Self-Consistent Moment-Conserving Decoupling Scheme and Its Application to the Heisenberg Ferromagnet

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A critique of the moment-conserving decoupling (MCD) procedure for linearizing Green's-function equations of motion is presented. It is shown that in its unembellished form this procedure is equivalent to an algorithm for constructing the relevant spectral function from the knowledge of its frequency moments. The nonuniqueness of this algorithm is discussed. Moreover, the limitations of this algorithm for predicting those frequency–wave-vector-dependent line shapes to which hydrodynamic modes make an important contribution is noted. To overcome some of these difficulties, the concept of a self-consistent moment-conserving decoupling procedure (SCMCD) is introduced. The SCMCD is then employed to study the behavior of the long-range order in a Heisenberg ferromagnet with nearest-neighbor exchange. The results in three dimensions are found to be similar to those following from the use of the random-phase approximation (RPA) and the Callen decoupling. In one and two dimensions, the spontaneous magnetization is found to be vanishing at all finite temperatures. For spin $\frac{1}{2}$, the SCMCD turns out to be identical to the Green's-function decoupling recently proposed by Mubayi and Lange.

1. INTRODUCTION

RECENTLY we proposed a scheme for generating moment-conserving decoupling approximations (MCD) for studying the properties of coupled many-body systems.[1] The crucial aspect of the MCD scheme was that it helped generate an expression for the basic Green's function such that the corresponding result for the relevant frequency and wave-vector-dependent correlation function automatically conserved the desired number of frequency moments. Because the conservation of the frequency moments is known[2,3] to be useful for predicting the frequency–wave-vector dependence of the correlation function, i.e., its line shape, such a procedure seemed to offer possibilities for understanding both the static and the time-dependent properties of statistical systems.

Unfortunately, it now appears that our initial hopes regarding the MCD were overly optimistic. We find, for example, that a straightforward application of the MCD procedure adequately generates only the most elementary type of line shapes, i.e., those that derive much of their spectral weight from a collection of highly peaked regions. The more complicated line shapes, e.g., those which incorporate hydrodynamic phenomena, etc., are quite possibly not well described by a simple application of our MCD.

This makes the MCD a relatively inferior procedure for analyzing situations where hydrodynamic modes, and possibly other similarly subtle collective modes, play a significant role. The reasons underlying this inadequacy of the MCD are twofold: First, the MCD in its original, unembellished form does not prescribe how the frequency moments themselves are to be computed. Second, the MCD is at best only an algorithm for constructing line shapes, so that they conserve an increasing number of the frequency moments. Indeed, since it is possible to have an infinite variety of such algorithms which are constructed to conserve any arbitrary number of frequency moments of the given line shape and yet all of which may differ in an arbitrary manner within any finite frequency interval from the original line shape,[4] the discovery of any one of these is not a scientific event. It is therefore clear that for constructing a physically meaningful line shape from the knowledge of frequency moments, more is needed than just a mathematical algorithm. For example, in situations where the contribution of such collective modes, such as can be described in terms of hydrodynamic analogs, is significant, the method of generalized diffusivity, introduced by Martin and co-workers,[5–7] perhaps offers the most rewarding theoretical machinery to work with.[8–11]

It appears to us that the foregoing weaknesses of the MCD are also shared by another procedure for decoupling many-body Green's functions as proposed by Roth.[12]

Although the usefulness of the MCD in its original form[1] is limited, an extension of the MCD to a self-consistent form (SCMCD) appears to have some promise. The philosophy behind the SCMCD is as follows: Rather than assuming that the frequency moments (which in themselves are time-independent thermodynamic averages) should be computed in an independent calculation, one requires that they be calculated

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[1] R. A. Tahir-Kheli and H. S. Jarrett, Phys. Rev. **180**, 544 (1969).

[2] J. H. Van Vleck, Phys. Rev. **74**, 1168 (1948); R. Kubo and K. Tomita, J. Phys. Soc. Japan **9**, 316 (1954).

[3] W. Marshall and R. D. Lowde, in *Reports on Progress in Physics* [The Institute of Physics and the Physical Society London, 1968), Vol. XXXI, Part II.

[4] See, for example, W. C. Grant, Physica **30**, 1433 (1964).

[5] L. P. Kadanoff and P. C. Martin, Ann. Phys. (N. Y.) **24**, 419 (1963).

[6] H. S. Bennett and P. C. Martin, Phys. Rev. **174**, 629 (1968).

[7] P. C. Martin and S. Yip, Phys. Rev. **170**, 151 (1968).

[8] H. S. Bennett, Phys. Rev. **174**, 629 (1968); **176**, 650 (1968).

[9] R. A. Tahir-Kheli, J. Appl. Phys. **40**, 1550 (1969).

[10] R. A. Tahir-Kheli and D. G. McFadden, Phys. Rev. **178**, 800 (1969); **182**, 604 (1969); and (to be published).

[11] D. G. McFadden and R. A. Tahir-Kheli (unpublished).

[12] L. Roth, Phys. Rev. Letters **20**, 1431 (1968); Phys. Rev. **184**, 451 (1969).

within the approximation scheme being used. For this procedure to be at all meaningful, however, the requirements of self-consistency should be completely satisfied. (For elaboration of this point see Sec. 4.) When these conditions can be satisfied, the decoupling of the basic Green's function is completely specified by the SCMCD.

We find that just this sort of a procedure can be used for studying the properties of Heisenberg spin systems with isotropic exchange interactions. When the exchange interactions are anisotropic, the conditions of self-consistency do not lead to a unique result. In other words, the SCMCD in its present form is not applicable to anisotropic spin systems except in the static Ising limit.[13]

The contents of this paper are organized as follows: In Sec. 2, the nature of the original[1] MCD is elaborated. In Sec. 3, we compare our MCD with the procedure suggested by Laura Roth.[12]

In Sec. 4, we describe the construction of SCMCD. From here on, we confine our attention exclusively to the study of the isotropic Heisenberg ferromagnet. We find that the application of the SCMCD leads to a Green's function, which is identical to that proposed by Mubayi and Lange[14] for a two dimensional Heisenberg ferromagnet with spin $\frac{1}{2}$. Section 5 discusses some of the mathematical details related to series expansion of some relevant functions.

In Sec. 6, we discuss the results in three dimensions following from the use of the SCMCD Green's function computed in Sec. 5. The quality of these results is similar to those obtained within the Callen decoupling scheme.[15] That is, the spontaneous magnetization contains an anomalous T^3 term for spin $\frac{1}{2}$, but for $S>1$, the results are similar to those obtained within the spin-wave approximation.[16–19] Just below the Curie temperature, the spontaneous magnetization has the classical form common to the molecular field approximation[20] and the simple random-phase approximation[21] (RPA). The behavior of the SCMCD results at very high temperature is also similar to those of the other approximate theories.[15,20,21] However, close to the critical temperature, the zero-field magnetic susceptibility has the classical divergence for $S=\frac{1}{2}$, while for $S>1$ the divergence is the same as given by other decoupling schemes[15,21] and the spherical model.[22]

In two dimensions, the consequences of the SCMCD are similar to those given by Mubayi and Lange.[14] The spontaneous magnetization is zero at all nonzero temperatures and therefore is in agreement with the rigorous predictions of Mermin and Wagner[23] that no long-range order obtains in the absence of an applied field. Moreover, in agreement with the prediction of Stanley and Kaplan,[24] within the SCMCD, the isotropic two-dimensional Heisenberg ferromagnet undergoes a second-order phase transition at a finite temperature T_c. In contrast to these very reasonable predictions made by the SCMCD, the usual decoupling schemes,[15,21] in two dimensions predict no phase transition at nonzero temperatures, whereas the molecular field theory,[20] which predicts a phase transition in all dimensions, gives nonvanishing spontaneous magnetization below T_c.

In one dimension, our SCMCD also predicts a phase transition. The reliability of this result seems to us to be questionable.

2. MOMENT-CONSERVING DECOUPLING

Let us define the retarded and advanced Green's functions as follows[25]:

$$\begin{aligned}\langle\langle A_g(t);B_p(t')\rangle\rangle^{\rm ret}&\equiv -i\Theta(t-t')\langle[A_g(t),B_p(t')]_\pm\rangle,\\ \langle\langle A_g(t);B_p(t')\rangle\rangle^{\rm adv}&\equiv +i\Theta(t'-t)\langle[A_g(t),B_p(t')]_\pm\rangle.\end{aligned}\tag{2.1}$$

Here we have used Dirac's units, i.e., $\hbar=1$; the time dependence is in the Heisenberg representation, the operators A_g and B_p refer to lattice positions g and p, the pointed brackets $\langle\cdots\rangle$ denote an ensemble average, and Θ is the Heaviside unit-step function. The choice of anti-commutator or the commutator, in the right-hand side of Eq. (2.1), is dictated by convenience.

The energy Fourier transform $\langle\langle A_g;B_p\rangle\rangle_{(E)}$ of the retarded (advanced) Green's function can be analytically continued into the upper (lower) complex energy plane, i.e.,

$$\begin{aligned}\langle\langle A_g;B_p\rangle\rangle_{(Z)}&\equiv G_{gp}{}^{AB}(Z)\\ &=\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\omega\,F_{gp}{}^{AB}(\omega)/(Z-\omega),\quad \mathrm{Im}Z\neq 0\end{aligned}\tag{2.2}$$

where $F_{gp}{}^{AB}(\omega)$ is the frequency Fourier transform of the anticommutator or the commutator time-correlation function

$$\langle[A_g(t),B_p(t')]_\pm\rangle=\int_{-\infty}^{+\infty}d\omega\,F_{gp}{}^{AB}(\omega)e^{-i\omega(t-t')}.\tag{2.3}$$

The structure of the Green's function $G_{gp}{}^{AB}(Z)$, which

[13] In the Ising limit, the simplest SCMCD reduces to the first-order RPA. The application of the SCMCD at a later stage also seems to reproduce the higher-order RPA's envisaged in the scheme of R. A. Tahir-Kheli [Progr. Theoret. Phys. (Kyoto) **40**, 1312 (1968)].

[14] V. Mubayi and R. V. Lange, Phys. Rev. **178**, 882 (1969).

[15] H. B. Callen, Phys. Rev. **130**, 890 (1963).

[16] F. J. Dyson, Phys. Rev. **102**, 1217 (1956); **102**, 1230 (1956).

[17] T. Oguchi, Phys. Rev. **117**, 117 (1960).

[18] F. Keffer and R. Loudon, J. Appl. Phys. **32**, 25 (1961).

[19] R. A. Tahir-Kheli and D. ter Haar, Phys. Rev. **127**, 95 (1962).

[20] J. H. Van Vleck, J. Chem. Phys. **9**, 85 (1941).

[21] R. A. Tahir-Kheli and D. ter Haar, Phys. Rev. **127**, 88 (1962).

[22] M. Lax and A. Levitas, Phys. Rev. **110**, 1016 (1958).

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

[24] H. E. Stanley and T. A. Kaplan, Phys. Rev. Letters **17**, 913 (1966); J. Appl. Phys. **48**, 975 (1967).

