Anisotropic triangular Ising model in the extended mean-field renormalization-group approach

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The recently proposed multi-interaction mean-field renormalization technique [C. N. Likos and A. Maritan, Phys. Rev. E **53**, 3303 (1996)] is applied to the Ising model on a triangular lattice with equal couplings in two directions and a different coupling in the third, a model equivalent to a square Ising model with additional second-neighbor interactions along a *single* diagonal direction. Three different clusters are considered and the possible mappings between them are discussed. The estimates for critical couplings and exponents are in satisfactory agreement with exact results. An explanation of the way in which the finite-size features of the method bring about a systematic overestimation of the critical temperature is also given. [S1063-651X(97)06402-7]

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Recently, an extension of the mean-field renormalization-group (MFRG) approach [1,2] has been proposed [3], which is capable of dealing with lattice Hamiltonians with two coupling constants, under certain restrictions on the geometry of the lattice and the ground states of the model. This extended MFRG (EMFRG) technique has been applied to a number of different Hamiltonians [3]; in this paper, we present another application of the method, this time to the anisotropic triangular Ising model. This is a system of Ising spins on a triangular lattice with nearest-neighbor interactions, but with the strength of the coupling being different along the three axes of the triangular lattice. An extensive study of the properties of this system, including the behavior of correlation functions, has been presented in a series of papers by Stephenson [4].

In this work we consider a special case of the model, in which the anisotropy is more restricted: we take the couplings to be equal in two directions in the triangular lattice but different from these, in general, along the third one. Thus we have a Hamiltonian with two coupling constants, which is the first prerequisite for the application of the EMFRG as it was presented in Ref. [3]; we establish the region in parameter space where the additional requirements for the application of the EMFRG are met, and derive the renormalization-group flows. We show that the EMFRG is successful in producing the qualitative features of the flows and the fixed points of the mapping. The quantitative accuracy is typical of MFRG types of techniques and, at the trivial fixed points of the iteration, the magnetic eigenvalues are exact. We find that the critical temperature of the model is consistently overestimated (in comparison with exact results) and we trace this overestimation to the fact that one eigenvalue in a particular fixed point is found in this method to be marginally relevant. This marginality is an artifact caused by the finite-cluster character of this approximate RG; this provides an understanding of the way in which the use of finite clusters affects the estimate of the critical temperature in this problem.

Let us consider a model Hamiltonian of Ising spins $s_i = \pm 1$ on a triangular lattice, of the form

$$\mathcal{H} = -\mathcal{J}\sum_{\langle ij\rangle} s_i s_j - \mathcal{K}\sum_{\langle\langle ij\rangle\rangle} s_i s_j - \mathcal{B}\sum_i s_i , \qquad (1)$$

where the first sum is carried over horizontal and right-leaning nearest-neighbor bonds, the second over left-leaning nearest-neighbor bonds (also called ''diagonals''), and the third over sites ($\mathcal{B}$ is the magnetic field.) Alternatively, the triangular lattice can be thought of as a square lattice with nearest-neighbor interactions (coupling constant $\mathcal{J}$) and a *single* second-neighbor interaction along left-leaning diagonals (coupling constant $\mathcal{K}$) [4,5]. This is the point of view which we adopt for the rest of the paper.

In the special case $\mathcal{J}=\mathcal{K}$, the usual triangular (anti)ferromagnetic Ising model is recovered, for ($\mathcal{J}<0$) $\mathcal{J}>0$. Similarly, the nearest-neighbor square Ising model with coupling constant $\mathcal{J}$ results when $\mathcal{K}=0$, whereas if $\mathcal{J}=0$ the model reduces to decoupled one-dimensional Ising chains along the diagonals, with nearest-neighbor coupling $\mathcal{K}$.

