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Ising model with antiferromagnetic next-nearest-neighbor coupling. V. Mean-field model and disorder points*

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A detailed account is given of the calculation of disorder points within the mean-field model on a variety of one-, two-, and three-dimensional Ising lattices. Comparison with exact solutions is made when feasible, and the limitations of the approximate method discussed.

I. INTRODUCTION

When a competing antiferromagnetic next-nearest-neighbor interaction is present in an Ising model, the pair correlation function may become oscillatory at high temperatures, above a precisely located temperature T_D, the disorder point. For soluble models in one and two dimensions,[1-3] the dependence of the disorder point on the relative strengths of the nearest-neighbor (nn) and next-nearest-neighbor (nnn) interactions may be determined explicitly. In three dimensions, where no exact solutions are available, we may resort to models, such as the mean-field model and the Bethe model which approximate the Ising model at high temperatures. The "mean-field" approximation has been used by Enting[4] to estimate disorder points for the spin-phonon interaction model of a compressible Ising magnet, as developed by Bolton and Lee.[5] Previously, as reported briefly elsewhere, the same approximate method has been used by the present author to estimate disorder points on Ising lattices.[6]

It is the purpose of the present paper to give details of the calculation of disorder points for the mean-field model on a variety of lattices in one, two, and three dimensions. We begin with the definition of a disorder point, and outline its calculation from the poles of the Fourier transform of the pair correlation function with special reference to the mean-field model. In the main body of the paper, we give details of the calculation (and methods) for a variety of Ising lattices, Secs. IV–VIII. A summary of our results is contained essentially in Table I.

II. DEFINITION AND CALCULATION OF THE DISORDER POINT

In the situation where the nn interaction determines the ground state, but a competing antiferromagnetic nnn interaction is present, pair correlations along a nnn axis will be antiferromagnetic at sufficiently high temperatures, and ferromagnetic at sufficiently low temperatures. Let $T_0(\vec{r})$ be the lowest temperature at which the pair correlation $\Gamma(\vec{r})$ vanishes. Then the disorder point is the large spin separation limit of $T_0(\vec{r})$. Explicitly,

$$T_D = \lim_{|\vec{r}|\to\infty} \inf\{T_0(\vec{r})\}\,. \tag{2.1}$$

To locate T_D, we observe that in the disordered phase the decay of pair correlations with increasing spin separation is dominated by an exponential factor $e^{-\kappa r}$, where κ is the reciprocal range of order. Following Fisher and Burford,[7] we may determine κ in a direction $\vec{e}$ (unit vector) by

$$\kappa = |\operatorname{Im} q(\vec{e}, T)|\,, \tag{2.2}$$

where $q\vec{e}$ is the solution of

$$1/\chi(\vec{q}, T) = 0\,, \tag{2.3}$$

which lies closest to the real axis. That is, q is located via the poles of the relative magnetic scattering intensity χ, which, in turn, is equal to the Fourier transform of the pair correlation function $\Gamma(\vec{r})$. When q is pure imaginary, the pair correlation decays monotonically, as in normal Ornstein-Zernike theory. But if q has a nonzero real part, an oscillatory factor modifies the exponential decay. The disorder point is located by the temperature at which q leaves the imaginary axis and acquires a nonzero real part. At higher temperatures q is complex, and the correlation decay is oscillatory exponential in appropriate directions $\vec{e}$.

For any fixed direction $\vec{e}$, the lowest temperature at which q acquires a nonzero real part will be denoted by T_1. The lowest value of T_1 over all directions, is equal to T_D.

III. MEAN-FIELD MODEL

The mean-field model can be derived as an approximation to the spin-$\frac{1}{2}$ Ising model, or to the Heisenberg model, or can be considered as a model with "weak long-range" interactions in its own right. The relevant scattering intensity, calculated via the Fourier transform of the pair correlation function,[4] is given by

$$1/\chi(\vec{q}, T) = 1 - \hat{K}(\vec{q}) , \tag{3.1}$$

where $\hat{K}(\vec{q})$ is the lattice Fourier transform of

$$K(\vec{r}) = J(\vec{r})/k_B T , \tag{3.2}$$

$J(\vec{r})$ being the interaction energy between spins separated by a lattice vector $\vec{r}$. To first order in $1/T$, this is in exact agreement with the Ising model expression for $\chi(\vec{q}, T)$. It is straightforward to calculate $\hat{K}(\vec{q})$ for various lattices, and the required formulas have already been listed in Table III of the preceding paper.[8] By solving the equation $1/\chi = 0$ for specific lattice directions $\vec{e}$, we can derive mean-field values for T_1 and hence for T_D.

