

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"*

RICHARD P. KENAN

Battelle Columbus Laboratories, 505 King Avenue, Columbus, Ohio 43201

(Received 27 October 1969)

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.

* Research supported in part by the U. S. Air Force Office of Scientific Research, Grant No. AF-AFOSR-68-1535.

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).

where $\omega_0 = g\mu_B H$ and $J_{ij} = J_{ji} > 0$, $J_{ii} = 0$, and we define a first-order Green's function by

$$G_{ij}(t-t') = \langle\langle S_i^+(t); S_j^-(t') \rangle\rangle \\ \equiv -i\theta(t-t') \langle [S_i^+(t), S_j^-(t')]_- \rangle. \quad (3)$$

The equation of motion of G is

$$[i(\partial/\partial t) - \omega_0]G_{ij}(t-t') = 2\langle S^z \rangle \delta_{ij} \delta(t-t') \\ + H_{ij}(t-t'), \quad (4)$$

where the second-order Green's function $H_{ij}(t-t')$ is given by

$$H_{ij}(t-t') = -2 \sum_l J_{il} \langle\langle S_l^+(t) S_i^z(t); S_j^-(t') \rangle\rangle \\ - \langle\langle S_l^z(t) S_i^+(t); S_j^-(t') \rangle\rangle. \quad (5)$$

Mubayi and Lange now proceed to write H_{ij} as a linear combination of G_{ij} 's. We prefer the more direct procedure of writing the decoupling in terms of the spectral densities, $g_{ij}(\omega)$ and $h_{ij}(\omega)$, defined by

$$G_{ij}(t-t') = -i\theta(t-t') \int_{-\infty}^{\infty} d\omega g_{ij}(\omega) \exp[-i\omega(t-t')] \quad (6)$$

and

$$H_{ij}(t-t') = -i\theta(t-t') \int_{-\infty}^{\infty} d\omega h_{ij}(\omega) \exp[-i\omega(t-t')], \quad (7)$$

in the form

$$h_{ij}(\omega) = \sum_l A_{il} g_{lj}(\omega) \quad (8)$$

since this form is more clearly related to the Roth procedure. g and h satisfy certain easily verified sum rules. Suppose we have a Green's function $\langle\langle A; B \rangle\rangle$ with spectral density $\rho_{AB}(\omega)$. Then

$$\int_{-\infty}^{\infty} d\omega \omega^n \rho_{AB}(\omega) = \langle\langle [\dots [A, \mathfrak{H}]_-, \dots \mathfrak{H}]_-, B \rangle\rangle, \quad (9)$$

where \mathfrak{H} appears n times in the nested commutator. Evaluation of (9) for $n=0$ gives, when (8) is used,

$$A_{ii} = \langle S^z \rangle^{-1} \sum_l J_{il} (2\langle S_i^z S_l^z \rangle + \langle S_i^- S_l^+ \rangle), \quad (10)$$

$$A_{il} = -\langle S^z \rangle^{-1} J_{il} (2\langle S_i^z S_l^z \rangle + \langle S_i^- S_l^+ \rangle), \quad i \neq l \quad (11)$$

in which we have assumed inversion symmetry for the lattice, so that the averages $\langle S_i^- S_j^+ \rangle$ are real. We therefore have for H_{ij}

$$H_{ij}(t-t') = \langle S^z \rangle^{-1} \sum_l J_{ij} (2\langle S_i^z S_l^z \rangle + \langle S_i^- S_l^+ \rangle) \\ \times [G_{ij}(t-t') - G_{lj}(t-t')]. \quad (12)$$

Equation (12) is identical to the decoupling used in I, but it has been derived for arbitrary spin. The form of the renormalization coefficient appearing in (12) is the result of the use of the Roth decoupling procedure. The

connection to the Roth decoupling can easily be seen by inserting Eq. (8) into Eq. (9) with $\rho = h$, which reproduces Eq. (5) of Roth's paper.

The inconvenient correlation function $\langle S_i^z S_l^z \rangle$ may be eliminated from the renormalization coefficient by direct evaluation of the correlation function $\langle BA \rangle$, using Eq. (8) and

$$\langle BA \rangle = \int_{-\infty}^{\infty} d\omega h_{ij}(\omega) [\exp(\beta\omega) - 1]^{-1}, \quad (13)$$

in the case of spin $\frac{1}{2}$. Further, restricting ourselves to nearest-neighbor interactions (for simplicity), we obtain

$$2\eta + \mu = 2\sigma^2 / (1 - 2\mu), \quad (14)$$

where η is defined by Eq. (1), the transverse correlation function μ is defined by

$$\mu = z^{-1} \sum_{\delta} \langle S_i^- S_{i+\delta}^+ \rangle, \quad (15)$$

$\langle S^z \rangle = \sigma$, and the identities $S^- S^+ = \frac{1}{2} - S^z$ and $S^- S^z = \frac{1}{2} S^-$ have been used.

