Unified first-order Green's-function theory of anisotropic Heisenberg ferromagnets for $S=\frac{1}{2}$

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A unified first-order Green's-function theory of anisotropic Heisenberg ferromagnets with $S=\frac{1}{2}$ is designed to decouple the higher-order Green's functions obtained in writing down the equations of motion of the first-order Green's functions. By defining the commutator and the anticommutator brackets, the equations of motion of the two kinds of Green's functions G^- and G^+ are written down. With the use of suitable decoupling parameters, a generalized decoupling scheme is suggested. In order to determine the relation between these decoupling parameters we define two conditions: (1) self-consistency and (2) vanishing of the equal-time correlation functions. Using this decoupling scheme, we calculate the thermodynamic properties of the anisotropic Heisenberg ferromagnets with $S=\frac{1}{2}$ at low temperatures. Finally, we also calculate the effect of the decoupling scheme on the magnon conductivity at low temperatures. We clearly find that the magnon conductivity is modified appreciably by the different decoupling parameters and by the anisotropy of the system.

I. INTRODUCTION

The double-time Green's functions have been[1] successfully used to calculate the thermodynamic properties of different Heisenberg ferromagnets. The basic idea is to write down the equation of motion of the first-order Green's function which involves the higher-order Green's functions. By writing down the equations of motion of these Green's functions we get a hierarchy of equations of motion which can be truncated by a suitable decoupling scheme. The decoupling scheme represents higher-order Green's functions in terms of the lower-order Green's functions. The simplest and the lowest-order decoupling scheme was suggested by Tyablikov[2] and is known as the random-phase approximation (RPA). Callen[3] has very ingeniously considered the spin deviation by introducing a suitable decoupling parameter. Since then many decoupling schemes have been suggested to calculate the thermodynamic properties of the magnetic systems. Kumar and Joshi[4] have attempted to generalize the different decoupling schemes which are the outcome of Callen's decoupling scheme.

Katsura and Horiguchi[5] have proposed a different coupling approximation by making use of the anticommutability of Pauli operators at the same lattice site. In the present work we generalize these ideas to unify the first-order Green's-functions theory for anisotropic Heisenberg ferromagnets with $S=\frac{1}{2}$, and compare it with the previously suggested decoupling schemes. We calculate the spontaneous magnetization and Curie temperature. We also derive these results for the simple cubic lattices. We calculate the low-temperature series expansion of the magnetization. Recently, Kumar[6] has suggested that the magnon conductivity also depends upon the decoupling scheme which we use to calculate the spin-wave energy. We therefore calculate the magnon conductivity by using the present decoupling scheme.

II. HAMILTONIAN AND GREEN'S FUNCTIONS

Following Katsura and Koriguchi,[5] and Tyablikov,[2] we can describe the Hamiltonian of the anisotropic Heisenberg ferromagnet for $S=\frac{1}{2}$ as

$$H=-g\mu_B H\sum_f S_f^z-\sum_{f,g}[J_\perp(f-g)(S_f^xS_g^x+S_f^yS_g^y)+J_{||}(f-g)S_f^zS_g^z]\ , \tag{2.1}$$

where $J_\perp(f-g)$ and $J_{||}(f-g)$ are the transverse and the longitudinal components of the exchange interaction between the spins at the sites f and g. S_f is the spin operator at the site f (in units of $\hbar$), g is the Landé g factor, and H is the external magnetic field. For $S=\frac{1}{2}$, the spin operators can be expressed in terms of Pauli operators as follows:

$$S_f^x+iS_f^y=S_f^+=a_f,\quad S_f^x-iS_f^y=S_f^-=a_f^\dagger\,,$$
$$S_f^z=\tfrac{1}{2}-a_f^\dagger a_f=\tfrac{1}{2}-n_f \tag{2.2}$$

obeying the following commutation and anticommutation relations:

$$[a_f,a_g]_\pm=[a_f^\dagger,a_g^\dagger]_\pm=0\,,$$
$$[a_g,a_f^\dagger]_+=2a_f^\dagger a_g+\delta_{gf}(1-2n_f)\,, \tag{2.3}$$
$$[a_g,a_f^\dagger]_-=\delta_{gf}(1-2n_f)\,.$$

