Ferromagnetic Curie Temperature in Cubic Lattices with Next-Nearest-Neighbor Interaction

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The Curie temperature for a Heisenberg ferromagnet with nearest-neighbor interaction J_1 and next-nearest-neighbor interaction J_2 is calculated by a Green's-function technique. The J_2/J_1 dependence is found to be significantly different from that given by molecular field theory. The Curie temperature approaches zero when $J_2/J_1 \to -1$ in a face-centered cubic magnetic lattice, and when $J_2/J_1 \to 0.6799$ in a body-centered cubic lattice. The face-centered cubic magnetic lattice is relevant to the chalcogenides of europium.

1. INTRODUCTION

WHILE most of the present theories of ferromagnetism and antiferromagnetism are based on the assumption of the nearest-neighbor exchange interaction only, the recent studies[1,2] of the magnetic properties of the europium chalcogenides indicate that in addition to the nearest-neighbor exchange the next-nearest-neighbor interaction is also appreciable. This picture has now been analyzed in the spin-wave theory.[3] However, the spin-wave theory adequately describes the behavior of magnetic systems only in the limit of low temperatures. Close to the transition temperature, the spin-wave picture becomes inappropriate[4] and therefore other approximate theories, such as the Weiss molecular field theory and the various cluster theories, are usually employed. The results of these theories are at best qualitatively satisfactory while sometimes they can be quite misleading.[5] The most reliable estimates of the critical properties are, of course, those obtained by extrapolating the exact high-temperature series-expansion results to the transition region.[6,7] This, however, is a very tedious procedure and the only systems adequately analyzed so far are those including a single exchange parameter.[8]

Recently the Green's-function methods have been successfully applied to the study of the magnetic systems.[9,10] It is found that, in general, a simple "random phase" decoupling approximation (RPA) leads to acceptable results for the Curie temperatures for both ferro[10] and antiferromagnetic[5] systems, while more sophisticated approximations can also be devised to yield even better results.[11] The extension of the Green's-function methods to the study of situations including, in addition to the nearest-neighbor exchange, the second-neighbor exchange also is the subject of the present note.

2. FERROMAGNETIC CURIE TEMPERATURES

Let the N spins, in the presence of a z-directed spatially uniform field H, be coupled via isotropic exchange interaction of the Heisenberg type

$$\mathcal{H}=-\mu H\sum_f S_f^z-\sum_{f,g} J_1(f-g)\mathbf{S}_f\cdot\mathbf{S}_g -\sum_{f,g} J_2(f-g)\mathbf{S}_f\cdot\mathbf{S}_g, \quad (2.1)$$

where f and g denote lattice sites, μS is the magnetic moment per site, $J_1(f-g)$ and $J_2(f-g)$, respectively, denote the nearest- and the next-nearest exchange integrals:

$$\begin{aligned} J_1(f-g)&=J_1, \quad f \text{ and } g \text{ nearest neighbors},\\ J_2(f-g)&=J_2, \quad f \text{ and } g \text{ next-nearest neighbors},\\ &=0, \quad \text{otherwise}. \end{aligned} \quad (2.2)$$

Following the method of Tahir-Kheli and ter Haar,[10-12] where an RPA type decoupling is employed, the statistical average $\langle S^z\rangle$ is found to be

$$\langle S^z\rangle=\frac{(S-\Phi)(1+\Phi)^{2S+1}+(S+1+\Phi)\Phi^{2S+1}}{(1+\Phi)^{2S+1}-\Phi^{2S+1}}, \quad (2.3)$$

where

$$\Phi=(1/N)\sum_k[\exp(\beta E_k)-1]^{-1}, \quad (2.4)$$

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$$E_k=\mu H+2\langle S^z\rangle[J_1z_1(1-\gamma_1(\mathbf{k}))+J_2z_2(1-\gamma_2(\mathbf{k}))], \quad (2.5)$$

$$\gamma_i(k)=(z_i)^{-1}\sum_{\delta_i}\exp(i\mathbf{k}\cdot\boldsymbol{\delta}_i) \quad (2.6)$$

($\boldsymbol{\delta}_i$ is the vector connecting ith nearest neighbors; the total number of such neighbors, to a given ion, being z_i).

