Irreducible-Green's-function theory of an anisotropic Heisenberg ferromagnet

K. G. Chakraborty
Department of Physics, Basirhat College, 24 Parganas (North), West Bengal 743412, India
(Received 24 July 1987; revised manuscript received 18 January 1988)

The exact Dyson equation for an anisotropic Heisenberg ferromagnet is derived using the irreducible-Green's-function technique. The spin-wave energy shift and damping are derived at low temperatures and are discussed with reference to earlier work. The results for the Curie temperature are derived and are critically analyzed with reference to those of the molecular-field approximation, the correlated effective-field approximation of Lines, the high-temperature series expansion of Wang and Lee, and the Green's-function diagrammatic theory of Yang and Wang.

I. INTRODUCTION

Observed data from magnetic resonance experiments and theoretical studies of the crystalline field, along with the perturbation calculation of the spin-orbit interaction,[1] have clearly established the fact that the exchange anisotropy and the single-ion anisotropy are two fundamentally important features existing in a wide variety of magnetic substances. Hence the static and dynamic properties of these substances can be studied by means of a generalized Heisenberg model expressed as

$$H=-\omega_0\sum_i S_i^z-D\sum_i (S_i^z)^2 -\sum_{i,j} J_{ij}[S_i^zS_j^z+\tfrac{1}{2}\eta(S_i^+S_j^-+S_i^-S_j^+)]\ , \quad (1)$$

where $\omega_0=g\mu_B H_a$; g being the Landé splitting factor, μ_B the Bohr magneton, and H_a the external field applied along the positive z direction. S_i and S_j are two spin operators at the lattice sites i and j, respectively. J_{ij} is the exchange integral and η measures the strength of the anisotropic exchange. D is a parameter measuring the strength of the single-ion anisotropy. The summation is assumed to extend over nearest-neighbor pairs i and j. In the present paper we restrict ourselves to the spin-1 case. We further assume at the outset that D is greater than zero which implies that the doublet is the ground state and the system orders along the z axis even if the exchange interaction is very weak compared to the single-ion anisotropy.

The above model has been extensively studied by a number of authors in the past[2–11] and some important results were obtained by them by several different methods. The model can be studied very simply by means of the molecular-field approximation[2] (MFA) and although it is the simplest of all the methods and it overestimates the interspin correlation, it gives fairly accurately the qualitative behavior of the model. More accurate quantitative results have been obtained by the method of double-time temperature-dependent Green's function.[2–11] In the early stage of application of Green's-function theory to magnetic problems, the equation-of-motion approach was adopted. In this approach one obtains a nonlinear differential equation in which the higher-order Green's functions are coupled with the lower-order ones. Each of the higher-order Green's functions is again written down in the form of a nonlinear equation and so on. This infinite hierarchy of equations is cut off by a decoupling approximation and the solution is achieved. However, these decoupling approximations are essentially intuitive or empirical in nature and cannot be justified from first principles. Often they lead to unphysical results. The problem becomes really serious for spins greater than $\frac{1}{2}$. A spin-1 Heisenberg model with single-ion anisotropy[2–11] and a spin-1 Heisenberg model with biquadratic exchange[12–17] are two well-known problems where the solutions obtained even by rigorous decoupling schemes are far from satisfactory. In both cases the problem of decoupling of single-site Green's functions causes much difficulty. However, it has been realized that the idea of decoupling of single-site Green's functions is erroneous and methods have been devised in which the single-ion terms were treated exactly.[4–6] In the present paper we restrict ourselves to the single-ion case and the biquadratic-exchange problem will be discussed in a later paper. A fairly long review of early works on the single-ion problem is presented in the paper of Yang and Wang[18] in which they clearly analyze the arbitrariness and inconsistencies in the calculations of earlier authors.

In order to remove the inconsistencies Yang and Wang developed a diagrammatic perturbation theory for standard basis operators (SBO) and summed up the diagrams to order $1/z$, where z is the number of nearest neighbors of a given spin. They showed that if one performs a correct summation of diagrams of a given order the redundancy problem of Murao and Matsubara[3] is removed. However, although their theory is a definite improvement over early works on the problem, there still seems to be objections. Haley[19] claims that Yang and Wang were only partially successful. In the formulation of Yang and Wang some arbitrariness remains in the Wick-like reduction theorem proposed to decouple the time-ordered products of SBO. Furthermore, it is felt that the use of SBO leads to unnecessary complications of the problem. A diagrammatic technique of Vaks, Larkin, and Pikin,[20] using the usual spin operators, was developed by Kaschenko *et al.*[21] and Balakhonov *et al.*[22]

However, a semi-invariant diagram method with the use of the reduction theorem of Care and Tucker[23] may be developed. A general formulation including the spin-phonon interaction has been recently developed by Chakraborty and Tucker.[24]

Recently, it has been realized that it is possible to formulate a systematic self-consistent many-body theory and to develop an exact Dyson equation for the system.[25–30] In this respect, two apparently dissimilar but essentially equivalent approaches were invented. One is the Zwanzig-Mori's projection-operator method[25–27] and the other is the method of irreducible Green's functions.[28–30] Micnas and Kishore,[31] using the former approach, treated the single-ion problem. However, they did not study many of the important aspects of the problem, and also they represented the spin operators in terms of SBO which complicates the problem. The method of irreducible Green's function is more advantageous due to its inherent simplicity.

The purpose of the present paper is to develop the irreducible-Green's-function theory of an anisotropic Heisenberg model expressed by Eq. (1) and to derive the results for some important thermodynamic quantities. To date no such calculation is apparently available in the literature.

The plan of the paper is as follows: Section II presents the formal developments of the equation of motion for the two-time temperature-dependent Green's function and the random-phase-approximation (RPA) results are studied. Section III employs some appropriate irreducible operators to obtain a solution. An exact Dyson equation is derived. In Sec. IV the low-temperature properties of the model are investigated. In Sec. V the results for the Curie temperature are derived and discussed with the results of MFA, of the diagrammatic technique of Yang and Wang, of the correlated effective-field approximation of Lines, and of the high-temperature series results of Wang and Lee. Some concluding remarks are presented in Sec. VI.