[25] A convenient review of the properties of retarded and advanced Green's functions is given by D. N. Zubarev, Usp. Fiz. Nauk **71**, 71 (1960) [English transl.: Soviet Phys.—Usp. **3**, 320 (1960)].

is of central interest for studying dynamic properties of the many-body system, was analyzed in Ref. 1 in terms of the frequency moments, $\omega_{\alpha\beta}{}^{(n)}(AB)$, of the spectral function $F_{\alpha\beta}{}^{AB}(\omega)$.

$$\omega_{\alpha\beta}{}^{(n)}(AB)=\int_{-\infty}^{+\infty}d\omega\left(\frac{F_{\alpha\beta}{}^{AB}(\omega)}{\omega}\right)\omega^n. \tag{2.4}$$

Since these moments are related to equilibrium time-independent thermodynamic averages, i.e.,

$$\omega_{\alpha\beta}{}^{(n+1)}(AB)$$
$$=\lim_{t=t'}\left\langle\left[\left(i\frac{d}{dt}\right)^{n-n'}A_\alpha(t),\left(-i\frac{d}{dt'}\right)^{n'}B_\beta(t')\right]_\pm\right\rangle, \tag{2.5}$$
$$n,n'\geqslant 0,\quad n-n'\geqslant 0$$

the hope is that the spectral function $F_{\alpha\beta}{}^{AB}(\omega)$ can be constructed from the knowledge of the frequency moments $\omega_{\alpha\beta}{}^{(n)}(AB)$. Note that if this hope is realized, it would be tantamount to expressing the system dynamics in terms of parameters, which in themselves are time-independent thermodynamic functions.

The procedure of Ref. 1 consists of terminating the hierarchy of the Green's functions (such a hierarchy is formed for coupled many-body systems, because the equation of motion of any Green's function always involves additional Green's functions of a higher order) at any one given stage by representing the additional Green's function in terms of all the functions corresponding to the previous stages. However, this termination is done in such a way that a maximum possible number of frequency moments of the spectral function $F_{\alpha\beta}{}^{AB}(\omega)$ are conserved.

To illustrate these statements schematically let us suppose the system Hamiltonian is $\mathcal{H}$ and the commutator of $A_\alpha(t)$ and $\mathcal{H}$ is $C_\alpha(t)$, i.e.,

$$[A_\alpha(t),\mathcal{H}]_-=C_\alpha(t). \tag{2.6}$$

Then

$$ZG_{\alpha\beta}{}^{AB}(Z)=(1/2\pi)\omega_{\alpha\beta}{}^{(1)}(AB)+G_{\alpha\beta}{}^{CD}(Z). \tag{2.7}$$

It is convenient to work in terms of the inverse-lattice Fourier transforms,

$$\gamma_{\alpha\beta}\equiv\frac{1}{N}\sum_{\mathbf{K}}e^{i\mathbf{K}(\mathbf{g}-\mathbf{p})}\gamma_{\mathbf{K}};\quad \gamma_{\alpha\beta}\equiv\omega_{\alpha\beta}{}^{(n)},G_{\alpha\beta}(Z),\ \text{etc.} \tag{2.8}$$

The Green's function $G_{\mathbf{K}}{}^{CB}(Z)$ is, in general, not exactly expressible in terms of the basic Green's function $G_{\mathbf{K}}{}^{AB}(Z)$ unless the system is noninteracting. However, if we decided to terminate the hierarchy of the Green's-function equations of motion [the rest of the hierarchy would be generated by writing the equation of motion of $G_{\mathbf{K}}{}^{CB}(Z)$, and so on] at the very first stage, then the MCD scheme gives the unique decoupling

$$G_{\mathbf{K}}{}^{CB}(Z)\sim[\omega_{\mathbf{K}}{}^{(2)}(AB)/\omega_{\mathbf{K}}{}^{(1)}(AB)]G_{\mathbf{K}}{}^{AB}(Z), \tag{2.9a}$$

which gives

$$G_{\mathbf{K}}{}^{AB}(Z)=\frac{1/2\pi\omega_{\mathbf{K}}{}^{(1)}(AB)}{Z-\omega_{\mathbf{K}}{}^{(2)}(AB)/\omega_{\mathbf{K}}{}^{(1)}(AB)}. \tag{2.9b}$$

This result is easily derived by writing

$$G_{\mathbf{K}}{}^{CB}(Z)=\alpha G_{\mathbf{K}}{}^{AB}(Z) \tag{2.10a}$$

and inserting it into the Fourier transform of Eq. (2.7) to get

$$G_{\mathbf{K}}{}^{AB}(Z)=(1/2\pi)\omega_{\mathbf{K}}{}^{(1)}(AB)[Z-\alpha]^{-1}. \tag{2.10b}$$

But, according to Eq. (2.2), we also have

$$G_{\mathbf{K}}{}^{AB}(Z)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\omega\,F_{\mathbf{K}}{}^{AB}(\omega)/(Z-\omega). \tag{2.10c}$$

Here the unknown coefficient α is chosen to conserve the maximum number of frequency moments $\omega_{\mathbf{K}}{}^{(n)}(AB)$. Moreover, since α is assumed to be independent of Z, therefore, for all choices of α, the right-hand sides of Eqs. (2.10b) and (2.10c) are identical to the first order in $(Z)^{-1}$ in the large Z expansion. Consequently, all Z independent choices for α will conserve the first frequency moment $\omega_{\mathbf{K}}{}^{(1)}(AB)$. To conserve the second frequency moment, i.e., to get the coefficients of the $(Z)^{-2}$ terms to be identical in the large Z expansions of the right-hand side of Eqs. (2.10b) and (2.10c), α must equal $\omega_{\mathbf{K}}{}^{(2)}(AB)/\omega_{\mathbf{K}}{}^{(1)}(AB)$.

In the above problem, if we had first written the equation of motion of the higher-order Green's function $G_{\alpha\beta}{}^{CB}(Z)$, i.e.,

$$ZG_{\alpha\beta}{}^{CB}(Z)=(1/2\pi)\omega_{\alpha\beta}{}^{(2)}(AB)+G_{\alpha\beta}{}^{DB}(Z), \tag{2.11a}$$

where

$$\left(i\frac{d}{dt}\right)^2A_\alpha(t)=[C_\alpha(t),\mathcal{H}]_-=D_\alpha(t), \tag{2.11b}$$

and then carried out the MCD at this second stage, we would have had the choice of decoupling $G_{\mathbf{K}}{}^{DB}(Z)$ in terms of the two lower-order Green's functions, i.e., $G_{\mathbf{K}}{}^{AB}(Z)$ and $G_{\mathbf{K}}{}^{CB}(Z)$. Such a decoupling, i.e.,

$$G_{\mathbf{K}}{}^{DB}(Z)=\alpha_1G_{\mathbf{K}}{}^{AB}(Z)+\alpha_2G_{\mathbf{K}}{}^{CB}(Z), \tag{2.12}$$

where both α_1 and α_2 are independent of Z, can at best be expected to conserve the first four frequency moments of the spectral function $F_{\mathbf{K}}{}^{AB}(\omega)$, i.e., $\omega_{\mathbf{K}}{}^{(n)}(AB)$ for $n=1,\ldots,4$. To see this, insert Eq. (2.12) into the Fourier transform of Eq. (2.11a) and substitute the results into the Fourier transform of Eq. (2.7). This immediately leads to

$$G_{\mathbf{K}}{}^{AB}(Z)=\frac{1}{2\pi}\frac{\omega_{\mathbf{K}}{}^{(1)}(AB)(Z-\alpha_2)+\omega_{\mathbf{K}}{}^{(2)}(AB)}{Z(Z-\alpha_2)-\alpha_1}. \tag{2.13}$$

Equating the right-hand side of the above to that of Eq. (2.10c), and comparing coefficients of $(Z)^{-n}$ in the large Z expansion of the two equations, we easily find that α_1 and α_2 have to be chosen as follows in order to con-

serve the maximum possible number of frequency moments:

$$\alpha_1=\{\omega_K^{(2)}(AB)\omega_K^{(4)}(AB)-[\omega_K^{(3)}(AB)]^2\}\times\{[\omega_K^{(2)}(AB)]^2-\omega_K^{(1)}(AB)\omega_K^{(3)}(AB)\}^{-1}, \quad (2.14a)$$

$$\alpha_2=[\omega_K^{(2)}(AB)\omega_K^{(3)}(AB)-\omega_K^{(1)}(AB)\omega_K^{(4)}(AB)]\times\{[\omega_K^{(2)}(AB)]^2-\omega_K^{(1)}(AB)\omega_K^{(3)}(AB)\}^{-1}. \quad (2.14b)$$

The above choice leads to an expression for $F_K^{AB}(\omega)$ which automatically conserves the four frequency moments $\omega_K^{(n)}(AB)$ for $n=1, \ldots, 4$.

By induction, the more general statement can now be made: Whenever the decoupling is made at the nth stage in the hierarchy of the Green's-function equations of motion, in such a way that the next order Green's function is represented in terms of a linear combination of all the lower-order Green's functions, then the optimal choice of the coefficients would be such that the resultant spectral function of the basic Green's function would conserve a total of $2n$ frequency moments. More specifically, when the MCD is carried out at the nth stage, the basic Green's function has the form

$$G_K^{AB}(Z)=\frac{1}{2\pi}\sum_{i=0}^{n-1}a_i(Z)^i/[Z^n+\sum_{i=0}^{n-1}b_i(Z)^i]. \quad (2.15)$$

The $2n$ parameters, a_i and b_i, can be determined completely from the knowledge of the first $2n$ frequency moments $\omega_K^{(p)}(AB)$, $p=1, \ldots, 2n$.

In the light of the above discussion, it is clear that the spectral line shapes $F_K^{AB}(\omega)$, generated by such a procedure, i.e., the MCD, are of a somewhat restricted variety. For instance, because the spectral function $F_K^{AB}(\omega)$ is related to the Green's function $G_K^{AB}(Z)$ in the manner

$$\lim_{\epsilon\to+0}2iG_K^{AB}(\omega+i\epsilon)=F_K^{AB}(\omega), \quad (2.16)$$

it is therefore possible for the resultant $F_K^{AB}(\omega)$ to be composed of n Dirac δ functions (this would happen when the polynomial

$$x^n+\sum_{i=0}^{n-1}b_ix^i=0$$

has n distinct, real roots).

It is instructive to compare the predictions of the above MCD procedure for the line shape $F_K^{zz}(\omega)$,

$$F_K^{zz}(\omega)=\frac{1}{2\pi}\sum_R e^{-i\mathbf{K}\cdot\mathbf{R}}\times\int_{-\infty}^{+\infty}\langle[S_R^z(t),S_0^z(0)]_-\rangle e^{+i\omega t}dt, \quad (2.17)$$

in a Heisenberg paramagnet at elevated temperatures. (For a complete discussion of this problem see Refs. 3 and 10.) For this case the first few frequency moments $\omega_K^{(n)}(zz)$,

$$\omega_K^{(n)}(zz)=\int_{-\infty}^{+\infty}d\omega\,[F_K^{zz}(\omega)/\omega]\omega^n d\omega, \quad (2.18)$$

are known. Moreover, because the function $F_K^{zz}(\omega)/\omega$ is even in ω [note that Eq. (2.17), unlike Eq. (2.3), only refers to a commutator correlation], its odd moments, $\omega_K^{(2n+1)}(zz)$, are vanishing and therefore, from Eqs. (2.13) and (2.16), we readily get

$$\langle\langle S_g^z(t);S_p^z(t')\rangle\rangle_{(K,Z)}\equiv G_K^{zz}(Z)=\frac{1}{2\pi}\omega_K^{(2)}(zz)[Z^2-\omega_K^{(4)}(zz)/\omega_K^{(2)}(zz)]^{-1}, \quad (2.19a)$$

$$F_K^{zz}(\omega)=\frac{[\omega_K^{(2)}(zz)]^{3/2}}{2[\omega_K^{(4)}(zz)]^{1/2}}\left\{\delta\left[\omega-\left(\frac{\omega_K^{(4)}(zz)}{\omega_K^{(2)}(zz)}\right)^{1/2}\right]-\delta\left[\omega+\left(\frac{\omega_K^{(4)}(zz)}{\omega_K^{(2)}(zz)}\right)^{1/2}\right]\right\}. \quad (2.19b)$$

The result (2.19b) does, of course, conserve the moments $\omega_K^{(n)}(zz)$ for $n=1, 2, 3$, and 4, but in the light of what is known about the structure of $F_K^{zz}(\omega)$ (see Refs. 3 and 11), this result is quite meaningless. On the other hand, the generalized diffusivity formulations,[5–11] lead to a much more meaningful result for $F_K^{zz}(\omega)$ even though they make use of somewhat similar basic information, i.e., the diffusivity formulations[5–11] make use of $\omega_K^{(n)}(zz)$ for $n=0, 1, \ldots, 4$. [Note that the expression (2.19b) does not conserve the zeroth frequency moment $\omega_K^{(0)}(zz)$. Indeed, it suggests that $\omega_K^{(0)}(zz)=[\omega_K^{(2)}(zz)]^2/\omega_K^{(4)}(zz)$.]

