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Onset of long-range order in a paramagnet

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The onset of long-range order in a paramagnet is studied using an expansion in powers of $1/z$, where z is the number of nearest neighbors. Rather than expand the correlation function itself, we expand the self-energy in powers of $1/z$. For both the Ising and Heisenberg models of ferromagnetism, the long-range correlations diverge at the true, shifted Curie temperaure. Therefore, the magnetic and paramagnetic results of the $1/z$ expansion are consistent.

I. INTRODUCTION

Expansion techniques[1] are quite useful in the study of ferromagnets, where exact results are difficult to obtain. In a recent paper[2] [by Fishman and Liu (FL)], we developed an expansion for the thermodynamic properties of the Ising and Heisenberg models of ferromagnetism. As argued in FL, the spin correlations in a ferromagnet produce $1/z$ corrections to mean-field (MF) theory, where z is the number of nearest neighbors in the lattice. In this paper, we use a related approach to study the onset of long-range order in a paramagnet. As expected, the long-range correlations of a paramagnet diverge at the same Curie temperature calculated in FL. So the paramagnetic and ferromagnetic results of the $1/z$ expansion are consistent.

It is not immediately obvious that a $1/z$ expansion can even be formulated for a spin-s paramagnet. In a ferromagnet, the MF Hamiltonian and the MF order parameter $M_0=\langle S_{1z}\rangle_{\mathrm{MF}}$ are nonzero. Because the $1/z$ correction to the order parameter is negative, the coupling of fluctuations suppresses the Curie temperature T_C/zJ from its MF value[3] of $T_0=s(s+1)/3$. But, in a paramagnet, the MF Hamiltonian and order parameter vanish while the MF correlation function $D_{ij}^{(0)}$ is nonzero only if $i=j$. So it may be difficult to incorporate long-range correlations in a consistent fashion.

Indeed, when the $1/z$ expansion is applied to the correlation function itself, the spin correlations remain short ranged. If the correlation function D_{ij} is expanded to order $1/z^m$, then the spin correlations vanish outside a sphere or radius ma, where a is the lattice constant. So, instead of directly expanding the correlation function $D(\mathbf{k})$, we expand a self-energy function $\Sigma(\mathbf{k})$ which is proportional to $[D(\mathbf{k})]^{-1}$. The self-energy embodies the coupling of fluctuations omitted by MF theory. This technique guarantees that the correlation function D_{ij} is long ranged, even if the self-energy Σ_{ij} is not. The major result of this paper is that the paramagnetic correlations diverge at the same Curie temperature obtained in the ferromagnet. So, the long-range correlations of a paramagnet can be studied self-consistently.

In a companion paper,[4] we use this expansion technique to study the dynamics of a ferromagnet below T_C. Although the formalism of that paper is complicated by the frequency dependence of the correlation function and self-energy, the basic methodology is the same as here. The paramagnetic calculations of this paper can be considered a test run of the self-energy expansion, prior to its application to the more complicated problem of spin dynamics. Of course, the paramagnet also poses unique challenges of its own.

Actually, the $1/z$ expansion in a ferromagnet has a very long history, dating back to the work of Horwitz and Callen,[5] Englert,[6] Stinchcombe,[7] Brout,[8] and Vaks *et al.*[9] Early work on the $1/z$ expansion was frustrated by the discovery of "anomalies" in the $1/z$ corrections to the order parameter and free energy at the MF Curie temperature T_0. In FL, we demonstrated that these so-called "anomalies" are required for the consistency of the theory and have no physical effects. Another such "anomaly" appears in this work: the $1/z$ correction to $\eta\equiv\langle S_{1z}^2\rangle$ is discontinuous across T_0. But, as shown in the Appendix, the total value of η is continuous across the true Curie temperature T_C, when both η and T_C are evaluated to order $1/z$. So, the discontinuity in the $1/z$ correction to η is required for the consistency of the expansion.

The original, unrenormalized $1/z$ expansion was abandoned because the Curie temperatures obtained from the onset of long-range order and from the divergence of the magnetic susceptibility were different.[6] To remedy this difficulty, the diagrams of the $1/z$ expansion were renormalized by the addition of higher-order terms. Unfortunately, the renormalized formalism no longer provided a well-defined expansion[7] of the thermodynamic variables. So, aside from testing the self-energy formalism, this paper serves another purpose: we demonstrate that an expansion of the self-energy yields the same Curie temperature as the expansions of the order parameter and susceptibility. So, we have finally established that the unrenormalized $1/z$ expansion is a reliable tool in condensed-matter physics.

Besides its applications to ferromagnets, the $1/z$ formalism has also successfully been applied to correlated electron systems[10–12] and to granular superconductors.[13,14] Indeed, it is possible to formulate the $1/z$ expansion for a general Hamiltonian[15] which reduces to either a ferromagnet or a granular superconductor.

This paper is divided into five parts. Section II introduces the basic formalism of the self-energy expansion. In Sec. III, we apply this formalism to the correlation function of the Ising model. Section IV is devoted to the Heisenberg model. Finally, Sec. V contains a conclusion. In the Appendix, we show that $\eta=\langle S_{1z}^2\rangle$ is continuous across the true Curie temperature, despite the discontinuity in the $1/z$ correction to η at the MF Curie temperature.

