Green's-function theory of the anisotropic Heisenberg model in a transverse field

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(Received 14 January 1987)

The $S=\frac{1}{2}$ anisotropic Heisenberg model in a transverse field (AHMTF) is studied by means of double-time Green's functions. A new approximation scheme is employed which is based upon the assumption of the statistical independence of the ordering operator. The basic approximations are required to satisfy all relevant operator and correlation identities. Emphasis is placed upon obtaining accurate approximations for those Green's functions which are related to the ordering susceptibility. The scheme is relatively simple to use and applicable to a wide variety of systems. Standard Green's-function techniques are shown to provide results for the critical transverse field for Ising-like systems which violate $S=\frac{1}{2}$ identities. They are also shown to be not applicable to the ordered phase of XY-like systems. In contrast, the new approximation provides reasonable results for all temperatures and couplings for the $S=\frac{1}{2}$ AHMTF.

I. INTRODUCTION

Double-time Green's functions[1] (DTGF) describe the linear response of many-body systems to external fields and treat quantum and thermal fluctuations on the same level. They provide a suitable framework for the consistent treatment of the physics of many-body systems at all temperatures. The development of approximation schemes for DTGF has focused on decoupling their equations of motion. Ideally, such schemes should be well defined (the decoupling criterion should be clear), consistent with all relevant operator identities, and generally applicable to a wide variety of systems.

The first step in the standard decoupling approach is to use the equations of motion of a basis set of operators to form the equations of motion of the DTGF. This results in a hierarchy of equations which must be decoupled to provide a closed set of equations for the DTGF. The approximate DTGF thus obtained are required to satisfy an identity in common with their exact counterparts. The decoupling is usually chosen for convenience or for reasons which are essentially *ad hoc*. The consistency of the basic decoupling approximation with relevant operator identities is not always assured.

This paper describes a new scheme which also begins by forming the DTGF equations of motion but, in addition, uses the operator equations of motion to form a set of correlation identities which are not considered in the standard procedure. The decoupling scheme is based upon the assumption of the statistical independence of the ordering operator and is, therefore, well defined and can be applied to a wide variety of systems. As part of the new procedure, the decoupling approximations are required to be consistent with all relevant operator identities. This requirement produces a set of correlation approximations. The decoupled hierarchy and correlation approximations are then used to determine the DTGF which are associated with the susceptibilities describing the response of the system to the ordering field. The accuracy of these approximate DTGF is assured by requiring them to satisfy an identity in common with their exact counterparts.

The $S=\frac{1}{2}$ anisotropic Heisenberg model in an external field transverse to the ordering direction (AHMTF) is an important application for any DTGF approximation scheme. The presence of the transverse field allows the determination of those DTGF which are directly related to the ordering susceptibilities of the system. Most currently available schemes have been developed for the case of vanishing transverse field[2–4] (AHM) and, thus, do not provide approximations for those DTGF which are directly related to the ordering susceptibilities. Those schemes proposed most recently[5–7] have improved on earlier versions through increasingly more complicated, *ad hoc* decouplings and are not generally applicable to other systems. Special cases of nonvanishing transverse field [i.e., the XY (Ref. 8) and Ising models[9] in a transverse field] have been treated within the standard approximation scheme by symmetric (random-phase) decoupling. It will be shown that adherence to the standard procedure forces unacceptable results for the Ising-type AHMTF [$\alpha_2>\alpha_1$ in Eq. (3.1)] and precludes the study of the ordered phase of the XY-type AHMTF [$\alpha_1>\alpha_2$ in Eq. (3.1)].

In contrast to previous approaches, the new general approximation scheme provides a DTGF-based treatment of the AHMTF which is valid for all T and all values of the coupling constants. Decoupling the DTGF equations of motion in first order, expressions are obtained for the critical curve and for the magnetization in the ordered phase. The parameters of the critical curve, i.e., the critical transverse field and the critical temperature in vanishing transverse field, compare very well in the pure Ising and pure XY limits with those obtained by high-temperature expansion techniques.[10,11] The ground-state order parameter is obtained for all values of the coupling constants.

II. DOUBLE-TIME GREEN'S FUNCTIONS

The retarded ($\rho=+1$) or advanced ($\rho=-1$) commutator ($\eta=-1$) or anticommutator ($\eta=+1$) double-time

Green's function is defined by

$$\langle\langle A(t);B(t')\rangle\rangle_{(\rho)}^{(\eta)} = -\frac{i}{2}[(\rho+1)\Theta(t-t') + (\rho-1)\Theta(t'-t)] \times \langle [A(t),B(t')]_\eta \rangle , \quad (2.1)$$

where

$$A(t)=e^{iHt}Ae^{-iHt} , \qquad [A,B]_\eta = AB+\eta BA , \quad (2.2)$$

and $\Theta(t)$ is unity for $t>0$ and zero for $t<0$. The single angular brackets in Eq. (2.1) denote thermal average. It follows from Eq. (2.1) that $\langle\langle A(t);B(t')\rangle\rangle_{(\rho)}^{(\eta)}$ is a function of $t-t'$ only.

The Fourier transform of $\langle\langle A(t);B\rangle\rangle_{(\rho)}^{(\eta)}$ is defined by

$$\langle\langle A;B\rangle\rangle_{E+i\rho\epsilon}^{(\eta)} = \int_{-\infty}^{\infty} dt \exp[i(E+i\rho\epsilon)t] \times \langle\langle A(t);B\rangle\rangle_{(\rho)}^{(\eta)}, \quad \epsilon\to 0^+ \quad (2.3)$$

and satisfies the equation of motion

$$E\langle\langle A;B\rangle\rangle_E^{(\eta)} = \langle [A,B]_\eta\rangle + \langle\langle [A,H]_-;B\rangle\rangle_E^{(\eta)} . \quad (2.4)$$

The Green's function (GF) on the right-hand side of Eq. (2.4) is generally of "higher order" than the GF on the left-hand side and must be decoupled so that a closed system of equations is obtained. The Fourier transformed GF as defined in Eq. (2.3) is sectionally holomorphic; the retarded (or advanced) GF is analytic in the upper (respectively, lower) half of the complex E plane.[12,13] It has been shown[12] that the commutator GF cannot have a pole at $E=0$, i.e.,

$$C^{(-)}=0 , \quad (2.5)$$

where

$$C^{(\eta)} = \lim_{E\to 0} E\langle\langle A;B\rangle\rangle_E^{(\eta)} . \quad (2.6)$$

The correlation $\langle BA(t)\rangle$ may be calculated from

$$\langle BA(t)\rangle = \tfrac{1}{4}(1-\eta)C^{(-\eta)} + \frac{i}{2\pi}\int_{-\infty}^{\infty} dE(e^{\beta E}+\eta)^{-1}e^{-iEt} \times \lim_{\epsilon\to 0^+}(\langle\langle A;B\rangle\rangle_{E+i\epsilon}^{(\eta)} - \langle\langle A;B\rangle\rangle_{E-i\epsilon}^{(\eta)}) , \quad (2.7)$$

where $\beta=1/k_BT$. The response of the system to an external field coupling to B is described by the generalized susceptibility[14,15]

$$\chi_{A,B}(E) = -\lim_{\epsilon\to 0^+}\langle\langle A;B\rangle\rangle_{E+i\epsilon}^{(-)} . \quad (2.8)$$