We note here that it is convenient to use the variable

$$\rho \equiv q_2 J_2 / q_1 |J_1| , \tag{3.3}$$

q_1, q_2 being coordination numbers for nn and nnn bonds, and that the mean-field value of the critical temperature is given by

$$k_B T/q_1 |J_1| = 1 + \rho . \tag{3.4}$$

Throughout our discussion, ρ is negative, and J_2 is antiferromagnetic:

$$\rho_c < \rho < 0 , \tag{3.5}$$

where ρ_c is the critical ratio above which the nn interaction determines the ground state. For cubic lattices the critical value of ρ is $-\frac{1}{2}$.[9]

IV. SIMPLE CUBIC LATTICE, sc(1,2)

A. [100] direction

Along a cube axis, we may set $\vec{e} = \vec{i}$ (x axis) with projection factor f equal to unity.[7] The nearest-neighbor distance a_1 is equal to the cube side a. The reciprocal scattering intensity is then

$$1/\chi = 1 - [4(K_1 + K_2) + 2(K_1 + 4K_2) \cos fqa] \tag{4.1}$$

and vanishes when

$$\cos fqa = [(3/q_1 K_1) - 2 - \rho]/(1 + 2\rho) . \tag{4.2}$$

At the critical temperature T_c, the cosine is unity, and at high temperatures remains real, and is greater than unity, so q is pure imaginary. In this direction $T_1 = \infty$. Clearly ρ must be restricted to the range $\rho > -\frac{1}{2}$, which it must in any case if the nn interaction is to determine the ground state.

B. [110] direction

Next, along a cube face diagonal $\vec{e} = (\vec{i} + \vec{j})/\sqrt{2}$, which is a nnn axis (in the x-y plane), we expect the pair correlation to oscillate in sign at sufficiently high temperatures. Also $f^2 = \frac{1}{2}$. Now

$$1/\chi = 1 - [2(K_1 + K_2) + 4(K_1 + 2K_2) \cos fqa + 2K_2 \cos 2fqa] \tag{4.3}$$

and vanishes when

$$\cos fqa = [-(1+\rho) \pm |\Delta|]/\rho , \tag{4.4}$$

with the discriminant Δ given by

$$\Delta^2 = 1 + \rho + \rho^2 + (3\rho/q_1 K_1) . \tag{4.5}$$

The + sign is needed here. The cosine is unity at T_c and increases with temperature until the discriminant becomes negative. This occurs at a temperature

$$k_B T_1/J_1 = (-2/\rho)(1 + \rho + \rho^2) \sim -2/\rho \quad \text{at small } \rho . \tag{4.6}$$

It is trivial to verify that $T_1 > T_c$, since

$$k_B(T_1 - T_c)/J_1 = (-2/\rho)(1 + 2\rho)^2 > 0 . \tag{4.7}$$

Also, at T_1, $\cos fqa = -(1+\rho)/\rho$, which is ≥ 1 when $-\frac{1}{2} \leq \rho < 0$. T_1 equals T_c when $\rho = -\frac{1}{2}$, and increases with ρ in the range $-\frac{1}{2} \leq \rho < 0$. Pair correlations in the [110] direction above T_1 will be oscillatory. The dependence of T_1 on the interaction ratio is graphed in Fig. 1.

C. [111] direction

Now along a cube body diagonal, connecting third-nearest-neighbor lattice sites, $\vec{e} = (\vec{i} + \vec{j} + \vec{k})/\sqrt{3}$, and $f^2 = \frac{1}{3}$:

$$1/\chi = 1 - [6K_2 + 6K_1 \cos fqa + 6K_2 \cos 2fqa] , \tag{4.8}$$

which vanishes when

$$\cos fqa = (-1 \pm |\Delta|)/2\rho , \tag{4.9}$$

with

$$\Delta^2 = 1 + (4\rho/q_1 K_1) , \tag{4.10}$$

and again the "+" sign is needed. At T_c the cosine is unity, and increases with temperature until the discriminant becomes negative. This occurs at a temperature which will be our best candidate for the disorder point T_D:

$$k_B T_D/J_1 = -3/2\rho . \tag{4.11}$$

It is trivial to verify that $T_1 > T_D > T_c$:

$$\begin{aligned} k_B(T_1 - T_D)/J_1 &= (-1/2\rho)(1 + 2\rho)^2 > 0 , \\ k_B(T_D - T_c)/J_1 &= (-3/2\rho)(1 + 2\rho)^2 > 0 . \end{aligned} \tag{4.12}$$

T_1, T_D, and T_c are all equal when $\rho = -\frac{1}{2}$, and increase with ρ in the range $-\frac{1}{2} \leq \rho < 0$. At T_D, $\cos fqa = -1/2\rho$ which is ≥ 1 when $-\frac{1}{2} \leq \rho < 0$.