In addition to the aforementioned limitation, the MCD also possesses the following rather disconcerting weaknesses: First, it is clear that instead of first finding $G_K^{AB}(Z)$ in terms of $\omega_K^{(n)}(AB)$, we can also determine $G_{gp}^{AB}(Z)$ directly in terms of $\omega_{gp}^{(n)}(AB)$. In that case, Eqs. (2.13), (2.14a) (2.14b), and (2.15) still retain the present form with the difference that the inverse-lattice label $\mathbf{K}$ is everwhere replaced by the real-lattice vector $(\mathbf{g}-\mathbf{p})$. It is clear that the two resultant expressions for $G_{gp}^{AB}(Z)$, obtained in these two alternative fashions, in general do not agree with each other.

The second disconcerting inconsistency that the MCD suffers from is that the two formulations of the problem obtained by using either a commutator or an anticommutator correlation function [see Eqs. (2.3)–(2.15)] are, in general, not mutually equivalent if the decoupling is carried out at an arbitrary stage. That this inconsistency can be quite disturbing is demonstrated by reanalyzing the problem of the spectral line shape in the Heisenberg paramagnet at elevated temperatures. Instead of using the commutator formulation employed in Eqs. (2.17)–(2.19b) above, we now use an anticommutator formulation throughout, i.e., beginning with

the Green's function. In view of the fact that we have already recorded some of the relevant mathematical details of the commutator formalism, we shall not repeat, in the following, the corresponding details for the anticommutator formulation. The only thing that need be mentioned here is that if we follow the foregoing procedure for the anticommutator case also, we are readily led to an expression for the spectral function of the anticommutator correlation function. This expression for the anticommutator spectral function is such that it automatically conserves its four frequency moments with $n=1, \ldots, 4$. At elevated temperatures the anticommutator spectral function is very simply related to the commutator spectral function $F_K{}^{zz}(\omega)$—it is equal to $2F_K{}^{zz}(\omega)/\beta\omega$—and the anticommutator frequency moments are also similarly simply related to the commutator frequency moments of one lower order than themselves—the nth anticommutator frequency moment is equal to $(2/\beta)$ times the $(n-1)$th commutator frequency moment. Therefore, the final result can be completely recast in terms of the commutator notation used in Eqs. (2.17)—(2.19b). One finds that the final result of the anticommutator procedure is quite different from Eq. (2.19b), being of the form

$$F_K{}^{zz}(\omega)=\tfrac{1}{2}\omega_K{}^{(0)}(zz)\omega\left\{\delta\left[\omega-\left(\frac{\omega_K{}^{(2)}(zz)}{\omega_K{}^{(0)}(zz)}\right)^{1/2}\right]+\delta\left[\omega+\left(\frac{\omega_K{}^{(2)}(zz)}{\omega_K{}^{(0)}(zz)}\right)^{1/2}\right]\right\}. \quad (2.20)$$

This result is such that it also conserves a total of four frequency moments of the commutator spectral function $F_K{}^{zz}(\omega)$, but these moments are $\omega_K{}^{(n)}(zz)$, with $n=0$, 1, 2, and 3 rather than with $n=1, \ldots, 4$ as was the case for the expression (2.19b).

It should perhaps be emphasized that the above example illustrates a point of general validity. Namely, the basic difference between the commutator and the anticommutator formulations is that the frequency moments being conserved are of different spectral functions. In the classical (or in the infinite temperature) limit, the two functions are simply related to each other, and then the commutator and the anticommutator formulations differ only in providing results which conserve one different frequency moment, i.e., the commutator formulation conserves the frequency moments $n=1, \ldots, 2p$, whereas the anticommutator formulation conserves the set of frequency moments $n=0, 1, \ldots, 2p-1$, where p is the order of the stage at which the decoupling is introduced. Moreover, the algorithm generated by the MCD procedure is such that the two resultant expressions for the line shape may be very different from each other.

To conclude this section it should be mentioned that the two aforementioned inconsistencies can be arbitrarily removed by making the following assumptions. First, the Green's function should always first be calculated in the inverse-lattice representation. The second inconsistency can also be similarly removed by making the arbitrary stipulation that, for boson operators, only the commutator formulation should be used, whereas for fermion operators, the relevant formulation should obviously be only in terms of the anticommutator correlation function. However, this stipulation still leaves the procedure for spin problems undefined because the spin operators obey neither the Bose nor the Fermi statistics.

3. ROTH'S ALGORITHM

In Sec. 2 we outlined in detail the various limitations of the MCD algorithm for constructing the spectral line shapes from the knowledge of their various lowest-order frequency moments. It is interesting to note that another procedure for linearizing many-body equations of motion in statistical mechanics has also been propounded. We shall call it Roth's algorithm (RA). This procedure was originally claimed to be well defined and to be related to a stationary principle.[12] However, recently Young[26] has noted that the variational aspect of the RA is nothing but a different definition for constructing frequency moment conserving line shapes. Moreover, Young has noted that when the RA is used optimally—meaning when the basis set is chosen so as to conserve the maximum number of frequency moments of the desired spectral function—then it reproduces the results of our MCD procedure.

The above description of the RA is in complete accord with our understanding. Therefore, it is clear that even the optimal use of the RA will have all the failings which we have noted in Sec. 2 with regard to the use of the MCD.

No general statement about the less than the best use of the RA can, however, be made since the quality of the result will then depend upon the choice of the basis set used.

4. SCMCD AND HEISENBERG SPIN SYSTEM

In this section the concept of self-consistent moment conserving decoupling (SCMCD) scheme is introduced. To illustrate the use of SCMCD, we have chosen to study a Heisenberg spin system. For the ease of computation, we assume the spatial range of the exchange interaction to be limited only to the nearest-neighbor separation. This is, of course, not an essential limitation and the same technique can also be applied to systems with longer-range exchange interactions.

It is instructive to consider first the more general case of anisotropic exchange interaction. The relevant Hamiltonian is assumed to have the form

$$\mathcal{H}=-\mu\sum_f S_f{}^z-\sum_{f_1,f_2} I_+(f_1f_2)(S_{f_1}{}^xS_{f_2}{}^x+S_{f_1}{}^yS_{f_2}{}^y)-\sum_{f_1,f_2} I_0(f_1f_2)S_{f_1}{}^zS_{f_2}{}^z. \quad (4.1)$$

[26] R. A. Young, Phys. Rev. 184, 601 (1969).

The assumption of only the nearest-neighbor interactions implies

$$I(f_1 f_2) = I_\alpha, \quad \text{when } f_1 \text{ and } f_2 \text{ are nearest neighbors} \tag{4.2a}$$

$$= 0, \quad \text{otherwise} \tag{4.2b}$$

$$\alpha \equiv +, \quad 0. \tag{4.2c}$$

The first term on the right-hand side of Eq. (4.1) refers to the Zeeman energy of the spin system in the presence of a spatially uniform z-directed external field proportional to μ. The second and the third terms, respectively, represent the exchange interaction between the transverse and the longitudinal components of the spins.

Under the Hamiltonian (4.1), the equation of motion of the retarded and the advanced Green's function [see Eq. (2.1) for the definition of the Green's function] $G_{gp}(t-t')$,

$$\langle\langle S_g^+(t); S_p^-(t')\rangle\rangle = G_{gp}(t-t'), \tag{4.3}$$

is

$$(Z-\mu)G_{gp}(Z) = (\sigma/\pi)\delta_{gp} + 2\sum_f I_0(gf)\langle\langle S_f^z S_g^+; S_p^-\rangle\rangle_{(Z)} - 2\sum_f I_+(gf)\langle\langle S_g^z S_f^+; S_p^-\rangle\rangle_{(Z)}, \tag{4.4}$$

where, as usual, the Green's function $G_{gp}(Z)$ is the analytic extension of the Fourier transform $G_{gp}(\omega)$,

$$G_{gp}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dt\, e^{i\omega t}\langle\langle S_g^+(t); S_p^-(0)\rangle\rangle, \tag{4.5}$$

to the complex frequency plane Z, and where

$$\sigma = \langle S_g^z\rangle. \tag{4.6}$$

The right-hand side of Eq. (4.4) contains higher-order Green's function, and if we carry out the MCD approximation at the very first stage, then we must represent these Green's functions in terms of a linear combination of the basic Green's function $G_{gp}(Z)$. The most general such linear combination with Z-independent parameters is of the type

$$I_0(gf)\langle\langle S_f^z S_g^+; S_p^-\rangle\rangle_{(Z)} - I_+(gf)\langle\langle S_g^z S_f^+; S_p^-\rangle\rangle_{(Z)} \sim C(gf)G_{gp}(Z) + D(gf)G_{fp}(Z). \tag{4.7}$$

The parameters $C(gf)$ and $D(gf)$ are not linearly independent, and they are fixed completely by only one requirement, namely, the first terms in the large Z expansion of the left- and the right-hand sides of Eq. (4.7) must coincide. This condition readily leads to the equation

$$[2I_0(gf)L^{(0)}(gf) + I_+(gf)\Psi^{(0)}(gf)]\delta_{g,f} - [I_0(gf)\Psi^{(0)}(gf) + 2I_+(gf)L^{(0)}(gf)]\delta_{f,p} = 2\sigma[C(gf)\delta_{g,p} + D(gf)\delta_{f,p}]. \tag{4.8}$$

Here, we have introduced the notation that for $g \neq f$

$$L^{(0)}(gf) = \langle S_g^z S_f^z\rangle,$$
$$\Psi^{(0)}(gf) = \langle S_g^\pm S_f^\mp\rangle = \langle S_f^\pm S_g^\mp\rangle. \tag{4.9}$$

Note that for the case not covered by Eq. (4.9), i.e., when $g=f$, the exchange integrals $I_\alpha(gf)$ are identically vanishing. Consequently, the above notation suffices for the present purposes.

