

Comments and Addenda

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Spin-Wave Theory for the Classical Heisenberg Antiferromagnet*

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A number of problems which beset the finite-spin Heisenberg antiferromagnet are eliminated by considering the infinite-spin, or classical case. Using a simple spin-wave treatment, the temperature dependence of the sublattice magnetization is found up to the leading effect due to spin-wave interactions. These new results are quite different from the finite-spin case but very similar to the magnetization of the classical ferromagnet.

SPIN-WAVE theory of the finite-spin Heisenberg model for the antiferromagnetic problem is complicated by three major difficulties—the kinematic effect (due directly to the finiteness of spin), bound-state effects, and the ground-state problem. The present calculation is an attempt to eliminate those effects and follows quite closely the philosophy of recent work on the corresponding ferromagnetic problem.¹

The classical models of magnetism may be obtained from the quantum-mechanical models by replacing the quantum-mechanical spin operators by classical unit vectors, or alternatively, and of interest for our purposes, by taking the large-spin limit $S = \infty$ of the finite-spin problem. Since the critical temperature is proportional to S^2 for large S , it is necessary to express the temperature in terms of T/S^2 , in fact we shall use¹

$$\tau = k_B T / S^2 |J| Z, \quad (1)$$

where the exchange interaction between two nearest-neighbor spins is $|J| \mathbf{S}_A \cdot \mathbf{S}_B$ and the number of nearest neighbors is Z .

The sublattice magnetization including the leading spin-wave interactions may be obtained simply by using the equations of the self-consistently renormalized spin-wave approximation of Bloch³ which we summarize by

$$m_A = \frac{M_A(T)}{g |\mu_B| N S} = 1 - \frac{c'}{2S} - \frac{1}{SN} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}}}{g_{\mathbf{k}}}, \quad (2)$$

where

$$n_{\mathbf{k}} = (e^{\alpha \beta \epsilon_{\mathbf{k}}} - 1)^{-1} \quad (3)$$

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¹ P. D. Loly, Ann. Phys. (N. Y.), **56**, 40 (1970).

² Our definition of J differs from some authors by a factor of $\frac{1}{2}$.

³ M. Bloch, J. Appl. Phys. **34**, 1151 (1963); S. H. Liu, Phys. Rev. **142**, 267 (1966).

and the renormalization due to spin-wave interactions by

$$\alpha = 1 + \frac{c}{2S} - \frac{1}{SN} \sum_{\mathbf{k}} g_{\mathbf{k}} n_{\mathbf{k}}. \quad (4)$$

Furthermore,

$$\epsilon_{\mathbf{k}} = Z |J| S g_{\mathbf{k}}, \quad g_{\mathbf{k}} = [1 - (\gamma_{\mathbf{k}}/\gamma_0)^2]^{1/2}, \quad (5)$$

$$\gamma_{\mathbf{k}} = \sum_{\rho}^{\text{nn}} e^{i\mathbf{k} \cdot \rho}.$$

In these equations, N is the number of spins on each sublattice and c and c' are constants which depend only on the lattice.

The crucial step now comes in using the correct expansion of the Planck function for the large-spin case—then $\alpha \beta \epsilon_{\mathbf{k}}$ is small for all \mathbf{k} . So for $T \gtrsim T_c/S$ we use^{1,4}

$$n(x) = 1/x - \frac{1}{2} + x/12 \dots \quad (6)$$

In the limit $S = \infty$ only the first term remains and the equations simplify to

$$m_A = 1 - c'' \tau / \alpha \quad (7)$$

and

$$\alpha = 1 - \tau / \alpha, \quad (8)$$

where

$$c'' = \frac{1}{N} \sum_{\mathbf{k}} (g_{\mathbf{k}})^{-2}. \quad (9)$$

In this approximation, Eq. (8) exhibits the Bloch³ cutoff temperature τ_M for real solutions of α . In fact, it differs from the classical ferromagnetic case only in

⁴ D. C. Mattis, *Theory of Magnetism* (Harper & Row Publishing Co., New York, 1965).

that τ in one case involves J while the other has $|J|$. This is perhaps not surprising in view of the relation noted by Rushbrooke and Wood⁵ for the classical case,

$$kT_c/J = kT_N/|J| \quad (10)$$

for the relationship of the Curie and Néel temperatures.