With the use of the Pauli operators the Hamiltonian reduces to

$$\bar{H}=E_0-\sum_{f,g}J_\perp(f-g)a_f^\dagger a_g+(zJ_{||}+g\mu_B H)\sum_f a_f^\dagger a_f$$
$$-\sum_{f,g}J_{||}(f-g)a_f^\dagger a_f a_g^\dagger a_g\,, \tag{2.4}$$

where

$$E_0=-\tfrac{1}{2}g\mu_B HN-\tfrac{1}{8}zJ_{||}N\,. \tag{2.5}$$

Here z is the number of nearest neighbors. Following Zubarev,[1] the Fourier-transformed equation of motion of the Green's function $G_{gf}^\pm(E)$, $\langle\langle \hat{a}_g \mid a_f^\dagger\rangle\rangle_E^\pm$, can be summarized as

$$(E-zJ_{||}-g\mu_B H)G_{gf}^+(E)=\tfrac{1}{2}\delta_{fg}\langle(1-2n_f)\rangle+\tfrac{1}{2}2\langle a_f^\dagger a_g\rangle-\sum_m J_\perp(g-m)G_{mf}^+(E)$$
$$+2\sum_m J_\perp(g-m)G_{ggmf}^+(E)-2\sum_m J_{||}(g-m)G_{mmff}^+(E)\,, \tag{2.6}$$

$$(E-zJ_{||}-g\mu_B H)G_{gf}^-(E)=\frac{1}{2\pi}\delta_{gf}\langle(1-2n)\rangle-\sum_m J_\perp(g-m)G_{mf}(E)$$
$$+2\sum_m J_\perp(g-m)G_{ggmf}^-(E)-2\sum_m J_{||}(g-m)G_{mmgf}^-(E)\,, \tag{2.7}$$

where $\langle a_{\vec f}^\dagger a_{\vec g}\rangle$ in Eq. (2.8) is the equal-time correlation function, and $G_{\vec g\,\vec g\,\vec m\,\vec f}^\pm(E)$, etc., are the Fourier transforms of second-order Green's functions as

$$G_{\vec g\,\vec l\,\vec m\,\vec f}^\pm(E)=\langle\langle a_{\vec g}(t)a_{\vec l}(t)a_{\vec m}(t)\mid a_{\vec f}^\dagger(t')\rangle\rangle_E^\pm$$
$$=-i\Theta(t-t')$$
$$\times\langle[a_{\vec g}^\dagger(t)a_{\vec l}(t)a_{\vec m}(t),a_{\vec f}^\dagger(t')]_\pm\rangle\,. \tag{2.8}$$

To simplify Eqs. (2.6) and (2.7), we require some suitable decoupling scheme in terms of the decoupling parameters.

III. DECOUPLING APPROXIMATIONS

Tyablikov[2] proposed a decoupling scheme, which is known as RPA, and the basic idea is to consider a self-consistent dynamic and kinematic interaction of the magnons at all temperatures however, as RPA ignores the fluctuations around $\langle S^z\rangle$. The series expansions of the magnetic susceptibility at low and high temperatures lead to a spurious T^3 temperature dependence. Oguchi and Honma[7] had improved the Tyablikov decoupling scheme of symmetric linearization in accordance with Wick's theorem for Bose operators. This is often known as the Hartree-Fock (HF) approximation and retains the T^3 term, and hence does not improve RPA appreciably. Callen[3] has successfully considered the fluctuations about $\langle S^z\rangle$ in a modified decoupling scheme. It incorporates the information about spin kinematics. Swendson[8] has been successful in eliminating the T^3 term in the series expansion of the magnetization by improving Callen's decoupling parameters. Katsura and Koriguchi,[5] on the other hand, had suggested modification to the HF-decoupling scheme to first eliminate its shortcoming of an infinite Curie temperature by using commutation and anticommutation of Pauli operators at different and the lattice sites, respectively.