III. ANISOTROPIC HEISENBERG MODEL

The anisotropic coupling of nearest-neighbor spins is represented by

$$H_0 = -\frac{\alpha_1}{2}\sum_{i,j} J_{ij}(S_i^xS_j^x+S_i^yS_j^y) - \frac{\alpha_2}{2}\sum_{i,j} J_{ij}S_i^zS_j^z , \quad (3.1)$$

where $\{S_i^\mu\}$, $\mu=x,y,z$ are the familiar dipolar spin operators which satisfy ($\hbar=1$)

$$[S_i^\mu,S_j^\nu] = i\delta_{ij}\mathcal{E}_{\mu,\nu,\lambda}S_j^\lambda , \quad (3.2)$$

where $\mathcal{E}_{\mu,\nu,\lambda}$ is the Levi-Civita symbol with $\mathcal{E}_{x,y,z}=1$. For $S=\frac{1}{2}$, $\{S_i^\mu\}$ also satisfies

$$S_i^\mu S_i^\nu = \frac{\delta_{\mu,\nu}}{4} + \frac{i}{2}\mathcal{E}_{\mu,\nu,\lambda}S_i^\lambda . \quad (3.3)$$

The effects of uniform fields coupling to S_i^x and S_i^z are described by

$$H_1 = -\Omega_1\sum_i S_i^x \quad (3.4)$$

and

$$H_3 = -\Omega_3\sum_i S_i^z . \quad (3.5)$$

The case of z ordering in the presence of a transverse x field, for which the full Hamiltonian is given by

$$H = H_0 + H_1 \quad (3.6)$$

is considered in detail in this section and in Secs. IV and V. In Sec. VI, results are also reported for the case of x-y ordering in the presence of a transverse z field, for which the full Hamiltonian is given by

$$H' = H_0 + H_3 . \quad (3.7)$$

Usually[2-7] z ordering in a system described by H_0 is studied by using H' and letting $\Omega_3\to 0$ and x-y ordering is studied by using H and letting $\Omega_1\to 0$. Such procedures clearly preclude the study of the effects of a transverse field on the ordering process. As will be seen in Sec. V, the presence of a transverse field also allows the determination of those Green's functions which are directly related to the susceptibilities which diverge at the critical point.

Using Eq. (3.2), the equations of motion of the spin operators are

$$[S_i^x,H] = -i\alpha_1\sum_m J_{im}S_i^zS_m^y + i\alpha_2\sum_m J_{im}S_i^yS_m^z , \quad (3.8a)$$

$$[S_i^y,H] = i\Omega_1S_i^z + i\alpha_1\sum_m J_{im}S_i^zS_m^x - i\alpha_2\sum_m J_{im}S_i^xS_m^z , \quad (3.8b)$$

$$[S_i^z,H] = -i\Omega_1S_i^y - i\alpha_1\sum_m J_{im}(S_i^yS_m^x - S_i^xS_m^y) . \quad (3.8c)$$

Taking the thermal averages of both sides of each member of Eqs. (3.8a)–(3.8c) yields the correlation identities

$$(\alpha_2-\alpha_1)\sum_m J_{im}\langle S_i^yS_m^z\rangle = 0 , \quad (3.9a)$$

$$\Omega_1 z - (\alpha_2-\alpha_1)\sum_m J_{im}\langle S_i^xS_m^z\rangle = 0 , \quad (3.9b)$$

$$\Omega_1 y = 0 , \quad (3.9c)$$

where, by definition and translational symmetry,

$$\mu \equiv \langle S_i^\mu \rangle, \quad \mu = x,y,z \ . \tag{3.10}$$

Equation (3.9c) clearly gives $y = 0$ for all T if $\Omega_1 \neq 0$.

Defining

$$G_{ij}^{\mu,R(\eta)} \equiv \langle\langle S_i^\mu ; R_j \rangle\rangle_E^{(\eta)}, \quad L_{ij}^{\mu,R(\eta)} \equiv \langle [S_i^\mu, R_j]_\eta \rangle \ , \quad \mu = x,y,z \ , \tag{3.11}$$

and using Eqs. (3.8a)–(3.8c) in Eq. (2.4) gives the Green's function equations of motion

$$EG_{ij}^{x,R(\eta)} = L_{ij}^{x,R(\eta)} - i\alpha_i \sum_m J_{im} \langle\langle S_i^z S_m^y ; R_j \rangle\rangle_E^{(\eta)} + i\alpha_2 \sum_m J_{im} \langle\langle S_i^y S_m^z ; R_j \rangle\rangle_E^{(\eta)} \ , \tag{3.12a}$$

$$EG_{ij}^{y,R(\eta)} = L_{ij}^{y,R(\eta)} + i\Omega_1 G_{ij}^{z,R(\eta)} + i\alpha_1 \sum_m J_{ij} \langle\langle S_i^z S_m^x ; R_j \rangle\rangle_E^{(\eta)} - i\alpha_2 \sum_m J_{im} \langle\langle S_i^x S_m^z ; R_j \rangle\rangle_E^{(\eta)} \ , \tag{3.12b}$$

$$EG_{ij}^{z,R(\eta)} = L_{ij}^{z,R(\eta)} - i\Omega_1 G_{ij}^{y,R(\eta)} - i\alpha_1 \sum_m J_{im} (\langle\langle S_i^y S_m^x ; R_j \rangle\rangle_E^{(\eta)} - \langle\langle S_i^x S_m^y ; R_j \rangle\rangle_E^{(\eta)}) \ . \tag{3.12c}$$

While Eq. (2.7) gives

$$\langle R_j S_i^\mu \rangle = \tfrac{1}{4}(1-\eta) \lim_{E \to 0} E \langle\langle S_i^\mu ; R_j \rangle\rangle_E^{(\eta)} + \frac{i}{2\pi} \int_{-\infty}^{\infty} dE (e^{\beta E} + \eta)^{-1} \lim_{\epsilon \to 0^+} (\langle\langle S_i^\mu ; R_j \rangle\rangle_{E+i\epsilon}^{(\eta)} - \langle\langle S_i^\mu ; R_j \rangle\rangle_{E-i\epsilon}^{(\eta)}) \ . \tag{3.13}$$

From Eq. (2.8), the response of the system to a uniform magnetic field in the μ direction ($\mu = x,y,z$) is given by

$$\chi_{\nu,\mu}(E) = - \lim_{\epsilon \to 0^+} \sum_{i,j} \langle\langle S_i^\nu ; S_j^\mu \rangle\rangle_{E+i\epsilon}^{(-)}, \quad \nu = x,y,z \ . \tag{3.14}$$