II. FORMALISM

This section describes the self-energy expansion technique, which can be applied to a general class of lattice Hamiltonians. In this paper, we specifically treat the Ising and Heisenberg models of ferromagnetism. The Hamiltonians of those two models are

$$H_I=-J\sum_{\langle i,j\rangle} S_{iz}S_{jz} \ , \tag{1}$$

$$H_H=-J\sum_{\langle i,j\rangle} \mathbf{S}_i\cdot\mathbf{S}_j \ , \tag{2}$$

where $J>0$ and the sums run over all nearest neighbors in the lattice. While the spins of the Ising model commute, the spin operators of the Heisenberg model obey the commutation relations

$$[S_{\alpha i},S_{\beta j}]=-i\delta_{ij}\varepsilon_{\alpha\beta\gamma}S_{i\gamma} \tag{3}$$

with $\hbar=1$. For future convenience, we define the operators

$$R_{ij}^I=S_{iz}S_{jz} \ , \tag{4}$$

$$R_{ij}^H=\mathbf{S}_i\cdot\mathbf{S}_j \ , \tag{5}$$

where the former commute but the latter do not. In a paramagnet, the expectation values of S_{iz} and $\mathbf{S}_i$ vanish. Hence, all the energy of a paramagnet is generated by the coupling of spin fluctuations on neighboring lattice sites.

In the magnetic state, the mean field experienced by every spin is zJM_0, where the MF order parameter $M_0=\langle S_{1z}\rangle_{\rm MF}$ is evaluated with the MF Hamiltonian. As z increases, the mean field also increases and the coupling of fluctuations on neighboring sites becomes less important. So, the effect of fluctuations can be studied with a $1/z$ expansion about MF theory. But, in a paramagnet, the mean field vanishes identically and this justification is lacking. Yet the effects of fluctuations still decrease with increasing z. In the limit $z\to\infty$, MF theory becomes exact and the spin correlations become short ranged. For finite z, the coupling of fluctuations induces long-range correlations among the spins.

The goal of this paper is to evaluate the correlation function

$$D(\mathbf{k})=\sum_i e^{-i\mathbf{k}\cdot\mathbf{R}_i}D_{1i} \ , \tag{6}$$

$$D_{ij}=-\langle S_{iz}S_{jz}\rangle \ , \tag{7}$$

where the lattice sites are located at $\mathbf{R}_i$ and $\mathbf{R}_1=0$. The expectation value of any operator A is defined by

$$\langle A\rangle=\frac{1}{Z}\mathrm{Tr}\{e^{-\beta H}A\} \ , \tag{8}$$

$$Z=\mathrm{Tr}\{e^{-\beta H}\} \ , \tag{9}$$

where the Hamiltonian H can stand for either H_I or H_H.

By expanding the exponents $e^{-\beta H}$ in Eqs. (8) and (9) and then collecting all the terms of a given order in $1/z$, we produce the $1/z$ expansion

$$\langle A\rangle=A_0(T^*)+\frac{1}{z}A_1(T^*)+\cdots \ . \tag{10}$$

Assuming A is dimensionless, each coefficient A_n is a function only of the dimensionless temperature $T^*=T/zJ$ and of the spin s. The zeroth-order term A_0 is the MF result, evaluated with $H=0$. The higher-order corrections embody the coupling of spin fluctuations on neighboring lattice sites. In the next two sections, this procedure is used to expand the correlation function of Eq. (7).

For both the Ising and Heisenberg models, the MF correlation function is given by

$$D_{ij}^{(0)}=-\tfrac{1}{3}s(s+1)\delta_{ij} \ . \tag{11}$$

Because the spin correlations vanish on different sites, the Fourier-transformed correlation function

$$D^{(0)}(\mathbf{k})=-\tfrac{1}{3}s(s+1) \tag{12}$$

is independent of $\mathbf{k}$.

In terms of the parameter $t=-s(s+1)/3$, the exact correlation function can be written as

$$D(\mathbf{k})=\frac{t}{1-t\Sigma(\mathbf{k})} \ , \tag{13}$$

where the self-energy $\Sigma(\mathbf{k})$ vanishes in MF theory. After a simple rearrangement, Eq. (13) defines the self-energy as

$$\Sigma(\mathbf{k})=\frac{1}{t}-\frac{1}{D(\mathbf{k})} \ . \tag{14}$$

Equation (13) can also be written in real space as

$$\underline{D}=t\underline{I}+t\underline{\Sigma}\,\underline{D} \ , \tag{15}$$

where $\underline{I}$ is the identity matrix, $\underline{D}$ is the correlation matrix, and $\Sigma(\mathbf{k})$ is related to the self-energy matrix $\underline{\Sigma}$ by

$$\Sigma(\mathbf{k})=\sum_i e^{-i\mathbf{k}\cdot\mathbf{R}_i}\Sigma_{1i} \ . \tag{16}$$

Equations (13) and (15) are entirely general expressions for the correlation function, provided that $[D(\mathbf{k})]^{-1}$ is nonzero for all $\mathbf{k}$ or, equivalently, that $\underline{D}$ is invertible. No other assumptions are made.

As discussed above, a $1/z$ expansion of the correlation function itself would never yield long-range order. If the correlation function $\underline{D}$ is expanded to order $1/z^n$, then the spin correlations would vanish outside a sphere of radius na. But, if the self-energy $\underline{\Sigma}$ is expanded to any finite order in $1/z$, then the spin correlations immediately become long ranged. Since the condition for long-range order is that $[D(\mathbf{k}=\mathbf{0})]^{-1}=0$, an expansion of $\Sigma(\mathbf{k})$ in powers of $1/z$ makes eminent sense.