The ground states of the model follow from a straightforward calculation. Keeping in mind that the problem has been recast in terms of spins on a *square* lattice we find the following $T=0$ phase diagram for the model: in the region $\{\mathcal{J}>0;\mathcal{K}>-\mathcal{J}\}$ the ground state is ferromagnetic (FM), whereas in the region $\{\mathcal{J}<0;\mathcal{K}>\mathcal{J}\}$ it is antiferromagnetic (AFM). The remaining region displays infinitely many ground states; within the domain $\mathcal{K}<-|\mathcal{J}|$, the randomness of the ground state is one dimensional (freedom of combining plaquettes is restricted along a single horizontal or vertical strip), the $T=0$ entropy scales as $N^{1/2}$ (where N is the number of lattice sites), and the entropy per site vanishes at the thermodynamic limit. On the other hand, *on the borderline* $\mathcal{K}=\mathcal{J}<0$ the ground states have a two-dimensional randomness, giving rise to the well-known extensive zero-temperature entropy of the AFM triangular model, which was calculated a long time ago by Wannier [6]. The same is true for the other borderline, $\mathcal{K}=-\mathcal{J}<0$.

According to the general requirements for the implementation of the EMFRG laid down in Ref. [3], we are going to consider the flows of the coupling constants only in the region $\mathcal{K}\geqslant 0$ where there are just the ordered FM and AFM ground states.

We first summarize the main ideas of the EMFRG, referring the reader to Ref. [3] for details. From Eq. (1) we obtain the reduced Hamiltonian

$$H\equiv-\beta\mathcal{H}=J\sum_{\langle ij\rangle} s_i s_j + K\sum_{\langle\langle ij\rangle\rangle} s_i s_j + h\sum_i s_i, \tag{2}$$

with $J=\beta\mathcal{J}$, $K=\beta\mathcal{K}$, and $h=\beta\mathcal{B}$. First, we separate the given bipartite lattice into two sublattices A and B. Let us consider, next, two clusters of N' and N sites with $N'<N$ (all primed symbols which appear hereafter refer to quantities pertaining to the small cluster, and all unprimed ones to the large one). The method *requires* the use of clusters in which the two sublattices are equivalent. If we denote the surrounding magnetizations on the A and B sublattices by b_1' (b_1) and b_2' (b_2) for the small (large) cluster, we can derive the usual mean-field expressions for the cluster sublattice magnetizations of the type $m'_{A(B)}(J',K',h',b_1',b_2')$ and $m_{A(B)}(J,K,h,b_1,b_2)$. A mapping $(J,K)\rightarrow(J',K')$ in the even subspace of the Hamiltonian is defined by requiring

$$m'_A(J',K',h',b_1',b_2')=l^{d-y_h}m_A(J,K,h,b_1,b_2) \tag{3}$$

along with

$$b_i'=l^{d-y_h}b_i, \quad i=1,2 \tag{4}$$

to hold to leading orders in h and b_i. In Eq. (3) above, d is the dimension of space, whereas the rescaling factor l is usually defined as $l=(N/N')^{1/d}$. From Eqs. (3) and (4) above, we now obtain the two flow equations in the even sector of the Hamiltonian in the form

$$\left.\frac{\partial m_A'(J',K',h',\mathbf{b}')}{\partial b_i'}\right|_{h'=\mathbf{b}'=0}=\left.\frac{\partial m_A(J,K,h,\mathbf{b})}{\partial b_i}\right|_{h=\mathbf{b}=0}, \quad i=1,2 \tag{5}$$

where $\mathbf{b}'$ [$\mathbf{b}$] is a shorthand for (b_1',b_2') [(b_1,b_2)]. It is here that the requirement for the equivalence of the sublattices in the clusters becomes crucial, because it guarantees that the flow equations are the same, regardless of the choice of the sublattice magnetization used in Eq. (5) above [3]. The even eigenvalues λ_i ($i=1,2$) are obtained from the linearization around the fixed point $\mathbf{J}_*\equiv(J_*,K_*)$ of Eq. (5). The magnetic exponent y_h is calculated from the scaling of the susceptibility χ at the fixed point, namely,

