PHYSICAL REVIEW B VOLUME 47, NUMBER 13 1 APRIL 1993-I

$1/z$ expansion for the Ising and Heisenberg models in an external field

X. W. Jiang and R. S. Fishman
Department of Physics, North Dakota State University, Fargo, North Dakota 58105-5566
(Received 2 October 1992)

Using an expansion in $1/z$, where z is the coordination number of the lattice, we examine the effects of fluctuations on the magnetic susceptibility and specific heat of a spin-s ferromagnet in an external field. As expected, the first-order fluctuation correction to the transition temperature calculated from the zero-field susceptibility agrees with previous results obtained from the expansion of the order parameter. The temperature of the peak in the fluctuation specific heat of the Heisenberg model increases linearly with the external field.

Expansions in $1/z$, where z is the number of nearest neighbors in the lattice, were first formulated[1–4] to study the properties of ferromagnets over 30 years ago. The original, unrenormalized $1/z$ expansion was abandoned for two reasons. First, "anomalies" were discovered[2] in the fluctuation corrections to the order parameter and free energy at the mean-field (MF) Curie temperature. Second, the Curie temperatures calculated from the $1/z$ expansions of the order parameter and magnetic susceptibility disagreed.[2] In order to circumvent these difficulties, each order of the expansion was renormalized[2,3] by including an infinite number of higher-order terms. Recent work[5,6] has demonstrated that the so-called anomalies of the unrenormalized expansion are, in fact, required to make the theory consistent. For example, the divergence of the $1/z$ correction to the order parameter at the MF Curie temperature signifies a shift in the transition temperature.[5] The discontinuity of the first-order correction to the entropy at the MF Curie temperature can be explained in a similar way.[6] In this Brief Report, we show that the second condition for the consistency of the expansion is also satisfied: We demonstrate that the expansions of the magnetic susceptibility and order parameter yield the same shifted Curie temperature, at least to first order in $1/z$.

The lowest-order term in any $1/z$ expansion is simply the MF result, which neglects the correlation of fluctuations on neighboring lattice sites. Higher-order corrections include the effects of spin correlations. In the formal limit $z\rightarrow\infty$ (only really possible in infinite dimension), the MF experienced by every spin diverges and MF theory is recovered. The fluctuation corrections become increasingly important as the coordination number z decreases. So a $1/z$ expansion is only sensible when MF theory already provides a good starting point for describing the physical properties of a system.[7] When MF theory is not qualitatively accurate, such as for a two-dimensional Heisenberg model, the $1/z$ expansion about MF theory is not meaningful.

In previous work, Fishman and Liu[5] (FL) developed the unrenormalized $1/z$ expansion for the order parameter $M=\langle S_{1z}\rangle$ and normalized free energy F/NzJ of the spin-s Heisenberg and Ising models with exchange constant J. The $1/z$ correction to the order parameter is evaluated by exactly summing an infinite series which couples the spin fluctuation over an increasing number of lattice sites. As shown by FL, the divergence of this first-order correction to $-\infty$ at the MF T_C signals the decrease in the Curie temperature from its MF value.

By expanding the free energy in powers of $1/z$, FL also found that the $1/z$ correction to the specific heat of the Heisenberg model contains a peak at the temperature $\overline{T}\approx 0.17zJs$. Fishman and Vignale[6] have associated this peak with a crossover from a low-temperature spin-wave regime to a high-temperature nonlinear regime. In the classical limit $s\rightarrow\infty$, the crossover temperature $\overline{T}\propto zJs$ vanishes on the scale of $T_C\propto zJs^2$. Above the crossover temperature, the strong coupling between longitudinal and transverse spin fluctuations produces new dynamical effects.[8]

We now generalize the work of FL for finite fields. Since the formalism is very similar to the one in zero field, we will primarily emphasize the effects of a finite field. The Hamiltonians of the Ising and Heisenberg models with external magnetic field $\mathbf{h}_{\rm ext}$ along the z direction are[9]

$$H_I=-J\sum_{\langle i,j\rangle}S_i\cdot S_j-h_{\rm ext}\sum_i S_{iz}\ , \tag{1}$$

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

where the sum runs over all nearest-neighbor sites. The spin operators $\mathbf{S}_i$ of the Heisenberg model obey the commutation relations

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

with $\hbar=1$. As usual, we separate the Hamiltonian into three terms:

$$H_{I,H}=H_{\rm eff}+H_1+H_2\ , \tag{4}$$

where

$$H_{\rm eff}=\sum_i H^i_{\rm MF}\ , \tag{5}$$

$$H^i_{\rm MF}=-(zJM_0+h_{\rm ext})S_{iz} \tag{6}$$

is the MF Hamiltonian, and $M_0=\langle S_{iz}\rangle_{MF}$ is the MF order parameter. Both the constant term $H_1=NzJM_0^2/2$ and the fluctuation Hamiltonian H_2 are the same as in the zero-field case. The fluctuation Hamiltonian H_2 couples spin fluctuations on neighboring lattice sites.