The $1/z$ expansion of the self-energy $\Sigma(\mathbf{k})$ is performed as follows. First, every correlation function D_{1j} is expanded to the required order in $1/z$. Then, Eq. (15) is used to solve for the real-space self-energy Σ_{ij}. Finally, the Fourier transform in Eq. (16) yields the $1/z$ expansion of $\Sigma(\mathbf{k})$:

$$\Sigma(\mathbf{k})=\sigma_0(T^*)+\frac{1}{z}\sigma_1(T^*)+\cdots \, . \tag{17}$$

Each coefficient σ_m is a function of the dimensionless temperature T^*, the spin s, and the dimensionless functions

$$\gamma_{\mathbf{k}}^{(n)}=\frac{1}{\mathcal{N}_n}\sum_{\delta^{(n)}} e^{i\mathbf{k}\cdot\delta^{(n)}} \, , \tag{18}$$

where the sum runs over the $\mathcal{N}_n$ different n-nearest-neighbor vectors $\boldsymbol{\delta}^{(n)}$.

Each function $\gamma_{\mathbf{k}}^{(n)}$ equals 1 when $\mathbf{k}=\mathbf{0}$ and reaches a minimum somewhere on the zone boundary. For example, in a cubic lattice with the lattice constant set to 1,

$$\gamma_{\mathbf{k}}^{(1)}=\tfrac{1}{3}[\cos(k_x)+\cos(k_y)+\cos(k_z)] \tag{19}$$

equals 1 when $\mathbf{k}=\mathbf{0}$ and equals -1 when $\mathbf{k}=(\pm\pi,\pm\pi,\pm\pi)$. Of course, $\mathcal{N}_1=z$ by definition. To lowest order in $1/z$, the number of nth-nearest neighbors is given by $\mathcal{N}_n=z^n/n!$ and $\gamma_{\mathbf{k}}^{(n)}=(\gamma_{\mathbf{k}}^{(1)})^n$. While the self-energy of the Ising model involves only the nearest-neighbor function $\gamma_{\mathbf{k}}^{(1)}$, the self-energy of the Heisenberg model also involves $\gamma_{\mathbf{k}}^{(2)}$ and $\gamma_{\mathbf{k}}^{(3)}$.

Unlike the MF term A_0 in the expansion of $\langle A \rangle$, the zeroth-order term σ_0 in the expansion of $\Sigma(\mathbf{k})$ is *not* the MF self-energy. In fact, σ_0 vanishes in MF theory but is nonzero due to the coupling of spin fluctuations on neighboring sites. To calculate σ_0, we must first evaluate D_{1j} to order $1/z^n$, where $\mathbf{R}_j$ is the nth-nearest neighbor of $\mathbf{R}_1$. Then, Eq. (15) is inverted to obtain Σ_{1j} to order $1/z^n$. Finally, the Fourier transform in Eq. (16) sums over the $z^n/n!$ equivalent lattice sites oriented about $\mathbf{R}_1$ to yield the zeroth-order term σ_0. To evaluate σ_1, we must expand D_{ij} to order $1/z^{n+1}$, then invert Eq. (15) to solve for the self-energy, and Fourier transform to obtain the final result.

Among the nth-nearest neighbors of $\mathbf{R}_1$, only lattice sites $\mathbf{R}_j$ which are linear combinations of n different $\boldsymbol{\delta}^{(1)}$ contribute to σ_0 and σ_1. For example, among the next-nearest neighbors in a two-dimensional square lattice, only the lattice sites $\mathbf{R}_j=\pm\hat{\mathbf{x}}\pm\hat{\mathbf{y}}$ fall into this class. The matrix elements D_{1j} with $\mathbf{R}_j=\pm 2\hat{\mathbf{x}}$ or $\pm 2\hat{\mathbf{y}}$ contribute to the $1/z^2$ correction σ_2 but not to the $1/z$ correction σ_1. Since we are only interested in σ_0 and σ_1, the correlation function may be evaluated within this subclass of the nth-nearest neighbors. Because D_{1j} and Σ_{1j} are the same for every nth-nearest neighbor in this subclass, we define D_n to be the correlation function D_{1j} and Σ_n to be the self-energy Σ_{1j}. Note that D_n and Σ_n are matrix elements of the correlation function and self-energy, not coefficients in the $1/z$ expansions of these quantities.

The $1/z$ corrections to the correlation function are evaluated by expanding Eq. (7) in powers of βH and then collecting all the terms of a given order in $1/z$. To lowest order in this expansion, D_n is of order $1/z^n$. The $1/z^n$ contribution to D_n is represented by Fig. 1(a). A solid line represents a factor of JR_{ij} which couples neighboring sites i and j. Because $\mathbf{R}_j$ is the linear combination of n different vectors $\boldsymbol{\delta}^{(1)}$, each of the n different lines in Fig. 1(a) must be oriented in a different direction. Hence, this diagram is proportional to $\beta^n J^n=\beta^{*n}/z^n$.