We should mention here that on all the other

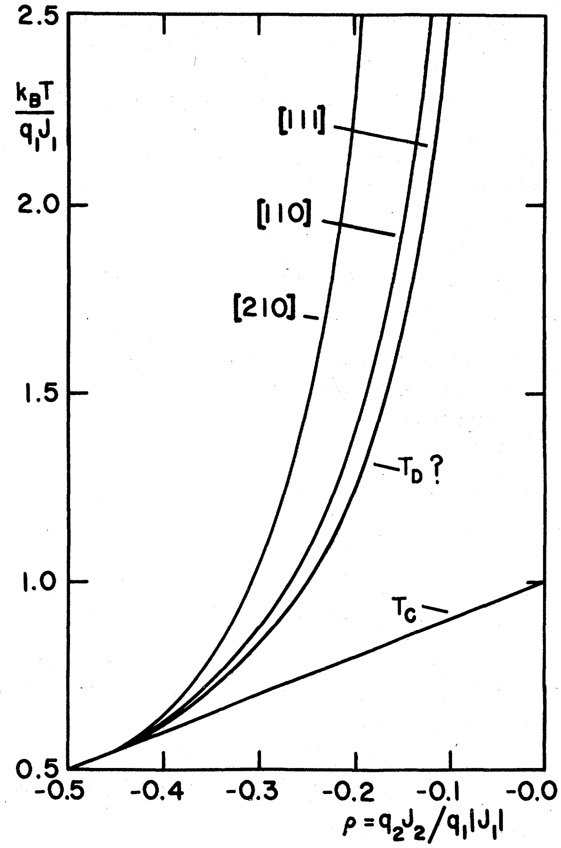

FIG. 1. Graphs of disorder-point estimates for the [111], [110], and [210] directions of the simple cubic lattice sc(1, 2), against interaction ratio ρ.

lattices considered, the most likely candidate for the disorder point comes from analysis of χ along the nnn axis. The simple cubic lattice is an exception, in that a better candidate comes from the third-nearest-neighbor axis. Spins in the [111] direction can be connected by a chain of alternate J_1 and J_2 bonds, and the leading term in the pair correlation contains a factor $(J_1J_2)^n$, so the correlation oscillates at sufficiently high temperatures. (Here $n=|\vec{r}|/\sqrt{3}a$.) We should investigate all other lattice directions in order to find out which one yields the lowest temperature T_1. This general problem will not be tackled here. Instead we consider just one more direction in order to illustrate techniques applicable to equations of cubic and higher degree.

D. [210] direction

In the [210] direction, the leading term in the pair correlation function again contains an oscillatory factor $(J_1J_2)^n$. Now $\vec{e}=(2\vec{i}+\vec{j})/\sqrt{5}$ and $f^2=\frac{1}{5}$:

$$1/\chi = 1-[2K_1(1+\cos fqa+\cos 2fqa) + 2K_2(3\cos fqa+2\cos 2fqa+\cos 3fqa)]. \tag{4.13}$$

The values of $\cos fqa$ at which $1/\chi$ vanishes satisfy a cubic equation. If we set

$$x=2\cos fqa \quad \text{and} \quad \mu = 1/\rho, \tag{4.14}$$

then the cubic for x is

$$1/K_2 = x^3+2(1+\mu)x^2+2\mu x-4. \tag{4.15}$$

The condition for a double root, at which a pair of real roots coalesce in order to change over to a complex pair, can easily be extracted via the standard form for a cubic

$$y^3+py+q=0, \tag{4.16}$$

with discriminant

$$4p^3+27q^2. \tag{4.17}$$

Equating this discriminant to zero yields the desired expression for T_1:

$$k_BT_1/J_1 = (2/27\mu)(4\mu^3+3\mu^2+3\mu-23-|\Delta|), \tag{4.18}$$

with

$$\Delta^2 = 2(2\mu^2+\mu+2)^3. \tag{4.19}$$

This expression for T_1 is plotted in Fig. 1 as a function of ρ. When $\rho=-\frac{1}{2}$, T_1 and T_c are equal.

For small ρ, T_1 has a quadratic dependence on $1/\rho$,

$$k_BT_1/J_1 \sim 16/27\rho^2. \tag{4.20}$$

This result may be obtained from an approximate treatment of the cubic equation, using a technique which is also applicable to higher-degree equations. To find the dependence of T_1 on the interaction ratio ρ, when ρ is very small, we seek the large-x solution of the equation which determines the condition for a double root. Differentiating the right-hand side of (4.15), equating the result to zero, and retaining leading terms of order x^2 and μx, one gets $x\sim(-\frac{4}{3}\mu)$. Resubstitution in (4.15), again keeping only leading terms, yields (4.20).