There are other intermediate decoupling schemes proposed by Mabayi and Lange,[9] Kenan,[10] Shimizu,[11] and Oguchi.[12] Other attempts had been to eliminate the T^3 term in magnetization as well as other shortcomings. All decoupling schemes[13-15] lead to some renormalization constant; the corresponding energy may be expressed as

$$E(\vec{k})=R[1-\gamma(\vec{k})]+\omega_0 .$$

One can obtain different values of decoupling parameters involved in the value of the renormalization constant R. We propose a unified decoupling scheme taking into account the kinematic interactions within the framework of first-order theories in order to eliminate the spurious T^3 term.

Following the concept of Callen's decoupling scheme with a suitable decoupling parameter,[3] we represent the decoupling approximation by taking a suitable combination of the three decoupling schemes as follows:

$$\langle\langle a^\dagger_{\vec{g}}(t)a_{\vec{g}}(t)a_{\vec{m}}(t)\,|\,a^\dagger_{\vec{f}}(t')\rangle\rangle^{\pm}_{E}\to f_{0gm}\langle a^\dagger_{\vec{g}}a_{\vec{g}}\rangle\langle\langle a_{\vec{m}}(t)\,|\,a^\dagger_{\vec{f}}(t')\rangle\rangle^{\pm}_{E}+f_{1gm}\langle a^\dagger_{\vec{g}}a_{\vec{m}}\rangle\langle\langle a_{\vec{g}}(t)\,|\,a^\dagger_{\vec{f}}(t')\rangle\rangle^{\mp}_{E}$$
$$+f_{2gm}\langle a^\dagger_{\vec{g}}a_{\vec{m}}\rangle\langle\langle a_{\vec{g}}(t)\,|\,a^\dagger_{\vec{f}}(t')\rangle\rangle^{\pm}_{E}+\rho(\vec{g},\vec{m},\vec{f})\delta(t-t') . \tag{3.1}$$

The corresponding Fourier transform of Eq. (3.1) can be expressed as

$$G^{\pm}_{\vec{g}\vec{g}\vec{m}\vec{f}}(E)=\langle\langle a^\dagger_{\vec{g}}a_{\vec{g}}a_{\vec{m}}\,|\,a^\dagger_{\vec{f}}\rangle\rangle^{\pm}_{E}\to f_{0gm}\langle a^\dagger_{\vec{g}}a_{\vec{g}}\rangle\langle\langle a_{\vec{m}}\,|\,a^\dagger_{\vec{f}}\rangle\rangle^{\pm}_{E}+f_{1gm}\langle a^\dagger_{\vec{g}}a_{\vec{m}}\rangle\langle\langle a_{\vec{g}}\,|\,a^\dagger_{\vec{f}}\rangle\rangle^{\mp}_{E}$$
$$+f_{2gm}\langle a^\dagger_{\vec{g}}a_{\vec{m}}\rangle\langle\langle a_{\vec{g}}\,|\,a^\dagger_{\vec{f}}\rangle\rangle^{\pm}_{E}+\rho(\vec{g},\vec{m},\vec{f}) , \tag{3.2}$$

where (f_0,f_1,f_2) are decoupling parameters which depend upon the magnetization and the transverse correlation function of the spins at the lattice sites $\vec{g}$ and $\vec{m}$, i.e., $\mu_{gm}=(\langle a^\dagger_{\vec{m}}a_{\vec{g}}\rangle)$. The last term, $\rho(\vec{g},\vec{m},\vec{f})$, is an additional term[16] which may depend upon the relative positions of the lattice sites $(\vec{g},\vec{m},\vec{f})$. We assume ρ to be symmetrical, i.e.,

