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Impurity distribution in a frustrated system

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Abstract

Results of Monte-Carlo simulations for the Falicov–Kimball (FK) model on a triangular lattice are presented. Half-filled neutral FK model on the triangular lattice is, at least in the large interaction regime, strongly frustrated. This results in disordered low-temperature impurity configurations. A pair distribution functions and frustrated-bond-graphs are used to quantitatively describe the formation of these states, when the temperature is lowered. The possibility of a phase transition is discussed.

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Keywords: Monte-Carlo simulations; Frustration; Falicov–Kimball model

1. Introduction

In geometrically frustrated systems, such as antiferromagnets on a triangular, Kagome, or pyrochlore lattice, a long-range ordering of spins is suppressed by the existence of a large number of minimal energy spin configurations. In classical frustrated systems the number of ground states grows exponentially with the system size, giving rise to an extensive zero-temperature entropy. On the other hand, the quantum dynamics may lift this enormous degeneracy by forming quantum superpositions of classical ground states, allowing for the existence of ordered states at finite temperatures.

The main aim of this paper is to analyze the Falicov–Kimball (FK) model [1] on a triangular lattice. In the strong interaction limit this model maps onto the antiferromagnetic spin-half Ising model, that does not exhibit a phase transition on the triangular lattice at any non-zero temperature [2]. On the other hand, it has been proved [3] that in $d \geqslant 2$ at low enough temperature the half-filled FK model possesses a long-range order. This statement, however, holds true only if the lattice is bipartite and the triangular lattice does not fulfill this requirement. Then, it is interesting to investigate the FK model on the triangular lattice away from the strong interaction limit, i.e, in the regime, where it is not equivalent to the Ising model and where the possibility of the presence of a long-range order is not excluded.

2. Model and method

The FK model describes a system consisting of two species of particles: itinerant electrons and classical, localized particles. The Hamiltonian of the spinless FK model is given by

$$H = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + U \sum_i n_i w_i, \tag{1}$$

where $c_i^\dagger$ (c_j) describe electron creation (annihilation) operators and w_i is equal to 0 or 1, according to whether the site i is occupied or unoccupied by a massive particle. This model has been investigated by means of various methods [4]. Here, we use the Monte-Carlo method adopted to investigate a system with both the classical as well as fermionic degrees of freedom [5]. The simulations were performed for the triangular lattice 21×21 clusters with periodic boundary conditions.

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3. Results and discussion

Fig. 1 presents "snapshots" of ionic configuration. Here we used frustrated-bond-graph (FB-graph) representations of the configurations, where all the neighboring pairs of sites in the same state (both occupied by ions or both unoccupied) are joined by line segments. These segments correspond to the frustrated pairs.

Comparing the upper and lower rows one can see the differences between configurations in the weak and strong coupling limits. In both these regimes at low temperature there are (almost) no triangles formed by neighboring occupied sites. However, for large-U also the unoccupied sites avoid to form triangles, what is not the case in the weak interaction regime. It can be explained by recalling that in the strong interaction limit the FK model maps onto the Ising model. Then the spin symmetry of the Ising model corresponds to the particle-hole symmetry of the FK model. As a result, in the FB-graph representations of the ionic configurations there are clusters consisting of empty sites encircled by lines connecting occupied sites as well as clusters of occupied sites surrounded by empty sites. In contradiction to this case, in the weak coupling regime at low temperature empty sites cluster together, whereas ions arrange themselves in a pattern around them forming closed lines. Such a distinct behavior in the strong and weak interaction regimes indicates, that the possibility of a finite-temperature phase transition in the FK model on the triangular lattice cannot be excluded on the basis of the mapping onto the Ising model. Such a distinction does not occurs in the half-filled FK model on a bipartite lattice, where the ground state is of a checkerboard character independently of the interaction strength.