Of course, the MF theory of the Ising and Heisenberg models is the same. For any operator A, the MF expectation value is

$$\langle A\rangle_{MF}=\frac{1}{Z_0}\mathrm{Tr}(e^{-\beta H_{eff}}A)\ , \tag{7}$$

where

$$Z_0=\mathrm{Tr}(e^{-\beta H_{eff}}) \tag{8}$$

is the MF partition function and $\beta=1/T$. It is easy to see that all MF expectation values depend only on the dimensionless temperature $T^*=T/zJ$ and field $h_{ext}^*=h_{ext}/zJ$. If H_i^{MF} is written as $-h_{eff}S_{iz}$, then the effective field is $h_{eff}=zJM_0+h_{ext}$ and the corresponding dimensionless effective field is $h_{eff}^*=M_0+h_{ext}^*$. The MF partition function can be written $Z_0=Z_{00}^N$, where

$$Z_{00}=\frac{\sinh[\beta^*h_{eff}^*(s+\frac{1}{2})]}{\sinh(\frac{1}{2}\beta^*h_{eff}^*)}\ , \tag{9}$$

with $\beta^*=1/T^*$. The MF order parameter $M_0(T^*,h_{eff}^*)$ is then obtained from the well-known self-consistent equation[9]

$$M_0=(s+\tfrac{1}{2})\coth[\beta^*h_{eff}^*(s+\tfrac{1}{2})]-\tfrac{1}{2}\coth(\tfrac{1}{2}\beta^*h_{eff}^*)\ . \tag{10}$$

Expanding for small M_0 in zero field, the MF transition temperature T_C^* is given by $T_0\equiv s(s+1)/3$.

The exact expectation value for any operator A is

$$\langle A\rangle=\frac{1}{Z}\mathrm{Tr}(e^{-\beta H_{eff}}e^{-\beta H_2}A)\ , \tag{11}$$

where

$$Z=\mathrm{Tr}(e^{-\beta H_{eff}}e^{-\beta H_2}) \tag{12}$$

is the exact partition function. The $1/z$ expansion is produced[5] by expanding both the numerator and the denominator of Eq. (11) in powers of the fluctuation Hamiltonian H_2. For any dimensionless operator A, the expectation value $\langle A\rangle$ can be expanded as

$$\langle A\rangle=A_0(T^*,h_{ext}^*)+\frac{1}{z}A_1(T^*,h_{ext}^*)+\cdots\ , \tag{13}$$

where $A_0=\langle A\rangle_{MF}$ is the MF value and the coefficients $A_n(T^*,h_{ext}^*)$ only depend on z through the dimensionless temperature and field. As discussed by FL, the first-order correction A_1 to any one-body expectation value such as $M=\langle S_{1z}\rangle$ can be written as the sum over bubble diagram and an infinite number of tadpole diagrams.

For example, the $1/z$ correction to the order parameter can be written as

$$M_1(T^*,h_{ext}^*)=\sum_{n=2}^{\infty}M_1^{(n)}(T^*,h_{ext}^*)\ , \tag{14}$$

where $M_1^{(n)}$ is produced by the H_2^n terms in the expansions of Eqs. (11) and (12). Because the series in Eq. (14) is geometric, the summation yields

$$M_1(T^*,h_{ext}^*)=\frac{M_1^{(2)}(T^*,h_{ext}^*)}{1-f(T^*,h_{ext}^*)}\ , \tag{15}$$

where the scaling function

$$\begin{aligned}f(T^*,h_{ext}^*)&=\beta^*\langle(S_{1z}-M_0)^2\rangle_{MF}\\&=\beta^*(G_1-M_0^2)\end{aligned} \tag{16}$$

is the same for the Ising and Heisenberg models. Here we have introduced the dimensionless functions

$$\begin{aligned}G_n(T^*,h_{ext}^*)&=\langle S_{1z}^{n+1}\rangle_{MF}\\&=\frac{1}{Z_{00}}\sum_{m=-s}^{s}m^{n+1}e^{\beta^*mh_{eff}^*}\ .\end{aligned} \tag{17}$$