Because the equality (4.8) is to hold for all locations p, the coefficients of the linearly independent constraints represented by $\delta_{g,p}$ and $\delta_{f,p}$ must separately be equal on the two sides of Eq. (4.8). This readily determines the unknown coefficients $C(gf)$ and $D(gf)$

$$C(gf) = (1/2\sigma)[2I_0(gf)L^{(0)}(gf) + I_+(gf)\Psi^{(0)}(gf)],$$
$$-D(gf) = (1/2\sigma)[I_0(gf)\Psi^{(0)}(gf) + 2I_+(gf)L^{(0)}(gf)]. \tag{4.10}$$

At this juncture it is convenient to postulate the basic requirement of the first-order self-consistent MCD. The moment conserving decoupling given in Eqs. (4.7) and (4.10) would be a self-consistent MCD if it leads to self-consistent results for the relevant time-independent statistical correlation functions which follow directly from the Green's functions on the two sides of Eq. (4.7). Clearly, this means that for the functions $C(gf)$ and $D(gf)$ given in Eq. (4.10) we must have[27]

$$I_0(gf)\langle S_f^z S_g^+ S_p^-\rangle - I_+(gf)\langle S_g^z S_f^+ S_p^-\rangle = C(gf)\langle S_g^+ S_p^-\rangle + D(gf)\langle S_f^+ S_p^-\rangle. \tag{4.11}$$

[This result follows directly by using the spectral representation of the Green's function given in Eqs. (2.2) and (2.16) into Eq. (4.7).] Because Eq. (4.11) is to hold for all locations p, it must in particular hold when $p=g$ and $p=f$.

While all the essential results of the present paper will be worked out for the case of general spin, to illustrate the derivation of a properly self-consistent MCD scheme, it is convenient first to specialize the following remarks only to the case of spin $\frac{1}{2}$. The great simplicity of the spin-$\frac{1}{2}$ result arises because in addition to the usual spin-commutation rules, for the case of spin $\frac{1}{2}$ the kinematic conditions are particularly easy to work with, i.e.,

$$S_g^+ S_g^- + S_g^- S_g^+ = 1,$$
$$S_g^z S_g^\pm = \pm\tfrac{1}{2} S_g^\pm, \tag{4.12}$$
$$S_g^\pm S_g^z = \mp\tfrac{1}{2} S_g^\pm.$$

For $S=\frac{1}{2}$ the consequences of using Eq. (4.10) into Eq. (4.11) for the case when $p=g$ are, in general, inconsistent with those when $p=f$. To see this let us first insert Eq. (4.10) into Eq. (4.11), put $p=g$, use the kinematic relations (4.12), and then solve for $L^{(0)}(gf)$ in terms of

[27] Note that the other time-independent relationship, which also follows directly from Eq. (4.7), i.e., $I_0(gf)\langle S_p^- S_f^z S_g^+\rangle - I_+(gf)\langle S_p^- S_g^z S_f^+\rangle = C(gf)\langle S_p^- S_g^+\rangle + D(gf)\langle S_p^- S_f^+\rangle$, is not linearly independent of Eq. (4.11) because of our conserving choice for functions $C(gf)$ and $D(gf)$ given in Eq. (4.10).

$\Psi^{(0)}(gf)$. This readily leads to the result

$$L^{(0)}(gf) = [I_+(gf)\Psi^{(0)}(gf) - 2I_0(gf)(\Psi^{(0)}(gf))^2 - 2\sigma^2 I_0(gf)] \times [4I_+(gf)\Psi^{(0)}(gf) - 2I_0(gf)]^{-1}. \quad (4.13a)$$

Now, if we repeat the same procedure and use the limit $p=f$, instead of the limit $p=g$, we are led to the following result:

$$L^{(0)}(gf) = [I_0(gf)\Psi^{(0)}(gf) - 2I_+(gf)(\Psi^{(0)}(gf))^2 - 2\sigma^2 I_+(gf)] \times [4I_0(gf)\Psi^{(0)}(gf) - 2I_+(gf)]^{-1}. \quad (4.13b)$$

Clearly, the results (4.13a) and (4.13b) are self-inconsistent, unless[28]

$$I_+(gf) = I_0(gf) \equiv I(gf). \quad (4.14)$$

The above illustration provides some insight into an important limitation of the SCMCD scheme. The requirement of self-consistency may indeed be used to determine the unknown frequency moments. However, unless the system Hamiltonian possesses additional internal symmetries which ensure that the various possible such determinations of the unknown moments are self-consistent within themselves, the SCMCD cannot be reliably used.

In the light of the above, we shall limit all further discussion to the case of isotropic exchange interaction $I(gf)$. Moreover, for convenience the only nonvanishing $I(gf)$ will be assumed to be between nearest-neighbor spins, and in order that it lead to a ferromagnetic ground state this exchange integral I will be assumed to be positive. It is now convenient to recast Eqs. (4.10) and (4.11) into the form

$$C = -D = (1/2\sigma)(2L^0 + \psi^0), \quad (4.15a)$$

$$C = [S(S+1)\sigma - L^0 - L' - \psi' - \psi^0] \times S[(S+1) - \sigma - M - \psi^0]^{-1}. \quad (4.15b)$$

Here we have introduced the abbreviated notation

$$C(\delta)/I(\delta) = C, \quad (4.16a)$$

$$D(\delta)/I(\delta) = D, \quad (4.16b)$$

$$L^0 = L^{(0)}(\delta), \quad (4.16c)$$

$$\psi^0 = \Psi^{(0)}(\delta), \quad (4.16d)$$

$$L' = \langle S_{g\pm\delta}{}^z (S_g{}^z)^2 \rangle = \langle S_g{}^z (S_{g\pm\delta}{}^z)^2 \rangle, \quad (4.16e)$$

$$\psi' = \langle S_g{}^z S_g{}^- S_{g\pm\delta}{}^+ \rangle = \langle S_{g\pm\delta}{}^+ S_g{}^z S_g{}^- \rangle, \quad (4.16f)$$

$$M = \langle (S_g{}^z)^2 \rangle. \quad (4.16g)$$

[28] In addition to the case given in Eq. (4.14), there possibly exists one other situation where Eqs. (4.13a) and (4.13b) are self-consistent. This would be the case in the Ising limit $I_+(gf) \to 0$ if the corresponding $\psi^{(0)}(gf)$ went to zero faster than $I_+(gf)$. The resultant $L^{(0)}(gf)$ would then be the molecular field expression, i.e., $=\sigma^2$.

Here δ denotes any of the z nearest-neighbor vectors (z is the coordination number of the lattice). [Note that because, of all possible $I(gf)$, only $I(\delta)$ is nonvanishing, the set of relations (4.15), (4.15b), and (4.16a)–(4.16g) suffice for all further discussions.]

The additional complexity of the general spin case is now clear. Whereas for the simple case of $S=\frac{1}{2}$ the only unknown parameters entering the Green's function Eq. of motion were ψ^0, L^0, and σ, for the general spin case the additional unknowns L', ψ', and M also appear in these equations of motion. Before we deal with this complexity it is convenient to write down the result for the Green's function $G_{\mathbf{K}}(Z)$ which follows from Eqs. (4.4), (4.7), and (4.15a),

$$G_{\mathbf{K}}(Z) = (\sigma/\pi)[Z - E_{\mathbf{K}}(S)]^{-1}, \quad (4.17)$$

$$E_{\mathbf{K}}(S) = \mu + 2C[J(0) - J(\mathbf{K})], \quad (4.18)$$

$$J(\mathbf{K}) = I \sum_{\delta} e^{i\mathbf{K}\cdot\delta}. \quad (4.19)$$

The above results now immediately lead to the following:

$$\langle S_g{}^- S_g{}^+ \rangle = S(S+1) - \sigma - M = 2\sigma\Phi(S), \quad (4.20)$$

$$\psi^0 = (2\sigma/N) \sum_{\mathbf{K}} [J(K)/J(0)]\Phi_{\mathbf{K}}(S), \quad (4.21)$$

$$\langle S_g{}^+ S_f{}^- \rangle = (2\sigma/N) \sum_{\mathbf{K}} [\Phi_{\mathbf{K}}(S) + 1] e^{i\mathbf{K}\cdot(\mathbf{g}-\mathbf{f})}, \quad (4.22)$$

where

$$\Phi_{\mathbf{K}}(S) = (e^{\beta E_{\mathbf{K}}(S)} - 1)^{-1}, \quad (4.23a)$$

$$\Phi(S) = 1/N \sum_{\mathbf{K}} \Phi_{\mathbf{K}}(S). \quad (4.23b)$$

The implicit dependence of $\Phi_{\mathbf{K}}$ and Φ on the spin S arises because the elementary excitation energy $E_{\mathbf{K}}$ is implicitly dependent upon S through its dependence upon C.

The results (4.17)–(4.23b) are of the same general form as those obtained within the usual decoupling schemes such as the RPA[21] and the Callen[15] decoupling. As shown by Callen and Shtrikman,[29] an implication of such a decoupling scheme, or alternatively of the Eqs. (4.17)–(4.23), is that the average $\langle (S_g{}^z)^n \rangle$ is related to $\Phi(s)$, i.e.,

$$\langle (S_g{}^z)^n \rangle = \left(\frac{d^n \Omega(x)}{dx^n} \right)_{x=0}, \quad (4.24a)$$

$$\Omega(x) = \langle e^{xS_g{}^z} \rangle = \frac{(\Phi(S))^{2S+1} e^{-xS} + (1+\Phi(S))^{2S+1} e^{(S+1)x}}{[(\Phi(S))^{2S+1} - (1+\Phi(S))^{2S+1}][(1+\Phi(S))e^x - \Phi(S)]}. \quad (4.24b)$$

[29] H. B. Callen and S. Shtrikman, Solid State Commun. 3, 5 (1965).

Similarly, it can be shown (see the Appendix) that under a similar assumption the correlations $\langle S_g^{\pm} e^{xS_f^z} S_f^{\mp}\rangle$ are related to the correlations $\langle S_g^{\pm} S_f^{\mp}\rangle$ through the relationships[30]:

$$\langle S_g^{\pm} e^{xS_f^z} S_f^{\mp}\rangle = \Gamma^{(\pm)}(x)\langle S_g^{\pm} S_f^{\mp}\rangle, \quad (4.25a)$$

where

$$\Gamma^{(\pm)}(x) = (1/2\sigma)\langle [S_g^{\pm}, e^{xS_g^z} S_g^{\mp}]_{-}\rangle. \quad (4.25b)$$

[Here we take either all the upper signs or all the lower signs on the two sides of Eqs. (4.25a) and (4.25b).]

