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LETTER TO THE EDITOR

Exact results for lattice models with pair and triplet interactions

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Abstract. We consider an Ising model and the related lattice gas on the Kagomé lattice with two- and three-site couplings. Using a transformation which effectively decimates the triplet interactions, we determine the exact phase diagram of the Ising model as well as the exact boundary of the two-phase region of the lattice gas.

One unresolved problem in statistical physics has been the determination of the effects of multi-particle interactions on properties of a thermodynamic system. In particular, it has proved extremely difficult to deduce exact information. The only non-trivial exact solution known to this date is the solution of the triangular Ising model with pure three-spin interactions [1]. Studies of systems with mixed pair and multi-site interactions have usually been carried out with the help of mean-field [2] and renormalisation group [3] approximations.

In this letter, we carry out an exact analysis of two lattice models with pair and triplet interactions for the Kagomé lattice. We consider the Ising model and the related lattice gas with two- and three-spin interactions and show that they can be related to systems without the triplet interactions. Using this transformation, we determine the phase diagram of the Ising model and the exact boundary of the two-phase region of the lattice gas.

Consider a Kagomé Ising lattice of N sites shown in figure 1 with the reduced Hamiltonian

$$-\beta\mathscr{H} = L\sum_i s_i + K\sum_{nn} ss' + M\sum_{\Delta} ss's'' \tag{1}$$

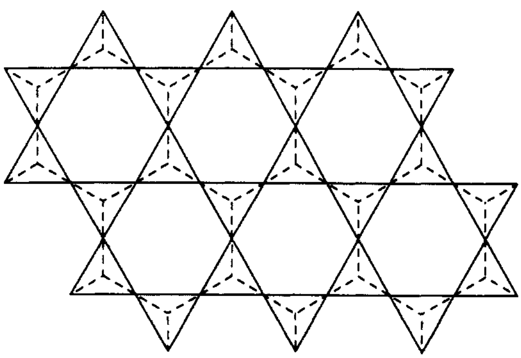

Figure 1. The Kagomé lattice (full lines) and the associated honeycomb lattice (broken lines).

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where $\beta = 1/kT$, the first summation is taken over all spins $s_i = \pm 1$, $i = 1, 2, \ldots, N$, the second summation over all nearest-neighbour pairs, and the third summation over the three spins surrounding each triangular face of the lattice. Thus, the Boltzmann factor of a triangular face is

$$\omega(s, s', s'') = \exp[\tfrac{1}{2}L(s + s' + s'') + K(ss' + s's'' + s''s) + Mss's''] \qquad (2)$$

and the partition function can be written as

$$Z(L, K, M) = \sum_{s_i = \pm 1} \prod_{\Delta} \omega(s, s', s''). \qquad (3)$$

The Kagomé lattice is the covering lattice of a honeycomb lattice, a situation shown in figure 1. Here, every spin of the Kagomé lattice resides on one edge of the honeycomb lattice. If we regard the spin variable $s = 1$ as implying that the edge on which the spin s resides is empty, and $s = -1$ as implying that the edge is covered by a bond, then the partition function (3) describes precisely an eight-vertex model on the honeycomb lattice [4] with the following vertex weights:

$$\begin{aligned} a &= \omega(1, 1, 1) = \exp(\tfrac{3}{2}L + 3K + M) \\ b &= \omega(1, 1, -1) = \omega(, -1, 1) = \omega(-1, 1, 1) = \exp(\tfrac{1}{2}L - K - M) \\ c &= \omega(, 1-1, -1) = \omega(-1, 1, -1) = \omega(-1, -1, 1) = \exp(-\tfrac{1}{2}L - K + M) \\ d &= \omega(-1, -1, -1) = \exp(-\tfrac{3}{2}L + 3K - M). \end{aligned} \qquad (4)$$

Now, the eight-vertex model on the honeycomb lattice is completely equivalent to an Ising model in an external magnetic field L_I and with a nearest-neighbour interaction K_I [4, 5]. The equivalent interaction K_I is given by† [4, 5]

$$\begin{aligned} \exp(4K_I) &= 1 + \Delta/(bd - c^2 + ac - b^2)^2 \\ &= 1 + \frac{u^2[4vw^4 + (v^{-2} - 6 - 3v^2)w^2 + 4v]}{[(u^2 - v)w^2 + 1 - u^2 v]^2} \end{aligned} \qquad (5)$$

where

$$\begin{aligned} &\Delta = (ad - bc)^2 - 4(bd - c^2)(ac - b^2) \\ &u = e^{-L} \qquad v = e^{-4K} \qquad w = e^{-2M}. \end{aligned} \qquad (6)$$

An explicit expression of the reduced magnetic field L_I has been given in [5]. Particularly, the trajectory $L_I = 0$ is, upon using (4),

$$\begin{aligned} 0 &= a(b^3 + d^3) - d(a^3 + c^3) + 3(ab + bc + cd)(c^2 - bd - b^2 + ac) \\ &= v^2w^2 + 3v^2(1 + u^2v + u^4)[1 + u^2v - (u^2 + v)w^2] + u^6(w^2 - v^3) - 1. \end{aligned} \qquad (7)$$

Thus, the Ising model (1) is transformed into one without three-spin interactions.