IV. CUMULANT DECOUPLING—STANDARD PROCEDURE

The Green's functions on the right-hand sides of Eqs. (3.12a)–(3.12c) are of the form $\langle\langle S_i^\mu S_m^\nu ; R_j \rangle\rangle_E^{(\eta)}$ and are of higher order than the basic Green's functions in Eq. (3.11). They must be approximately decoupled to provide a closed, soluble set of equations to replace Eqs. (3.12a)–(3.12c). The decoupling scheme used in this treatment is based upon the concepts of cumulants and statistical independence. The cumulant averages of $\langle S_i^\mu(t) S_m^\nu(t) R_j \rangle$ and $\langle R_j S_i^\mu(t) S_m^\nu(t) \rangle$, the correlations appearing in $\langle\langle S_i^\mu S_m^\nu ; R_j \rangle\rangle_E^{(\eta)}$, are defined by[16]

$$\langle S_i^\mu(t) S_m^\nu(t) R_j \rangle = \mu \langle S_m^\nu(t) R_j \rangle + \nu \langle S_i^\mu(t) R_j \rangle + R (\langle S_i^\mu S_m^\nu \rangle - 2\mu\nu) + \langle S_i^\mu(t) S_m^\nu(t) R_j \rangle_c \tag{4.1a}$$

and

$$\langle R_j S_i^\mu(t) S_m^\nu(t) \rangle = \mu \langle R_j S_m^\nu(t) \rangle + \nu \langle R_j S_i^\mu(t) \rangle + R (\langle S_i^\mu S_m^\nu \rangle - 2\mu\nu) + \langle R_j S_i^\mu(t) S_m^\nu(t) \rangle_c \ , \tag{4.1b}$$

where $i \neq m$, $\mu \neq \nu$, $R = \langle R_i \rangle$ and the subscript c stands for cumulant average. The cumulant averages can be written in terms of the fluctuations

$$\Delta_i^\mu(t) = S_i^\mu - \mu, \quad \mu = x,y,z$$

$$\Delta_i^R = R_i - R \ ,$$

as

$$\langle S_i^\mu(t) S_m^\nu(t) R_j \rangle_c = \langle \Delta_i^\mu(t) \Delta_m^\nu(t) \Delta_j^R \rangle \ , \tag{4.2a}$$

$$\langle R_j S_i^\mu(t) S_m^\nu(t) \rangle_c = \langle \Delta_j^R \Delta_i^\mu(t) \Delta_m^\nu(t) \rangle \ . \tag{4.2b}$$

The assumption that one of the operators appearing in $\langle\langle S_i^\mu S_m^\nu ; R_j \rangle\rangle_E^{(\eta)}$ is statistically independent of the others gives[16]

$$\langle S_i^\mu(t) S_m^\nu(t) R_j \rangle_c = \langle R_j S_i^\mu(t) S_m^\nu(t) \rangle_c = 0 \tag{4.3}$$

and is equivalent to the assumption (in the calculation of the fluctuation correlations) that two of the fluctuation operators interact with the average of the third. When used in Eqs. (4.1a) and (4.1b), Eq. (4.3) gives the approximations ($i \neq m, \mu \neq \nu$)

$$\langle S_i^\mu(t) S_m^\nu(t) R_j \rangle = \mu \langle S_m^\nu(t) R_j \rangle + \nu \langle S_i^\mu(t) R_j \rangle + R (\langle S_i^\mu S_m^\nu \rangle - 2\mu\nu) \ , \tag{4.4a}$$

$$\langle R_j S_i^\mu(t) S_m^\nu(t) \rangle = \mu \langle R_j S_m^\nu(t) \rangle + \nu \langle R_j S_i^\mu(t) \rangle + R (\langle S_i^\mu S_m^\nu \rangle - 2\mu\nu) \ . \tag{4.4b}$$

Using Eqs. (4.4a) and (4.4b) gives the cumulant decoupling approximation

$$\langle\langle S_i^\mu S_m^\nu ; R_j \rangle\rangle_E = \mu G_{mj}^{\nu,R(\eta)} + \nu G_{ij}^{\mu,R(\eta)} + \frac{(1+\eta)R}{E} (\langle S_i^\mu S_m^\nu \rangle - 2\mu\nu) \ . \tag{4.5}$$

Inspection of Eqs. (3.12a)–(3.12c) shows that R_j is the only operator that appears in all of the Green's functions which are to be decoupled by Eq. (4.5). Therefore, the assumption that a single operator of the set $\{S_i^x, S_i^y, S_i^z\}$ is statistically independent of the others requires that R_j be chosen to be the statistically independent operator. Using Eq. (4.5) in Eqs. (3.12a)–(3.12c), solving the resulting decoupled equations, and requiring that the commutator Green's functions ($\eta = -1$) have no zero-frequency poles [cf. Eq. (2.5)] gives the conditions

$$xL_{\mathbf{k}}^{x,R(-)} + zL_{\mathbf{k}}^{z,R(-)} = 0 \tag{4.6}$$

(which is an identity in this case for all $R_i = S_i^x, S_i^y, S_i^z$) and

$$[\Omega_1 + (\alpha_1 - \alpha_2) X J_0] L_{\mathbf{k}}^{x,R(-)} = 0 \tag{4.7}$$

and the cumulant decoupling approximation Green's functions

$$G_{\mathbf{k}}^{x,R(\eta)}=\frac{1}{\Phi_{\mathbf{k}}(E)}[EL_{\mathbf{k}}^{x,R(\eta)}+i\alpha_2 zJ_0(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)L_{\mathbf{k}}^{y,R(\eta)}]$$
$$-\frac{(1+\eta)}{E\Phi_{\mathbf{k}}(E)}\{z^2(\alpha_2-\alpha_1)RJ_0[2(\alpha_2-\alpha_1)xJ_0-\Omega_1]N\delta_{\mathbf{k},0}+[\Omega_1+\alpha_1 xJ_0(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)]A_{\mathbf{k}}^R\}\ , \tag{4.8}$$

$$G_{\mathbf{k}}^{y,R(\eta)}=\frac{1}{\Phi_{\mathbf{k}}(E)}\{EL_{\mathbf{k}}^{y,R(\eta)}+i(1+\eta)Rz[2(\alpha_2-\alpha_1)xJ_0-\Omega_1]N\delta_{\mathbf{k},0}$$
$$-i[\alpha_2 zJ_0(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)L_{\mathbf{k}}^{x,R(\eta)}-[\Omega_1+\alpha_1 xJ_0(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)]L_{\mathbf{k}}^{z,R(\eta)}]\}\ , \tag{4.9}$$

$$G_{\mathbf{k}}^{z,R(\eta)}=\frac{1}{\Phi_{\mathbf{k}}(E)}\{EL_{\mathbf{k}}^{z,R(\eta)}-i[\Omega_1+\alpha_1 xJ_0(1-\gamma_{\mathbf{k}})]L_{\mathbf{k}}^{y,R(\eta)}\}$$
$$+\frac{(1+\eta)z}{E\Phi_{\mathbf{k}}(E)}\{\Omega_1 R[2(\alpha_2-\alpha_1)xJ_0-\Omega_1]N\delta_{\mathbf{k},0}-\mu J_0(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)A_{\mathbf{k}}^R\}\ . \tag{4.10}$$