In terms of these functions, the bubble contributions $M_1^{(2)}$ for the Ising and Heisenberg models are

$$M_1^{(2)}(T^*,h_{ext}^*)^I=\frac{1}{2T^{*2}}\{-2M_0^5+M_0^3G_1-M_0^2G_2-3M_0G_1^2+G_1G_2\}\ , \tag{18a}$$

$$\begin{aligned}M_1^{(2)}(T^*,h_{ext}^*)^H=\frac{1}{2T^{*2}}(&-2M_0^5+M_0^3(\tfrac{1}{2}+5G_1)-M_0^2G_2\\&+M_0\{\tfrac{1}{2}G_1[s(s+1)-1]-\tfrac{7}{2}G_1^2\}\\&-\tfrac{1}{2}s(s+1)G_2+\tfrac{3}{2}G_1G_2)\ .\end{aligned} \tag{18b}$$

These results are the same as in FL except that M_0 and G_n now depend on field h_{ext}^* as well as on temperature T^*. Because the external field suppresses the correlation of spin fluctuations, M_1 decreases with increasing h_{ext}^*. For any nonzero field, M_1 no longer diverges to $-\infty$ at T_0 and the Curie temperature is no longer defined.

In general, the MF magnetic susceptibility is given by

$$\chi=\frac{dM}{dh_{ext}^*}\ , \tag{19}$$

which like the order parameter can also be expanded in $1/z$. Identical results for the zero-field susceptibility would be obtained with the definition $\chi=[M(h_{ext}^*)-M(0)]/h_{ext}^*$. It is straightforward to show that the MF susceptibility defined by Eq. (19) is given by

$$\chi_0(T^*,h_{ext}^*)=\frac{\beta^*(G_1-M_0^2)}{1-\beta^*(G_1-M_0^2)}\ . \tag{20}$$

In zero field, χ_0 diverges to $+\infty$ both above and below T_0, as shown in the inset to Fig. 1. In a nonzero field, however, the MF susceptibility is continuous with a peak near T_0.

By differentiating M_1 with respect to the external field and expressing the result in terms of M_0 and G_n, we have also evaluated the $1/z$ correction χ_1, which is plotted in Fig. 1 versus $T^*/s(s+1)$ for the Heisenberg model with three different fields. In zero field, χ_1 diverges to $+\infty$

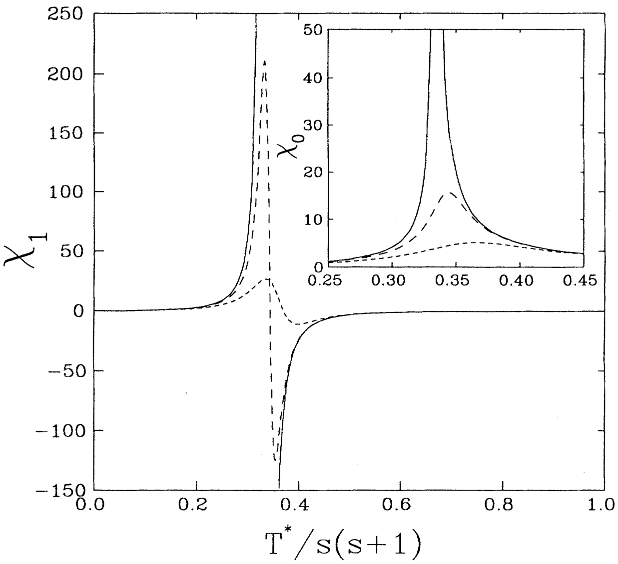

FIG. 1. First-order susceptibility χ_1 vs $T^*/s(s+1)$ for the spin-$\frac{3}{2}$ Heisenberg model, with $h^*_{\rm ext}=0$ (solid curve), 0.05 (long-dashed curve), and 0.1 (short-dashed curve). Inset is the MF susceptibility near T_0 for the same fields.

below T_0 and to $-\infty$ above T_0. As discussed below, these divergences signify a decrease in the Curie temperature from its MF value. In a nonzero field, the susceptibility becomes a continuous function of temperature as shown in Fig. 1.