As a result of the relationships (4.24a)–(4.25b), the additional functions ψ' and M are no longer unknown but are determined in terms of $\Phi(S)$ and ψ^0, i.e.,

$$M = S^2 + (1-2S)\Phi(S) + 2[\Phi(S)]^2 - \frac{(1+2S)[1+2\Phi(S)][\Phi(S)]^{2S+1}}{[1+\Phi(S)]^{2S+1} - [\Phi(S)]^{2S+1}}, \quad (4.26)$$

$$\psi' = [3M - \sigma - S(S+1)]\psi^0/2\sigma, \quad (4.27)$$

where

$$\sigma = \frac{[S-\Phi(S)][1+\Phi(S)]^{2S+1} + [1+S+\Phi(S)][\Phi(S)]^{2S+1}}{[1+\Phi(S)]^{2S+1} - [\Phi(S)]^{2S+1}}. \quad (4.28)$$

The only additional function that enters the discussion of the general spin case and is still unspecified, is L'. In the Appendix we sketch an argument—within a scheme similar in spirit to the Callen and Shtrikman algorithm—in which the correlations $\langle (S_g^z)(S_f^z)^n\rangle$ are all related to the lowest-order longitudinal correlation $\langle S_g^z S_f^z\rangle$ through the generating function relationship

$$\langle S_f^z e^{xS_g^z} S_g^z\rangle - \sigma\frac{d\Omega(x)}{dx} = \left(\frac{\langle S_f^z S_g^z\rangle - \sigma^2}{M-\sigma^2}\right)\left(\frac{d^2\Omega(x)}{dx^2} - \sigma\frac{d\Omega(x)}{dx}\right). \quad (4.29)$$

Therefore, we get

$$L' = \sigma M + (L^0 - \sigma^2)(\rho - \sigma M)/(M-\sigma^2), \quad (4.30)$$

where

$$\rho = \langle (S_g^z)^3\rangle = S^3 + (3S-1-3S^2)\Phi(S) + 6(S-1)[\Phi(S)]^2 - 6[\Phi(S)]^3 + (2S+1)[\Phi(S)]^{2S+1} \times \{S^2+S+1+6\Phi(S)[1+\Phi(S)]\} \times \{[1+\Phi(S)]^{2S+1} - [\Phi(S)]^{2S+1}\}^{-1}. \quad (4.31)$$

The relationships (4.26)–(4.31) are all functions of only three unknowns L^0, ψ', and $\Phi(S)$. However, if we now equate the right-hand sides of Eqs. (4.15a) and (4.15b), we get an additional relationship which reduces the unknowns to only two, i.e., $\Phi(S)$ and ψ^0. These quantities, however, are in turn determined from the knowledge of $E_K(S)$ [see Eqs. (4.21)–(4.23b)] which itself depends upon C. Therefore, let us next attend to the job of expressing C in terms of $\Phi(S)$ and ψ^0.

Following the scheme proposed in the preceding paragraph, i.e., using Eqs. (4.15a), (4.15b), and (4.30) to eliminate L' and L^0, we find

$$C = \frac{\sigma[S(S+1) - M + \gamma] + [S(S+1) - 3M + \gamma]\psi^0/2\sigma}{S(S+1) - M - \psi^0 + \gamma}, \quad (4.32)$$

where

$$\gamma = \sigma(\rho - \sigma M)/(M-\sigma^2). \quad (4.33)$$

The set of equations (4.18), (4.21), (4.23a), (4.23b), (4.28), (4.31), (4.32a), and (4.32b) lead to a closed scheme, involving implicit transcendental relationships from which $\Phi(S)$, ψ^0—and in turn the magnetization σ, the longitudinal correlation, and the system energy, etc.—may be calculated.

The foregoing remarks are applicable to the case of general spin. It is interesting, however, to ask what these results look like in the extreme limit of spin $\frac{1}{2}$. For spin $\frac{1}{2}$, the spin kinematics require that

$$M = \tfrac{1}{4}; \quad \rho = \tfrac{1}{4}\sigma. \quad (4.33')$$

Therefore

$$\gamma = 0, \quad (4.34)$$

and C reduces to the extremely simple form

$$C = (\tfrac{1}{2}\sigma)[\tfrac{1}{2} - \psi^0]^{-1}, \quad \text{for} \quad S = \tfrac{1}{2} \quad (4.35)$$

Moreover, Eq. (4.20) also simplifies, and we get

$$\sigma = (\tfrac{1}{2})[1 + 2\Phi(\tfrac{1}{2})]^{-1}, \quad \text{for} \quad S = \tfrac{1}{2} \quad (4.36)$$

The relationships (4.18), (4.21), (4.35), and (4.36) are identical with those obtained by Mubayi and Lange[14] (ML) in their study of the properties of a two-dimensional spin-$\frac{1}{2}$ Heisenberg ferromagnet. To the extent that the present work achieves the same decoupling as recently derived by ML, it may be considered to be an extension of their decoupling to general spin values as well as an extension of their results to one and three dimensions. However, since the arguments used by ML were rather different than those presented here, this paper may also be considered to provide further insights into the decoupling proposed by ML.

5. SERIES EXPANSION SCHEMES

The coupled, implicit relationships involving σ, ψ^0, and L^0 obtained in Sec. 4 cannot in general be solved analytically. However, since these quantities are themselves functions of $\Phi(S)$, it is possible to derive series expansions for them which are valid in the extreme limits $\Phi(S) \ll 1$ and $\Phi(S) \gg 1$.

[30] See also, M. E. Lines, Phys. Rev. 156, 534 (1967).

First, let us consider the case of $\Phi(S)\ll 1$. Here from Eqs. (4.28), (4.26), and (4.31), we get

$$\begin{aligned}\sigma&=S-\Phi(S)+(2S+1)[\Phi(S)]^{2S+1}+O,\\ M&=S^2+(1-2S)\Phi(S)+2[\Phi(S)]^2\\&\quad-(1+2S)[\Phi(S)]^{2S+1}+O,\\ \rho&=S^3+(3S-1-3S^2)\Phi(S)+6(S-1)[\Phi(S)]^2\\&\quad+(2S+1)(S^2+S+1)[\Phi(S)]^{2S+1}+O,\\ O&\equiv O([\Phi(S)]^{2S+2},[\Phi(S)]^3).\end{aligned}\tag{5.1}$$

Inserting the above into Eq. (4.32b) we get

$$\gamma=S(2S-1)+(1-6S)\Phi(S)+2S^2(2S+1)^2[\Phi(S)]^{2S}+O([\Phi(S)]^2,[\Phi(S)]^{2S+1}).\tag{5.2}$$

Using Eqs. (5.1) and (5.2), Eq. (4.32a), we find the appropriate result for C:

$$C=S-\Phi(S)+\psi^0/2S+O(\psi^0\Phi(S),[\Phi(S)]^2),\quad\text{for}\quad\Phi(S)\ll 1.\tag{5.3}$$

For the opposite limiting case of $\Phi(S)\gg 1$, the algebra is quite tedious. The relevant results are

$$\begin{aligned}\sigma&=X\Phi^{-1}(S)[1-\tfrac{1}{2}\Phi^{-1}(S)+\tfrac{1}{10}(3-2X)]\Phi^{-2}(S)]\\&\quad+O(\Phi^{-4}(S)),\\ M&=X+\tfrac{1}{10}[\Phi^{-2}(S)]X(4X-1)[1-\Phi^{-1}(S)\\&\quad-(2/7)(X-3)\Phi^{-2}(S)]+O(\Phi^{-5}(S)),\\ \rho&=\tfrac{1}{5}X(3X-1)\Phi^{-1}(S)[1-\tfrac{1}{2}\Phi^{-1}(S)]\\&\quad-(X/210)\Phi^{-3}(S)(6S^4+12S^3-28S^2-34S+9)\\&\quad+O(\Phi^{-4}(S)),\end{aligned}\tag{5.4}$$

where we have used the notation

$$X=\tfrac{1}{3}S(S+1).\tag{5.5}$$

Using the above expansions into Eq. (4.32b), we get

$$\gamma=\tfrac{1}{5}X\Phi^{-2}(S)\{(4X-1)[1-\Phi^{-1}(S)]+[\Phi^{-2}(S)/420](-32S^4-64S^3+476S^2+508S-363)\}+O(\Phi^{-5}(S)),\quad\text{for}\quad\Phi(S)\gg 1.\tag{5.6}$$

The relevant expression for C can now be obtained

$$\begin{aligned}C&=C(\text{num})/C(\text{denom}),\\ C(\text{num})&=\Phi^{-1}(S)\{2X^2[1-\tfrac{1}{2}\Phi^{-1}(S)+\tfrac{1}{4}\Phi^{-2}(S)]\\&\quad-[(4X-1)/20](1-\tfrac{1}{2}\Phi^{-1}(S)\\&\quad-[\Phi^{-2}(S)/140][(44X-41)\psi^0]\}\\&\quad+O(\Phi^{-3}(S)),\\ C(\text{denom})&=2X\{1+[\Phi^{-2}(S)/20](4X-1)\}-\psi^0\\&\quad+O(\Phi^{-3}(S)).\end{aligned}\tag{5.7}$$

6. RESULTS IN THREE DIMENSIONS

In the present section the series expansion solutions, outlined in Sec. 5, will be used to study three-dimensional lattices. For simplicity we shall limit our discussion to lattices of cubic symmetry only.

A. Low Temperatures

The limiting case of $\Phi(S)\ll 1$ is self-consistently satisfied in the limit of low temperatures,[31] i.e., when

$$k_BT=\beta^{-1}\ll 4SJ(0),\tag{6.1}$$

where k_B is the Boltzmann constant. Here a straightforward iteration procedure, which uses a power expansion in the ratio

$$\theta=3k_BT/4\pi\nu_0SJ(0),\tag{6.2a}$$

$$\begin{aligned}\nu_0&=1,\quad\text{for sc lattice}\\&=\tfrac{3}{4}(2)^{2/3},\quad\text{bcc}\\&=(2)^{1/3},\quad\text{fcc}\end{aligned}\tag{6.2b}$$

is found to be rapidly convergent. The details of this calculation are in many ways similar to those used relating to spin-wave theories[16–19] and will not be given here. For the zeroth-order results we put $C=S$ and find:

$$\Phi(S)=a_0\theta^{3/2}+a_1\theta^{5/2}+O,\quad\text{for}\quad\theta\ll 1\tag{6.3a}$$

$$\psi^0=2S[a_0\theta^{3/2}-\tfrac{1}{3}a_1\theta^{5/2}]+O,\quad\text{for}\quad\theta\ll 1\tag{6.3b}$$

where

$$a_0=\mathbf{Z}(\tfrac{3}{2}),\tag{6.4a}$$

$$a_1=\tfrac{3}{4}\pi\nu_0\mathbf{Z}(\tfrac{5}{2}),\tag{6.4b}$$

$$\mathbf{Z}(n)=\sum_{r=1}^{\infty}(r)^{-n}\exp(-\beta\mu r),\tag{6.4c}$$

and where O in Eqs. (6.3a) and (6.3b) denotes terms of order θ^3 or smaller. [These a_0 and a_1 should not be confused with those occurring in Eq. (2.15)]. Now, to begin the second cycle of iteration we compute the corresponding result for C. This gives

$$C=S-\pi\nu_0\mathbf{Z}(\tfrac{5}{2})\theta^{5/2}+O,\quad\text{for}\quad\theta\ll 1.\tag{6.5}$$

Using the above result for C, we find

$$\Phi(S)=a_0\theta^{3/2}+a_1\theta^{5/2}+a_2\theta^{7/2}+(2a_0a_1/S)\theta^4+O(\theta^{9/2}),\quad\text{for}\quad\theta\ll 1\tag{6.6a}$$

where

$$a_2=\pi^2\nu_0^2\omega_0\mathbf{Z}(\tfrac{5}{2}),\tag{6.6b}$$

$$\omega_0=33/32,\ \text{sc};\quad 281/288,\ \text{bcc};\quad 15/16,\ \text{fcc}.\tag{6.6c}$$

Since the accuracy of $\Phi(S)$ is now adequate, no further iteration for calculating ψ^0 and C is necessary. The cor-

[31] A point often missed in the literature is that the condition (6.1) is more stringent than the condition $T\ll T_c$ (where T_c is of the order of the Curie temperature), especially when $S\gg 1$. The reason for this is that T_c is essentially proportional to $S(S+1)J(0)$. As such, for a system of classical spins where the effective-spin quantum number is infinity, finite temperatures are not low in the sense implied by Eq. (6.1). Consequently, for such classical spin systems, the low-temperature expansions discussed in Sec. 6 are not applicable and a more careful expansion procedure has to be devised.

responding result for the magnetization is

$$\sigma=S-a_0\theta^{3/2}-a_1\theta^{5/2}-a_2\theta^{7/2}-(2a_0a_1/S)\theta^4 -O(\theta^{9/2})+(2S+1)(a_0)^{2S+1}\theta^{3(2S+1)/2} \times[1+(2S+1)(a_0/a_1)\theta+O(\theta^2)], \quad \text{for} \quad \theta\ll 1. \quad (6.7)$$

The above result is identical (to the order of accuracy maintained here) to that given by the Callen[15] decoupling. It, therfore, also suffers from the same deficiency as Callen's work, i.e., that for spin $\frac{1}{2}$ it contains the anaomalous θ^3 term. Similarly, the present result for the elementary excitation energy is dominantly correct for all spins [To see this insert the C given in Eq. (6.5) into Eq. (4.18)] just as Callen's result also is.