$$\chi_*'=l^{d-2y_h}\chi_*. \tag{6}$$

The square lattice is separated into the two interpenetrating square sublattices formed by the diagonals of the original one. The two-sublattice EMFRG imposes, clearly, the choice of clusters with even number of spins, and we will consider the three smallest values, 2, 4, and 6 in this work. For $N=2$ the nearest-neighbor bond is an appropriate cluster. On the other hand, the form of the present Hamiltonian rules out the choice of the elementary plaquette as a possible $N=4$ cluster because in this case there appears within the cluster a K coupling between two of the spins of the same sublattice which is absent for the two spins of the other sublattice. Thus for $N=4$ we are led to the choice of the parallelogram whose short sides are nearest-neighbor bonds and long sides are the next-nearest-neighbor diagonals along which the coupling $\mathcal{K}$ exists; the latter couples spins in the same sublattice. Finally, for $N=6$ we consider the rectangle which is formed by two adjacent elementary plaquettes.

At first sight, it appears that we can now define three possible mappings, namely, $6\rightarrow4$, $6\rightarrow2$, and $4\rightarrow2$. If the nearest-neighbor coupling vanishes, then the A and B sublattices completely decouple from each other. Then, $J'=J=0$ satisfies one of the two equations (5) above for arbitrary K,K' in a trivial way, because both sides vanish. This is the equation which relates the derivatives of the sublattice magnetizations with respect to the boundary magnetizations of the other sublattice. The remaining one is then the flow equation for the parameter K. If we use the $4\rightarrow2$ mapping, the mapping is equivalent to a $2\rightarrow1$ MFRG flow for the one-dimensional Ising model. On the other hand, the geometry of the $N=6$ cluster is such that for the case $J=0$ the cluster degenerates (for each sublattice) into a two-spin cluster and an additional one-spin cluster. In other words, the maximum number of interacting spins in the cluster is, in this case, *the same* as that for the $N=4$ cluster. In that respect, the $N=6$ cluster is not ''larger'' than the $N=4$ one along the $J=0$ direction in Hamiltonian space, and it is at first doubtful whether the $6\rightarrow4$ mapping will be meaningful at all. Indeed, it turns out that if one attempts such a mapping, one obtains the *erroneous result* that at the high-temperature fixed point $\mathbf{J}_*=(0,0)$ there exists *one relevant eigenvalue* along the (0,1) direction. This pathology is due to the reasons explained above, and therefore a $6\rightarrow4$ mapping is ruled inadmissible. Hence only the $4\rightarrow2$ and $6\rightarrow2$ mappings will be considered here.

We begin with the simpler mapping, $4\rightarrow2$. The recursion relations expressing the renormalized couplings (J',K') in terms of the original ones (J,K) read as

$$3J'\tanh(J')+2K'=\frac{e^{2K}[5J\sinh(3J)+2K\cosh(3J)]-J\sinh(J)+2K\cosh(J)}{e^{2K}\cosh(3J)+(2+e^{-2K})\cosh(J)} \tag{7}$$

and

$$3J'+2K'\tanh(J')=\frac{e^{2K}[2K\sinh(3J)+5J\cosh(3J)]+5J\cosh(J)}{e^{2K}\cosh(3J)+(2+e^{-2K})\cosh(J)}. \tag{8}$$

TABLE I. The ferromagnetic critical fixed points of the RG transformation and the associated critical exponents, the critical couplings for the square and triangular ferromagnetic Ising models as predicted by the present work, and the exact results for comparison.