The first-order correction to the transition temperature can now be calculated from χ_1. Near the MF Curie temperature, χ_1 approaches the limits

$$\chi_1^I \to \frac{3}{10}\frac{1}{1-f}\frac{2s(s+1)+1}{s(s+1)}\chi_0 , \tag{21}$$

$$\chi_1^H \to -\frac{1}{4}\frac{1}{1-f}\frac{4s(s+1)+3}{s(s+1)}\chi_0 , \tag{22}$$

above T_0, and

$$\chi_1^I \to \frac{3}{5}\frac{1}{1-f}\frac{2s(s+1)+1}{s(s+1)}\chi_0 , \tag{23}$$

$$\chi_1^H \to \frac{1}{2}\frac{1}{1-f}\frac{4s(s+1)+3}{s(s+1)}\chi_0 , \tag{24}$$

below T_0.

In zero field, the total susceptibility must diverge at the shifted Curie temperature T_C^*. Therefore we impose the condition

$$\left[\chi_0+\frac{1}{z}\chi_1\right]^{-1}\Bigg|_{h^*_{\rm ext}=0,\,T^*=T_C^*}=0 . \tag{25}$$

Since the zero-field MF susceptibility $\chi_0(T^*=T_0+T_1/z)$ contains terms of order $1/z$, this condition can be written

$$T_1=-\lim_{T^*\to T_0}\frac{\chi_1(T^*)}{d\chi_0/dT^*} , \tag{26}$$

which can be evaluated either above (using Eqs. (21) and (22)] or below [using Eqs. (23) and (24)] the MF Curie temperature. In either case, the results for T_1 are the same and given by

$$T_1^I=-\tfrac{1}{5}s(s+1)-\tfrac{1}{10} , \tag{27}$$

$$T_1^H=-\tfrac{1}{3}s(s+1)-\tfrac{1}{4} . \tag{28}$$

These expressions agree with the corrections obtained by expanding the order parameter in zero field.[5] The same results can also be obtained from the correlation function[10] in the paramagnetic regime above T_C.

We have further extended the work of FL to calculate the fluctuation free energy in a finite field. Following the same methodology as before, we find that the first-order free energies for the Ising and Heisenberg models are

$$\frac{F_1^I(T^*,h^*_{\rm ext})}{NzJ}=-\tfrac{1}{4}\beta^*(M_0^2-G_1)^2 , \tag{29}$$

$$\frac{F_1^H(T^*,h^*_{\rm ext})}{NzJ}=-\tfrac{1}{4}\beta^*\{(M_0^2-G_1)^2+\tfrac{1}{2}[s(s+1)-G_1]^2-\tfrac{1}{2}M_0^2\} . \tag{30}$$

Again, the only difference between these expressions and those in FL is that M_0 and G_n now depend on the external field. In zero field, the first derivative of F_1 is discontinuous at $T^*=T_0$. As explained in FL, however, the total entropy $S=-dF/dT=S_0+S_1/z$ is continuous across the shifted Curie temperature $T_C^*=T_0+T_1/z$. In a finite field, the first derivative of the free energy becomes continuous, but the second derivative becomes very large and positive near T_0.

The first-order correction to the specific heat is given in terms of F_1 by

$$\frac{C_1(T^*,h^*_{\rm ext})}{N}=-T^*\frac{d^2}{dT^{*2}}\frac{F_1}{NzJ} . \tag{31}$$

Evaluating this expression numerically, we plot C_1/N for the spin-$\frac{3}{2}$ Heisenberg model in Fig. 2. As expected, the fluctuation specific heat is suppressed by an external field. More surprisingly, for small nonzero fields, C_1/N becomes very negative in the vicinity of T_0. This behavior is produced by the large second derivative of the free energy F_1/NzJ in this region.

The most interesting feature of C_1/N is the small peak below the transition temperature. In zero field, the temperature of the peak is given by $\bar{T}\approx 0.177zJs$. As discussed by Fishman and Vignale,[6] this peak marks the crossover from a low-temperature spin-wave regime to a high-temperature nonlinear regime. Within the spin-wave approximation, the peak is produced when the transverse free energy enters an equipartition regime[6] in which spin waves of all momenta contribute to the free energy. For the Ising model, the peak is absent. In a nonzero field, the temperature of the peak is given by $\bar{T}=0.177(zJs+h_{\rm ext})$, which increases linearly with the field. As shown in the inset to Fig. 2, the peak is both flattened and shifted by the external field. So by suppressing quantum fluctuations of the spin, the exter-