E. Results for simple cubic lattice

The temperatures above which pair correlations in the [110], [111], and [210] directions become oscillatory are plotted against ρ in Fig. 1, with the [111] direction yielding the estimate for T_D. At small nnn interaction strengths, T_D is large, and we surmise that the asymptotic form

$$k_BT_D/J_1 \sim -3/2\rho \tag{4.21}$$

will be in exact agreement with the (unknown) Ising-model value. Similarly, for small ρ along the [110] direction, $k_B T_1/J_1 \sim -2/\rho$.

V. SOME OTHER THREE-DIMENSIONAL LATTICES

We shall limit our discussion of other three- (and also two-) dimensional lattices to points of interest pertinent to the specific lattice and directions under consideration. The relevant formulas for $1/\chi$ can easily be obtained via (3.1), taking $\hat{K}(\vec{q})$ from Table III of the preceding paper.[8] A summary of disorder point estimates is presented in Table I.

A. Body-centered-cubic lattice, bcc(1,2)

The disorder-point estimate comes from the [100] nnn direction. Equating to zero the discriminant of the quadratic equation for $\cos f q a_1$, we obtain

$$k_B T_D/J_1 = (-3/\rho)\,(1-\tfrac{8}{9}\rho^2)\,. \tag{5.1}$$

Pair correlations in the [110] and [111] directions are ferromagnetic for all $T > T_c$. In the [110] direction the leading terms in the pair correlation function are like K_1^{2n} and K_2^{2n}, which are always positive. In the [111] direction the discriminant of the relevant cubic for $\cos f q a_1$ can vanish, but does so at a temperature which lies below T_c when ρ is in the physical range $-\frac{1}{2} \leq \rho < 0$. In the [311] direction the leading term in the pair correlation contains a factor $(J_1 J_2)^n$, and there will be an estimate T_1 for the disorder point. Analysis of the relevant sextic shows that $T_1 \gg T_D$.

B. Face-centered-cubic lattice, fcc(1,2)

The disorder-point estimate comes from the [100] nnn direction, and is

$$k_B T_D/J_1 = (-2/\rho)\,(1-2\rho-2\rho^2)\,. \tag{5.2}$$

There are no disorder-point estimates from the [110] and [111] directions. In the [310] direction the high-temperature form of the pair correlation function contains an oscillatory factor $(J_1 J_2)^n$. The disorder-point estimate, obtained by treating the sextic for $\cos f q a_1$ by the approximate method of Sec. IV D, is

$$k_B T_1/J_1 \sim 1/27\rho^2 \tag{5.3}$$

for small ρ, which is larger than T_D.

C. Face-centered-cubic lattice as body-centered-cubic lattice plus simple quadratic layers

This lattice is of interest in connection with the problem of antiferromagnetism in the fcc lattice.[9] A bcc lattice with interaction J_1 is augmented by simple quadratic layers of nnn bonds with interaction J_2. The extra bonds are those sides of the basic cubic lattice which lie parallel to the x-y plane. This lattice can be expanded parallel to the z axis to become a regular fcc lattice, without altering the disorder point estimate. We treat the bcc lattice as regular and periodic with cube side a. The nn bond has length $a_1 = (\frac{1}{2}\sqrt{3})\,a$, and the nnn quadratic layer bonds have length a. The coordination numbers are $q_1 = 8$ and $q_2 = 4$. The disorder-point estimate comes from the [100] nnn direction, in which the discriminant of the quadratic for $\cos f q a_1$ vanishes when

$$k_B T_D/J_1 = -2/\rho\,. \tag{5.4}$$

A higher estimate is obtained from the [210] direction, with $T_1 \sim -1/\rho^3 \gg T_D$ for small ρ.

VI. SOME TWO-DIMENSIONAL LATTICES

A. Simple quadratic lattice, sq(1,2)

The disorder-point estimate for this unsolved two-dimensional lattice comes from the [11] nnn direction, and is

$$k_B T_D/J_1 = -1/\rho\,. \tag{6.1}$$

Another estimate from the [21] direction comes from solving a cubic for $\cos f q a_1$ (Table I). Graphs of these T_D estimates are presented in Fig. 2.