II. BASIC FORMALISM

There exist in the literature sufficient sources of information about the equation-of-motion approach for two-time temperature-dependent Green's functions and so it is not very useful to repeat it here. Following Zubarev[32] we employ a two-time thermal-retarded Green's function $G_{fg}(t-t')$ defined by

$$G_{fg}(t-t')=\langle\langle S_f^+;S_g^-\rangle\rangle = -i\Theta(t-t')\langle[S_f^+(t),S_g^-(t')]\rangle , \tag{2}$$

where f and g are lattice sites and $\Theta(x)$ is the step function having the property

$$\Theta(x)=\begin{cases}0, & \text{for } x<0\\ 1, & \text{for } x>0 .\end{cases} \tag{3}$$

Considering differentiation with respect to the first time t, the equation of motion for the Green's function may be shown to be

$$\omega\langle\langle S_f^+;S_g^-\rangle\rangle_\omega=(1/2\pi)\langle[S_f^+,S_g^-]\rangle + \langle\langle[S_f^+,H];S_g^-\rangle\rangle_\omega , \tag{4}$$

where we have chosen units such that $\hbar=1$. The suffix ω attached to the Green's function implies that we have taken the time-energy Fourier transform of the Green's function $G_{fg}(t-t')$. Henceforth we omit this suffix.

Using Eq. (1) for H in Eq. (4), we get, after simplifications,

$$(\omega-\omega_0)\langle\langle S_f^+;S_g^-\rangle\rangle=(1/\pi)\langle S_f^z\rangle\delta_{fg}+D\langle\langle\sigma_f^+;S_g^-\rangle\rangle +2\sum_i J_{if}\langle\langle(S_i^zS_f^+-\eta S_i^+S_f^z);S_g^-\rangle\rangle, \tag{5}$$

where

$$\sigma_f^+=S_f^zS_f^++S_f^+S_f^z \tag{6}$$

is treated as a single operator.

The right-hand side of Eq. (5) contains higher-order Green's function of two kinds. One is the exchange Green's function like $\langle\langle S_i^zS_f^+;S_g^-\rangle\rangle$ and the other is the single-site Green's function like $\langle\langle\sigma_f^+;S_g^-\rangle\rangle$. The random-phase approximation used to decouple the former type gives very good results throughout a wide range of temperatures. Much more rigorous decoupling schemes were also devised. Similar attempts were also made to decouple the single-site Green's functions. However, it has been realized by some authors that there is no need to decouple this kind of Green's function and that the single-ion term can be treated exactly. Actually, σ_f^+ is a single operator and one can readily set up the following equation of motion for $S=1$:

$$(\omega-\omega_0)\langle\langle\sigma_f^+;S_g^-\rangle\rangle=(1/\pi)\lambda_f\delta_{fg}+D\langle\langle S_f^+;S_g^-\rangle\rangle +2\sum_i J_{if}\langle\langle(S_i^z\sigma_f^+-\eta S_i^+\lambda_f);S_g^-\rangle\rangle, \tag{7}$$

where

$$\lambda_f=3(S_f^z)^2-2 . \tag{8}$$

In deriving Eq. (7) we have used the following spin-1 identities:

$$S_f^+S_f^+=0 , \qquad (S_f^z)^2S_f^++S_f^+(S_f^z)^2=S_f^+ . \tag{9}$$

Because of the translational invariance of the lattice we can use the following Fourier transforms:

$$S_i^z=(1/N^{1/2})\sum_k S_k^z\exp(-i\mathbf{k}\cdot\mathbf{R}_i) ,$$
$$S_i^\pm=(1/N^{1/2})\sum_k S_k^\pm\exp(\mp i\mathbf{k}\cdot\mathbf{R}_i) , \tag{10}$$
$$J_{ij}=(1/N)\sum_k J_k\exp[-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)] .$$

The Fourier transforms of σ_i^+ is like S_i^+ and λ_i is like S_i^z.

Equations (5) and (7), therefore, take the following forms:

$$(\omega-\omega_0)\langle\langle S_k^+;S_{q'}^-\rangle\rangle = \langle S_{k-q'}^z\rangle/(\pi\sqrt{N})+D\langle\langle\sigma_k^+;S_{q'}^-\rangle\rangle + (2/N^{1/2})\sum_{k'}J_{k'}\langle\langle(S_{k'}^zS_{k-k'}^+-\eta S_{k-k'}^zS_{k'}^+);S_{q'}^-\rangle\rangle , \tag{11}$$

$$(\omega-\omega_0)\langle\langle\sigma_k^+;S_{q'}^-\rangle\rangle = \langle\lambda_{k-q'}\rangle/(\pi N^{1/2})+D\langle\langle S_k^+;S_{q'}^-\rangle\rangle + (2/N^{1/2})\sum_{k'}J_{k'}\langle\langle(S_{k'}^z\sigma_{k-k'}^+-\eta\lambda_{k-k}S_{k'}^+);S_{q'}^-\rangle\rangle . \tag{12}$$

Equations (11) and (12) are the results of straightforward derivation and were obtained in these forms by Potapkov.[6] These equations may also be seen to follow from the works of Devlin[4] and Tanaka and Kondo.[5]

Now within the RPA one can write

$$\langle\langle S_{k'}^zS_{k-k'}^+;S_{q'}^-\rangle\rangle = N^{1/2}b\delta_{k'}\langle\langle S_{k-k'}^+;S_{q'}^-\rangle\rangle , \tag{13}$$

$$\langle\langle S_{k'}^z\sigma_{k-k'}^+;S_{q'}^-\rangle\rangle = N^{1/2}b\delta_{k'}\langle\langle\sigma_{k-k'}^+;S_{q'}^-\rangle\rangle . \tag{14}$$

Equations (11) and (12) may, therefore, be written in the following forms:

$$\{(\omega-\omega_0)-2b(J_0-\eta J_k)\}G_1-DG_2=(b/\pi)\delta_{k-q'} , \tag{15}$$

$$-(D-2\eta\lambda J_k)G_1+(\omega-\omega_0-2bJ_0)G_2=(\lambda/\pi)\delta_{k-q'} , \tag{16}$$

where

$$G_1=\langle\langle S_k^+;S_{q'}^-\rangle\rangle ,$$
$$G_2=\langle\langle\sigma_k^+;S_{q'}^-\rangle\rangle ,$$
$$b=\langle S^z\rangle;\quad \lambda=\langle\lambda\rangle . \tag{17}$$

For $\eta=1$, Eqs. (15) and (16) reduce to those of Potapkov, and generate two spin-wave branches, one is the usual spin-wave excitation and the other is the optical excitation. Equations (15) and (16), along with the use of the spectral theorem, enable one to derive all the necessary thermodynamic quantities with correct qualitative behavior.