B. Just Below Critical Point

Next let us consider the temperature region immediately below the critical temperature. For convenience we shall consider the situation here in the absence of an applied field, i.e., for $\mu=0$. Because in this region we expect σ to be small compared with its zero-temperature saturated value S, therefore it follows from Eq. (5.1) that here $\Phi(S)$ is large compared with unity. Therefore, we use the relevant expansion for C given in Eq. (5.7) and calculate $\Phi(S)$ and ψ^0 self-consistently from the relations

$$\Phi(S)=F(0)\Phi(S)P(S)/2\beta J(0)-\tfrac{1}{2} +\beta J(0)\Phi^{-1}(S)/6P(S)+O, \quad (6.8)$$

$$\psi^0=[X/\beta J(0)][1-\tfrac{1}{2}\Phi^{-1}(S)+\tfrac{1}{5}\Phi^{-2}(S)(\tfrac{3}{2}-X)] \times[F(0)-1]P(S)-[\beta J(0)/3z][X/P(S)] \times\Phi^{-2}(S)+O, \quad (6.9)$$

where O stands for terms of higher order in the powers of $\Phi^{-1}(S)$ than those retained. Here we have used the notation that for any Q

$$F(Q)=(1/N)\sum_{\mathbf{K}}[Q+1-J(K)/J(0)]^{-1}. \quad (6.10)$$

Also, $P(S)$ is defined as

$$P(S)=\Phi^{-1}(S)/C, \quad (6.11)$$

and z is the coordination number given by the relation

$$z^{-1}=\frac{1}{N}\sum_{\mathbf{K}}[J(K)/J(0)]^2. \quad (6.12)$$

The set of relations (6.8)–(6.11) can now be simultaneously solved to derive self-consistent power series expansions in powers of $\Phi^{-1}(S)$ or, alternatively, in powers of σ. The details are quite tedious, and only the final results are quoted below. One finds that for $T<T_c$ and $(T_c-T)\ll T_c$,

$$\sigma=\left(\frac{A(S)k_BT_c}{J(0)B(S)}\right)^{1/2}\left(1-\frac{T}{T_c}\right)^{1/2}+O\left(1-\frac{T}{T_c}\right), \quad (6.13)$$

where

$$k_BT_c=(J(0)/10)[(16X+1)+(4X-1)/F(0)], \quad (6.14)$$

$$A(S)=10X^2, \quad (6.15a)$$

$$B(S)=\tfrac{1}{12}[4X-1+(16X+1)F^2(0)] +\frac{F(0)-1}{F(0)}\frac{(4X-1)}{70}[3-22X] +(1/20)(4X-1)[(16X+1)F(0)+(4X-1)] +\frac{F(0)}{2X}(16X+1)\left(\frac{4X-1}{(16X+1)F(0)+4X-1} +\frac{F(0)X}{6z}\right). \quad (6.15b)$$

For cubic lattices, the function $F(0)$ is well known,[32]

$$F(0)=1.51638, \quad \text{for sc}$$
$$=1.39320, \quad \text{for bcc} \quad (6.16)$$
$$=1.34466, \quad \text{for fcc}.$$

It is instructive to compare the structure of the foregoing result for the limiting cases of $S=\frac{1}{2}$ and $S=\infty$. For $S=\frac{1}{2}$, $X=\frac{1}{4}$, and we get

$$k_BT_c/J(0)=\tfrac{1}{2}, \quad \text{for} \quad S=\tfrac{1}{2} \quad (6.17a)$$

$$\frac{\sigma}{\frac{1}{2}}=\left(\frac{3z}{(z+1)F(0)}\right)^{1/2}\left(1-\frac{T}{T_c}\right)^{1/2} +O\left(1-\frac{T}{T_c}\right), \quad \text{for} \quad S=\tfrac{1}{2}. \quad (6.17b)$$

For $S\to\infty$, $X\gg 1$, and we get

$$k_BT_c/J(0)=\tfrac{2}{5}X[4+1/F(0)], \quad \text{for} \quad S=\infty, \quad (6.18a)$$

$$\frac{\sigma}{S}=\left(\frac{35}{3}\right)^{1/2}\left[\frac{4F(0)+1}{28F^2(0)-4F(0)+1}\right]^{1/2} \times\left(1-\frac{T}{T_c}\right)^{1/2}+O\left(1-\frac{T}{T_c}\right), \quad \text{for} \quad S=\infty. \quad (6.18b)$$

It is amusing to note that in the above equations the dimensionality of the lattice enters through only two parameters, namely, $F(0)$ and z. Therefore, the form of the corresponding results in other dimensionalities may be guessed by simply making an appropriate choice for $F(0)$ and z. Now, in one and two dimensions $F(0)\to\infty$, while z shows no dramatic behavior. Therefore, as the temperature is decreased below the corresponding critical temperature, the spontaneous magnetization σ may be expected to continue to remain zero in one and two dimensions. In the following sections, where we carry

[32] G. N. Watson, Quart. J. Math. 10, 266 (1939).

out more careful analysis of these cases, this guess will be verified.

Let us next study the region above the critical temperature, i.e., $T>T_c$. In the presence of a vanishingly small external field, it is appropriate to recast the energy $E_{\mathbf{K}}$ [see Eq. (4.18)] into the following form:

$$E_K(S)=\mu[1+Q^{-1}\eta(\mathbf{K})], \tag{6.19}$$

where

$$Q=XU/2J(0)\chi, \tag{6.20a}$$

$$U=[2X-\psi^0(0)]\times[2X^2-(1/20)(4X-1)\psi^0(0)]^{-1}, \tag{6.20b}$$

$$\chi=\lim_{\mu=0}(\sigma/\mu), \tag{6.20c}$$

$$\psi^0(0)=\lim_{\mu=0}[\psi^0], \tag{6.20d}$$

$$\eta(\mathbf{K})=1-J(\mathbf{K})/J(0). \tag{6.20e}$$

In the limit of vanishingly small μ, Eqs. (4.23) and (4.21) for $\Phi(S)$ and ψ^0 lead to the following simple expressions:

$$\lim_{\mu=0}(\Phi(S)\mu/X)=\chi^{-1}=QF(Q)/\beta X \tag{6.21}$$

and

$$\psi^0(0)=[2X/F(Q)][(1+Q)F(Q)-1], \tag{6.22}$$

where $F(Q)$ is as defined in Eq. (6.10). Solving Eqs. (6.20a)–(6.22) simultaneously and using Eq. (6.14), we are led to the convenient expression

$$\begin{aligned}10k_B(T-T_c)/J(0)&=(16X+1)[(1-\beta X\chi^{-1})^{-1}-1]\\&\quad+Q(1-4X)(1-\beta X\chi^{-1})^{-1}\\&\quad+(4X-1)[F^{-1}(Q)(1-\beta X\chi^{-1})^{-1}-F^{-1}(0)].\end{aligned} \tag{6.23}$$

For the particular case of spin $\frac{1}{2}$, the solution of the above equation is straightforward for all temperatures $T>T_c$. For this case the terms involving $(1-4X)$ vanish identically, and one readily gets

$$\chi=\frac{1}{4k_B}\left(\frac{1}{T-T_c}\right), \quad \text{for} \quad S=\tfrac{1}{2}. \tag{6.24}$$

This result is identical to the molecular field theory prediction. We note also that since the above expression does not involve any parameters which depend upon the dimensionality, this result is likely to hold also in one and two dimensions.

For the case of $S>\frac{1}{2}$, it is not possible to derive the result for χ in a closed form valid for all paramagnetic temperatures. Instead, for this general case it is convenient to separate the regions $(T-T_c)\ll T_c$ and $T\gg T_c$.

In the first region, the susceptibility χ is expected to be large and as such Q may be expected to be a small parameter [see Eqs. (6.20)–(6.22)]. Therefore, we can use the well-known expansion[33] for (FQ):

$$F(Q)=F(0)-bQ^{1/2}+\cdots, \tag{6.25}$$

where

$$\begin{aligned}b&=3\sqrt{3}/\pi\sqrt{2}, \quad \text{for sc}\\&=2\sqrt{2}/\pi, \quad \text{for bcc}\\&=3\sqrt{3}/2\pi, \quad \text{for fcc}.\end{aligned} \tag{6.26}$$

Substitution of Eq. (6.25) into Eqs. (6.20)–(6.23) leads to the following result:

$$[\chi]_{(T-T_c)\ll T_c}=\frac{(4X-1)^2b^2(10X)(T/T_c-1)^{-2}}{J(0)[(16X+1)F^2(0)+(4X-1)]^3}, \quad \text{for} \quad S>\tfrac{1}{2}. \tag{6.27}$$

Therefore, in three dimensions for $S\geqslant 1$, the structure of the zero-field susceptibility just above the critical temperature is similar to that predicted by the spherical model[22] and the usual Green's-function decoupling approximations.[15,21] As before it might be guessed that since the crucial dependence upon the dimensionality in the above result is through $F(0)$ then in one and two dimensions the $(T/T_c-1)^{-2}$ behavior will be absent, even for $S>\frac{1}{2}$, and that the structure of the susceptibility will have the classical form[2] for all spins.

Next let us consider the regime of elevated temperatures where $T\gg T_c$. Here $Q\gg 1$ and the following expansion of $F(Q)$ is therefore the appropriate one:

$$F(Q)=Q^{-1}[1-Q^{-1}+(1+1/z)Q^{-2}]+O(Q^{-4}). \tag{6.28}$$

Inserting (6.27) into Eqs. (6.20)–(6.23) finally leads to the results

$$\chi^{-1}=(k_BT/X)[1-Q^{-1}+(1+1/z)Q^{-2}]+O(Q^{-4}), \quad \text{for} \quad T\gg T_c \tag{6.29a}$$

$$\frac{k_BT}{2J(0)X}=Q+\frac{(16X+1)(1+1/z)+(4X-1)}{20X}+O(Q^{-1}), \quad \text{for} \quad T\gg T_c. \tag{6.29b}$$

Equations (6.28a) and (6.28b) can now be solved simultaneously to give

$$\chi=\beta X\{1+2\beta J(0)X+4\beta^2J^2(0)X^2[1-(4X-1)(20zX)^{-1}]\}+O(\beta^4), \quad \text{for} \quad T\gg T_c. \tag{6.30}$$

The above result relates to all values of the spin. It agrees with the exact[34] series expansion only to the first two powers in $\beta J(0)$ much as the results of the other decoupling theories.[15,21]

[33] See for example, I. Mannari and C. Kawabata, Research Note No. 15, Okayama University, Okayama, Japan, 1964 (unpublished).