B. Triangular lattice, t(1,2)

We orient the lattice relative to Cartesian axes as in Fig. 4(d) of the preceding paper.[8] From the nnn axis, $\vec{e} = \vec{j}$ (y axis) we obtain the disorder-point estimate

$$k_B T_D/J_1 = (-1/\rho)\,(1+3\rho^2)\,. \tag{6.2}$$

When $\rho = -\frac{1}{3}$, T_c and T_D are equal, and this expression for T_D is valid only for $-\frac{1}{3} < \rho < 0$, even though $\rho_c = -\frac{1}{2}$ for the Ising model. Along the nn axis, $\vec{e} = \vec{i}$ (x axis) the discriminant of the cubic for $\cos\frac{1}{2} q a_1$ vanishes at a temperature T_1 which satisfies $T_1 > T_D > T_c$ in the range $-\frac{1}{3} < \rho < 0$, with equality holding when $\rho = -\frac{1}{3}$.

C. Union-jack lattice

Now we turn to some soluble one- and two-dimensional models, for which the disorder point may be located exactly. This will serve as a test for the validity of the mean-field-theory results when J_2 is small and T_D is at a high temperature.

By inspection of the lattice, Fig. 4(e) of the preceding paper, we see that nnn bonds spread out only from alternate lattice sites. Accordingly we take the mean-field calculation for sq (1, 2) and replace J_2 by $\frac{1}{2}J_2$ everywhere to obtain the cor-

TABLE I. Mean-field values of T_D and T_1.[a]

Lattice	Direction	$1/K_1$ at T_D or T_1	Comments
lc(1, 2)	Along chain	$(-1/4\rho)(1+8\rho^2)$	Asymptotically equal to exact T_D for small ρ
lca(1, 2)	Along chain	$(-1/4\rho)(1+8\rho^2)$	Disagrees with exact T_D for small ρ
sq(1, 2)	nn axis, sq edge [10]	∞	Ferromagnetic short-range order
	nnn axis, sq diagonal [11]	$-1/\rho$	T_D
	[21] direction	$(2\mu^3-9\mu^2-36\mu-2\lvert\Delta\rvert)/27\mu$, $\Delta^2=(\mu^2-3\mu+6)^3$, $\mu=1/\rho$	$k_B T_1/J_1 \sim 4/27\rho^2$, ρ small
h(1, 2)	nn direction	∞	Ferromagnetic short-range order
	nnn direction	$(1/2\rho)(1+3\rho^2)$	T_D
t(1, 2)	nn axis	$1/27\rho^2-2/3\rho+1-2\rho$	T_1
	nnn axis	$(-1/\rho)(1+3\rho^2)$	T_D
sc(1, 2)	nn axis, cube edge [100]	∞	Ferromagnetic short-range order
	nnn axis, face diagonal [110]	$(-2/\rho)(1+\rho+\rho^2)$	T_1
	third-nn axis, body diagonal [111]	$-3/2\rho$	T_D
	[210] direction	$2(4\mu^3+3\mu^2+3\mu-23-\lvert\Delta\rvert)/27\mu$, $\Delta^2=2(2\mu^3+\mu+2)^3$, $\mu=1/\rho$	$k_B T_1/J_1 \sim 16/27\rho^2$, ρ small
bcc(1, 2)	nnn axis, cube edge [100]	$(-3/\rho)(1-\frac{8}{9}\rho^2)$	T_D, [110] and [111] ferromagnetic short-range order
fcc(1, 2)	nnn axis, cube edge [100]	$(-2/\rho)(1-2\rho-2\rho^2)$	
d(1, 2)	nnn axis, cube edge [100]	$(-3/4\rho)(1+\frac{16}{9}\rho^2)$	T_D
Triangular lattice or sq plus one set of nnn bonds	nnn axis, sq diagonal	$(-1/2\rho)(1+8\rho^2)$	Asymptotically equal to exact T_D for small ρ. Sq edge and diagonal: ferromagnetic short-range order
union-jack	nnn axis, sq diagonal	$-1/\rho$, same as sq(1, 2)	Asymptotically equal to exact T_D for small ρ
fcc as bcc plus sq layers	nnn axis, sq edges [100]	$-2/\rho$	T_D

[a] Results for the honeycomb h(1, 2) and diamond d(1, 2) lattices are included in the table. Results for only some of the lattice directions considered in the text have been entered in the table.

responding result for the union-jack lattice.

$$k_B T_D/J_1 = -1/\rho \,, \tag{6.3}$$

with $q_1 = 4$ and $q_2 = 2$ (average coordination number). This can be compared with the exact result[3]

$$\tanh 2K_2 + (\tanh 2K_1)^2 = 0 \,, \tag{6.4}$$

which at high temperatures, for small J_2, takes the form

$$2K_2 + 4K_1^2 \sim 0 \,, \tag{6.5}$$

whence the validity of (6.3) for small J_2 is confirmed.