However, the calculations done in the above way are subject to serious criticisms from another corner. It may be noted that in addition to the Green's functions G_1 and G_2, there are other pair of Green's functions G_3 and G_4 which are, respectively, the Fourier transforms of the Green's functions $\langle\langle S_f^+;\sigma_g^-\rangle\rangle_\omega$ and $\langle\langle\sigma_f^+;\sigma_g^-\rangle\rangle_\omega$. The equations of motion for these Green's functions can be found to be

$$(\omega-\omega_0)\langle\langle S_f^+;\sigma_g^-\rangle\rangle = (b/\pi)\delta_{fg}+D\langle\langle\sigma_f^+;\sigma_g^-\rangle\rangle + 2\sum_i J_{if}\langle\langle(S_i^zS_f^+-\eta S_i^+S_f^z);\sigma_g^-\rangle\rangle , \tag{18}$$

$$(\omega-\omega_0)\langle\langle\sigma_f^+;\sigma_g^-\rangle\rangle = (\lambda/\pi)\delta_{fg}+D\langle\langle S_f^+;\sigma_g^-\rangle\rangle + 2\sum_i J_{if}\langle\langle(S_i^z\sigma_f^+-\eta\lambda_fS_i^+);S_g^-\rangle\rangle . \tag{19}$$

Fourier transforming to momentum space we get

$$(\omega-\omega_0)\langle\langle S_k^+;\sigma_{q'}^-\rangle\rangle = \langle\lambda_{k-q'}\rangle/(\pi N^{1/2})+D\langle\langle\sigma_k^+;\sigma_{q'}^-\rangle\rangle + (2/N^{1/2})\sum_{k'}J_{k'}\langle\langle(S_{k'}^zS_{k-k'}^+-\eta S_{k'}^+S_{k-k'}^z;\sigma_{q'}^-\rangle\rangle , \tag{20}$$

$$(\omega-\omega_0)\langle\langle\sigma_k^+;\sigma_{q'}^-\rangle\rangle = \langle S_{k-q'}^z\rangle/(\pi N^{1/2})+D\langle\langle S_k^+;\sigma_{q'}^-\rangle\rangle + (2/N^{1/2})\sum_{k'}J_{k'}\langle\langle(S_{k'}^z\sigma_{k-k'}^+-\eta\lambda_{k-k'}S_k^+);\sigma_{q'}^-\rangle\rangle . \tag{21}$$

Using RPA one can linearize the above equations of motion and one obtains two coupled equations in G_3 and G_4. Using this set of equations it is again possible to derive necessary thermodynamic quantities. The interesting point is that the results obtained from this set do not agree with those derived from Eqs. (15) and (16). This redundancy problem was discussed by many authors. When one uses the SBO an additional problem develops. This is the one related to the breakdown of kinematical consistency of SBO.[19]

One interesting point should be noted. Two sets of equations mentioned above are actually coupled with each other. When one uses the RPA this coupling breaks down and two sets become essentially independent and this leads to redundancy. So, to remove this redundancy we have to retain this coupling and this is what is done in a diagram technique.

III. IRREDUCIBLE GREEN'S FUNCTIONS

It is possible to formulate the equation-of-motion technique with the use of irreducible operators first introduced by Plakida,[28] and later studied by other authors.[29,30] Like the diagrammatic technique the irreducible Green's function theory, in principle, enables one to formulate the problem exactly. However, as in a diagram technique, only a certain class of diagrams are summed up in practice, likewise in the irreducible Green's function theory specific approximations are found to be necessary for reducing or evaluating the irreducible operators.

In the present problem we use the following irreducible operators:[30]

$$(S^z_{k'})^{ir}=S^z_{k'}-bN^{1/2}\delta_{k'}\,,$$
$$\phi_1=(S^z_{k'}S^+_{-k'}-\eta S^z_{k-k'}S^+_{k'})^{ir}\,, \tag{22}$$
$$\phi_2=(S^z_{k'}\sigma^+_{-k'}-\eta\lambda_{k-k'}S^+_{k'})^{ir}\,.$$

Therefore, we can write

$$\langle\langle(S^z_{k'}S^+_{-k'}-\eta S^z_{k-k'}S^+_{k'});S^-_{q'}\rangle\rangle = \langle\langle(\phi_1+bN^{1/2}\delta_{k'}S^+_{-k'}-\eta bN^{1/2}\delta_{k-k'}S^+_{k'});S^-_{q'}\rangle\rangle\,, \tag{23}$$

$$\langle\langle(S^z_{k'}\sigma^+_{-k'}-\eta\lambda_{k-k'}S^+_{k'});S^-_{q'}\rangle\rangle = \langle\langle(\phi_2+bN^{1/2}\delta_{k'}\sigma^+_{-k'}-\eta\lambda N^{1/2}\delta_{k-k'}S^+_{k'});S^-_{q'}\rangle\rangle\,. \tag{24}$$

The equations of motion for G_1, G_2, G_3, and G_4 can, therefore, be written in the following matrix form:

$$\begin{bmatrix}G_1 & G_2\\ G_3 & G_4\end{bmatrix}\begin{bmatrix}\omega-\gamma+2\eta bJ_k & -(D-2\eta\lambda J_k)\\ -D & \omega-\gamma\end{bmatrix} = \begin{bmatrix}I_{1,S^-_{q'}} & I_{2,S^-_{q'}}\\ I_{1,\sigma^-_{q'}} & I_{2,\sigma^-_{q'}}\end{bmatrix}, \tag{25}$$

where

$$\gamma=\omega_0+2bJ_0\,, \tag{26}$$

$$\left.\begin{matrix}I_{1(2),S^-_{q'}}\\ I_{1,(2),\sigma^-_{q'}}\end{matrix}\right\} = \begin{Bmatrix}b(\lambda)/\pi\\ \lambda(b)/\pi\end{Bmatrix}\delta_{k-q'} + (2/N^{1/2})\sum_{k'}J_{k'}\left\langle\!\left\langle\phi_{1(2)};\begin{Bmatrix}S^-_{q'}\\ \sigma^-_{q'}\end{Bmatrix}\right\rangle\!\right\rangle\,. \tag{27}$$