Returning to Eq. (9) we expand in powers of τ for $\tau < \tau_M$ finding

$$m_A = 1 - c''\tau - c''\tau^2 - O(\tau^3) \dots \quad (11)$$

Experience with the ferromagnetic case suggests that the error will lie in the τ^3 term, and moreover, that the only contributions are of the form $a_n\tau^n$, $n \geq 0$.

In this infinite-spin limit the kinematic effect vanishes and we assume that the bond states disappear by analogy with the ferromagnetic situation. We see from Eq. (11) that the classical ground state has the full alignment of the Néel state as should be expected,

⁵ G. S. Rushbrooke and P. J. Wood, *Mol. Phys.* **6**, 409 (1963).

i.e., the zero-point deviation of the finite-spin case has been removed. Furthermore, what is left in the temperature dependence of the sublattice magnetization is quite different from the finite-spin results of Oguchi,⁶ specifically for noninteracting spin waves one has a linear effect instead of T^2 , T^4 , T^6 , ... dependences and the leading interaction term is quadratic rather than T^6 .

There exists a strong similarity between the sublattice magnetization of Eq. (11) and the magnetization of the classical ferromagnet, at least to the order τ^2 treated here—for the ferromagnet we find Watson's integral⁷ instead of c'' . For the CsCl or bcc type of antiferromagnet (s.c. sublattices and Brillouin zone) preliminary computations give $c'' \sim 1.393 \pm 0.002$ which is close to the value of Watson's integral on the bcc lattice, namely, 1.39320. Further work on a number of aspects of this problem are underway.

⁶ T. Oguchi, *Phys. Rev.* **117**, 117 (1960).

⁷ G. N. Watson, *Quart. J. Math.* **10**, 266 (1939).

Comment on "Phase Transition in the Two-Dimensional Ferromagnet"*

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It is shown that the decoupling procedure used by Mubayi and Lange leads to the onset of antiferromagnetic short-range order in ferromagnetic systems. This defect occurs in both two- and three-dimensional lattices and occurs over a temperature range that includes the supposed transition temperatures. Any conclusions drawn about the behavior of the systems over this temperature range, including the existence of a transition, must, therefore, be regarded as questionable.

I. INTRODUCTION

RECENTLY, Mubayi and Lange¹ presented a theory for a two-dimensional ferromagnet that exhibited a phase transition, in accord with the conjectures of Stanley and Kaplan,² without the appearance of any spontaneous magnetization, in accord with the proof of Mermin and Wagner³ that a two-dimensional isotropic ferromagnet cannot support a finite magnetization in zero field. Their theory consists of a linearized Green's-function theory in which the second-order Green's function is written as a linear combination of first-order functions. The coefficients in the expansion are chosen by requiring that the replacement be exact in certain limiting cases.

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¹ V. Mubayi and R. V. Lange, *Phys. Rev.* **178**, 882 (1969); hereafter referred to as I.

² H. E. Stanley and T. A. Kaplan, *Phys. Rev. Letters* **17**, 913 (1966).

³ N. D. Mermin and H. Wagner, *Phys. Rev. Letters* **17**, 1133 (1966).

In this paper, we point out that the procedure used in I, which is equivalent to the use of the Roth⁴ decoupling procedure, always leads to the result that at some temperature in the range $(0, T_c)$, the longitudinal correlation function

$$\eta \equiv z^{-1} \sum_{\delta} \langle S_i^z S_{i+\delta^z} \rangle \quad (1)$$

changes sign. Here, z is the coordination number of the lattice, and the δ 's connect nearest-neighboring sites. Furthermore, at $T = T_c$, the symmetry remains broken, and this persists into the paramagnetic region. Since negative η corresponds to antiferromagnetic order, the conclusions of I are open to question.

II. LINEARIZED EQUATIONS OF MOTION

We begin with the Hamiltonian used in I,

$$\mathcal{H} = -\omega_0 \sum_i S_i^z - \sum_{i,j} J_{ij} S_i \cdot S_j, \quad (2)$$

⁴ L. M. Roth, *Phys. Rev. Letters* **20**, 1431 (1968).