D. Triangular lattice

The exactly soluble Ising triangular lattice may be regarded as a nn square lattice with interaction J_1, plus a single set of diagonal bonds J_2. Figures 4(d) and 4(f) of the preceding paper illustrate the triangular lattice in its regular triangular form and in the distorted square lattice form. The form of χ depends on the shape of the lattice. The disorder-point estimate is the same for both forms

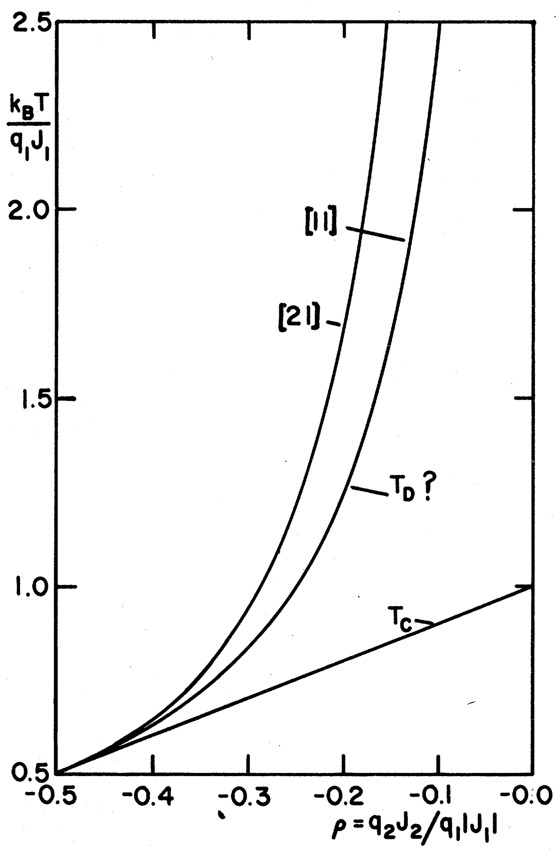

FIG. 2. Graphs of disorder-point estimates for the [11] and [21] directions of the simple quadratic (square) lattice sq(1, 2), against interaction ratio ρ.

of the triangular lattice, since it depends only on the connectivity of the lattice and not on its geometrical shape. In the nnn directions we obtain (different) quadratic equations for $\cos f q a_1$ (and different f values), but the condition that the discriminants vanish yields the *same* estimate for the disorder point:

$$k_B T_D/J_1 = (-1/2\rho)(1 + 8\rho^2) \,. \tag{6.6}$$

Along nn directions, correlations are ferromagnetic.

For the general triangular lattice (in triangular shape) with three interactions J_1, J_2, and J_3 along the three lattice axes, one readily obtains, parallel to the J_3 direction,

$$1/\chi = 1 - [2(K_1 + K_2)\cos q a_1 + 2K_3 \cos 2 q a_1] \,, \tag{6.7}$$

which reduces correctly on equating appropriate pairs of interactions to J_1, and calling the remaining interaction J_2. In general, if J_3 is the antiferromagnetic interaction, then the disorder point is given by the vanishing of the discriminant, so that

$$(K_1 + K_2)^2 + 4K_3(1 + 2K_3) = 0 \,. \tag{6.8}$$

When J_3 is small, (6.8) becomes

$$-K_3 \sim \tfrac{1}{4}(K_1 + K_2)^2 \,. \tag{6.9}$$

This should be compared with the exact result[2,3]

$$\tanh K_1 \tanh K_2 + \tanh K_3 = 0 \,, \tag{6.10}$$

which for small J_3 at high temperatures takes the form

$$-K_3 \sim K_1 K_2 \,, \tag{6.11}$$

which differs from the mean-field result (6.9). This is an unsatisfactory property of the mean-field model.

VII. ONE-DIMENSIONAL LATTICES

A. lc(1,2), mean-field formula for χ

For the linear chain with all nnn interactions, lc (1, 2), Fig. 4(a), Ref. 8,

$$1/\chi = 1 - [2K_1 \cos q a + 2K_2 \cos 2 q a] \,, \tag{7.1}$$

with $\vec{e} = \vec{i}$, parallel to the chain along the x axis. The disorder point is at

$$k_B T_D/J_1 = (-1/4\rho)(1 + 8\rho^2) \,, \tag{7.2}$$

with $\rho > -\frac{1}{4}$ so $T_D > T_c$. For small ρ,

$$k_B T_D/J_1 \sim -1/4\rho \,, \tag{7.3}$$

in agreement with the high-temperature small-ρ form of the exact formula locating T_D,[3,10]