The expressions for $\langle\langle\phi_1;S^-_{q'}\rangle\rangle$ etc., can be written down by setting up the equations of motion with respect to the second time t' appearing in the Green's functions. Using the irreducible operators

$$\psi_1=(S^z_{k'}S^-_{k'+q'}-\eta S^z_{k'-q'}S^-_{k'})^{ir}\,, \tag{28}$$
$$\psi_2=(S^z_{k'}\sigma^-_{k'+q'}-\eta\lambda_{k'-q'}S^-_{k'})^{ir}\,, \tag{29}$$

and after necessary simplifications Eq. (25) can be thrown into the following matrix Dyson equation

$$\underline{G}=\underline{G}^0+\underline{G}^0\underline{P}\underline{G}^0 \tag{30}$$

where G^0 is the mean field or zeroth-order Green's function and P is the polarization operator. These are given by

$$G^0_1=\frac{b(\omega-\gamma)+\lambda D}{\pi(\omega-\omega^+_k)(\omega-\omega^-_k)}\,,$$
$$G^0_4=G^0_1+\frac{2J_k(b^2-\eta\lambda^2)}{\pi(\omega-\omega^+_k)(\omega-\omega^-_k)}\,, \tag{31}$$

$$G^0_2=G^0_3=\frac{1}{\pi}\frac{\lambda(\omega-\gamma)+bD}{(\omega-\omega^+_k)(\omega-\omega^-_k)}\,, \tag{32}$$

$$P_n=C_nI_{k'k''}\,, \tag{33}$$

$$C_1=\left[\frac{2\pi(\omega-\gamma)}{b(\omega-\gamma)+\lambda D}\right]^2\,, \tag{34}$$

$$C_2=\frac{4\pi^2(\omega-\gamma)(D-2\eta\lambda J_k)}{[\lambda(\omega-\gamma)+bD]^2}\,, \tag{35}$$

$$C_3=\frac{4\pi^2(\omega-\gamma)(D-2\eta\lambda J_k)}{[b(\omega-\gamma)+\lambda D]^2}\,, \tag{36}$$

$$C_4=\left[\frac{2\pi(D-2\eta\lambda J_k)}{\lambda(\omega-\gamma)+bD+2(1-\eta)b\lambda J_k}\right]^2\,, \tag{37}$$

$$I_{k'k''}=(1/N)\sum_{k',k''}J_{k'}J_{k''}\left\langle\!\left\langle\left[\phi_1+\frac{D\phi_2}{(\omega-\gamma)}\right];\left[\psi_1+\frac{D\psi_2}{(\omega-\gamma)}\right]\right\rangle\!\right\rangle\,, \tag{38}$$

$\omega^\pm_k$ give two branches of excitation spectra expressed as

$$\omega^\pm_k=\gamma-\eta bJ_k\pm[\eta^2b^2J_k^2+D(D-2\eta\lambda J_k)]^{1/2}\,. \tag{39}$$

For $\eta=1$, the above equation coincides with that obtained by previous authors.

Equation (30) can be written down as the exact Dyson equation

$$\underline{G}=\underline{G}^0+\underline{G}^0\Sigma\underline{G}\,, \tag{40}$$

where Σ is the self-energy operator given by

$$\Sigma=(P)^c\,, \tag{41}$$

c denoting the connected or proper part.

Knowing (41), one can calculate G exactly from Eq. (40), but the problem is that there exists no procedure for calculating (41) exactly and we have to employ approximations. It can be readily shown that in the lowest-order approximation the results obtained agree exactly with those obtained from $(1/z)^0$ order diagrams. In the lowest order we have only two Green's functions $G^0_1=G^0_3$ and $G^0_2=G^0_4$, and so the thermodynamic properties can be calculated uniquely and hence no redundancy arises. It may be noted that identical results were also obtained by Yang and Wang to order $(1/z)^0$.

Furthermore, we note that G^0_1 can be rearranged as

$$G^0_1=\frac{\Delta(\omega)}{1+\eta J_{k'}\Sigma(\omega)} \tag{42}$$

where

$$\Delta(\omega)=\frac{1}{2\pi}\frac{2b}{\omega-\gamma-D}-\frac{1}{2\pi}\frac{2D(b-\lambda)}{(\omega-\gamma)^2-D^2}\,, \tag{43}$$
$$\Sigma(\omega)=2\pi\Delta(\omega)\,. \tag{44}$$

For $\eta=1$, the above equations reduce exactly to those of Tanaka and Kondo[5] and Potapkov.[6]

Again, as the correspondence with the semi-invariant

diagrammatic formalism, we may rewrite G_1^0 in the following form:

$$G_1^0 = g(1+2\pi\eta J_k g)^{-1} , \tag{45}$$

where g stands for

$$g = \frac{b+\lambda}{2\pi(\omega-\gamma-D)} + \frac{b-\lambda}{2\pi(\omega-\gamma+D)} , \tag{46}$$

g is thus identical with the second-order semi-invariant and Eq. (45) is the same as that obtained in a semi-invariant diagrammatic formalism[21,24] to order $(1/z)^0$.

IV. RENORMALIZED GREEN'S FUNCTION AND LOW-TEMPERATURE RESULTS

From Eq. (40) one can write down the expression for the renormalized Green's function in a straightforward way. The result is

$$G_m(k,\omega) = A_m^+[\omega - E_m^+(k)]^{-1} + A_m^-[\omega - E_m^-(k)]^{-1} , \tag{47}$$

where $E_m^{\pm}(k)$ stand for the renormalized energy and are given by

$$E_m^{\pm}(k) = \omega_k^{\pm} + A_m^{\pm}\Sigma_m(k,\omega_k^{\pm}+i\epsilon) , \tag{48}$$

with $m = 1-4$ and

$$A_1^{\pm} = \pm\frac{b(\omega_k^{\pm}-\gamma)+\lambda D}{\pi(\omega_k^+-\omega_k^-)}, \quad A_4^{\pm} = \pm A_1^{\pm} \pm \frac{2J_k(b^2-\eta\lambda^2)}{\pi(\omega_k^+-\omega_k^-)} , \tag{49}$$

$$A_2^{\pm} = A_3^{\pm} = \pm\frac{\lambda(\omega_k^{\pm}-\gamma)+bD}{\pi(\omega_k^+-\omega_k^-)} . \tag{50}$$

The energy shift and damping are given by

$$\Delta\omega_k^{\pm}(m) - i\Gamma_k(m) = A_m^{\pm}\Sigma_m(k,\omega_k^{\pm}+i\epsilon) , \tag{51}$$

where $\Delta\omega_k$ is the shift in energy and Γ_k is the spin-wave damping.

