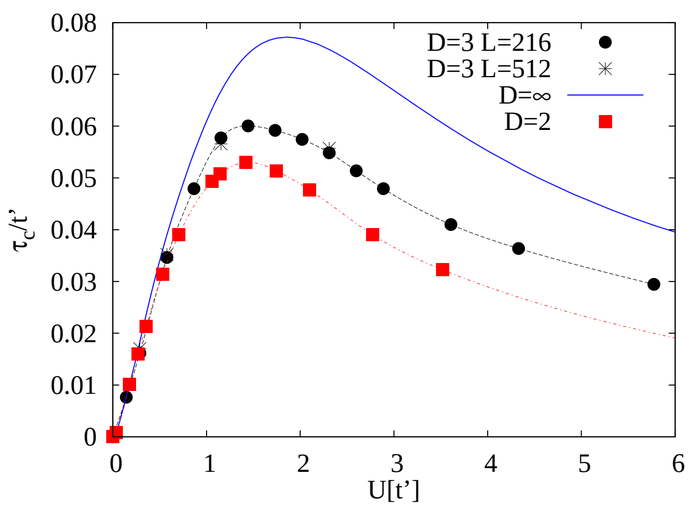


Fig.1 Specific heat as a function of τ for $U = 2$ and different lattice sizes. The insets represent the temperature dependencies of the structure factor $S_q(\pi,\pi) = \frac{1}{2L} \sum_{j,k} e^{i\mathbf{Q}(\mathbf{R}_j - \mathbf{R}_k)} (w_j w_k)$.

$C_{V,N}$ as a function of τ shows sharp low-temperature peak which scales with the lattice size. Hereby the structure factor $S_q(\pi,\pi)$ changes rapidly from 1 to ~ 0 (insets in Fig.1), near the temperature where the maximum of $C_{V,N}$ appears. This indicates that the sharp maxima can be used to estimate the critical temperature of the phase transition from the ordered phase to the disordered phase.

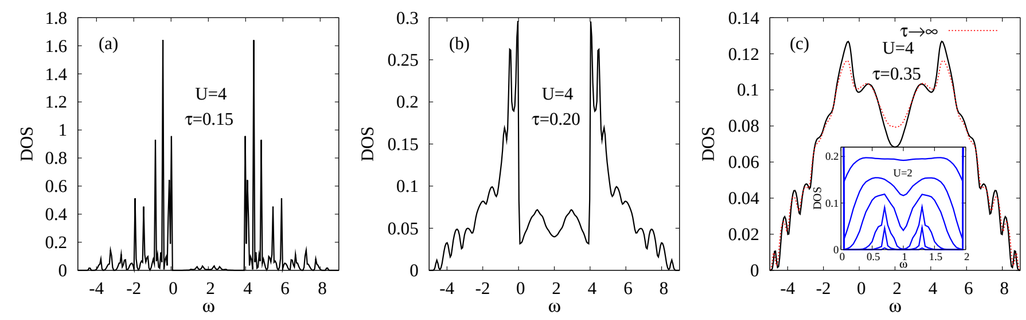


Fi.2 The transition temperature τ_c of the half-filled FKM as a function of U obtained for $D = 2$ [3], $D = \infty$ [4] and $D = 3$. Units of $t' = 2t\sqrt{D}$ are used.

It is evident that outside the weak coupling limit the critical temperature in $D = 3$ is considerably enhanced in comparison to $D = 2$, and it is considerably smaller than in $D = \infty$.