In Eqs. (4.6)–(4.10),

$$G_{\mathbf{k}}^{\mu,R(\eta)}=\frac{1}{N}\sum_{i,j}e^{i\mathbf{k}\cdot\mathbf{r}_{ij}}G_{ij}^{\mu,R(\eta)}\ , \tag{4.11a}$$

$$L_{\mathbf{k}}^{\mu,R(\eta)}\equiv\frac{1}{N}\sum_{i,j}e^{i\mathbf{k}\cdot\mathbf{r}_{ij}}L_{ij}^{\mu,R(\eta)}\ , \tag{4.11b}$$

$$J_{\mathbf{k}}=\frac{1}{N}\sum_{i,j}e^{i\mathbf{k}\cdot\mathbf{r}_{ij}}J_{ij}\ , \tag{4.11c}$$

$$a_{\mathbf{k}}^{R,\mu}=\frac{1}{N}\sum_{i,j}e^{i\mathbf{k}\cdot\mathbf{r}_{ij}}\langle R_i S_j^{\mu}\rangle\ , \tag{4.11d}$$

$$\gamma_{\mathbf{k}}=J_{\mathbf{k}}/J_0\ , \tag{4.11e}$$

$$\Phi_{\mathbf{k}}(E)=E^2-\omega_{\mathbf{k}}^2\ , \tag{4.11f}$$

$$A_{\mathbf{k}}^R=[\Omega_1+\alpha_1 xJ_0(1-\gamma_{\mathbf{k}})]a_{\mathbf{k}}^{R,x}$$
$$+\alpha_2 zJ_0(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)a_{\mathbf{k}}^{R,z}\ , \tag{4.11g}$$

and

$$\omega_{\mathbf{k}}^2=[\Omega_1+\alpha_1 xJ_0(1-\gamma_{\mathbf{k}})][\Omega_1+\alpha_1 xJ_0(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)]$$
$$+(\alpha_2 zJ_0)^2(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)^2\ . \tag{4.11h}$$

The standard procedure for implementing the approximate Green's functions, Eqs. (4.8)–(4.10) is to use them in Eq. (3.13) and apply the $S=\frac{1}{2}$ identity, Eq. (3.3), to obtain approximate correlation expressions. Following this procedure (cf. Appendix) forces the choice $R_i=S_i^y$ in order to obtain useful information. All information is then generated from the approximate $G_{\mathbf{k}}^{y,y(\eta)}$. Serious difficulties with this standard procedure become apparent when its predictions for the critical curve are considered. In particular, the result for the critical field, i.e., the value of Ω_1 for which the critical temperature vanishes, violates the fundamental property of $S=\frac{1}{2}$ systems

$$\mu\leq\tfrac{1}{2},\quad \mu=x,y,z\ . \tag{4.12}$$

Thus, while the standard procedure has apparent advantages (e.g., cumulant and symmetric decoupling coincide and commutator and anticommutator Green's functions provide the same result), because of the violation of inequality (4.12), the standard procedure must be considered unsatisfactory.

The source of the failure of the standard procedure is the choice $R_i=S_i^y$, i.e., the assumption that S_i^y is the statistically independent operator of the set $\{S_i^x,S_i^y,S_i^z\}$. This choice leads to the determination of all information from $G_{\mathbf{k}}^{y,y(\eta)}$. From another point of view, the use of Eq. (3.13) within the standard procedure serves to assure that the approximate version of $G_{\mathbf{k}}^{y,y(-)}$ satisfies Eq. (3.13) in common with the exact $G_{\mathbf{k}}^{y,y(-)}$. However, on the critical curve for z ordering,

$$\chi_{z,z}=-G_0^{z,z(-)}(E=0) \tag{4.13}$$

is diverging, while $G_0^{y,y(-)}(E=0)$ remains finite. The dominant Green's function in the neighborhood of the critical curve is thus $G_{\mathbf{k}}^{z,z(-)}$, not $G_{\mathbf{k}}^{y,y(-)}$. An improved approximation scheme would allow the use of Eq. (3.13) to assure the accuracy of an approximate version of $G_{\mathbf{k}}^{z,z(-)}$. Such a scheme would clearly require the choice $R_i=S_i^z$, i.e., the assumption of the statistical independence of the ordering operator. In addition, the standard procedure for implementing $G_{\mathbf{k}}^{z,z(-)}$ and Eq. (3.13) must be replaced since the standard procedure only yields useful results for the choice $R_i=S_i^y$.

V. NEW APPROXIMATION SCHEME

The new approximation scheme is based upon the assumption of the statistical independence of the ordering operator. As discussed in Sec. IV, this dictates the choice $R_i=S_i^z$ and is equivalent to the assumption that in the fluctuation correlation, $\langle\Delta_i^{\mu}(t)\Delta_m^{\nu}(t)\Delta_j^z\rangle$, the fluctuations $\Delta_i^{\mu}(t)$ and $\Delta_m^{\nu}(t)$ interact with the mean ordering field. For $R_i=S_i^z$, the basic decoupling approximations, Eqs. (4.4a) and (4.4b), become ($i\neq m$).

$$\langle S_i^{\mu}(t)S_m^{\nu}(t)S_j^z\rangle=\mu\langle S_m^{\nu}(t)S_j^z\rangle+\nu\langle S_i^{\mu}(t)S_j^z\rangle$$
$$+z(\langle S_i^{\mu}S_m^{\nu}\rangle-2\mu\nu)\ , \tag{5.1}$$

and

$$\langle S_j^z S_i^{\mu}(t)S_m^{\nu}(t)\rangle=\mu\langle S_j^z S_m^{\nu}(t)\rangle+\nu\langle S_j^z S_i^{\mu}(t)\rangle$$
$$+z(\langle S_i^{\mu}S_m^{\nu}\rangle-2\mu\nu)\ . \tag{5.2}$$

In the new scheme, the basic decoupling approxima-

tions are required to be consistent with the $S=\frac{1}{2}$ identity, Eq. (3.3). Using Eq. (3.3) in the $t=0$ forms of Eqs. (5.1) and (5.2) gives the two-site correlation approximations

$$\langle S_i^z S_m^\nu \rangle = \nu z, \quad i \neq m, \quad \nu = x,y,z \ . \tag{5.3}$$

Using Eq. (5.3) in Eq. (4.11d) gives

$$a_{\mathbf{k}}^{z,\mu} = \frac{\delta_{\mu,z}}{4} - z\mu(1-N\delta_{\mathbf{k},0}) + \frac{i\lambda}{2}\mathcal{E}_{z,\mu,\lambda} \ . \tag{5.4}$$

Using Eq. (5.3) in the correlation identities Eqs. (3.9a)–(3.9c) yields

$$z[\Omega_1 - (\alpha_2 - \alpha_1)xJ_0] = 0 \ . \tag{5.5}$$

Next, the cumulant decoupling approximation for $G_{\mathbf{k}}^{z,z(-)}$, the Green's function associated with the ordering susceptibility, $\chi_{z,z}$ is obtained by setting $R_i = S_i^z$ in Eq. (4.10) with $\eta = -1$, i.e.,

$$G_{\mathbf{k}}^{z,z(-)} = \frac{x}{\Phi_{\mathbf{k}}(E)}[\Omega_1 + \alpha_1 xJ_0(1-\gamma_{\mathbf{k}})] \ . \tag{5.6}$$

Using Eqs. (5.4) and (5.5) with Eq. (4.10) gives

$$\lim_{E\to 0} EG_{\mathbf{k}}^{z,z(+)} = 2z^2 N\delta_{\mathbf{k},0} + \frac{2z^2(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)}{x^2(1-\gamma_{\mathbf{k}}) + z^2(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)} \times (\tfrac{1}{4} - x^2 - z^2) \ . \tag{5.7}$$

Finally, the approximate $G_{\mathbf{k}}^{z,z(-)}$ is required to satisfy Eq. (3.13) in common with its exact counterpart. Thus, using Eqs. (5.6) and (5.7) in Eq. (3.13) and summing over $\mathbf{k}$ gives

$$\frac{1}{4} = \frac{x}{2N}\sum_{\mathbf{k}} \frac{\Omega_1 + \alpha_1 xJ_0(1-\gamma_{\mathbf{k}})}{\omega_{\mathbf{k}}} \coth\frac{\beta\omega_{\mathbf{k}}}{2} + z^2\left[1 + (\tfrac{1}{4} - x^2 - z^2)\frac{1}{N}\sum_{\mathbf{k}} \frac{1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2}{x^2(1-\gamma_{\mathbf{k}}) + z^2(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)}\right] \ . \tag{5.8}$$

Equations (5.8) and (5.5) determine the single site terms x and z in the new procedure and together with Eq. (5.6) determine the DTGF associated with the ordering susceptibility.