Because the expectation values $\langle S_{1x}S_{1z}\rangle$ and $\langle S_{1y}S_{1z}\rangle$ both vanish, only the longitudinal terms in H contribute to Fig. 1(a). So, for either the Ising or Heisenberg models, $D_n^{(a)}$ involves the product of expectation values $\langle S_{1z}^2\rangle_{\mathrm{MF}}^{n+1}=-(-1)^n t^{n+1}$. After a straightforward calculation, we find that

$$D_n^{(a)}=\frac{n!}{z^n}(-1)^n\beta^{*n}t^{n+1} \, . \tag{20}$$

The factor of $n!$ reflects the different possible orderings of the n lines which join $\mathbf{R}_1$ to $\mathbf{R}_j$. For $n=0$, the contribution of this diagram equals t, as expected from MF theory. By inverting Eq. (15), we solve for the self-energy matrix elements Σ_n. To order $1/z^n$, the only nonzero matrix element is

$$\Sigma_1=-\frac{1}{z}\beta^* \, . \tag{21}$$

Finally, after summing over the z-nearest neighbors in the Fourier transform of Eq. (16), we find that

$$\sigma_0=-\beta^*\gamma_{\mathbf{k}}^{(1)} \, . \tag{22}$$

Because the other self-energy matrix elements $\Sigma_{n\neq 1}$ are of order $1/z^{n+1}$ or higher, they do not contribute to σ_0. The Curie temperature is obtained by setting

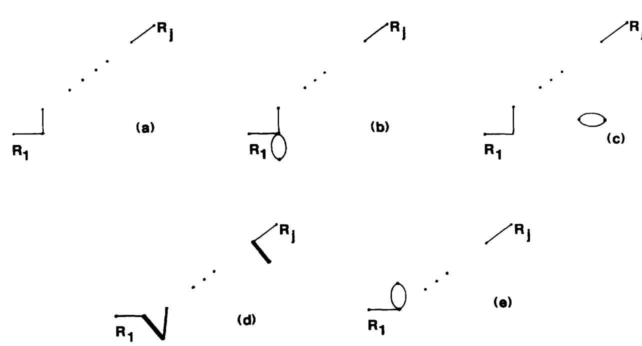

FIG. 1. The diagrams which contribute to the correlation function D_n. (e) is absent in the Ising model.

$D(\mathbf{k}=0)^{-1}=0$, with the result

$$T_C^*=T_0\equiv\tfrac{1}{3}s(s+1)\ . \tag{23}$$

Since the self-energy $\Sigma(\mathbf{k})$ is only accurate to order 1, this MF expression[3] for the Curie temperature neglects $1/z$ corrections.

To evaluate the $1/z$ corrections to the Curie temperature requires the $1/z^{n+1}$ corrections to the correlation function D_n. These are represented by Figs. 1(b)–1(e). In Fig. 1(b), a loop connects any site on the "backbone" to the $z-2$ sites around it. In Fig. 1(c), this loop is disconnected from the backbone. Since the loop can occupy $Nz/2$ different positions on the lattice, Fig. 1(c) includes extensive terms from both the denominator and the numerator of Eq. (7). The extensive terms in the numerator cancel the extensive terms in the partition function, leaving a finite contribution. As shown in Fig. 1(d), lines in the $\pm\boldsymbol{\delta}$ directions may be inserted at any two points on the backbone. In Fig. 1(e), a line is replaced by a loop. Because three lines join at one point, the contribution of this diagram is proportional to $\langle S_{1z}^3\rangle$, which vanishes in the Ising model.

Compared to the backbone diagram, each of these diagrams is smaller by a factor of $1/z$. For example, the contribution of the loop in Fig. 1(b) is proportional to zJ^2 or to $1/z$ in dimensionless units. In Fig. 1(d), the darkened lines may be inserted at any two lattice sites in z different directions. So, the contribution of these inserted lines is proportional to zJ^2 or to $1/z$ in dimensionless units. In the same way, it can be shown that Figs. 1(c) and 1(e) are also of order $1/z^{n+1}$. These diagrams are evaluated in the next two sections.

III. ISING MODEL

It is straightforward to apply this formalism to the Ising model. To order $1/z^{n+1}$, the contributions of Figs. 1(b)–1(d) are

$$D_n^{(b)}=\frac{(n+1)!}{10z^{n+1}}(-1)^n\beta^{*n+2}t^{n+2}(9t+1)\ , \tag{24}$$

$$D_n^{(c)}=-\frac{(n+1)!}{2z^{n+1}}(-1)^n\beta^{*n+2}t^{n+3}\ , \tag{25}$$

$$D_n^{(d)}=\frac{n(n+1)!}{2z^{n+1}}\beta^{*n+2}t^{n+3}\ . \tag{26}$$

As mentioned earlier, $D_n^{(e)}=0$ for the Ising model. The total correlation function D_n is obtained by simply adding Eq. (20) for $D_n^{(a)}$ with Eqs. (24)–(26).

For $n=0$, the total correlation function is given by

$$D_0\equiv D_{11}=t+\frac{1}{10z}\beta^{*2}t^2(4t+1)\ , \tag{27}$$

which is valid to order $1/z$. Rewritten as the $1/z$ expansion of $\eta\equiv\langle S_{1z}^2\rangle$, Eq. (27) becomes

$$\eta=\eta_0+\frac{1}{z}\eta_1\ , \tag{28}$$

where $\eta_0=-t$ and $\eta_1=-\beta^{*2}t^2(4t-1)/10$. In the Heisenberg model, $\eta=s(s+1)/3$ is exact because of the identity $\mathbf{S}_i\cdot\mathbf{S}_i=s(s+1)$ and the equivalence of all three spin components. Since this identity is absent in the Ising model, η only reaches the MF value of $s(s+1)/3$ in the limit of infinite temperature. In the Appendix, we evaluate η_1 below T_0. Although η_1 is discontinuous across T_0, the total value of η is continuous across the true, shifted Curie temperature.