	(J_*,K_*)	y_t	y_h	J_c^{sq}	J_c^{tr}
$4\to 2$	(0.2605,0.1355)	0.648	1.434	0.334	0.218
$6\to 2$	(0.1770,0.3160)	0.694	1.474	0.353	0.224
Exact		1.000	1.875	0.441	0.275

The fixed points (J_*,K_*) of the flows in the subspace $K\geqslant 0$ are the following: there are two low-temperature stable fixed points, $L_1=(+\infty,+\infty)$ representing the FM ground state and $L_2=(-\infty,+\infty)$ representing the AFM ground state. There is also the high-temperature fixed point $P=(0,0)$ representing the paramagnetic phase, which is stable as well. At L_1, the magnetic exponent is $y_h=2=d$ as it should be, since this point is a ''discontinuity fixed point'' and $y_h=d$ is a signal of a first-order phase change [7]. At the paramagnetic fixed point, we obtain $y_h=d/2$, again in agreement with the exact result arising from the consideration that the paramagnetic-phase zero-field susceptibility is a finite constant. In addition, there exists an unstable fixed point $L_3=(0,+\infty)$ which represents the zero-temperature ordered state of the one-dimensional Ising chains. Clearly, any departure from this fixed point drives the flows away from it. Finally, there exist two critical points, which are mirror images of each other with respect to the $J=0$ axis: the point $C_1=(0.2605,0.1335)$ which corresponds to FM criticality and the point $C_2=(-0.2605,0.1335)$ which corresponds to AFM criticality. For both C_1 and C_2 we find one relevant eigenvalue $\lambda_1=1.252$ yielding the estimate $y_t=0.648$ for the thermal exponent (cf. $y_t=1$ is the exact value), whereas the irrelevant eigenvalue is $\lambda_2=0.509$. The magnetic exponent at C_1 is $y_h=1.434$, to be compared with the exact result $y_h=1.875$. At C_2, we obtain $2y_h-d=-0.131<0$, a characteristic of AFM critical points, also found in earlier work [3] on different models.

From the intersection of the ferromagnetic critical line with the $K=0$ and $K=J$ lines we also obtain the estimates for the critical couplings of the square and triangular ferromagnetic Ising models, respectively, which read $J_c^{sq}=0.334$ (cf. 0.441 exact) and $J_c^{tr}=0.218$ (cf. 0.275 exact). These results, along with the ones obtained from the other mapping are summarized, for comparison, in Table I.

The $6\to 2$ mapping yields the same low- and high-temperature fixed points L_1,L_2,L_3, and P as the $4\to 2$ mapping, also with the correct magnetic exponent $y_h=d$ at L_1 and $y_h=d/2$ at P. The two critical fixed points are $C_1=(0.1770,0.3160)$ and $C_2=(-0.1770,0.3160)$, with eigenvalues $\lambda_1=1.464$ and $\lambda_2=0.567$. The thermal exponent is now $y_t=0.694$ and the magnetic exponent at C_1 is $y_h=1.474$; at C_2 we have again $0>2y_h-d=-0.238$. The estimates for the square and triangular Ising critical couplings read $J_c^{sq}=0.353$ and $J_c^{tr}=0.224$. The flow diagram is shown in Fig. 1; the flow pattern for the previous, $4\to 2$, mapping is identical to that shown in Fig. 1.

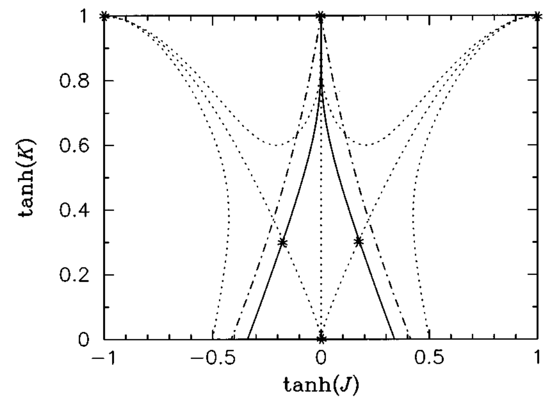

FIG. 1. RG flows of the present model obtained by the $6\to 2$ mapping. The stars denote fixed points. The dotted lines are attracted to either the low- or the high-temperature fixed points. The solid curves denote the basins of attraction of the two critical points. The dash-dotted curves denote the exact critical lines, Eq. (9).