The Curie temperatures are determined by investigating the limit when, in the absence of the applied field H, the statistical average $\langle S^z\rangle$, being proportional to the system magnetization, approaches zero. In this limit we get

$$2S(S+1)/3=\lim_{T=T_c,H=0}[2\langle S^z\rangle\Phi] \quad (2.7)$$

and therefore

$$(k_BT_c)_{\mathrm{RPA}}=\tfrac{2}{3}S(S+1)J_1z_1/F(J_2/J_1), \quad (2.8)$$

where

$$F\left(\frac{J_2}{J_1}\right)=\left(\frac{1}{N}\right)\sum_k\left\{1-\gamma_1(k)+\left(\frac{J_2z_2}{J_1z_1}\right)[1-\gamma_2(k)]\right\}^{-1}. \quad (2.9)$$

The sums $F(J_2/J_1)$ have been calculated for fcc and bcc lattices, on an IBM-1620 system, for a range of values of the ratio (J_2/J_1) and are listed in Tables I and II. These sums over the Brillouin zones were performed using Gauss' approximate quadrature method. For most of the values shown in the tables, the sums were obtained by use of the real roots of the Legendre polynomial of order 10, which corresponds to evaluating the sum at about 8000 points within the zone. Near the divergent points, however, the sum is slowly convergent and more points within the zone must be taken. For these cases the roots of the Legendre polynomial of order 32 were used, which corresponds to evaluating the sum at about 250 000 points within the zone. These sums are correct to three significant figures.

In Ref. 11, an interpolation Green's-function method was developed which led to an improvement of the

TABLE I. Face-centered cubic lattice.

J_2/J_1	$F(J_2/J_1)$	J_2/J_1	$F(J_2/J_1)$
2.00	0.603	−0.05	1.39
1.80	0.636	−0.10	1.44
1.60	0.673	−0.15	1.50
1.40	0.715	−0.20	1.56
1.20	0.763	−0.25	1.63
1.15	0.776	−0.30	1.71
1.10	0.790	−0.35	1.80
1.05	0.804	−0.40	1.89
1.00	0.819	−0.45	2.00
0.95	0.834	−0.50	2.13
0.90	0.850	−0.55	2.28
0.85	0.867	−0.60	2.46
0.80	0.885	−0.65	2.67
0.75	0.903	−0.70	2.94
0.70	0.922	−0.75	3.29
0.65	0.943	−0.80	3.76
0.60	0.964	−0.85	4.46
0.55	0.986	−0.90	5.64
0.50	1.01	−0.95	8.35
0.45	1.03	−0.96	9.46
0.40	1.06	−0.97	11.1
0.35	1.09	−0.98	14.0
0.30	1.12	−0.99	20.9
0.25	1.15	−0.994	28.6
0.20	1.18	−0.998	61.5
0.15	1.22	−0.9992	130
0.10	1.26	−0.9996	242
0.05	1.30	−1.00	∞
0.00	1.34		

TABLE II. Body-centered cubic lattice.

J_2/J_1	$F(J_2/J_1)$	J_2/J_1	$F(J_2/J_1)$
2.0	0.517	0.1	1.28
1.9	0.533	0.00	1.39
1.8	0.551	−0.10	1.53
1.7	0.569	−0.20	1.71
1.6	0.589	−0.30	1.93
1.5	0.610	−0.40	2.23
1.4	0.633	−0.50	2.67
1.3	0.658	−0.60	3.39
1.2	0.685	−0.65	4.06
1.1	0.714	−0.66	4.25
1.0	0.746	−0.667	4.51
0.9	0.781	−0.670	4.66
0.8	0.820	−0.675	5.12
0.7	0.863	−0.679	5.97
0.6	0.912	−0.6794	6.91
0.5	0.966	−0.6795	7.43
0.4	1.03	−0.6797	10.1
0.3	1.10	−0.6798	16.3
0.2	1.18	−0.67985	33.