After inverting Eq. (15), we solve for the matrix elements Σ_n. To order $1/z^{n+1}$, the only nonzero matrix elements are

$$\Sigma_0=\frac{1}{10z}\beta^{*2}(-6t+1)\ , \tag{29}$$

$$\Sigma_1=-\frac{1}{z}\beta^*\ . \tag{30}$$

While Eq. (29) neglects the $1/z^2$ corrections to Σ_0, Eq. (30) neglects the $1/z^3$ corrections to Σ_1. Finally, after Fourier transforming with Eq. (16), we find that the coefficients in the $1/z$ expansion of the self-energy $\Sigma(\mathbf{k})$ are

$$\sigma_0=-\beta^*\gamma_{\mathbf{k}}^{(1)}\ , \tag{31}$$

$$\sigma_1=\tfrac{1}{10}\beta^{*2}(-6t+1)\ . \tag{32}$$

Setting $[D(\mathbf{k}=0)]^{-1}=0$, we find that the Curie temperature of the Ising model is

$$T_C^*=T_0+\frac{1}{z}T_1\equiv\tfrac{1}{3}s(s+1)-\frac{1}{5z}s(s+1)-\frac{1}{10z}\ , \tag{33}$$

in agreement with FL.

The self-energy expansion technique is totally different than the method used in FL to evaluate the Curie temperature. In FL, we calculated the lowest-order correction M_1/z to the MF order parameter M_0. The $1/z$ expansion of the Curie temperature is obtained by demanding that the total order parameter M_0+M_1/z vanishes at T_C. In the paramagnet, however, the MF correlation function is short ranged and the MF Hamiltonian vanishes. Nonetheless, an expansion of the self-energy in the paramagnet yields the same Curie temperature as the expansion of the order parameter in the ferromagnet. Therefore, the results of the $1/z$ expansion for the paramagnet and the ferromagnet are consistent.

Using Eqs. (31) and (32) for the self-energy, we now solve for the correlation length of a paramagnet. In a d-dimensional hypercubic lattice with $z=2d$ nearest neighbors, the long-wavelength limit of $\gamma_{\mathbf{k}}^{(1)}$ is given by

$$\gamma_{\mathbf{k}}^{(1)}\approx 1-\frac{1}{z}k^2\ , \tag{34}$$

where the lattice constant is set to 1. So, when $|\mathbf{R}_j|>>1$, the correlation function becomes

$$\langle S_{1z}S_{jz}\rangle\approx\frac{zT^*}{N}\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{R}_j}\frac{1}{k^2+\kappa^2}\ , \tag{35}$$

where

$$\kappa^2=z\left[\frac{T^*}{T_0}-1\right]+\tfrac{1}{10}\beta^*(-6t+1) \tag{36}$$

defines the correlation length κ^{-1}. Near the Curie temperature, $\langle S_{1z}S_{jz}\rangle$ is proportional to $e^{-\kappa|\mathbf{R}_j|}/|\mathbf{R}_j|$. So the spin correlations persist within a sphere of radius κ^{-1}.

Near T_C, the correlation length diverges like the square root of $1/(T^*-T_C^*)$. Hence, the critical exponents are not changed by the $1/z$ expansion. This is not really surprising. Because the critical exponents are nonanalytic functions[1] of $1/z$, they are not shifted by a $1/z$ expansion. The shifts in the critical exponents can only be obtained through a nonperturbative, renormalization-group analysis.

The basic idea of this calculation is to expand the inverse of the correlation function rather than the correlation function itself. Expanded to any finite order in $1/z$, the correlation function never diverges. But if the self-energy is expanded in powers of $1/z$, then the correlation function diverges at the true Curie temperature, expanded to the same order in $1/z$.

IV. HEISENBERG MODEL

This same technique can easily be applied to the Heisenberg model, which contains both transverse and longitudinal fluctuations. The $1/z^{n+1}$ corrections to the correlation function D_n now involve four diagrams instead of three and the correlation functions with $n=0$ and $n=1$ must now be treated separately from the general case $n\geq 2$.

For $n=0$, the contributions of Figs. 1(b) and 1(c) are

$$D_0^{(b)}=\frac{3}{2z}\beta^{*2}t^3\ , \tag{37}$$

$$D_0^{(c)}=-\frac{3}{2z}\beta^{*2}t^3\ . \tag{38}$$

Since Figs. 1(d) and 1(e) do not contribute for $n=0$, we find that $D_0=t$. So, as expected, fluctuations do not shift $\eta=\langle S_{1z}^2\rangle$ from its MF value of $s(s+1)/3$.

For $n=1$, we find that

$$D_1^{(b)}=-\frac{1}{3z^2}\beta^{*3}t^3(9t+1)\ , \tag{39}$$

$$D_1^{(c)}=\frac{3}{z^2}\beta^{*3}t^4\ , \tag{40}$$

$$D_1^{(d)}=-\frac{1}{z^2}\beta^{*3}t^4\ , \tag{41}$$

$$D_1^{(e)}=\frac{1}{4z^2}\beta^{*2}t^2\ . \tag{42}$$

Finally, for $n\geq 2$,

$$D_n^{(b)}=\frac{(n+1)!}{6z^{n+1}}(-1)^n\beta^{*n+2}t^{n+2}(9t+1)\ , \tag{43}$$

$$D_n^{(c)}=-3\frac{(n+1)!}{2z^{n+1}}(-1)^n\beta^{*n+2}t^{n+3}\ , \tag{44}$$

$$D_n^{(d)}=\frac{n(n+1)!}{2z^{n+1}}\beta^{*n+2}t^{n+3}\ , \tag{45}$$

$$D_n^{(e)}=-\frac{n!n}{12z^{n+1}}\beta^{*n+1}(-1)^n t^{n+1}\ . \tag{46}$$

Once again, the total value for D_n is obtained by adding the contributions of Figs. 1(a)–1(e).