A few remarks can already be made by looking at the summary of the results shown in Table I. It can be seen that the quantitative accuracy of the method is typical of the family of MFRG type of techniques with the use of small clusters. The critical couplings are off by about 20%, with an improvement from 24% to 20% for J_c^{sq} and from 20% to 18% for J_c^{tr} as the order of the mapping is increased. The critical temperature is overestimated systematically (see below.) The fractional errors on the critical exponents are larger than those for the critical couplings, but again a slow improvement is observed as the order of the mapping increases.

A more detailed analysis of the predictions for the critical temperature T_c (Curie point) is allowed by the existence of an exact expression for this quantity, based on generalized duality transformations [5]. The locus of critical points is given by the equation

$$e^{-2K}=\sinh(2|J|). \tag{9}$$

On the other hand, the locus of critical points obtained from our approximate RG analysis is given by the critical lines of the fixed points C_1, C_2; in Fig. 1 we plot for comparison the exact result (9) together with the critical lines obtained from the $6\to 2$ mapping (the ones obtained from the $4\to 2$ mapping run very close to those shown). Although the RG gives correctly the ''starting point'' of these lines at $T=0$ for vanishing nearest-neighbor coupling, for finite values of J the approximate critical line runs systematically *below* the exact one, thus giving rise to a consistent overestimation of the critical temperature. However, we observe that the shape of the approximate critical line is correct for values of J that are not too close to the origin; the deviation from the exact one is caused chiefly by its wrong behavior for small J, where it ''sticks'' close to the K axis. It can be seen now that this behavior is closely connected to the eigenvalues associated with the fixed point L_3. By symmetry, the two eigenvectors at this point are along the (1,0) and (0,1) directions. The eigenvalue associated with the latter direction is thus the ‘‘thermal eigenvalue’’ of the one-dimensional Ising chain. The RG gives for this eigenvalue the erroneous prediction that it is marginally relevant; this can easily be seen by introducing the variables $v = \tanh(K)$ and $t = 1 - v$ which measure the deviation from the one-dimensional critical point, and confirming that the present method gives to linear order $t' = t$ close to L_3. As a result of this marginality, the trajectories in the vicinity of this fixed point (including the critical line) ‘‘stick’’ on the K axis [8]. On the other hand, exact RG transformations for the Ising chain yield the relation $t' = 2t$, i.e., the correct eigenvalue $\lambda_t = 2$ is strictly relevant [9]. The marginality of the thermal eigenvalue in the one-dimensional Ising model is one of the shortcomings of the MFRG and stems from the use of finite clusters for performing the mapping. Indeed, as was pointed out in the original MFRG paper [1], the exact thermal eigenvalue in one dimension would involve, in this method, the comparison of two chains with L and $L' = L - 1$ spins in the limit $L \to \infty$. So we can now see how the finite-size feature of the MFRG affects (at least in this application) the trajectories: it brings about a distortion of the flow lines due to the wrong prediction of a marginal field which, however, can be cured only by considering *infinite* clusters. This, in turn, results in the systematic overestimation of T_c as explained above.

We have presented a further application of the multi-interaction mean-field renormalization method to the anisotropic triangular Ising model, finding that the method is qualitatively successful in describing the phases of this model. From the quantitative aspect, we found the typical deviations of the predictions from the exact results. We presented an explanation for the overestimation of the critical temperature of this model, arising from the finite-size nature of the approach. The study was limited, at present, to the region of ferromagnetic diagonal couplings, consistently with the general restrictions of the method presented in Ref. [3]. The investigation of the region of antiferromagnetic diagonal interactions, where an infinity of ground states exists, is an obvious challenge and a strong test for the applicability of MFRG ideas in such ‘‘unusual’’ and interesting cases. This would also allow for the study of the antiferromagnetic triangular lattice and the associated peculiarities of its zero-temperature critical point. This problem is currently under investigation.

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