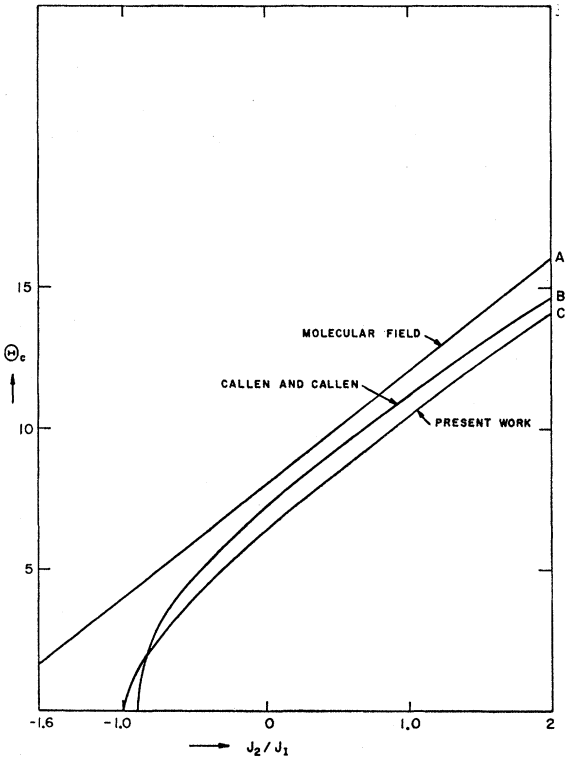

FIG. 1. $\Theta_c=k_BT_c/S(S+1)J_1$ for $S=\frac{7}{2}$ in fcc lattice.

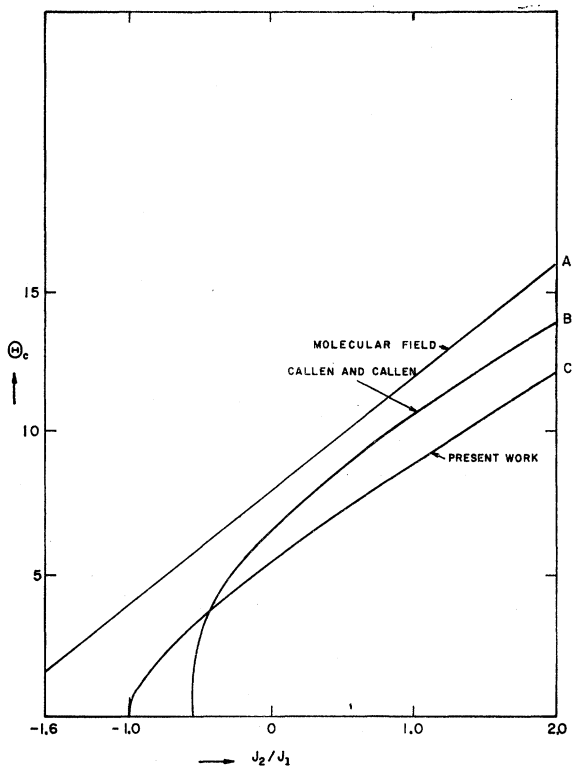

FIG. 2. $\Theta_c = k_B T_c / S(S+1) J_1$ for $S = \frac{1}{2}$ in fcc lattice.

RPA results. For Curie temperatures, the results of reference (11) can in our notation be written as follows:

$$(k_B T_c) = (k_B T_c)_{\mathrm{RPA}} \left[1 + \frac{F(0)-1}{F(0)} \frac{S-1}{3S} \right]. \quad (2.10)$$

In Figs. 1 and 2 we have plotted the

$$[k_B T_c / S(S+1) J_1] \equiv \Theta_c$$

obtained from Eqs. (2.8)–(10) for a fcc lattice and for the cases $S = \frac{7}{2}$ and $S = \frac{1}{2}$. [The corresponding results for the bcc lattice can easily be obtained from Eqs. (2.8)–(2.10) and from Table II.] Included for comparison are the plots obtained from the molecular field theory[13] which gives

$$\Theta_c \underset{\text{mol. field}}{=} (2z_1/3)[1 + J_2 z_2 / J_1 z_1]$$

and also from the recent extension by Callen and Callen[14] of the "consistent" two-particle cluster approximation of Strieb, Callen, and Horwitz.[15] We observed that for $J_2/J_1 > 0$, our Θ_c, like the molecular field result, varies roughly linearly with J_2/J_1, while for $J_2/J_1 < 0$ the variation is more rapid. In fact, $\Theta_c \to 0$ in the fcc lattice when $J_2/J_1 \to -1$, and in the bcc lattice when $J_2/J_1 \to -0.6799$. This should be compared with the limiting conditions, $J_2/J_1 \to -1$ and -0.667, which, according to Smart's interpretation of molecular field theory,[13,16] separate the region of ferromagnetic order from antiferromagnetic order of the second kind in the fcc and the bcc lattices, respectively.[13]

We feel that in the absence of the detailed exact high-temperature series expansion results, our results, which are in semiquantitative agreement with Callen and Callen's cluster approximation results, probably provide the most reliable available estimates of the Curie temperatures.

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[16] A detailed discussion of the limiting behavior of the ferro-, anti-, and paramagnetic phases in systems with next-nearest-neighbor exchange interaction has now been carried out in the spin wave as well as the Green's-function theories and will be presented in a future publication by R. A. Tahir-Kheli and H. B. Callen.