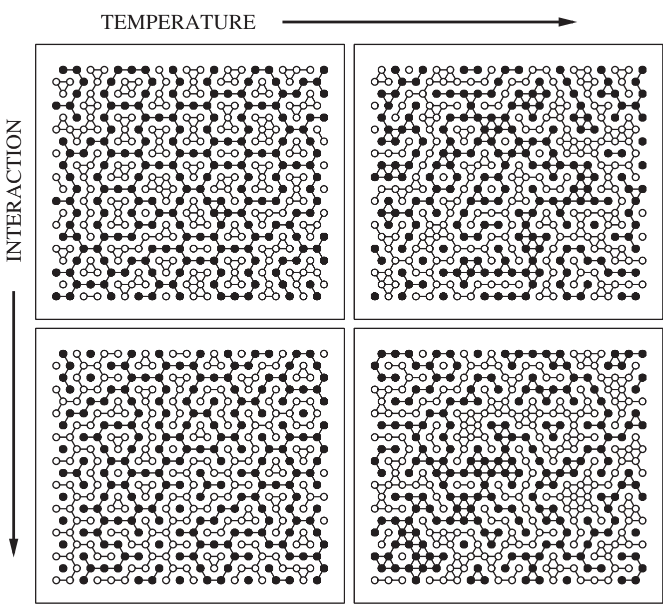

Fig. 1. Examples of ionic configurations in various regimes: Upper left panel—$U/t=1$, $k_{\mathrm{B}}T/t=0.0001$, upper right—$U/t=1$, $k_{\mathrm{B}}T/t=0.02$, lower left—$U/t=10$, $k_{\mathrm{B}}T/t=0.005$, lower right—$U/t=10$, $k_{\mathrm{B}}T/t=0.3$.

Another indication for different behavior of the FK model in the strong and weak interaction regimes comes from the pair distribution function (PDF) analysis, that is a powerful technique for revealing the real space ionic arrangement in nonperiodic matter. Given a reference occupied site, PDF gives the occupancy probability as a function of the distance. Fig. 2 demonstrates PDFs for $U/t=1$ and 10.

Despite the fact that the short-range correlations are stronger for large U, the oscillations of the PDF reaches much farther in the weak interaction regime. This may suggest the existence of a low-temperature long-range order in the weakly interacting FK model on the triangular lattice.

And finally, the MC simulations indicate the presence of a sharp peak in the specific heat for small and intermediate U. At small U ($U/t \lesssim 2$) the specific heat is featureless

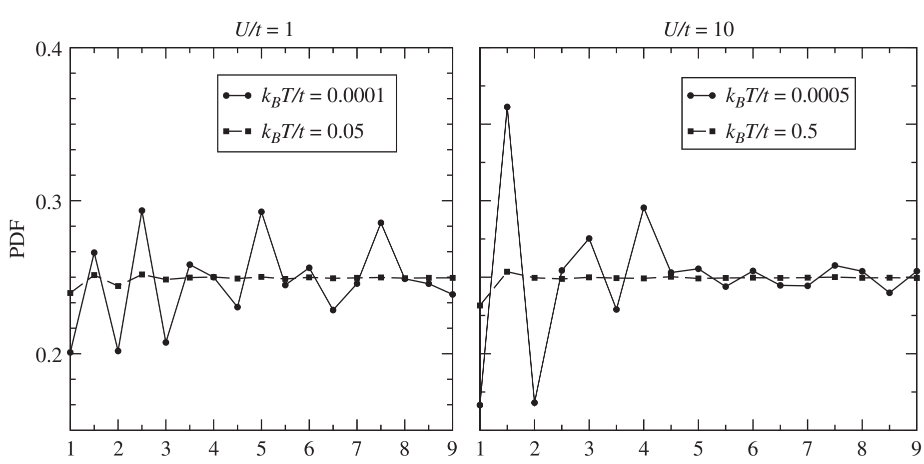

Fig. 2. PDFs for $U/t=1$ and 10 at low (solid lines) and high (dashed lines) temperatures.

except for this single peak. For larger U a gap opens in the electronic density of states and a Schottky-type anomaly develops in the temperature dependence of the specific heat. With increasing U the temperature at which the peak occurs decreases, going to zero in the large-U limit, thus recovering the exact Wannier result, that the triangular Ising antiferromagnet is known to exhibit a phase transition at $T = 0$ [2].

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