Above the critical temperature (T_3), $z=0$ and Eqs. (5.6) and (4.13) give the z susceptibility

$$\chi_{z,z} = \frac{x}{\Omega_1 - (\alpha_2 - \alpha_1)xJ_0} \ , \tag{5.9}$$

while Eq. (5.8) becomes

$$\frac{1}{2} = \frac{x}{N}\sum_{\mathbf{k}} \frac{\Omega_1 + \alpha_1 xJ_0(1-\gamma_{\mathbf{k}})}{\omega_{\mathbf{k}}} \coth\frac{\beta\omega_{\mathbf{k}}}{2}, \quad T > T_3 \tag{5.10}$$

where

$$\omega_{\mathbf{k}}^2 = [\Omega_1 + \alpha_1 xJ_0(1-\gamma_{\mathbf{k}})] \times [\Omega_1 + \alpha_1 xJ_0(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)] \ . \tag{5.11}$$

The critical curve is determined by the divergence of $\chi_{z,z}$, i.e., from Eq. (5.9),

$$\Omega_1 - (\alpha_2 - \alpha_1)xJ_0 \to 0, \quad T \to T_3^+ \ . \tag{5.12}$$

Using Eq. (5.12) in Eq. (5.10) gives the expression for the critical curve

$$\frac{1}{2} = \frac{1}{N}\sum_{\mathbf{k}} \left[\frac{1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2}{1-\gamma_{\mathbf{k}}}\right]^{1/2} \coth\frac{\beta_3\omega_{\mathbf{k}3}}{2} \ , \tag{5.13}$$

where $\beta_3 = 1/k_B T_3$ and

$$\omega_{\mathbf{k}3} = \alpha_2 xJ_0(1-\gamma_{\mathbf{k}})^{1/2}(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)^{1/2} \ . \tag{5.14}$$

Since

$$1 - \alpha_1\gamma_{\mathbf{k}}/\alpha_2 > 0 \tag{5.15}$$

for all $\mathbf{k}$ only if

$$\alpha_1 < \alpha_2 \ , \tag{5.16}$$

real solutions for β_3 and $\omega_{\mathbf{k}3}$ are obtained from Eqs. (5.13) and (5.14) only if inequality (5.16) is satisfied. Thus, this solution predicts z ordering only if $\alpha_2 > \alpha_1$.

The critical value of x, again denoted by x_3, is obtained from Eq. (5.13) by letting $\beta_3 \to \infty$ this gives

$$x_3 = \frac{1/2}{\frac{1}{N}\sum_{\mathbf{k}} \left[\frac{1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2}{1-\gamma_{\mathbf{k}}}\right]^{1/2}} \ . \tag{5.17}$$

Equation (5.17) gives for $\alpha_1 < \alpha_2$

$$x_3 < \tfrac{1}{2} \tag{5.18}$$

as required by the basic spin-$\frac{1}{2}$ relation, Eq. (4.12). The dependence of x_3 on α_1/α_2 is depicted in Fig. 1. The value of T_3 for vanishing Ω_1, denoted by T_3^0 is obtained by letting $x \to 0$ in Eq. (5.13) to give

$$\frac{k_B T_3^0}{\alpha_2 J_0} = \frac{1/4}{F(-1)} \ , \tag{5.19}$$

where the Watson sums, $F(n)$, are given by[17]

$$F(n) = \frac{1}{N}\sum_{\mathbf{k}} (1-\gamma_{\mathbf{k}})^n \ . \tag{5.20}$$

For the isotropic-Heisenberg-zero-field case ($\Omega_1 = 0$, $\alpha_1 = \alpha_2$), Eq. (5.19) reduces to the result of Tahir-Kheli.[18] These results for T_3^0 agree to about 1% with the results of high temperature series expansions.[19] The results of the new scheme for the critical curve parameters x_3 and T_3 in the special case $\alpha_1 = 0$, $\alpha_2 = 1$ (IMTF) are presented in Table I along with the results of high-temperature series expansions (HTE) and other current approximation schemes. Only the two-spin cluster variation result compares more favorably than the current scheme with the HTE results. However, the two-spin cluster approximation is suitable only at higher temperatures[20] while the

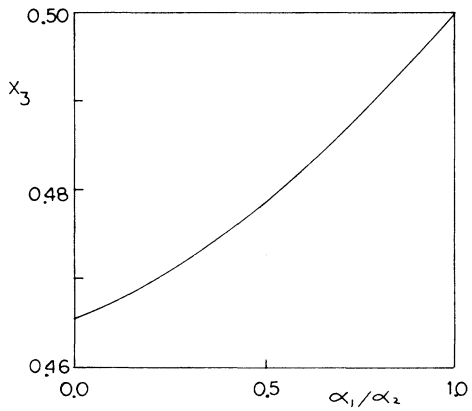

FIG. 1. Dependence of critical field (x_3) on coupling ratio (α_1/α_2) for a bcc lattice, Ising-like coupling ($\alpha_1/\alpha_2<1$).

present scheme is appropriate for all temperatures.

For $T<T_3$, $z\neq 0$ and Eq. (5.5) gives

$$\Omega_1=(\alpha_2-\alpha_1)xJ_0 \ . \tag{5.21}$$

Using Eq. (5.21), Eq. (5.8) becomes

$$\tfrac{1}{4}=z^2+z^2(\tfrac{1}{4}-x^2-z^2)\frac{1}{N}\sum_{\mathbf{k}}D_{\mathbf{k}}+\frac{x^2}{2N}\sum_{\mathbf{k}}D_{\mathbf{k}}^{1/2}\coth\frac{\beta\omega_{\mathbf{k}}}{2} \ , \tag{5.22}$$

where

$$D_{\mathbf{k}}=\frac{1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2}{x^2(1-\gamma_{\mathbf{k}})+z^2(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)} \tag{5.23}$$

and

$$\omega_{\mathbf{k}}^2=(\alpha_2 J_0)^2(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)\times[x^2(1-\gamma_{\mathbf{k}})+z^2(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)] \ . \tag{5.24}$$

The ground-state magnetization in the bcc lattice as a function of x for $\alpha_1/\alpha_2=0.5$, obtained by taking $\beta\rightarrow\infty$ in Eq. (5.22), is presented in Fig. 2.