Using the spectral theorem

$$\langle S_k^- S_k^+(t)\rangle = i\lim_{\epsilon\to 0}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega t}(e^{\beta\omega}-1)^{-1} \times(\langle\langle S_k^+;S_k^-\rangle\rangle_{\omega+i\epsilon} - \langle\langle S_k^+;S_k^-\rangle\rangle_{\omega-i\epsilon}) \tag{52}$$

we get the following relations:

$$\tfrac{4}{3} - b - (\lambda/3) = (1/N)\sum_k (N_1^+ b_r^+ + N_1^- b_r^-) \tag{53}$$

$$= (1/N)\sum_k (N_4^+ b_r^+ + N_4^- b_r^-) , \tag{54}$$

$$b - \lambda = (1/N)\sum_k (N_2^+ \lambda_r^+ + N_2^- \lambda_r^-) \tag{55}$$

$$= (1/N)\sum_k (N_3^+ \lambda_r^+ + N_3^- \lambda_r^-) , \tag{56}$$

where

$$N_x^{\pm} = (e^{\beta E_x^{\pm}(k)}-1)^{-1} , \tag{57}$$

$$b_r^{\pm} = b \pm [(\lambda D - b^2 J_k)/M(k)] ,$$
$$\lambda_r^{\pm} = \pm[(bD - b\lambda J_k)/M(k)] ,$$
$$M(k) = [\eta^2 b^2 J_k^2 + D(D - 2\eta\lambda J_k)]^{1/2} . \tag{58}$$

For the case $\eta = 1$ and when we use the unrenormalized energy values, i.e., $E_m^{\pm}(k) = \omega_k^{\pm}$ we may readily recover the expressions derived by Potapkov[6] and Devlin.[4]

Equations (53)–(56) enable us to study the statistical-mechanical properties of the model at any arbitrary temperature, but the complicated structure of these equations prevent us from having exact estimates. However, the low-temperature case can be treated very easily. This is mainly due to the fact that at low temperatures we can neglect the upper branch ω_k^+ and that we have to consider only the lower branch ω_k^-, and one gets after simplifications

$$b = \left[1 + (2/N)\sum_k (e^{\beta\omega_k^-}-1)^{-1}\right] , \tag{59}$$

$$\lambda = b^2 , \tag{60}$$

$$\omega_k^- = \omega_0 + D + 2(J_0 - J_k)b , \tag{61}$$

where we have quoted the results only for $\eta = 1$. These are well-known results.

For the spin-1 case we get, using $\lambda \approx 1, b \approx \lambda$, the simple relationship

$$P_1 = P_2 = P_3 = P_4 \tag{62}$$

which implies

$$G_1 = G_2 = G_3 = G_4 , \tag{63}$$

and

$$P_1 = \left[\frac{(D-2J_k)}{D-J_k}\right]^2 I_{k'k''} , \tag{64}$$

$$\Sigma(k,\omega_k^-) = \left[\frac{\pi(D-2J_k)}{D-J_k}\right]^2 (1/N) \times \sum_{k',k''} J_{k'} J_{k''} \left\langle\!\!\left\langle \phi_1 + \frac{D\phi_2}{D-2J_k}; \psi_1 + \frac{D\psi_2}{D-2J_k}\right\rangle\!\!\right\rangle . \tag{65}$$

Equation (65) can be written down in a very simple form. We note that at any arbitrary temperature $I_{k'k''}$ may be expressed as

$$I_{k'k''}=(1/N)\sum_{k',k''} J_k J_{k''}\int_{-\infty}^{\infty}\frac{d\omega'}{\omega-\omega'}(e^{\beta\omega'}-1)\int_{-\infty}^{\infty}dt\, e^{i\omega' t}\left[\langle\psi_1\phi_1(t)\rangle+\frac{D}{D-2J_k}\langle\psi_2\phi_1(t)\rangle\right.$$
$$\left.+\frac{D}{D-2J_k}\langle\psi_1\phi_2(t)\rangle+\left[\frac{D}{D-2J_k}\right]^2\langle\psi_2\phi_2(t)\rangle\right]. \quad (66)$$

Let us use a simple decoupling approximation of the form

$$\langle(S^z_{k''}S^-_{k''+q'})^{ir}[S^z_{k'}(t)S^+_{-k'}(t)]^{ir}\rangle \sim\langle S^z_{k''}S^z_{k'}(t)\rangle\langle S^-_{k''+q'}S^+_{-k'}(t)\rangle\,, \quad (67)$$

along with a single-pole approximation $\omega\simeq\omega_k^-$ we get the following low-temperature expression for the self-energy:

$$\Sigma_1(k,\omega_k^-+i\epsilon)\simeq(4b\pi^2/N)\sum_{k'}\frac{(J_{k'}-J_{k+k'})^2\langle S^z_{k'}S^z_{k'}\rangle}{\omega_k^--\omega_{k-k'}+i\epsilon}\,. \quad (68)$$

The expressions for the energy shift and damping are given by

$$\Delta\omega_k=(4b^2\pi/N)\sum_{k'}[(J_{k'}-J_{k+k'})^2/(J_{k-k'}-J_k)]\langle S^z_k S^z_{k'}\rangle\,, \quad (69)$$

$$\Gamma_k=(4b^2\pi^2/N)\sum_{k'}(J_{k'}-J_{k+k'})^2\langle S^z_{k'}S^z_{k'}\rangle\delta(J_{k-k'}-J_k)\,. \quad (70)$$

The resonance linewidth is related to Γ_0 and we see in this case that $\Gamma_0=0$. Also, $\Delta\omega_0=0$. These results agree with those obtained by Chakraborty and Tucker.[24] But these results are not in accordance with the results of Kaschenko *et al.*[21] and Yang and Wang[18] in diagrammatic framework, and of Micnas and Kishore[31] in a projection-operator framework.