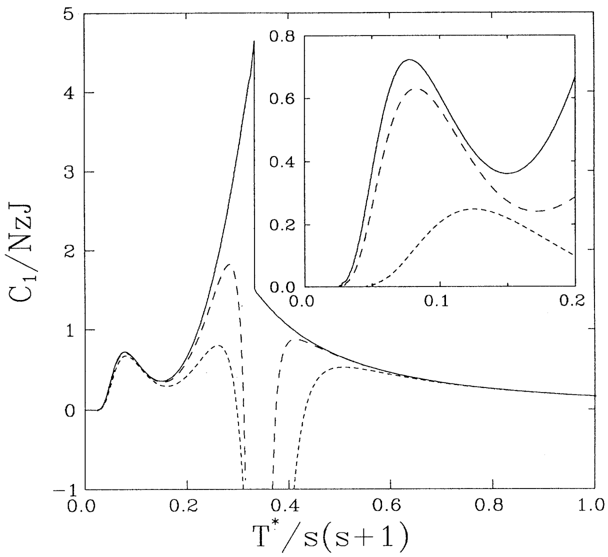

FIG. 2. First-order specific heat C_1/N vs $T^*/s(s+1)$ for the same spin and fields as in Fig. 1. Inset is the quantum peak for the Heisenberg model with $h^*_{\text{ext}}=0$ (solid curve), 0.05 (long-dashed curve), and 0.1 (short-dashed curve).

nal field also increases the crossover temperature above which quantum fluctuations play a crucial role.

Very close to $\overline{T}$, the MF specific heat C_0/N contains a hump.[5] When C_0/N is added to the fluctuation specific heat C_1/zN for $z \geq 6$, the total specific heat also contains a hump near the crossover temperature $\overline{T}$. This hump has been observed experimentally in gadolinium and terbium compounds.[11,12] Of course, it would be most interesting to observe the peaks in C_1/N directly by subtracting off the MF contribution to the specific heat.

A troubling feature of these results is the large negative contribution to the specific heat and susceptibility near T_0 for a nonzero field. In zero field, the divergence of χ_1 and the discontinuity in $S_1=-dF_1/dT$ at T_0 signify the shift in T_C^* from T_0 to $T_0+T_1/z<T_0$. But in a finite field, no such interpretation is possible. Although χ_1 and S_1 are now continuous at T_0, the large negative contributions of χ_1 and $C_1/N=(T/N)dS_1/dT$ near T_0 are difficult to interpret physically.

To summarize, this Brief Report has examined the effects of an external field on the fluctuation contributions to the magnetic susceptibility and specific heat. As expected, the external field suppresses quantum fluctuations of the spin. In this Brief Report, we find that the first-order corrections of the Curie temperatures evaluated from the order parameter and susceptibility are identical. Hence the final objection to the unrenormalized $1/z$ expansion has been removed.

We would like to acknowledge support from the EPSCOR (Experimental Program to Stimulate Cooperative Research) program of the National Science Foundation, administered in North Dakota. Enlightening conversations with M. Bartkowiak, who independently arrived at similar results, are also gratefully acknowledged.

[1]F. Englert, Phys. Rev. Lett. **5**, 102 (1960).
[2]G. Horwitz and H. B. Callen, Phys. Rev. **124**, 1757 (1961).
[3]R. B. Stinchcombe, G. Horwitz, F. Englert, and R. Brout, Phys. Rev. **130**, 155 (1963).
[4]R. Brout, in *Magnetism,* edited by G. T. Rado and H. Suhl (Academic, New York, 1965), Vol. 2A, p. 43.
[5]R. S. Fishman and S. H. Liu, Phys. Rev. B **40**, 11 028 (1989).
[6]R. S. Fishman and G. Vignale, Phys. Rev. B **44**, 658 (1991); J. Phys. Condens. Matter **3**, 4381 (1991).
[7]R. S. Fishman, Int. J. Mod. Phys. B **22**, 3483 (1992).
[8]R. S. Fishman and S. H. Liu, J. Phys. Condens. Matter **3**, 8313 (1991); Phys. Rev. B **45**, 5414 (1992).
[9]See, for example, R. M White, *Quantum Theory of Magnetism* (Springer-Verlag, Berlin, 1963); D. C. Mattis, *The Theory of Magnetism I* (Springer, Berlin, 1988), Chap. 5.
[10]R. S. Fishman and S. H. Liu, Phys. Rev. B **45**, 5406 (1992).
[11]M. Griffel, R. E. Skochdopole, and F. H. Spedding, Phys. Rev. **93**, 657 (1954); L. D. Jennings, R. M. Stanton, and F. H. Spedding, J. Chem. Phys. **27**, 909 (1957).
[12]M. Bouvier, P. Lethuillier, and D. Schmitt, Phys. Rev. B **43**, 13 137 (1991); J. A. Blanco, D. Gignoux, and D. Schmitt, *ibid.* **43**, 13 145 (1991).