[34] H. A. Brown and J. M. Luttinger, Phys. Rev. **100**, 685 (1955).

7. RESULTS IN ONE DIMENSION

The algebraic manipulations necessary for finding a properly self-consistent solution of the various equations given in Sec. 4 are, as in three dimensions, a lot more cumbersome for the general case of $S>\frac{1}{2}$ than they are for the simple case of $S=\frac{1}{2}$. However, in one and two dimensions, unlike in three dimensions, the structure of the results for $S=\frac{1}{2}$ and $S>\frac{1}{2}$ is not expected to be so different from each other. Therefore, for convenience and brevity, we shall describe in detail only the solution for the case of $S=\frac{1}{2}$. For the general spin case, only some results will be quoted.

For spin $\frac{1}{2}$, we first recast the relevant expressions given in Sec. 4 into convenient form

$$\sigma^{-1}=\pi^{-1}\int_{-\pi}^{+\pi}\coth[\tfrac{1}{2}\beta E_K(\tfrac{1}{2})]dK, \tag{7.1}$$

$$\psi^0\sigma^{-1}=(2\pi)^{-1}\int_{-\pi}^{+\pi}\coth[\tfrac{1}{2}\beta E_K(\tfrac{1}{2})]\times[J(K)/J(0)]dK, \tag{7.2}$$

where

$$J(K)=2I\cos K, \tag{7.3a}$$

$$E_K=\mu+4CI(1-\cos K), \tag{7.3b}$$

$$C^{-1}=\sigma^{-1}-2\psi^0\sigma^{-1}=\pi^{-1}\int_{-\pi}^{+\pi}dK(1-\cos K)\coth[\tfrac{1}{2}\beta E_K(\tfrac{1}{2})] \tag{7.3c}$$

Knowing that[14] $0\leqslant\sigma\leqslant\frac{1}{2}$ and $0\leqslant|\psi^0|\leqslant\frac{1}{2}$, we gather that C is non-negative. Moreover, the inequality

$$\coth[\tfrac{1}{2}\beta E_K(\tfrac{1}{2})]\geqslant|2/\beta E_K(\tfrac{1}{2})| \tag{7.4}$$

renders Eq. (7.3c) into the inequality

$$1\geqslant\frac{1}{2\pi\beta I}\int_{-\pi}^{+\pi}\frac{dK(1-\cos K)}{(\mu/4IC)+(1-\cos K)}, \tag{7.5a}$$

which gives

$$(1-T_c/T)\leqslant(1+8IC/\mu)^{-1/2}. \tag{7.5b}$$

Here we have for convenience put

$$\beta I=T_c/T. \tag{7.6}$$

We shall shortly recognize the T_c, defined by Eq. (7.6), to be the system's critical temperature.

From the inequality (7.5b) it is clear that for $T>T_c$, the ratio (C/μ) must approach a finite limit as $\mu\to 0$ (note that we have assumed I to be positive), i.e.,

$$\lim_{\mu=0}C=d(T/T_c,I)\mu, \quad \text{for} \quad T>T_c. \tag{7.7}$$

This relationship is easily seen to be self-consistently correct for all $T>T_c$ because then Eq. (7.4) is an exact equality.

It is clear that the solution (7.7) breaks down at the point $T=T_c$ unless we assume $d(1,I)$ to be divergent. Instead, the inequality (7.5b) can be satisfied only if

$$\lim_{\mu=0,T=T_c}[C]=\alpha\mu^{1/n}, \quad n>1. \tag{7.8}$$

To fix the value of n, it is necessary to employ at least one additional term in the series (7.4), i.e., to use the inequality

$$\coth[\tfrac{1}{2}\beta E_K(\tfrac{1}{2})]\leqslant 2/\beta E_K(\tfrac{1}{2})+\tfrac{1}{6}\beta E_K(\tfrac{1}{2}). \tag{7.9}$$

The consequences of Eqs. (7.3c) and (7.9) are

$$\beta I\leqslant[1-(1+8IC/\mu)^{-1/2}]+\tfrac{1}{3}\beta^2 I\mu C+2\beta^2 I^2C^2. \tag{7.10}$$

At $T=T_c$, i.e., $\beta I=1$, the relevant solution of the above equation is of the form (7.8), with

$$n=5, \quad \alpha=\tfrac{1}{2}(I)^{-1/5}. \tag{7.11}$$

[Note that for C given by Eqs. (7.8) and (7.11), Eq. (7.10) self-consistently becomes an equality, hence (7.11) is the correct solution.]

Let us next examine the structure of the susceptibility χ as a function of the applied field μ at the critical point, i.e., when $\beta I=1$. To do this we express Eq. (7.1) into the form of an equality in a manner similar to that used for deriving Eq. (7.10) from Eq. (7.3c). This gives

$$\lim_{T=T_c}(\chi^{-1})=4I(1+8IC/\mu)^{-1/2}+\mu^2/3I+\tfrac{4}{3}C\mu. \tag{7.12}$$

Now using Eqs. (7.8) and (7.11), we find

$$\lim_{T=T_c}(\chi)=\text{const}\mu^{-2/5}, \quad \text{for} \quad (\mu\to 0). \tag{7.13}$$

The behavior of the zero-field susceptibility χ just above the critical point is also analyzed by proceeding from Eq. (7.1) and taking the limit $\mu=0$. This leads to the equality (note that here the temperature T is assumed to be above that of the critical temperature, i.e., $T\geqslant T_c+\epsilon$, where $\epsilon\to+0$),

$$\chi^{-1}=4k_BT(1+8IC/\mu)^{-1/2}. \tag{7.14}$$

Under these conditions Eq. (7.5b) is also reduced to an equality, and therefore we get

$$\lim_{\mu=0}[\chi]=[4k_B(T-T_c)]^{-1}, \quad \text{for} \quad T\geqslant T_c+\epsilon. \tag{7.15}$$

This is the same result that was derived in the case of three dimensions [see Eq. (6.24)].

Let us next examine the behavior of C and σ below the critical temperature. For simplicity we assume the absence of the applied field, i.e., $\mu=0$.

For $T<T_c$, the parameter C is found to have a finite value even in the absence of the field. To see this let us use Eq. (7.3c), the inequality (7.9) and put $\mu=0$. In this fashion we are led to the inequality

$$\lim_{\mu=0}C^2\geqslant(T/T_c)(1-T/T_c), \tag{7.16}$$

which proves our assertion.

Next let us examine the behavior of the long-range order parameter σ, i.e., the magnetization, below the temperature T_c. Using Eq. (7.1) and the inequality (7.4), we readily find that in the limit of a small field, i.e., $\mu \ll I$, we have

$$\sigma \leqslant \text{const}\mu^{1/2}/T. \tag{7.17}$$

This inequality suggests that except in the trivial limit of absolute zero temperature, the magnetization σ vanishes more rapidly than $\mu^{1/2}$ throughout the temperature range $T<T_c$. Though this inequality is somewhat weaker than the rigorous inequality of Mermin and Wagner,[23] it is quite consistent with it.

It is clear that the behavior of the system is characterized largely by whether the system is above or below the critical point, i.e., whether the system temperature T is greater than T_c, equal to T_c, or less than T_c. The existence of such a critical point signifies the occurrence of a phase transition at a finite temperature.

When we consider the case of general spin, i.e., $S>\frac{1}{2}$, the structure of the foregoing results remains largely unaltered. The relevant algebra, however, becomes extremely tedious. Therefore in the following, we quote only the results for the zero-field susceptibility just above the critical point.

For general spin the result is

$$\chi=[X/(T-T_c)][1+2(4X-1)/(16X+1)], \tag{7.18}$$

where

$$5k_BT_c=I(16X+1). \tag{7.19}$$

This result is in complete accord with our conjecture based upon an extrapolation of the corresponding results in three dimensions. [Compare Eqs. (6.14) and the remarks following Eq. (6.26).]

8. RESULTS IN TWO DIMENSIONS

For spin $\frac{1}{2}$, the results of our SCMCD are identical to those following from the ML decoupling.[14] The consequences of this decoupling have been discussed by ML, and we refer the reader to their paper[14] for the corresponding details. For the present purposes it is convenient to quote only the results.

The system distributed over a square lattice undergoes a phase transition at $T=T_c$, where

$$k_BT_c=2I, \quad \text{for} \quad S=\tfrac{1}{2}. \tag{8.1}$$

The parameter C has the limiting behavior

$$\begin{aligned} C&=\text{const}\mu, \quad \text{for} \quad T>T_c \\ &=(\text{const}|\log\mu|^{1/3})\mu^{1/3}, \quad \text{for} \quad T=T_c \\ &=\text{independent of } \mu \text{ and of the form:} \\ &\qquad \text{const}(T_c-T)^{1/2}+\cdots, \quad \text{for} \quad T<T_c. \end{aligned} \tag{8.2}$$

Similarly, the zero-field susceptibility behaves as follows:

$$\begin{aligned} \chi&=\text{const}(T-T_c)^{-1}, \quad \text{for} \quad T>T_c \\ &=\text{const}\mu^{-1/6}, \quad \text{for} \quad T=T_c. \end{aligned} \tag{8.3}$$

As in one dimension, at nonzero temperature the spontaneous magnetization is also vanishing in two dimensions and is found to follow the inequality

$$\sigma \leqslant (\text{const}/T)\cdot 1/|\log\mu|. \tag{8.4}$$

For general spin, the essential structure of the above results is expected to be similar. The magnitude of the critical temperature is

$$5k_BT_c=2I(16X+1). \tag{8.5}$$

9. DISCUSSION

We have given a critique of the moment conserving decoupling approximations and shown that they generate only a limited class of line shapes which may be of interest when the system properties are well described in terms of long-lived elementary excitations. The corresponding line shape is then made up of peaked regions at appropriate positions indicating the dispersion energies of the elementary excitations.

The nonuniqueness of the resultant line shapes has been noted. A self-consistent MCD procedure, which reduced some of this nonuniqueness, has been outlined. The use of this SCMCD—at the first nontrivial stage—has been discussed in connection with the study of the long-range order parameter (LRO) in isotropic Heisenberg spin system. The results for the LRO are found to be reasonable in three dimensions. In one and two dimensions, they are found to be consistent with the rigorous inequalities given by Mermin and Wagner.[23]

Our results have suggested the existence of a phase transition in all the three dimensionalities studied. For two and three dimensions, this is not in contradiction with the accepted notions. In one dimension, however, the situation is not very clear. According to a recent conjecture of Dyson,[35] one expects that an infinite linear isotropic Heisenberg ferromagnet will have a phase transition at a finite temperature provided that the range of the exchange interaction $I(R)$ is long enough, and $I(R)$ is positive and monotonically decreasing, and provided the sums $J(0)$ and J_3,

$$J(0)=\sum_{n=1}^{\infty} I(na), \tag{9.1}$$

$$J_3=\sum_{n=1}^{\infty} [\log\log(n+4)][n^3I(na)]^{-1}, \tag{9.2}$$

converge. (Here a is the nearest-neighbor distance.) Unfortunately, the Dyson conjecture does not straightforwardly refer to the case under study, because here the range of the exchange interaction is limited only to the nearest-neighbor distance.