Furthermore, at low temperatures one can readily derive the following result:

$$G_1(0)=\frac{2b}{2\pi(\omega-\omega_0-D)}\,. \quad (71)$$

The resonance frequency is thus $\omega_r=\omega_0+D$ which is the same as that of Potapkov.[6]

V. HIGH-TEMPERATURE RESULTS

As in a diagrammatic theory for a magnetic system it is also very difficult in the present theoretical framework to derive quantitatively accurate results at high temperatures. However, some sensibly accurate values of Curie temperatures can be derived with the use of some approximations. Equations (53)–(56) are exact expressions for b and λ, but it is impossible, in practice, to perform computations from these equations. The simplified forms for the self-energy are necessary for computation. However, we shall consider an easier problem of computing the results for the Curie temperature. We first see that since $E_1(k)=E_4(k)$, $E_2(k)=E_3(k)$, Eqs. (53)–(56) reduce to the following two identities:

$$\frac{(4-\lambda)}{3}-b=(1/N)\sum_k\left[bn_1^+ +\frac{D-b^2J_k}{M(k)}n_1^-\right], \quad (72)$$

$$b-\lambda=(1/N)\sum_k\left[n_1^+ +\frac{b(D-b^2J_k)}{M(k)}n_2^-\right], \quad (73)$$

where

$$n_x^{\pm}=(e^{\beta E_x^+(k)}-1)^{-1}\pm(e^{\beta E_x^-(k)}-1)^{-1}\,. \quad (74)$$

After straightforward simplifications we can write the following explicit expressions for n_1 and n_2:

$$n_1^+=-1-\tfrac{1}{2}\beta(\gamma-bJ_k)\operatorname{cosech}^2[\tfrac{1}{2}\beta M(k)]$$
$$-\frac{\pi\beta}{2M(k)}\operatorname{cosech}^2[\tfrac{1}{2}\beta M(k)]\left[\frac{f^+}{b(-bJ_k+M(k))+\lambda D}+\frac{f^-}{b(bJ_k+M(k))-\lambda D}\right], \quad (75)$$

$$n_1^-=\coth[\tfrac{1}{2}\beta M(k)]-\frac{\pi\beta}{2M(k)}\operatorname{cosech}^2[\tfrac{1}{2}\beta M(k)]\left[\frac{f^+}{b(-bJ_k+M(k))+\lambda D}-\frac{f^-}{b(bJ_k+M(k))-\lambda D}\right], \quad (76)$$

$$n_2^+=-1-\tfrac{1}{2}\beta(\gamma-bJ_k)\operatorname{cosech}^2[\tfrac{1}{2}\beta M(k)]$$
$$-\frac{\beta\pi(D-2\lambda J_k)}{2M(k)}\operatorname{cosech}^2[\tfrac{1}{2}\beta M(k)]\left[\frac{f^+P^+}{\lambda(-bJ_k+M(k))+bD}+\frac{f^-P^-}{\lambda(bJ_k+M(k))-bD}\right], \quad (77)$$

$$n_2^-=\coth[\tfrac{1}{2}\beta M(k)]-\frac{\beta\pi(D-2\lambda J_k)}{2M(k)}\operatorname{cosech}^2\left[\frac{\beta M(k)}{2}\right]\left[\frac{f^+P^+}{\lambda(-bJ_k+M(k))+bD}-\frac{f^-P^-}{\lambda(bJ_k+M(k))-bD}\right], \quad (78)$$

where

$$f^{\pm}=(1/N)\sum_{k',k''} J_{k'}J_{k''}\langle\langle [bJ_k \mp M(k)]\phi_1 - D\phi_2 ;$$
$$[bJ_k \mp M(k)]\psi_1 - D\psi_2\rangle\rangle_{\omega_k^{\pm}+i\epsilon} , \quad (79)$$
$$P^{\pm}=-bJ_k \pm M(k) .$$

The elimination or the determination of λ from Eqs. (72) and (73) in the limit $b\to 0$ and the subsequent derivation for an expression for the Curie temperature are evidently complicated. However, approximate results for the Curie temperature may be obtained readily using a single-pole approximation which is consistent with the observation of Kaschenko *et al.*[21] stating that even at temperatures close to the Curie point one of the modes becomes highly damped in comparison to the other mode. They identified ω_k^+ as this highly damped mode. So, considering only a single pole at $\omega=\omega_k^-$ and taking the limit $b\to 0$ we arrive at the following two equations (for $\eta=1$):

$$1=U(\beta_c)-\lambda V(\beta_c)+W_2(\beta_c) , \quad (80)$$
$$\lambda=\frac{4+3W_1(\beta_c)}{1+3U(\beta_c)} . \quad (81)$$

Combining (80) and (81) we arrive at the final expression for the Curie temperature

$$1=U(\beta_c)-W_2(\beta_c)+\frac{4+3W_1(\beta_c)}{1+3U(\beta_c)}V(\beta_c)=0 . \quad (82)$$

This equation is structurally similar to the form obtained by Tanaka and Kondo.[5] Different parameters appearing in the above equation are given by

$$U(\beta_c)=(1/N)\sum_k \frac{D}{M_0(k)}\coth[\tfrac{1}{2}\beta_c M_0(k)] , \quad (83)$$
$$V(\beta_c)=(1/N)\sum_k \{(J_k/M_0(k)]\coth[\tfrac{1}{2}\beta_c M_0(k)]+\tfrac{1}{2}\beta_c(2J_0-J_k)\operatorname{cosech}^2[\tfrac{1}{2}\beta_c M_0(k)]\} , \quad (84)$$
$$W_1(\beta_c)=\frac{\pi\beta_c}{2N}\sum_k \frac{\gamma_2}{M_0^2(k)}\operatorname{cosech}^2[\tfrac{1}{2}\beta_c M_0(k)] , \quad (85)$$
$$W_2(\beta_c)=-\frac{\pi\beta_c}{2N}\sum_k \frac{(D-2\lambda J_k)}{m_0^3(k)}\left[\gamma_1-\left[\frac{(D-2\lambda J_k)(D-\lambda J_k)}{M_0(k)}\gamma_2\operatorname{cosech}^2[\tfrac{1}{2}\beta_c M_0(k)]\right]\right] , \quad (86)$$

where

$$\gamma_1=\lim_{b\to 0}\left[\frac{f^+-f^-}{b}\right] ,$$
$$\gamma_2=\lim_{b\to 0}(f^++f^-) ,$$
$$M_0(k)=[D(D-2J_k(\lambda)_{b\to 0})]^{1/2} .$$