The cases $n=0$ and $n=1$ must be treated differently from the general case $n\geq 2$ because D_0 and D_1 involve the unsymmetrized expectation values of operators. For $n=1$, $D_1^{(e)}$ is proportional to

$$\langle R_{12}^2 S_{2z}S_{1z}\rangle_{\rm MF}=-\tfrac{1}{2}t^2\ , \tag{47}$$

with R_{12}^2 operating to the left of the spin operators. But for $n>1$, $D_n^{(e)}$ is proportional to the symmetrized sum

$$\tfrac{1}{3}\{\langle R_{12}^2S_{2z}S_{1z}\rangle_{\rm MF}+\langle R_{12}S_{2z}R_{12}S_{1z}\rangle_{\rm MF}+\langle S_{2z}R_{12}^2S_{1z}\rangle_{\rm MF}\}=-\tfrac{1}{6}t^2\ . \tag{48}$$

Hence, an additional factor of $\frac{1}{3}$ appears in the expression for $D_{n>1}^{(e)}$. Similarly, $D_{n>0}^{(b)}$ is proportional to the symmetrized average

$$\tfrac{1}{3}\{\langle R_{12}^2S_{1z}^2\rangle_{\rm MF}+\langle R_{12}S_{1z}R_{12}S_{1z}\rangle_{\rm MF}+\langle S_{1z}R_{12}^2S_{1z}\rangle_{\rm MF}\}=-\tfrac{1}{3}t^2(9t+1)\ . \tag{49}$$

But, for $n=0$,

$$D_0^{(b)}+D_0^{(c)}=-\frac{1}{2z}\beta^{*2}\langle R_{12}^2(S_{1z}^2-\langle S_{1z}^2\rangle_{\rm MF})\rangle_{\rm MF}=0\ , \tag{50}$$

with R_{12}^2 operating only to the left. So, unlike the correlation functions with $n>0$, the correlation function D_0 is not affected by fluctuations.

Because the operators in the Ising model commute, the unsymmetrized expectation values are equivalent to the symmetrized expectation values. Consequently, a general expression for the correlation function D_n is possible. In the Heisenberg model, on the other hand, the R_{ij} operators do not commute. Therefore, the symmetrized expectation values are different than the unsymmetrized ones and a general expression for D_n is not possible.

In order to calculate the self-energy, we invert Eq. (15) and solve for the matrix elements Σ_n. To order $1/z^{n+1}$, the nonzero matrix elements are

$$\Sigma_0=-\frac{1}{z}\beta^{*2}t\ , \tag{51}$$

$$\Sigma_1=-\frac{1}{z}\beta^{*}+\frac{1}{4z^2}\beta^{*2}-\frac{1}{3z^2}\beta^{*3}t\ , \tag{52}$$

$$\Sigma_2=-\frac{1}{3z^2}\beta^{*4}t^2+\frac{2}{3z^3}\beta^{*3}t\ , \tag{53}$$

$$\Sigma_3=\frac{1}{z^4}\beta^{*4}t^2\ . \tag{54}$$

Once again, Eqs. (51)–(54) ignore corrections of order $1/z^2$, $1/z^3$, $1/z^4$, and $1/z^5$, respectively.

Using Eqs. (16) and (17) for the Fourier transform and $1/z$ expansion of the self-energy, we find that

$$\sigma_0 = -\gamma_{\mathbf{k}}^{(1)}\beta^* , \tag{55}$$

$$\sigma_1 = -\beta^{*2}t + \gamma_{\mathbf{k}}^{(1)}\beta^{*2}\{\tfrac{1}{4} - \tfrac{1}{3}\beta^* t\} + \tfrac{1}{3}\gamma_{\mathbf{k}}^{(2)}\beta^{*3}t\{1 - \tfrac{1}{2}\beta^* t\} + \tfrac{1}{6}\gamma_{\mathbf{k}}^{(3)}\beta^{*4}t^3 , \tag{56}$$

where the functions $\gamma_{\mathbf{k}}^{(n)}$ were previously defined by Eq. (18). After setting $[D(\mathbf{k}=\mathbf{0})]^{-1}=0$, we finally obtain the Curie temperature

$$T_C^* = T_0 + \frac{1}{z}T_1 \equiv \tfrac{1}{3}s(s+1) - \frac{1}{3z}s(s+1) - \frac{1}{4z} , \tag{57}$$

in agreement with FL.

While the self-energy of the Ising model only involves the nearest-neighbor function $\gamma_{\mathbf{k}}^{(1)}$, the self-energy of the Heisenberg model also involves the functions $\gamma_{\mathbf{k}}^{(2)}$ and $\gamma_{\mathbf{k}}^{(3)}$. Hence, a self-consistent treatment of the Heisenberg model must incorporate next, next-nearest-neighbor correlations in the self-energy. Actually, the correlation function of the Heisenberg model can be simplified considerably if the special cases $n=0$ and $n=1$ are treated as corrections. An alternative self-energy $\Pi(\mathbf{k})$ is then defined through the relation

$$D(\mathbf{k}) = \frac{t}{1 - t\Pi(\mathbf{k})} - \frac{1}{6z}\beta^{*2}t^2(1-\gamma_{\mathbf{k}}^{(1)}) . \tag{58}$$