$$\rho(\vec{g},\vec{m},\vec{f})=\rho(\vec{m},\vec{g},\vec{f}) . \tag{3.3}$$

The relation between the decoupling parameters (f_0,f_1,f_2) can be obtained by making use of the conditions of self-consistency and the vanishing of the correlation function

$$\langle a^\dagger_{\vec{f}}(t')a^\dagger_{\vec{g}}(t)a_{\vec{g}}(t)a_{\vec{m}}(t)\rangle ,$$

automatically at $\vec{f}=\vec{g}$ and $t=t'$, because of the anticommutability of the Pauli operators at the same lattice site. Writing the following contractions of the related correlation functions, we find that

$$\langle a^\dagger_{\vec{f}}(t')a^\dagger_{\vec{g}}(t)a_{\vec{g}}(t)a_{\vec{m}}(t)\rangle\to f_0\langle a^\dagger_{\vec{g}}(t)a_{\vec{g}}(t)\rangle\langle a^\dagger_{\vec{f}}(t')a_{\vec{m}}(t)\rangle-f_1\langle a^\dagger_{\vec{g}}(t)a_{\vec{m}}(t)\rangle\langle a^\dagger_{\vec{f}}(t')a_{\vec{g}}(t)\rangle$$
$$+f_2\langle a^\dagger_{\vec{g}}(t)a_{\vec{m}}(t)\rangle\langle a^\dagger_{\vec{f}}(t')a_{\vec{g}}(t)\rangle . \tag{3.4}$$

It should vanish at $\vec{f}=\vec{g}$ and $t=t'$, if

$$f_0+f_2=f_1 . \tag{3.5}$$

The other relationships between the different decoupling parameters can be determined by using the condition of self-consistency. It can be done by evaluating the expression

$$\lim_{t-t'\to 0^+}[G^{\pm}_{\vec{g}\vec{g}\vec{m}\vec{m}}(t,t')-G^{\pm}_{\vec{m}\vec{m}\vec{g}\vec{m}}(t,t')] \tag{3.6}$$

and by introducing the decoupling scheme in Eq. (3.6), which gives

$$f_0(\bar{n}\langle a_{\vec{m}}a^\dagger_{\vec{f}}\rangle\pm\bar{n}\langle a^\dagger_{\vec{f}}a_{\vec{m}}\rangle-\bar{n}\langle a_{\vec{g}}a^\dagger_{\vec{f}}\rangle\mp\bar{n}\langle a^\dagger_{\vec{f}}a_{\vec{g}}\rangle)$$
$$+f_1(\langle a^\dagger_{\vec{g}}a_{\vec{m}}\rangle\langle a_{\vec{g}}a^\dagger_{\vec{f}}\rangle\mp\langle a^\dagger_{\vec{g}}a_{\vec{m}}\rangle\langle a^\dagger_{\vec{f}}a_{\vec{g}}\rangle-\langle a^\dagger_{\vec{m}}a_{\vec{g}}\times a_{\vec{m}}a^\dagger_{\vec{f}}\rangle\pm\langle a^\dagger_{\vec{m}}a_{\vec{g}}\rangle\langle a^\dagger_{\vec{f}}a_{\vec{m}}\rangle)$$
$$+f_2(\langle a^\dagger_{\vec{g}}a_{\vec{m}}\rangle\langle a_{\vec{g}}a^\dagger_{\vec{f}}\rangle\pm\langle a^\dagger_{\vec{g}}a_{\vec{m}}\rangle\langle a^\dagger_{\vec{f}}a_{\vec{g}}\rangle-\langle a^\dagger_{\vec{m}}a_{\vec{g}}\rangle\langle a_{\vec{m}}a^\dagger_{\vec{f}}\rangle-\langle a^\dagger_{\vec{m}}a_{\vec{g}}\rangle\langle a^\dagger_{\vec{f}}a_{\vec{m}}\rangle) . \tag{3.7}$$