If one ignores $W_1(\beta_c)$ and $W_2(\beta_c)$ one can recover the results of Tanaka and Kondo.[5] Thus in the present framework the results for the Curie temperature are substantially modified by the presence of the parameters $W_1(\beta_c)$ and $W_2(\beta_c)$. The estimates for these parameters may be made by means of calculating γ_1 and γ_2. Exact calculation is not possible at present. We resort to approximations. Using Tyablikov's approximation[33] for infinite energy we may write for $D>0$ and at $T=T_c$

$$G_1(\omega_k^-)\sim -\lambda_0/(4\pi D) , \quad (87)$$

where $\lambda_0=(\lambda)_{b\to 0}$. We have assumed that the mode ω_k^+ is highly damped. The expressions for γ_1 and γ_2 thus become

$$\gamma_1\approx\frac{\lambda^2 D}{\pi}J_k(J_0-J_k) , \quad (88)$$
$$\gamma_2\approx\frac{\lambda^3 D}{2\pi}J_k^2 . \quad (89)$$

The expressions for $W_1(\beta_c)$ and $W_2(\beta_c)$ take the forms

$$W_1(\beta_c)=-\frac{\lambda^3\beta_c}{4N}\sum_k \frac{D^3J_k^2}{M_0^4(k)}\operatorname{cosech}^2[\tfrac{1}{2}\beta_c M_0(k)] , \quad (90)$$
$$W_2(\beta_c)=\frac{\beta_c\lambda^2}{4N}\sum_k \frac{D^5J_k^2}{M_0^6(k)} \times\{1+2[M_0^2(k)/D^2][1-(J_0/J_k)]\} , \quad (91)$$

For the case $W_1(\beta_c)=0$, $W_2(\beta_c)=0$, and

$$M_0(k)=D, \quad \lambda=\frac{2(e^{\beta_{cD}}-1)}{e^{\beta_c D}+1} ,$$

one can get the MFA result

$$4\beta_c J_0=\gamma , \quad (92)$$

where $\gamma=2+\exp(-\beta_c D)$, and $J_0=Jz$, J being the nearest-neighbor exchange constant and z being the number of nearest neighbors.

Using (92) as a first step of iteration and ignoring

$W_1(\beta_c)$ and $W_2(\beta_c)$, we arrive at the RPA result

$$4\beta_c J_0=\gamma F \ , \tag{93}$$

where

$$F=(1/N)\sum_k[1-(J_k/J_0)]^{-1} \ . \tag{94}$$

We shall now include the effects of the parameters W_1 and W_2. Using (93) we get the following equation for the Curie temperature:

$$24aPK_c^2+2\gamma(2+aC)-F\gamma^2=0 \ , \tag{95}$$

where

$$a=Q/\alpha, \quad C=(1+4a)(1+2a), \quad \alpha=D/J_0 \ ,$$
$$Q=1-(3/\gamma), \quad P=1-(2/\gamma) \ .$$

The results are shown in Fig. 1 where K_c has been plotted against D/J_0. For comparison the results of other calculations are also quoted. These results correspond to those of the MFA, of correlated-effective-field (CEF) approximation[34] and of the high-temperature-series (HTS) expansion derived by Wang and Lee. Results of diagrammatic theory of Yang and Wang are not shown in Fig. 1 since they are not very distinguishable from those of Wang and Lee.[35] Figure 1 shows that the results of the present calculation are very close to those of CEF theory of Lines.[34]

VI. CONCLUDING REMARKS

The irreducible Green's function (IRG) theory for a spin-1 anisotropic Heisenberg model developed in the preceding sections has been found to be more satisfactory than the conventional equation-of-motion technique. Like a diagram technique, the IRG theory is, in principle, able to reproduce exact results. An additional advantage of an IRG theory is its simplicity in application to complicated magnetic systems. It has been realized that for a Heisenberg model with complicated interactions it is not really easy to carry out high-temperature-series expansion, Monte Carlo simulation, or a renormalization-group calculation. Indeed, the results of such calculations are still not available. Wang-Lee's results of HTS expansion[35] are actually based on the diagrammatic perturbation formalism of standard basis operators, which has some disadvantages as mentioned in the Introduction. So the results calculated from this expansion should not be considered as exact. Still, considering these results as the best available estimates for the Curie temperature, we find that the results of the present paper do not differ very widely from the results of Wang and Lee. An additional feature to be noted is that the present results agree nicely with those of CEF theory of Lines.[34]

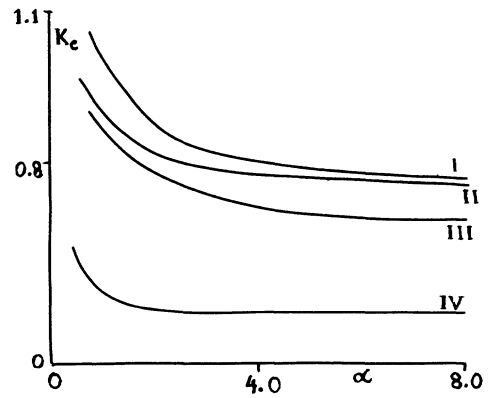

FIG. 1. The variation $K_c=J_0/k_BT_c$ with respect to $\alpha=D/J_0$, for a spin-1 simple-cubic Heisenberg ferromagnet. Curve I represents the results of the present paper. Curve II shows the results of CEF of Lines. Curve III represents the results of HTS expansion of Wang and Lee. Curve IV corresponds to the results of MFA.

However, it is clear that the most difficult part of an IRG theory is the calculation of the self-energy operator and no systematic method has been invented for this. Combining with the formalities of the diagrammatic technique, it might be possible to devise an appropriate reduction theorem for the irreducible operators. The problem may also be considered with reference to the recent work of Singer and Weeks,[36] who, starting from Kubo's generalized cumulant formalism, developed renormalized finite cluster expansions for a class of statistical systems in which the degrees of freedom can be grouped according to their degrees of correlation. They were able to show that when the expansion is truncated at different orders the final result is found to be a hierarchy of mean-field approximations and a number of terms of the exact series expansion is reproduced. In the present IRG formulation the mean-field contribution is first extracted out from the higher-order Green's functions and the effects of the remaining terms are all left with the irreducible operators which are then decoupled by RPA. So, the results might not be expected to agree with the results obtained from the first few terms of the exact series. A systematic way of extracting mean-field contributions successfully from the irreducible operators may possibly reproduce an increasing number of terms of the exact series expansion. A formulation of the problem in this manner will be considered in future.