VI. APPLICATION TO *XY*-LIKE COUPLING ($\alpha_1>\alpha_2$)

In this case the Hamiltonian is given by Eq. (3.7) and the operator equations of motions are

$$[S_i^x,H']=i\Omega_3 S_i^y-i\alpha_1\sum_m J_{im}S_i^zS_m^y+i\alpha_2\sum_m J_{im}S_i^yS_m^z \ , \tag{6.1a}$$

$$[S_i^y,H']=-i\Omega_3 S_i^x+i\alpha_1\sum_m J_{im}S_i^zS_m^x-i\alpha_2\sum_m J_{im}S_i^xS_m^z \ , \tag{6.1b}$$

$$[S_i^z,H']=-i\alpha_1\sum_m J_{im}(S_i^yS_m^x-S_i^xS_m^y) \ . \tag{6.1c}$$

Taking the thermal average of both sides of Eqs. (6.1a) and (6.1b) yields the correlation identities

$$\Omega_3 y-(\alpha_1-\alpha_2)\sum_m J_{im}\langle S_i^zS_m^y\rangle=0 \ , \tag{6.2}$$

$$\Omega_3 x-(\alpha_1-\alpha_2)\sum_m J_{im}\langle S_i^zS_m^x\rangle=0 \ , \tag{6.3}$$

Using cumulant or symmetric decoupling within the standard procedure as described in Sec. IV provides two equations for the three unknowns $a_{\mathbf{k}}^{R,x}$, $a_{\mathbf{k}}^{R,y}$ and $a_{\mathbf{k}}^{R,z}$ which, in the ordered phase, do not provide a unique solution for any member of the set $(a_{\mathbf{k}}^{R,x},a_{\mathbf{k}}^{R,y},a_{\mathbf{k}}^{R,z})$ for any R. Thus, the standard procedure does not allow the study of the ordered phase for *XY*-like coupling in a transverse field.

The new approximation procedure is based upon the assumption of the statistical independence of the ordering operators, S^x and S^y. Using cumulant decoupling under this assumption requires, as in Sec. V, the choices $R_i=S_i^x$ and $R_i=S_i^y$. Requiring that cumulant decoupling be consistent with the $S=\frac{1}{2}$ identity, Eq. (3.3), now gives

$$\langle S_i^xS_l^\nu\rangle=x\nu, \quad i\neq l, \quad \nu=x,y,z \ , \tag{6.4}$$

$$\langle S_i^yS_l^\nu\rangle=y\nu, \quad i\neq l, \quad \nu=x,y,z \ . \tag{6.5}$$

Using Eqs. (6.4) and (6.5) in Eqs. (6.2) and (6.3) gives

$$y[\Omega_3-(\alpha_1-\alpha_2)zJ_0]=0 \ , \tag{6.6}$$

$$x[\Omega_3-(\alpha_1-\alpha_2)zJ_0]=0 \ , \tag{6.7}$$

while using Eqs. (6.4) and (6.5) in Eq. (4.11d) gives

TABLE I. Comparison of results obtained by high-temperature expansion and various current-approximation schemes for the critical field (x_3) and the critical temperature in vanishing applied field ($k_BT_3^0/J_0$) for the IMTF, sc lattice.

	x_3	$k_BT_3^0/J_0$
High temperature expansion (Refs. 10 and 21)	0.430	0.188
Cluster-variation (Refs. 20 and 22)	0.446	0.206
Present (DTGF)	0.449	0.165
Effective field (Ref. 23)	0.392	0.212
Mean field	0.5	0.25

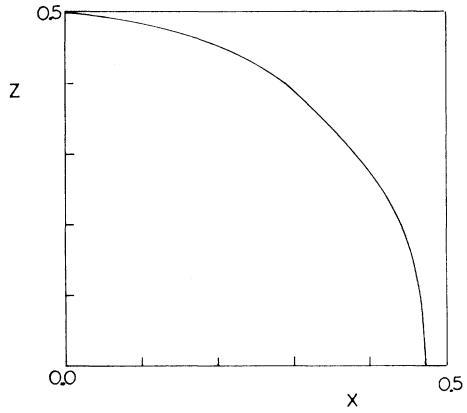

FIG. 2. Dependence of ground-state magnetization (z) on applied field (x) for a bcc lattice, Ising-like coupling, $\alpha_1/\alpha_2=0.5$.

$$a_{\mathbf{k}}^{x,\mu}=\frac{\delta_{\mu,x}}{4}-x\mu(1-N\delta_{\mathbf{k},0})+\frac{i\lambda}{2}\mathcal{E}_{x,\mu,\lambda}\ , \tag{6.8}$$

$$a_{\mathbf{k}}^{y,\mu}=\frac{\delta_{\mu,y}}{4}-y\mu(1-N\delta_{\mathbf{k},0})+\frac{i\lambda}{2}\mathcal{E}_{y,\mu,\lambda}\ . \tag{6.9}$$

Forming the Green's function equations of motion with Eqs. (6.1a)–(6.1c) and using the cumulant decoupling approximation, Eq. (4.5) gives

$$G_{\mathbf{k}}^{x,x(-)}=\frac{1}{E^2-\eta_{\mathbf{k}}^2}\{z[\Omega_3+\alpha_2 zJ_0(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)]+y^2\alpha_1 J_0(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)\}\ , \tag{6.10}$$

$$G_{\mathbf{k}}^{y,y(-)}=\frac{1}{E^2-\eta_{\mathbf{k}}^2}\{z[\Omega_3+\alpha_2 zJ_0(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)]+x^2\alpha_1 J_0(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)\}\ , \tag{6.11}$$

and

$$\lim_{E\to 0} EG_{\mathbf{k}}^{x,x(+)}=2x^2N\delta_{\mathbf{k},0}+2x^2(\tfrac{1}{4}-x^2-y^2-z^2)B_{\mathbf{k}}\ , \tag{6.12}$$

$$\lim_{E\to 0} G_{\mathbf{k}}^{y,y(+)}=2y^2N\delta_{\mathbf{k},0}+2y^2(\tfrac{1}{4}-x^2-y^2-z^2)B_{\mathbf{k}}\ , \tag{6.13}$$

where

$$\eta_{\mathbf{k}}^2=[\Omega_3+\alpha_2 zJ_0(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)]^2+(\alpha_1 J_0)^2(x^2+y^2)(1-\gamma_{\mathbf{k}})(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)\ , \tag{6.14}$$

and

$$B_{\mathbf{k}}=\frac{(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)}{z^2(1-\gamma_{\mathbf{k}})+(x^2+y^2)(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)}\ . \tag{6.15}$$

Using Eqs. (6.10)–(6.13) in Eq. (3.13) and summing over $\mathbf{k}$ gives

$$x^2=y^2 \tag{6.16}$$

and

$$\frac{1}{4}=\frac{1}{2N}\sum_{\mathbf{k}}\frac{1}{\eta_{\mathbf{k}}}\{z[\Omega_3+\alpha_2 zJ_0(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)]+x^2\alpha_1 J_0(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)\}\coth\frac{\beta\eta_{\mathbf{k}}}{2}+x^2+x^2(\tfrac{1}{4}-2x^2-z^2)\frac{1}{N}\sum_{\mathbf{k}}B_{\mathbf{k}}\ . \tag{6.17}$$