$$\tanh K_2 + (\tanh \tfrac{1}{2} K_1)^2 = 0 \,. \tag{7.4}$$

It is of interest to note that the mean-field model is also an approximation to the Heisenberg model. In one dimension, the classical spin (Heisenberg) model undergoes a change in the nature of its ground state at precisely the ratio $\rho_c = -\frac{1}{4}$. For $\rho_c < \rho < 0$, spin correlations show a "spiral" structure.[11] A similar behavior occurs for the Heisenberg chain with antiferromagnetic nnn interactions, with apparently the same critical value for ρ_c.[11,12]

B. lca(1,2), mean-field formula for χ

For the linear chain with alternate nnn interactions, Fig. 4(b), Ref. 8, we replace J_2 by $\frac{1}{2}J_2$ in all the formulas for lc(1, 2), and use an average coordination number $q_2 = 1$, so for small ρ,

$$k_B T_D/J_1 \sim -1/4\rho . \tag{7.5}$$

This is now in disagreement with the high-temperature small-ρ form of the exact formula for T_D

$$\tanh K_2 + (\tanh K_1)^2 = 0 . \tag{7.6}$$

The cause of this discrepancy is discussed below.

C. Exact and approximate formulas for χ

The exact expression for the Fourier transform of the pair correlation function for these one-dimensional models takes the form[8,13]

$$\chi = N/D . \tag{7.7}$$

In the case of the lca(1, 2), the numerator contains terms in $1/T$, whereas for lc(1, 2) the first temperature-dependent term is of order $(1/T)^2$. The reciprocal range of order and the disorder point can be extracted *correctly* from the requirement that the denominator vanish, to give χ a simple pole. But, in the mean-field model, all terms in $1/T$ are collected together in the denominator, so setting $1/\chi = 0$ gives a wrong result for the lca(1, 2). Of course, to order $1/T$, there is agreement between the expansions of χ from the mean-field and the exact formulas.

D. lca(1,2), exact formula for χ

Reference to the preceding paper[8] shows that the exact denominator for χ is, putting $a = 1$,

$$D = 1 - 2x \cos 2q + x^2 , \tag{7.8}$$

where

$$x = \frac{\cosh 2K_1 - e^{-2K_2}}{\cosh 2K_1 + e^{-2K_2}} , \tag{7.9}$$

so the solution of $1/\chi = 0$ is

$$\cos 2q = \tfrac{1}{2}(x + x^{-1}) \quad \text{or} \quad x = e^{2iq} . \tag{7.10}$$

The reciprocal range of order is now

$$\kappa = -iq = -\tfrac{1}{2}\ln|x| , \tag{7.11}$$

as derived previously from direct inspection of the correlation decay.[10] Expansion of the numerator to order $1/T$ yields

$$N \sim 1 + 2K_1 \cos q - K_2 \cos 2q , \tag{7.12}$$

On the other hand, expansion of χ to order $1/T$ yields

$$\chi \sim 1 + 2K_1 \cos q + K_2 \cos 2q + \cdots , \tag{7.13}$$

which is the same as one obtains from the mean-field expression.

E. lc(1,2), exact formula for χ

Again, reference to the preceding paper[8] shows that the exact denominator for χ is

$$D = (1 - 2x \cos q + x^2)(1 - 2y \cos q + y^2) , \tag{7.14}$$

with x and y defined as in (5.7), and (5.8) of Ref. 8:

$$x = \mu_+/\lambda_+ , \quad y = \mu_-/\lambda_+ . \tag{7.15}$$

Now χ has simple poles when

$$e^{iq} = x, \quad 1/x, \quad y, \quad \text{or} \quad 1/y . \tag{7.16}$$

The solution for q with the smallest imaginary part is then

$$q = i \ln(1/x) , \tag{7.17}$$

so the reciprocal range of order below T_D is[10]

$$\kappa = \ln(1/x) \tag{7.18}$$

as expected. Above T_D, x and y become complex, and $|x| = |y|$. We may set $\mu_\pm = \mu e^{\pm i\theta}$ so

$$q = i \ln(\lambda_+/\mu) + \theta . \tag{7.19}$$

q acquires a real part at T_D. In previously introduced notation,[8,10] we have

$$\tan\theta = |\Delta'|/(a - b) , \tag{7.20}$$

with θ (and Δ') vanishing at T_D.

The expansion of the numerator N in powers of $1/T$ contains no terms of first order, $1/T$. Therefore the denominator D and the mean-field expression for χ are in agreement to first order in $1/T$. Consequently, the mean-field disorder-point estimate is in agreement with the high-temperature small-ρ form of the exact result, as discussed earlier.