We conclude by mentioning the major difficulties at present to formulate the problem using renormalization-group technique. Recently, the Heisenberg models are studied on the basis of Migdal[37]-Kadanoff[38] (MK) approximation which has the following basic problem.[39–42] The MK approximation consists of two main steps—one is the bond moving and the other is the site decimation. For quantum-spin models site decimation cannot be carried out exactly and one has to resort to a suitable approximation. Recent modified approximate schemes for site decimation done by Chen, Chen, and Lee[42] may be applied to the present problem. Under these circumstances IRG theory may be granted as an acceptable approach since it has been found from the present calculations that this method has got the potential to reproduce the results with reasonable accuracy.

ACKNOWLEDGMENT

The author wishes to thank Dr. J. W. Tucker of the Department of Physics, University of Sheffield, Sheffield, England, for many helpful discussions.

[1]K. W. H. Stevens, in *Magnetism,* edited by G. T. Rado and H. Suhl (Academic, New York, 1963), Vol. 1, p. 1; J. Kanamori, *ibid.*, p. 127.
[2]M. E. Lines, Phys. Rev. **156**, 534 (1967).
[3]T. Murao and T. Matsubara, J. Phys. Soc. Jpn. **25**, 352 (1968).
[4]J. F. Devlin, Phys. Rev. B **4**, 136 (1971).
[5]M. Tanaka and Y. Kondo, Prog. Theor. Phys. **48**, 1815 (1972).
[6]N. A. Potapkov, Teor. Mat. Fiz. **8**, 381 (1971).
[7]S. B. Haley and P. Erdos, Phys. Rev. B **5**, 1106 (1972).
[8]S. L. Ginzburg, Fiz. Tverd. Tela **12**, 1805 (1970) [Sov. Phys.—Solid State **12**, 1429 (1970)].
[9]L. M. Noskova, Fiz. Met. Mettalloved **33**, 698 (1972).
[10]A. Narath, Phys. Rev. **140**, A854 (1965).
[11]F. B. Anderson and F. B. Callen, Phys. Rev. **136**, A1068 (1964).
[12]L. Biegala, Phys. Status Solidi **40**, 1249 (1969).
[13]K. G. Chakraborty, J. Phys. C **9**, 1499 (1976); **10**, 2197 (1977).
[14]M. Tiwari and R. N. Srivastava, Nuovo Cimento **58B**, 323 (1980).
[15]A. M. Stewart and J. Adler, J. Phys. C **13**, 6227 (1980).
[16]V. Kumar and K. C. Sharma, J. Phys. C **10**, 1511 (1977).
[17]R. G. Munro and M. D. Girardeau, J. Magn. Magn. Mater. **2**, 319 (1976).
[18]D. H. Y. Yang and Y.-L. Wang, Phys. Rev. B **12**, 1057 (1975).
[19]S. B. Haley, Phys. Rev. **17**, 337 (1978).
[20]V. G. Vaks, A. I. Larkin, and S. A. Pikin, Zh. Eksp. Teor. Fiz. **53**, 1089 (1967) [Sov. Phys.—JETP **26**, 188 647 (1968)].
[21]M. P. Kaschenko, N. F. Balakhonov, and L. V. Kurbatov, Zh. Eksp. Teor. Fiz. **64**, 391 (1973) [Sov. Phys.—JETP **37**, 201 (1973)].
[22]N. F. Balakhonov, M. P. Kaschenko, V. N. Kitaev, and L. V. Kurbatov, Teor. Mat. Fiz. **19**, 102 (1974).
[23]C. M. Care and J. W. Tucker, J. Phys. C **10**, 2773 (1977).
[24]K. G. Chakraborty and J. W. Tucker, Physica A (to be published).
[25]R. Zwanzig, in *Lectures in Theoretical Physics, Boulder, Colorado, 1960,* edited by W. E. Bittin, D. W. Downs, and Downs (Interscience, New York, 1961), Vol. III.
[26]H. Mori, Prog. Theor. Phys. **33**, 423 (1965).
[27]M. Ichyanagi, J. Phys. Soc. Jpn. **32**, 604 (1972).
[28]N. M. Plakida, J. Phys. C **4**, 1680 (1971); Phys. Lett. **43A**, 481 (1973).
[29]A. L. Kuzmensky, Theor. Math. Phys. **36**, 208 (1978).
[30]D. I. Marvakov, J. P. Vlahov, and A. L. Kuzmensky, J. Phys. C **18**, 2871 (1985).
[31]R. Micnas and R. Koshore, Physica **108A**, 180 (1981).
[32]D. N. Zubarev, Usp. Fiz. Nauk **71**, 71 (1960) [Sov. Phys.—Usp. **3**, 320 (1960)].
[33]S. V. Tyablikov, *Methods in the Quantum Theory of Magnetism,* translated from Russian by A. Tybulewicz (Plenum, New York, 1967), Chap. VII, p. 236.
[34]M. E. Lines, Phys. Rev. B **9**, 3766 (1975).
[35]Y. L. Wang and F. Lee, Phys. Rev. Lett. **38**, 913 (1977).
[36]S. J. Singer and J. D. Weeks, Phys. Rev. B **36**, 215 (1987).
[37]A. A. Migdal, Zh. Eksp. Teor. Fiz. **69**, 810 (1975); **69**, 1457 (1975).
[38]L. P. Kadanoff, Ann. Phys. (N.Y.) **100**, 359 (1976).
[39]H. H. Chen, F. Lee, and H. C. Tseng, Phys. Rev. B **34**, 6448 (1986).
[40]M. Suzuki and H. S. Takano, Phys. Lett. **69A**, 426 (1979).
[41]H. S. Takano and M. Suzuki, J. Stat. Phys. **26**, 635 (1981).
[42]H. H. Chen, Y. C. Chen, and F. Lee, Phys. Lett. A **125**, 235 (1987).