Above the critical temperature (denoted by T_1), $x=y=0$ and Eqs. (6.10), (6.11), and (3.14) give the susceptibilities

$$\chi_{x,x}=\chi_{y,y}=\frac{z}{\Omega_3-(\alpha_1-\alpha_2)zJ_0}\ , \tag{6.18}$$

while Eq. (6.17) becomes

$$\frac{1}{2}=\frac{z}{N}\sum_{\mathbf{k}}\coth\frac{\beta\eta_{\mathbf{k}}}{2}\ , \tag{6.19}$$

where

$$\eta_{\mathbf{k}}=\Omega_3+\alpha_2 zJ_0(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)\ . \tag{6.20}$$

The critical curve is determined by the divergence of $\chi_{x,x}$ and $\chi_{y,y}$, i.e., from Eq. (6.18)

$$\Omega_3-(\alpha_1-\alpha_2)zJ_0\to 0 \quad \text{as } T\to T_1^+\ . \tag{6.21}$$

Using Eq. (6.21) in Eq. (6.19) gives the expression for the critical curve

$$\frac{1}{2}=\frac{z}{N}\sum_{\mathbf{k}}\coth\frac{\beta_1\eta_{\mathbf{k}1}}{2}\ , \tag{6.22}$$

where $\beta_1=1/k_BT_1$ and

$$\eta_{\mathbf{k}1}=\alpha_1 zJ_0(1-\gamma_{\mathbf{k}})\ . \tag{6.23}$$

The critical value of z, denoted by z_1, is obtained from Eq. (6.22) by taking $\beta_1\to\infty$. This gives $z_1=\frac{1}{2}$ for all α_2/α_1. The value of T_1 for vanishing Ω_3, denoted by T_1^0, is obtained by taking $z\to 0$ in Eq. (6.22) to obtain

$$\frac{k_BT_1^0}{\alpha_1 J_0}=\frac{1/4}{F(-1)}\ . \tag{6.24}$$

For the special case $\alpha_2=0$ (pure XY model in a transverse field), Eq. (6.24) is identical to the result of Austen[8] and is within 2%, 1.7%, and 1.4% of the HTE results[11] for the sc, bcc, and fcc lattices, respectively.

For $T<T_1$, x and y do not vanish and Eqs. (6.6) and (6.7) give

$$\Omega_3=(\alpha_1-\alpha_2)zJ_0,\quad T<T_1\ . \tag{6.25}$$

Eq. (6.17) now becomes

$$\frac{1}{4}=x^2+x^2(\tfrac{1}{4}-2x^2-z^2)\frac{1}{N}\sum_{\mathbf{k}}B_{\mathbf{k}}+\frac{\alpha_1 J_0}{2N}\sum_{\mathbf{k}}\frac{1}{\eta_{\mathbf{k}}}[z^2(1-\gamma_{\mathbf{k}})+x^2(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)]\times\coth\frac{\beta\eta_{\mathbf{k}}}{2}\ , \tag{6.26}$$

where, now,

$$\eta_{\mathbf{k}}^2=(\alpha_1 J_0)^2(1-\gamma_{\mathbf{k}})[z^2(1-\gamma_{\mathbf{k}})+2x^2(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)]\ , \quad T<T_1\ . \tag{6.27}$$

The ground-state magnetization in the bcc lattice as a function of z for $\alpha_2/\alpha_1=0.5$ is presented in Fig. 3 and the dependence of the ground-state magnetization on α_2/α_1 for $z\to 0$ is shown in Fig. 4.

VII. CONCLUSION

The new DTGF approximation scheme is based upon the assumption of the statistical independence of the ordering operator, requires the consistency of the basic approximation with all relevant operator and correlation identities, and emphasizes the accuracy of the DTGF which are related to the ordering susceptibility. It has been used to study the AHMTF for all T and all values of α_2/α_1. In contrast to the standard approach, it provides

reasonable results for the AHMTF critical transverse field for all values of α_2/α_1 and is applicable to the ordered phase in the case of XY-like coupling. The results obtained in the special cases of pure Ising and pure XY couplings in a transverse field compare very favorably with those obtained by HTE in these special cases. The new scheme is reasonably simple to apply and is based upon ideas which are well defined and generally applicable to a wide variety of systems.

APPENDIX: STANDARD APPROXIMATION PROCEDURE ($\alpha_2 > \alpha_1$)

The standard procedure uses Eqs. (4.8)–(4.10) in Eq. (3.13) and applies Eq. (3.3) to obtain approximate correlation expressions. Following this procedure, both $G_{\mathbf{k}}^{x,R(\eta)}$ and $G_{\mathbf{k}}^{z,R(\eta)}$ when used in Eq. (3.13) lead to the same expression, i.e.

$$\alpha_2 z J_0(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)a_{\mathbf{k}}^{R,x}-[\Omega_1+\alpha_1 x J_0(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)]a_{\mathbf{k}}^{R,z} = \frac{i\omega_{\mathbf{k}}}{2}L_{\mathbf{k}}^{y,R(-)}\coth\frac{\beta\omega_{\mathbf{k}}}{2}+\frac{\omega_{\mathbf{k}}^2 L_{\mathbf{k}}^{z,R(-)}}{2[\Omega_1+\alpha_1 x J_0(1-\gamma_{\mathbf{k}})]}+Rz[2(\alpha_2-\alpha_1)xJ_0-\Omega_1]N\delta_{\mathbf{k},0}\ , \tag{A1}$$

while using $G_{\mathbf{k}}^{y,R(\eta)}$ in Eq. (3.13) gives

$$a_{\mathbf{k}}^{R,y}=-\frac{L_{\mathbf{k}}^{y,R(-)}}{2}-\frac{i}{2\omega_{\mathbf{k}}}\{\alpha_2 z J_0(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)L_{\mathbf{k}}^{x,R(-)}-[\Omega_1+\alpha_1 x J_0(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)]L_{\mathbf{k}}^{z,R(-)}\}\coth\frac{\beta\omega_{\mathbf{k}}}{2}\ . \tag{A2}$$

Equations (A1) and (A2) must be supplemented by the analyticity condition, Eq. (4.7).

Clearly, Eq. (A1) does not generally permit the determination of separate solutions for $a_{\mathbf{k}}^{R,x}$ and $a_{\mathbf{k}}^{R,z}$. Attention is thus focused on Eq. (A2) which becomes, for $R_i=S_i^x$, S_i^y, and S_i^z, respectively,

$$a_{\mathbf{k}}^{x,y}=iz/2\ , \tag{A3}$$

$$a_{\mathbf{k}}^{y,y}=\frac{1}{2\omega_{\mathbf{k}}}\{\alpha_2 J_0(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)z^2+[\Omega_1+\alpha_1 x J_0(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)]x\}\coth\frac{\beta\omega_{\mathbf{k}}}{2}\ , \tag{A4}$$

$$a_{\mathbf{k}}^{z,y}=-ix/2\ . \tag{A5}$$

Summing over $\mathbf{k}$ and using Eq. (3.3), Eqs. (A3) and (A5) give identities while Eq. (A4) gives

$$\frac{1}{2}=\frac{1}{N}\sum_{\mathbf{k}}\frac{1}{\omega_{\mathbf{k}}}\{\alpha_2 J_0(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)z^2+[\Omega_1+\alpha_1 x J_0(1-\alpha_2\gamma_{\mathbf{k}}/\alpha_1)]x\}\coth\frac{\beta\omega_{\mathbf{k}}}{2}\ . \tag{A6}$$

Thus, practical considerations [the extraction of useful information, i.e., Eq. (A6)] within the standard procedure dictate the choice $R_i=S_i^y$. Use of the standard procedure within other decoupling schemes (e.g., symmetric decoupling[9]) leads to the same conclusion. For $R_i=S_i^y$, the results of cumulant and symmetric decoupling are identical and the analyticity condition, Eq. (4.7), becomes

$$[\Omega_1+(\alpha_1-\alpha_2)xJ_0]z=0\ . \tag{A7}$$

Equations (A6) and (A7) represent the standard cumulant-symmetric decoupling solution for this case.