For $\Delta > 0$ or, equivalently,

$$\cosh 2M > (3v^4 + 6v^2 - 1)/8v^3 \qquad (8)$$

† More precisely, $\exp(2K_I)$ is given by equation (25) of [5], where the sign on the RHS of (25) is chosen so as to make $\exp(2K_I) > 0$, subject to the condition (32) of [5]. In the present case, it can be shown that the condition (32) of [5] is always satisfied along the critical surface (7), $K_I > K_c$, so we can, instead, use (5) for $\exp(4K_I)$.

which is satisfied when the nearest-neighbour interaction K is ferromagnetic†, we have $K_I > 0$ so that the equivalent Ising model is ferromagnetic. In this case it is known that the Ising free energy is singular only at $L_I = 0$, the locus (7), for

$$\exp(2K_I) \geqslant \exp(2K_c^{HC}) \equiv 2+\sqrt{3}. \tag{9}$$

Thus (7) in the regime (9) gives rise to a critical surface across which the Ising model exhibits a first-order transition and along which there is a non-zero spontaneous magnetisation. This critical surface is shown in figure 2.

Conversely, the above critical surface occurs only for $K > 0$. To see this, we eliminate w between (5) and (7) to obtain

$$\exp(2K_I) = \frac{(u^2+v)(u^2v+1)}{v(u^4+2u^2v+1)} \geqslant 2+\sqrt{3} \tag{10}$$

where the last inequality follows from (9). Since u^2 is positive, the inequality (10) then implies

$$v = \exp(-4K) \leqslant \exp(-4K_c^{Kag}) \equiv (3+2\sqrt{2})^{-1} < 1 \tag{11}$$

hence $K > 0$. The regime (10) is the projection of the critical surface (7) onto the (u, v) plane; the broken curve in figure 2.

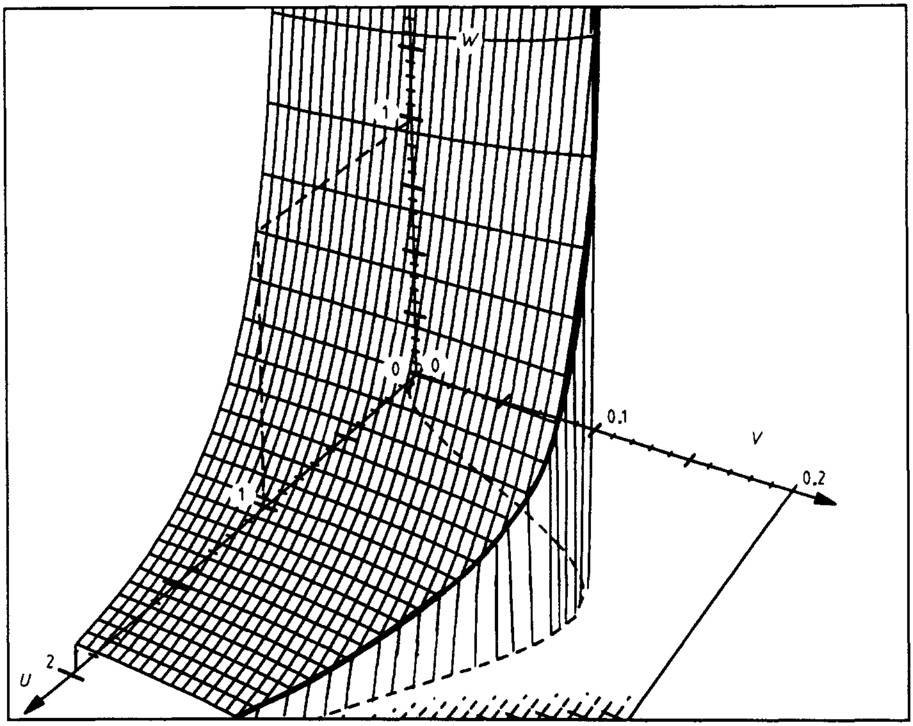

Figure 2. The phase diagram of the Kagomé Ising model. The shaded surface denotes a first-order surface $L_I = 0$, $K_I > K_c$, which terminates on the critical line $L_I = 0$, $K_I = K_c$ (the full line). The critical surface contains the line segment $u = 1$, $w = 1$, $v < (3+2\sqrt{3})^{-1} = 0.1547$, the critical line for pure pair interactions.