The additional term in this expression guarantees that Eqs. (37)–(42) for D_0 and D_1 are satisfied but does not affect the correlation functions D_n with $n>1$. Comparing Eqs. (14) and (58) for $D(\mathbf{k})$ and using Eqs. (55) and (56) for $\Sigma(\mathbf{k})$, we find that

$$\Pi(\mathbf{k}) = -\beta^*\gamma_{\mathbf{k}}^{(1)}\left\{1 - \frac{1}{12z}\beta^*\right\} + \frac{1}{z}\beta^{*2}\{\tfrac{1}{6} - t\} \tag{59}$$

only contains the nearest-neighbor function $\gamma_{\mathbf{k}}^{(1)}$. The denominator of $D(\mathbf{k}=\mathbf{0})$ still vanishes at the Curie temperature given by Eq. (57).

Using Eq. (59) for the self-energy, we can solve for the correlation function of a hypercubic lattice in the long-wavelength limit. When $|\mathbf{R}_j| >> 1$, the last term in Eq. (59) does not contribute and

$$\langle S_{1z}S_{jz}\rangle \approx \frac{zT^*}{N}\left\{1 + \frac{1}{12z}\beta^*\right\}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_j}\frac{1}{k^2+\kappa^2} , \tag{60}$$

where

$$\kappa^2 = z\left\{\frac{T^*}{T_0} - 1\right\} + \tfrac{1}{6}\beta^*(-6t+1) - \frac{1}{12t} \tag{61}$$

defines the correlation length κ^{-1}. Once again, κ^{-1} diverges at the Curie temperature like the square root of $1/(T^* - T_C^*)$, with the Curie temperature now given by Eq. (57).

Since $\eta = s(s+1)/3$, the correlation function of the Heisenberg model must satisfy the sum rule[3]

$$\frac{1}{N}\sum_{\mathbf{k}} D(\mathbf{k}) = D_0 = -\tfrac{1}{3}s(s+1) . \tag{62}$$

Summing the correlation function over all momentum, we find that this sum rule is violated to order $1/z^2$. However, the correlation function $D(\mathbf{k})$ of Eqs. (58) and (59) is only exact to order $1/z$. Therefore, D_n is only exact to order $1/z^{n+1}$ and D_0 is only exact to order $1/z^2$. Of course, the identity in Eq. (62) could be ensured by adding the appropriate constant term to the right-hand side of Eq. (60). But that procedure is not justified by a $1/z$ expansion.

Although the $1/z$ correction to $\eta = \langle S_{1z}^2\rangle$ vanishes in the paramagnet, η_1 reaches a finite value as T_0 is approached from below. But, as shown in the Appendix, the total $\eta_0 + \eta_1/z$ is continuous across the shifted Curie temperature T_C^* given by Eq. (59). So the discontinuity in η_1 at T_0 is required for the continuity of η across T_C^*.

V. CONCLUSION

This paper has demonstrated a method for studying the onset of long-range order in a paramagnet. After expanding the self-energy $\Sigma(\mathbf{k})$ in powers of $1/z$, we find that the inverse correlation function $[D(\mathbf{k}=\mathbf{0})]^{-1}$ vanishes at the same Curie temperature obtained in FL.

There are, or course, other ways to study the onset of long-range order in a paramagnet. The $1/z$ approach can also be used to calculate the linear susceptibility $\chi = M/h$ in the presence of a small magnetic field h. After expanding the order parameter $M = \langle S_{1z}\rangle$ to order $1/z$, we have evaluated[16] χ^{-1} to order $1/z$. For the Heisenberg model,

$$\frac{1}{\chi} = \frac{1}{\chi_0}\left\{1 + t\beta^* - \frac{1}{4z}t\beta^{*2}(-4t+1)\right\} , \tag{63}$$

where the MF susceptibility is

$$\chi_0 = -\frac{t}{T} . \tag{64}$$

This expression for the susceptibility diverges at the Curie temperature of Eq. (57). For the Ising model, the susceptibility diverges at the Curie temperature of Eq. (33).

In a companion paper,[4] we use the self-energy expansion to study the dynamical correlation function $D(\omega,\mathbf{k})$ in a Heisenberg ferromagnet. Although complicated by the frequency dependence of the correlation function, the formalism of that paper is quite similar to the one demonstrated here. First, we construct a self-energy $\Sigma(\omega,\mathbf{k})$ which is proportional to the inverse of the correlation function. Then, after expanding the real-space correlation functions $D_n(\omega)$ to order $1/z^{n+1}$, we evaluate the self-energy matrix elements $\Sigma_n(\omega)$ to the same order. Finally, a Fourier transformation yields the $1/z$ expansion of the self-energy $\Sigma(\omega,\mathbf{k})$. The mode frequencies $\omega_{\mathbf{k}}$ are determined by the poles of the correlation function. Using this technique, we find that the coupling between the longitudinal and transverse fluctuations causes a splitting of the spin-wave resonance above the crossover temperature[17] $\overline{T} \approx 0.2zJs$.

A related expansion technique has been used by Johnson, Gros, and von Szczepanski[18] to study the mode frequencies of a spin-$\frac{1}{2}$ antiferromagnet at zero temperature. For $s=\frac{1}{2}$, the spin operators can be replaced by a set of fermion operators and Wick's theorem can be used to evaluate the correlation diagrams. Unlike the approach of Johnson *et al.*, the technique described here can be used for any value of the spin. Wick's theorem is not needed to evaluate the correlation diagrams because each contribution factors into the product of expectation values on single sites. For the Heisenberg ferromagnet, each expectation value is evaluated with the full commutation relations of Eq. (3).