Serious difficulties with this solution become apparent

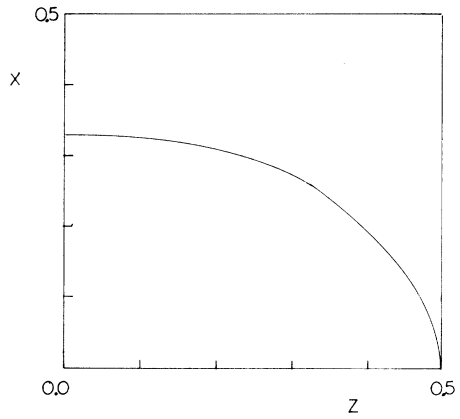

FIG. 3. Dependence of ground-state magnetization (x) on applied field (z) for a bcc lattice, XY-like coupling, $\alpha_2/\alpha_1=0.5$.

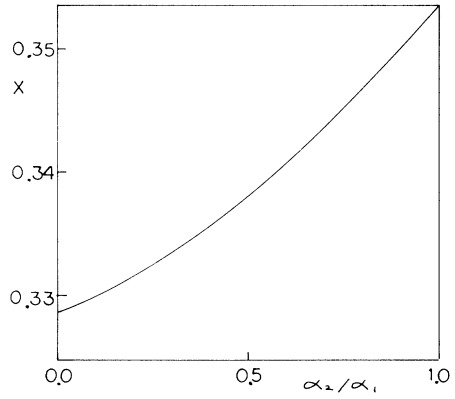

FIG. 4. Dependence of ground-state magnetization (x) on coupling ratio (α_2/α_1) for $z\to 0$, bcc lattice, XY-like coupling ($\alpha_2/\alpha_1<1$).

when its predictions for the critical curve are considered. For $z \neq 0$, Eq. (A7) gives

$$\Omega_1 = (\alpha_2 - \alpha_1) x J_0 \tag{A8}$$

and Eq. (A6) becomes

$$\frac{1}{2} = \frac{1}{N} \sum_{\mathbf{k}} \left[\frac{(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)z^2 + (1-\gamma_{\mathbf{k}})x^2}{1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2} \right]^{1/2} \coth\frac{\beta\omega_{\mathbf{k}}}{2} . \tag{A9}$$

While using Eq. (A8) in Eq. (4.11h) gives

$$\omega_{\mathbf{k}}^2 = (\alpha_2 J_0)^2 (1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2) \times [(1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)z^2 + (1-\gamma_{\mathbf{k}})x^2] . \tag{A10}$$

The expression for the critical curve is obtained by letting $z \to 0$ to obtain

$$\frac{1}{2} = \frac{x}{N} \sum_{\mathbf{k}} \left[\frac{1-\gamma_{\mathbf{k}}}{1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2} \right]^{1/2} \times \coth \left[\frac{\beta_3}{2} \alpha_2 x J_0 (1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2)^{1/2} (1-\gamma_{\mathbf{k}})^{1/2} \right] , \tag{A11}$$

where T_3 denotes the critical temperature and $\beta_3 = 1/k_B T_3$.

The critical field is defined as that value of Ω_1 for which $\beta_3 \to \infty$. For values of Ω_1 greater than the critical value, no ordering takes place. Since Ω_1 and x are related by Eq. (A8), a critical value of Ω_1 implies a critical value of x (denoted by x_3) which is obtained by letting $\beta_3 \to \infty$ in Eq. (A11) to give

$$x_3 = \frac{1/2}{\frac{1}{N} \sum_{\mathbf{k}} \left[\frac{1-\gamma_{\mathbf{k}}}{1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2} \right]^{1/2}} . \tag{A12}$$

Since, for $\alpha_1 < \alpha_2$,

$$\frac{1}{N} \sum_{\mathbf{k}} \left[\frac{1-\gamma_{\mathbf{k}}}{1-\alpha_1\gamma_{\mathbf{k}}/\alpha_2} \right]^{1/2} < 1 , \tag{A13}$$

Eq. (A12) gives

$$x_3 > \tfrac{1}{2} \tag{A14}$$

which violates the fundamental property of $S = \frac{1}{2}$ systems, Eq. (4.12).

[1] D. N. Zubarev, Usp. Fiz. Nauk. **71**, 71 (1960) [Sov. Phys.—Usp. **3**, 320 (1960)].
[2] S. V. Tyablikov, *Methods in the Quantum Theory of Magnetism* (Plenum, New York, 1967).
[3] H. B. Callen, Phys. Rev. **130**, 890 (1963).
[4] S. Katsura and T. Horiguchi, J. Phys. Soc. Jpn. **25**, 60 (1968).
[5] T. Oguchi and A. Honma, J. Appl. Phys. **34**, 1153 (1963).
[6] R. H. Swendsen, Phys. Rev. B **5**, 116 (1972).
[7] A. Kumar and A. Gupta, Phys. Rev. B **28**, 3968 (1983).
[8] D. J. Austen, Can. J. Phys. **52**, 1660 (1974).
[9] V. Ramakrishnan and T. Tanaka, Phys. Rev. B **16**, 422 (1977).
[10] R. J. Elliot and C. Wood, J. Phys. C **4**, 2359 (1971).
[11] D. D. Betts, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1974), Vol. III, p. 569.
[12] P. E. Bloomfield and N. Nafari, Phys. Rev. A **5**, 806 (1972).
[13] P. E. Bloomfield, R. Hecht, and P. Sievert, Phys. Rev. B **2**, 3714 (1970).
[14] R. Kubo, J. Phys. Soc. Jpn. **12**, 570 (1957).
[15] K. M. Van Vliet, J. Math. Phys. (N.Y.) **19**, 1345 (1978).
[16] R. Kubo, J. Phys. Soc. Jpn. **17**, 1100 (1962).
[17] G. N. Watson, Q. J. Math. **10**, 266 (1939).
[18] R. A. Tahir-Kheli, Phys. Rev. **132**, 689 (1963).
[19] C. Domb and M. F. Sykes, Phys. Rev. **128**, 168 (1962).
[20] V. K. Saxena, Phys. Rev. B **27**, 6884 (1983).
[21] J. Zinn-Justin, J. Phys. **40**, 969 (1979).
[22] J. A. Plascak, Phys. Status Solidi B **120**, 215 (1983).
[23] F. C. Sa Barreto and I. P. Fittipalid, Physica (Utrecht) **129A**, 360 (1985).