† Since the RHS of (8) is less than 1 for $0 < v < 1$.

For $\Delta<0$ we have $K_1<0$, which is possible only when $K<0$, and L_1 is pure imaginary [4]. In this case there exists no rigorous result on the critical behaviour of the equivalent Ising model. However, we have found numerical evidence that the correlation length does not diverge. We therefore conjecture that the free energy of the Ising model is actually analytic in this regime. This implies that the only singularity of the Kagomé Ising free energy is that of the first-order surface (7) shown in figure 2. The phase diagram in the $(T, L/K, M/K)$ space is similar and is not shown.

The preceding results also lead to the determination of exact results for a lattice gas with pair and triplet interactions. Again, we consider the Kagomé lattice. It is well known that an Ising model is equivalent to a lattice gas [6], an equivalence which is effected by introducing

$$s_i = 2n_i - 1 \tag{12}$$

where $n_i = 0, 1$ is the occupation number of the lattice site. The partition function (3) then becomes

$$Z(L, K, M) = \exp[N(-L+2K-2M/3)]\Xi(z, J, J_3) \tag{13}$$

which is the grand partition function of the Kagomé lattice gas with reduced nearest-neighbour interactions $-J=4(M-K)$, three-site interactions $-J_3=-8M$ and the fugacity $z=\exp(4M-8K+2L)$. For this lattice gas the equation of state is

$$\frac{p}{kT}=\frac{1}{N}\ln \Xi(z, J, J_3) \tag{14}$$

where p is the pressure, T the temperature, and the fugacity z is to be eliminated from the expression of the density

$$\rho = z\frac{\partial}{\partial z}\left(\frac{p}{kT}\right). \tag{15}$$

Along $L_1=0$, namely (7), we use (13), (3), the known free energy for the zero-field honeycomb Ising model [7] (see also equation (131) of [8]), and (14) of [5], to specialise (14) as

$$\begin{aligned}\frac{p}{KT} &= \tfrac{2}{3}\ln \tilde{a} - \tfrac{1}{6}\ln 2 - \ln\cosh K_I + \frac{1}{24\pi^2}\int_0^{2\pi} \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi \\ &\quad \times \ln\{1+\cosh^3(2K_I) - \sinh^2(2K_1)[\cos\theta + \cos\phi + \cos(\theta+\phi)\}\end{aligned} \tag{16}$$

where $\tilde{a}$ is a function of a, b, c, d given by (10) and (20) of [5]. Along the critical surface of $L_I=0$, $K_I>K_c$, the expression (15) for ρ splits into two branches ρ_l and ρ_g, where ρ_l and ρ_g are the respective densities of the liquid and gas phases, corresponding to the spontaneous magnetisation I_0 being taken to be positive or negative [6]. Thus, (15) and (16) give rise to a parametric equation for the boundary of the two-phase region. We have computed this phase boundary numerically using the following explicit expression for I_0 [9]:

$$I_0=\left(1-\frac{16\exp(-6K_I)[1+\exp(-6K_I)]}{[1-\exp(-2K_I)]^3[1-\exp(-4K_I)]^3}\right)^{1/8}. \tag{17}$$

This result is plotted in figure 3 for two values of $J_3=0$ and $J_3=0.2\,J$.

In summary, we have considered the Ising model on the Kagomé lattice with two- and three-spin interactions, and obtained its exact phase boundary. We have also considered a Kagomé lattice gas with pair and triplet interactions, and obtained its exact boundary of the two-phase region.

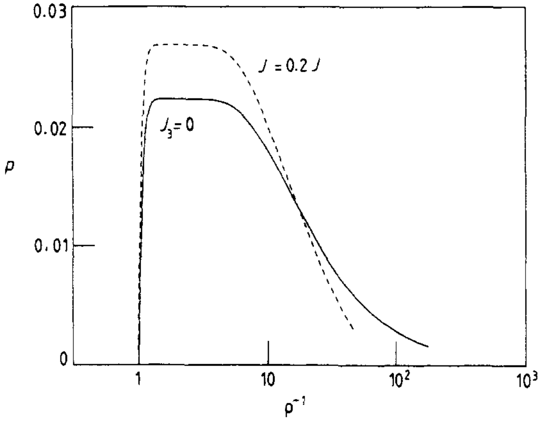

Figure 3. The exact boundary of the two-phase region of the Kagomé lattice gas for $J_3 = 0$ and $J_3 = 0.2J$. p is in units of kTJ.

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