VIII. EFFECTS OF CHANGING THE SHAPE OF A LATTICE

The lattices discussed in this paper can be drawn in a variety of different shapes. For example, consider the triangular lattice of Sec. VID. Any reasonable formula for the disorder point must of course be unaltered by a change in the shape of a lattice, since disorder points, and critical points too, depend only on the connectivity and interactions within a lattice structure. On the other hand, χ can undergo changes in form when a lattice is distorted. The question arises as to how the poles of χ move, and how, nevertheless, the disorder-point estimates remain the same, under lattice distortion.

In general,

$$\chi(\vec{q}, T) = \sum_{\vec{r}} e^{i\vec{q}\cdot\vec{r}}\Gamma(\vec{r}) . \tag{8.1}$$

Now $\Gamma(\vec{r})$ can be expressed in such a way that the actual vector $\vec{r}$ is no longer explicitly involved, but only the connectivity of the lattice points is important. Suppose for a given wave vector $\vec{q} = q\vec{e}$ we alter all the lattice vectors $\vec{r}$ in such a way that

$$\vec{r} \to \vec{r} + \lambda(\vec{r})\vec{e}_\perp , \tag{8.2}$$

where $\lambda(\vec{r})$ depends on $\vec{r}$, but $\vec{e}_\perp$ is perpendicular to $\vec{e}$, so all the lattice displacements are perpendicular to the wave vector. Then $\vec{q}\cdot\vec{e}_\perp = 0$ and χ is unaltered by the lattice distortion for the particular wave vector $\vec{q}$ under consideration. In particular, estimates of T_D from the condition $1/\chi = 0$ in the direction $\vec{e}$ will be unchanged.

A. Linear chain, lc(1,2)

Referring to Fig. 4(a) of the preceding paper, we take $\vec{e} = \vec{i}$ parallel to the chain, and distort the chain in a perpendicular direction ($\vec{j}$). The projections of nn and nnn lattice vectors $\vec{a}_1$ and $\vec{a}_2$ onto $\vec{e}$ are unaltered, and χ is unchanged.

B. Triangular lattice

As discussed in Sec. VID, we wish to consider a distorted form of triangular lattice which is square in shape, as in Figs. 4(d) and 4(f) of the preceding paper. When $\vec{q}$ is parallel to a nnn diagonal axis with interaction J_2, we obtain the disorder point estimate of Sec. VID, (6.6). The distortion may be achieved by (relative) movement of all lattice sites in a direction perpendicular to $\vec{e}$, thereby altering the nn distances a_1 but keeping a_2 unchanged. χ is unaltered by this process (Table III, Ref. 8, entries under t, triangular lattice, in nnn directions). Similarly if $\vec{e}$ is perpendicular to a nnn lattice axis, then a distortion can again be made from square to triangular form. On the other hand, when $\vec{e}$ is parallel to the x axis, the expressions for χ differ (Table III, Ref. 8, entries under t, in nn directions with $\vec{e} = \vec{i}$).

C. Face-centered cubic

The face-centered-cubic lattice as a body-centered-cubic lattice plus simple quadratic (square) lattice layers has been discussed in Sec. VII. If the nn bcc distance is a_1, then the nnn sq lattice side is $a_2 = (2/\sqrt{3})a_1$. A distortion parallel to the z axis, $\vec{k}$ direction, converts the lattice to a regular fcc lattice with all bond lengths equal. All the bcc bonds of length a_1 are stretched by the *same* amount. The disorder-point estimates from directions of the wave vector lying in the x-y plane are unaffected by this lattice distortion.

IX. CONCLUSION

A summary of our disorder-point calculations is presented in Table I. The disorder point has been obtained by locating the temperature at which the reciprocal range of order becomes complex. For the mean-field model, the range of order is given by the zeros of $1/\chi$ in (3.1). Even though the mean-field-model expression for $1/\chi$ is in exact agreement with the Ising-model to order $1/T$, it does not necessarily follow that the zeros of $1/\chi$ are in such agreement. Therefore, the mean-field values of the disorder point are not necessarily in exact agreement with the Ising-model values when ρ has small negative values. However, fortuitous agreement is obtained for some exactly soluble Ising lattices, triangular, union-jack, and lc(1, 2), but not for the lca(1, 2), for reasons given in Sec. VII. It is to be hoped, therefore, that a more reliable way of estimating the small-ρ high-temperature behavior of T_D can be devised, possibly via a direct analysis of power series expansions for the correlation functions themselves.

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