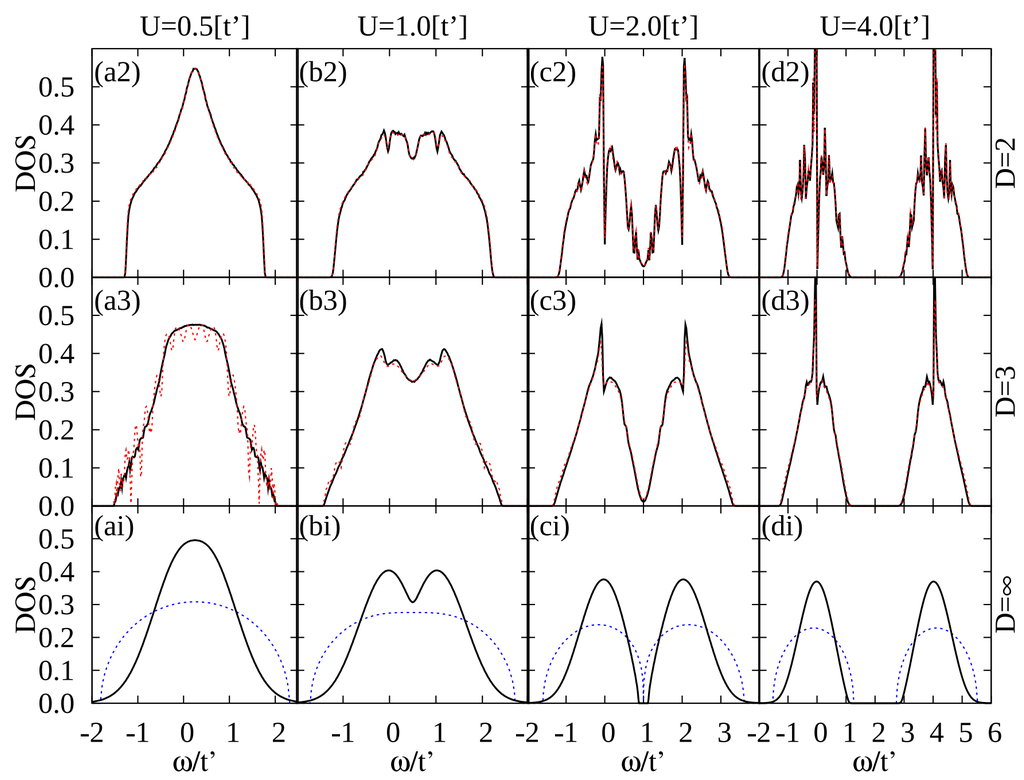
Density of States

In Fig.3 the single-particle DOS for the three dimensional FKM is shown. A fine structure appears in the DOS in the region of $0 < \omega < U$ (Fig.3(a)), that with increasing τ transforms to a pseudo-gap. In the limit of the weak Coulomb interaction the sufficiently high temperature closes the pseudo-gap (inset of Fig.3(c)). For an intermediate U a pseudo-gap persists even for $\tau \to \infty$ (Fig.3(c)). Finally, for the strong coupling limit the fine structure reduces the width of the gap but it still remains open.



DOS for $U = 4$ at various temperatures for $L = 512$. Dotted line in figure (c) represents the solutions for $\tau \to \infty$. Inset in (c) is a detail of the temperature evolution of the fine structure of DOS in the region of $0 \leq \omega <\leq U$ for a weak Coulomb interaction $U = 2$ and various τ.

Fig.4(a3-d3) illustrates the finite temperature Mott-Hubbard transition as a function of U in the real dimension and for the homogeneous phase. Moreover, with increasing dimension the fine structure becomes smoother, and finally, transforms in the smooth maxima for $D = \infty$. In the weak coupling limit the character of DOS in $D = \infty$ is even closer to the realistic $D = 3$ case than the $D = 2$ case. The opposite is true in the strong coupling limit, where the DOS in infinite dimensions lacks the peaks and local minima near $\omega = \mu \pm U/2$. This fact can play an important role in the correct description of electronic correlations of real materials in $D = 3$ since these details are connected with the interaction between f and d electrons.



DOS in the homogenous phase computed for different U and different dimensions. Both open (black) and periodic (red) boundary conditions and units of $t' = 2t\sqrt{D}$ are used. In the infinite dimension the DOS (computed by DMFT [5]) for hypercubic lattice (black solid line) and Bethe lattice (blue dashed line) are plotted.

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References

[1] L.M. Falicov and J.C. Kimball, Phys. Rev. Lett. 22 (1969) 997
[2] P. de Vries, K. Michielsen, H. De Raedt, Z. Phys. B 92 (1993) 353
[3] M.M. Maśka, K. Czajka, Phys. Rev. B 74 (2006) 035109
[4] L. Chen, J.K. Freericks, B.A. Jones, Phys. Rev. B 68 (2003) 153102
[5] J.K. Freericks, V. Zlatić, Rev. Mod. Phys. 75 (2003) 1333

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