It should be mentioned here that the results of our SCMCD for the short-range order phenomena, e.g., the system specific heat, etc., are not as satisfactory as those for the LRO. To see how this comes about, first

[35] F. J. Dyson, Commun. Math. Phys. (to be published).

note that our result for the longitudinal correlation L^0 [see Eqs. (4.13a), (4.13b), and (4.14) to find L^0 for the case of spin $\frac{1}{2}$. For general spin, the corresponding L^0 can be obtained from using Eqs. (4.15a), (4.15b), (4.25a), (4.25b), and (4.30)], does not attain isotropy at $T \to T_c$ and $\mu \to 0$, i.e.,

$$\lim_{T=T_c;\,\mu=0} L^0 \neq \tfrac{1}{2}\psi^0. \tag{9.3}$$

This makes all direct predictions based upon L^0 suspect and indeed the corresponding results for the specific heat have the same unsatisfactory features as those obtained in the work of Tahir-Kheli and Callen.[36]

The foregoing shortcoming of our SCMCD is not unexpected but rather is in accord with the well-known observation that, in general, any given decoupling approximation leads to results of differing accuracies for the longitudinal and the transverse correlations.[37,38]

In conclusion it should be mentioned that the real usefulness of the SCMCD procedure will not lie in its application to standard three-dimensional ferromagnets where the exchange strength along all directions is nearly equally strong, because for these systems the accuracy of the SCMCD results is not compellingly greater than that of the corresponding results obtained in the usual decoupling approximations.[15,19] Rather, the great advantage of the SCMCD procedure over the usual decoupling theories lies in its (possible) application to those systems where the intraplanar exchange interactions are strong and the interplanar interactions comparatively weak, e.g., in $CrBr_3$.[39,40] Here the usual decoupling schemes[41] would be expected to give a relatively poor representation of both the LRO parameter σ and the spin correlation function $\langle S_g^+ S_p^- \rangle$. The reason for this is that in the limit of vanishing interplanar interaction, the results of the usual decoupling approximations are known to be drastically inaccurate[41] because they predict no phase transition at nonzero temperatures, and moreover they yield too low a value for the short-range order parameter, i.e., of the correlation ψ^0.

However, for the case of the other interesting limiting situation where the magnetic structure is dominantly linear, i.e., where the intrachain exchange is much greater than the interchain interaction, the present method affords an inferior description[42] as compared to the usual decoupling procedures.[43]

[36] R. A. Tahir-Kheli and H. B. Callen, J. Appl. Phys. **35**, 946 (1964); Phys. Rev. **135**, A679 (1964).
[37] H. S. Bennett, Ann. Phys. (N. Y.) **39**, 127 (1966).
[38] R. A. Tahir-Kheli, Phys. Rev. **159**, 439 (1967).
[39] A. C. Gossard, V. Jaccarino, and J. P. Remeika, Phys. Rev. Letters **7**, 122 (1961).
[40] H. L. Davis and A. Narath, Phys. Rev. **134**, A433 (1964).
[41] M. E. Lines, J. Appl. Phys. **40**, 1352 (1969).
[42] Indeed, in the limit when the interchain exchange is vanishing, the result of the SCMCD procedure—namely, that there occurs a phase transition at finite temperature—is quite likely to be in error, whereas the usual decoupling-procedure result—namely, that the transition temperature for such a system is 0°K—is physically more reasonable.
[43] T. Oguchi, Phys. Rev. **133**, A1098 (1964).

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APPENDIX

It was stated in Sec. 4 in the text that Eqs. (4.17) and (4.18)—which are valid for all spins within the first-order MCD scheme—implied that the averages $\langle (S^z)^n \rangle$ for various n values were implicitly related with each other through their dependence upon the function $\Phi(S)$. Similarly, the assertion was made that within a similar scheme the existence of Eqs. (4.25a), (4.25b), and (4.29) was also implied. In this Appendix we elaborate upon the assumptions under which the above assertions are valid.

The peculiar dependence of $\langle (S^z)^n \rangle$ upon $\Phi(S)$ given in Eqs. (4.24a) and (4.24b) is based upon the assumption that the Green's function

$$\langle\langle S_g^+(t);\, e^{xS_p^z(t')} S_p^-(t') \rangle\rangle \equiv G_{gp}{}^x(t-t') \tag{A1}$$

will have the following truncated equation of motion within the first-order MCD scheme

$$G_{\mathbf{K}}{}^x(Z)[Z - E_{\mathbf{K}}(S)] = \Gamma^+(x)/2\pi, \tag{A2}$$

where $E_{\mathbf{K}}(S)$ is again given by Eq. (4.18). Once the above assertion is made, it can be shown in a manner analogous to that expounded in Refs. 15, 29, and 30 (for brevity we do not repeat these arguments here) that Eqs. (4.24a)–(4.25b) indeed follow.

It should, however, be emphasized that Eq. (A2) is not quite what the MCD procedure would lead to—except, of course, when $x=0$. Indeed the correct equation of motion of $G_{gp}{}^x(Z)$ for arbitrary x is the following:

$$G_{gp}{}^x(Z)[Z-\mu] = \delta_{g,p}\Gamma^+(x)/2\pi + 2\sum_f I(gf)\langle\langle S_f{}^z S_g^+ - S_g{}^z S_f^+;\, e^{xS_p^z} S_p^- \rangle\rangle_{(Z)}. \tag{A3}$$

Therefore according to the actual MCD procedure (see Sec. 4 for the relevant details of the MCD) the above Eq. (A3) would take the decoupled form

$$G_{\mathbf{K}}{}^x(Z)[Z - E_{\mathbf{K}}{}^x(S)] = \Gamma^+(x)/2\pi, \tag{A4}$$

where

$$E_{\mathbf{K}}{}^x(S) = \mu + 2C^x(S)[J(0) - J(\mathbf{K})], \tag{A5}$$

$$\begin{aligned} C^x(S) = {} & [(e^{-x}-1)S(S+1)\langle S_{f+\delta}{}^z e^{xS_f{}^z}\rangle \\ & + \langle e^{xS_f{}^z} S_f{}^- S_{f+\delta}{}^+\rangle + (e^{-x}+1)\langle S_{f+\delta}{}^z e^{xS_f{}^z} S_f{}^z\rangle \\ & - (e^{-x}-1)\langle S_{f+\delta}{}^z e^{xS_f{}^z}(S_f{}^z)^2\rangle] \\ & \times [S(S+1)(e^{-x}-1)\Omega(x) + (e^{-x}+1)\langle e^{xS_f{}^z} S_f{}^z\rangle \\ & - (e^{-x}-1)\langle e^{xS_f{}^z}(S_f{}^z)^2\rangle]^{-1}. \end{aligned} \tag{A6}$$

In Eq. (A6), δ as usual denotes the vector separation of any two neighboring sites in the lattice. Clearly, the differential equations obeyed by the correlations, $\langle e^{xS_f{}^z} S_f{}^- S_g^+ \rangle$, that we would obtain from the above Green's function are exceedingly more complex than

those solved in Ref. 15. This is caused by the implicit x dependence that the above $E_{\mathbf{K}}{}^{x}(S)$ possesses. In contrast, the corresponding differential equations obtained within the usual decoupling approximations[15,21] are tractable because $E_{\mathbf{K}}(S)$, and in turn $\Phi(S)$, are not implicit functions of x. Indeed, within the usual decoupling schemes, we always have

$$E_{\mathbf{K}}{}^{x}(S)=E_{\mathbf{K}}{}^{0}(S)\equiv E_{\mathbf{K}}(S). \tag{A7}$$

To make the mathematical manipulations of the present paper tractable, we have been forced to make the assumption of the validity of Eq. (A7). We feel that this is a plausible assumption in view of the fact that almost the entire elementary excitation spectrum—at least in the spin-wave regime—is the one that is generated by the propagation of a single spin flip. In other words, the spin-wave spectrum is determined in large part by the poles of the Green's function $G_{\mathbf{K}}{}^{0}(Z)=G_{\mathbf{K}}(Z)$. In other words, while the poles of the more general Green's function $G_{\mathbf{K}}{}^{x}(Z)$ are not necessarily identical to those of $G_{\mathbf{K}}{}^{0}(Z)$ [because the renormalization of the spectrum $E_{\mathbf{K}}{}^{x}(S)$ will contain different contributions from the two and higher number of spin-flip processes than does $E_{\mathbf{K}}{}^{0}(S)$] to an approximation which is possibly not much worse than the one which makes use of nondecaying elementary excitation energies, we may assume $E_{\mathbf{K}}{}^{0}(S)$ to be the same as $E_{\mathbf{K}}{}^{x}(S)$. And since the MCD gives only nondecaying elementary excitations, i.e.,

$$\mathrm{Im}[E_{\mathbf{K}}{}^{x}(S)]\equiv 0, \tag{A8}$$

the inordinately heavy additional effort necessary for solving Eqs. (A4)–(A6) is clearly not warranted.

Let us next turn to the verification of Eq. (4.29). Once the plausible assumption of the validity of Eq. (A7) has been made, and consequently the interrelationship of $\langle(S^{z})^{n}\rangle$ for various n values has been established via Eqs. (4.24a) and (4.24b), then we can use the same algebraic manipulations as given by Tahir-Kheli and Callen[36] and Tahir-Kheli[38] to derive a differential equation of the form

$$\left[\frac{d^{2}}{dx^{2}}+\frac{[1+\Phi(S)]e^{x}+\Phi(S)}{[1+\Phi(S)]e^{x}-\Phi(S)}\frac{d}{dx}-S(S+1)\right]\Lambda^{x}(gp)$$
$$=\Gamma^{+}(x)[1-\Phi(S)(e^{-x}-1)]^{-1}R(gp), \tag{A9}$$

where

$$\Lambda^{x}(gp)=\langle S_{g}{}^{z}e^{xS_{p}{}^{z}}\rangle \tag{A10}$$

and $R(gp)$ is independent of x. The important point to note here is that while the actual form of the function $R(gp)$ is implicitly dependent upon precisely how the formulation leading to Eq. (A10) is carried out [compare Refs. 36 and 38], the structure of the differential equation (A9) is invariant for all decoupling procedures which assume (A7).

The solution of the differential equation (A9) is clearly

$$\Lambda^{x}(gp)=\sigma\Omega(x)+\left(\frac{d\Omega(x)}{dx}-\sigma\Omega(x)\right)R(gp). \tag{A11}$$

The above solution automatically satisfies the boundary condition that

$$\Lambda^{x}(gp)=\sigma, \quad \text{for} \quad x=0 \tag{A12}$$

because $\Omega(0)=1$. A suitable form for the remaining boundary condition which fixes the unknown function $R(gp)$ is

$$\left(\frac{d\Lambda^{x}(gp)}{dx}\right)_{x=0}=\langle S_{g}{}^{z}S_{p}{}^{z}\rangle. \tag{A13}$$

The satisfaction of this boundary condition by the solution (A1) guarantees that

$$R(gp)=(\langle S_{g}{}^{z}S_{p}{}^{z}\rangle-\sigma^{2})/(M-\sigma^{2}). \tag{A14}$$

Note that the crucial point in the above derivation is that although the actual magnitude of the function $L^{0}(gp)$ is dependent upon how we use the Green's-function theory for its computation, the interdependence of functions $\langle S_{g}{}^{z}(S_{p}{}^{z})^{n}\rangle$ for $n=1,2,3,\ldots$, is completely independent of the technique of computation used. This observation is very close to the spirit of the argument presented by Callen and Shtrikman[28] (in a somewhat different context) and its validity arises only because of the assumption of quasi-independent collective excitations $E_{\mathbf{K}}(S)$ with the behavior shown in Eq. (A7).

Using Eqs. (A10), (A11), and (A14), we readily derive Eq. (4.29) given in the text.