To summarize, this paper has shown that the $1/z$ expansions of the paramagnet and of the ferromagnet are consistent. The self-energy expansion technique has wide applications to problems in ferromagnets and paramagnets, including the study of spin dynamics below T_C and the study of spin correlations above T_C. In future papers we also hope to apply this method to other systems, such as granular superconductors.

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APPENDIX

In this appendix we show that $\eta=\langle S_{1z}^2\rangle$ is continuous across the Curie temperature T_C^*, when both η and T_C^* are evaluated to order $1/z$.

For both the Heisenberg and Ising modes, the MF value of η is given by

$$\eta_0=G_1(T^*)\ , \tag{A1}$$

where the functions $G_n(T^*)$ are defined by

$$G_n(T^*)=\frac{1}{Z_{00}}\sum_{m=-s}^{s} m^{n+1}e^{\beta^* m M_0}\ , \tag{A2}$$

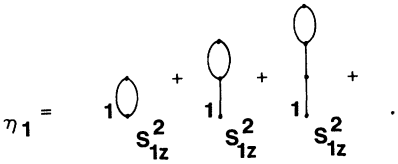

FIG. 2. The diagrams which contribute to the $1/z$ correction to $\eta=\langle S_{1z}^2\rangle$.

$$Z_{00}=\sum_{m=-s}^{s} e^{\beta^* m M_0}\ . \tag{A3}$$

Of course, the MF order parameter M_0 is equivalent to G_0.

For either model, η_1 involves the sum over diagrams shown in Fig. 2. Each diagram in Fig. 2 is of order $1/z$. For example, the "bubble" diagram has two lines joining site 1 with any of the z neighboring sites. So its contribution is proportional to $J^2 z=(zJ)^2/z$ or, in dimensionless units, to $1/z$.

While the "bubble" diagram is simple to evaluate, the infinite sum over "tadpole" diagrams reduces to a geometric series. In terms of the R_{ij} operators, η_1 is given by

$$\eta_1=\tfrac{1}{2}\beta^{*2}\langle R_{12}^2(S_{1z}^2-G_1)\rangle_{\mathrm{MF}} + \tfrac{1}{6}\beta^{*3}\langle P(R_{12}R_{23}^2)S_{1z}^2\rangle_{\mathrm{MF}}\frac{1}{1-f}\ , \tag{A4}$$

where

$$f=\beta^*(G_1-M_0^2) \tag{A5}$$

and P sums over the three distinct permutations of $R_{12}R_{23}^2$. In the Ising model, the R_{ij} operators commute so that P simply multiplies the last term by 3. The bubble diagram is responsible for the first term in η_1; the sum over tadpole diagrams produces the second term. Below T_0, the MF expectation values are evaluated using the MF Hamiltonian $H_{\mathrm{eff}}=-zJM_0\sum_i S_{iz}$. Since f equals 1 at the MF Curie temperature T_0, $1-f$ vanishes at T_0 and the second term in η_1 tends to a finite value as T^* approaches T_0 from below. But this term vanishes above T_0, where $M_0=0$. So η_1 discontinuous across the MF Curie temperature.

But the total discontinuity of η across the true Curie temperature is given by

$$\begin{aligned}\Delta\eta&=\eta(T_C^{*+})-\eta(T_C^{*-})\\&=\eta_0\left[T_0+\frac{1}{z}T_1+\varepsilon\right]-\eta_0\left[T_0+\frac{1}{z}T_1-\varepsilon\right]+\frac{1}{z}\{\eta_1(T_0+\varepsilon)-\eta_1(T_0-\varepsilon)\}\\&=\frac{1}{z}T_1\left\{\frac{dG_1}{dT^*}\bigg|_{T_0^+}-\frac{dG_1}{dT^*}\bigg|_{T_0^-}\right\}+\frac{1}{z}\{\eta_1(T_0^+)-\eta_1(T_0^-)\}\ .\end{aligned} \tag{A6}$$

So $\Delta\eta$ contains two $1/z$ corrections: one due to the discontinuity in η_1 across T_0, the other due to the shift in the Curie temperature from T_0 to T_0+T_1/z. Above T_0, $G_1=-t$ is a constant and the derivative of G_1 vanishes. Just below T_0, the derivative of G_1 is given by

$$\left.\frac{dG_1}{dT^*}\right|_{T_0^-}=-\frac{4s(s+1)-3}{2s(s+1)+1} . \tag{A7}$$

Of course, the discontinuity in η_1 is different for the two models.

For the Ising model, the discontinuity of η_1 across T_0 is given by

$$\eta_1(T_0^+)-\eta_1(T_0^-)=\tfrac{1}{10}[4s(s+1)-3] . \tag{A8}$$

So, using Eq. (33) for T_i, we find from Eq. (A6) that $\Delta\eta=0$, as expected.

For the Heisenberg model, η_1 now contains the effects of the transverse terms in the fluctuation Hamiltonian. Since η_1 vanishes above T_0, we find that

$$\eta_1(T_0^+)-\eta_1(T_0^-)=\tfrac{1}{12}[4s(s+1)-3]\frac{4s(s+1)+3}{2s(s+1)+1} . \tag{A9}$$

Using Eq. (57) for the Curie temperature, we again find that $\Delta\eta=0$. So, for either model, the discontinuity of η vanishes across the true Curie temperature.

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