III. TRANSITION TEMPERATURE

The solution of Eq. (4) using Eqs. (12) and (14) is straightforward for spin- $\frac{1}{2}$ systems and nearest-neighbor interactions. Fourier-transforming in space and time, we obtain

$$G(\mathbf{k}, E) = [2\sigma / 2\pi N^{1/2}] [E - \omega_0 - \epsilon(\mathbf{k})]^{-1}, \quad (16)$$

with

$$\epsilon(\mathbf{k}) = [2\sigma / (1 - 2\mu)] J_z (1 - \gamma_{\mathbf{k}}), \quad (17)$$

$$\gamma_{\mathbf{k}} = z^{-1} \sum_{\delta} e^{i\mathbf{k} \cdot \delta}. \quad (18)$$

The spectral density obtained from (16) is

$$g(\mathbf{k}, \omega) = 2\sigma N^{-1/2} \delta[\omega - \omega_0 - \epsilon(\mathbf{k})]. \quad (19)$$

We therefore obtain the following equations for σ and μ :

$$\frac{1}{2} - \sigma = (2\sigma/N) \sum_{\mathbf{k}} \{ \exp\beta[\omega_0 + \epsilon(\mathbf{k})] - 1 \}^{-1} \quad (20)$$

and

$$\mu = (2\sigma/N) \sum_{\mathbf{k}} \gamma_{\mathbf{k}} \{ \exp\beta[\omega_0 + \epsilon(\mathbf{k})] - 1 \}^{-1}. \quad (21)$$

Setting $\omega_0 = 0$ and allowing $\sigma \rightarrow 0$, we obtain

$$kT_c / J_z = [2\mathfrak{F} (1 - 2\mu)]^{-1} \quad (22)$$

and

$$kT_c / J_z = [\mathfrak{F} - 1]^{-1} [1 - 2\mu]^{-1} \quad (23)$$

from Eqs. (20) and (21), respectively. Here,

$$\mathfrak{F} = N^{-1} \sum_{\mathbf{k}} (1 - \gamma_{\mathbf{k}})^{-1}. \quad (24)$$

For two-dimensional systems, \mathfrak{F} diverges to ∞ , and one must resort to more careful analysis of the equations, as was done in I. For three-dimensional systems,

\mathfrak{F} is finite and greater than 1. Solving Eqs. (22) and (23) gives, for these systems,

$$\mu = (\mathfrak{F} - 1)/(2\mathfrak{F}) > 0; \quad kT_c/Jz = \frac{1}{2}. \quad (25)$$

It should be noted that the transition temperature is identical to that predicted by the molecular-field theory. The fact that μ is positive at T_c indicates that η must be negative since $2\eta + \mu = 0$ [by Eq. (14)]. Near $T=0$, we find that $\mu=0$, $\eta=1$. Thus, η changes sign between $T=0$ and $T=T_c$. Furthermore, the symmetry of the system under rotations of the crystal as a whole remains broken above T_c since we do not have $2\eta = +\mu$.

Mubayi and Lange give the necessary analysis for the two-dimensional case. They find that above T_c the renormalization coefficient vanishes linearly with the field H . At $T=T_c$, it vanishes like $(H \ln|H|)^{1/3}$. Finally, below T_c , it is independent of H and proportional to $(T_c - T)^{1/2}$, and $\mu \equiv \frac{1}{2}$. Thus, above T_c , we again have $\eta < 0$, while just below T_c , $2\eta + \mu$ can be made arbitrarily small by approaching T_c . We can conclude, therefore, that even in the two-dimensional case, there exists a range of temperatures for which $\eta < 0$, and that this range includes the transition temperature. Indeed, it can be shown that Eqs. (14) and (15) of I can be solved directly for η , giving (in our notation)

$$\eta = -\frac{1}{4} + \sigma + \frac{(\frac{1}{2} - \sigma - \mu)^2}{(1 + 2\mu)}, \quad (26)$$

so that, when $\sigma=0$, we obtain $\eta = -\frac{1}{2}\mu$, and, below T_c , we find $\eta \equiv -\frac{1}{4}$. Thus, η is less than 0 over the entire temperature range considered, a stronger conclusion than the arguments beginning this paragraph reach.

IV. CONCLUSIONS

We have shown that there exists a range of temperatures surrounding the transition temperature over which the theory of I gives the result that the longitudinal correlation function η is negative. η is essentially the

same thing as the short-range order, and $\eta < 0$ means that the order is antiferromagnetic, which is unacceptable in a ferromagnet (where $\eta > 0$ at low temperatures). At the same time, the theory fails to restore the correct symmetry of the $H=0$ states. Since the object of the theory was to establish the existence (or probable existence) of the transition temperature, and since the theory appears to fail before the proposed transition temperature is reached, we think that any conclusions drawn about the behavior of the system in the region of negative η must be viewed with suspicion.

The origin of the difficulty is not clearly exposed, but we can suggest the following. Linearization of the equations of motion of a spin system is inconsistent with the continued assumption that the operators with which we are dealing are spin operators, unless the Hamiltonian is a Zeeman Hamiltonian. It is consistent with the assumption that, along with the linearization, we change the operators into something closely resembling bosons. In using the Roth procedure, we (and the authors of I) have made full use of the spin kinematics, assuming, in effect, that while we are not obtaining the correct equations of motion for the spin system under consideration, we are, nonetheless, obtaining the equations of motion for *some spin system*. We are not, for no such *spin* Hamiltonian exists. The more common linearization procedures, on the other hand, use what amounts to a Wick-type theorem on the spin-raising and -lowering operators in order to determine the expansion coefficients. Such theorems hold for bosons (in some degree of approximation), and this is just the direction in which linearization takes the spin operators. We therefore suggest that the problems of the theory of I are due to the attempt to force the linearized equations for the Green's functions to obey (for $t=t'$) the relations obeyed by the exact equations. The resulting difficulties are reminiscent of the familiar oscillations often produced by forcing a polynomial of degree $N-1$ to pass through N specified points.