We assume

$$i \lim_{t-t'\to 0^+} G^{\pm}_{\vec{m}\,\vec{f}}(t,t') = \langle a_{\vec{m}} a^{\dagger}_{\vec{f}} \rangle \pm \langle a^{\dagger}_{\vec{f}} a_{\vec{m}} \rangle$$

and (3.8)

$$\rho(\vec{g},\vec{m},\vec{f}) = \rho(\vec{m},\vec{g},\vec{f}) \; .$$

In Eq. (3.7), $\bar{n} = \langle a^{\dagger} a \rangle$ because $\langle a^{\dagger}_{\vec{g}} a_{\vec{g}} \rangle$ is independent of the lattice site due to translational invariance. We now consider the equal-time correlation function which can be expressed as

$$i \lim_{t-t'\to 0^+} [G^{\pm}_{\vec{g}\,\vec{g}\,\vec{m}\,\vec{f}}(t,t') - G^{\pm}_{\vec{m}\,\vec{m}\,\vec{g}\,\vec{f}}(t,t')]$$
$$(\langle a^{\dagger}_{\vec{g}} a_{\vec{g}} a_{\vec{m}} a^{\dagger}_{\vec{f}} \rangle \pm \langle a^{\dagger}_{\vec{f}} a^{\dagger}_{\vec{g}} a_{\vec{g}} a_{\vec{m}} \rangle - \langle a^{\dagger}_{\vec{m}} a_{\vec{m}} a_{\vec{g}} a^{\dagger}_{\vec{f}} \rangle \mp \langle a^{\dagger}_{\vec{f}} a^{\dagger}_{\vec{m}} a_{\vec{m}} a_{\vec{g}} \rangle) \; . \quad (3.9)$$

Putting $\vec{f} = \vec{m}$ and using the commutation relation we find

$$i \lim_{t-t'\to 0^+} [G^{\pm}_{\vec{g}\,\vec{g}\,\vec{m}\,\vec{m}}(t,t') - G^{\pm}_{\vec{m}\,\vec{m}\,\vec{g}\,\vec{m}}(t,t')] = \bar{n} - \langle a^{\dagger}_{\vec{m}} a_{\vec{g}} \rangle \quad (3.10)$$

and

$$i \lim_{t-t'\to 0^+} [G^{-}_{\vec{g}\,\vec{g}\,\vec{m}\,\vec{m}}(t,t') - G^{-}_{\vec{m}\,\vec{m}\,\vec{g}\,\vec{m}}(t,t')] = n - \langle a^{\dagger}_{\vec{m}} a_{\vec{g}} \rangle - 2\langle a^{\dagger}_{\vec{g}} a_{\vec{g}} a^{\dagger}_{\vec{m}} a_{\vec{m}} \rangle \; . \quad (3.11)$$

Putting $\vec{f} = \vec{m}$ in Eq. (3.7) and comparing it with Eqs. (3.11) and (3.10), we get

$$f_0 \bar{n}(1 - 2\langle a^{\dagger}_{\vec{m}} a_{\vec{g}} \rangle) - f_1 \langle a^{\dagger}_{\vec{m}} a_{\vec{g}} \rangle (1 - 2\pi) - f_2 \langle a^{\dagger}_{\vec{m}} a_{\vec{g}} \rangle (1 - 2\langle a^{\dagger}_{\vec{g}} a_{\vec{m}} \rangle) = \bar{n} - \langle a^{\dagger}_{\vec{m}} a_{\vec{g}} \rangle \quad (3.12)$$

and

$$f_0 \bar{n}(1 - 2\bar{n}) - f_1 \langle a^{\dagger}_{\vec{m}} a_{\vec{g}} \rangle (1 - 2\langle a^{\dagger}_{\vec{g}} a_{\vec{m}} \rangle) - f_2 \langle a^{\dagger}_{\vec{m}} a_{\vec{g}} \rangle (1 - 2\bar{n}) = \bar{n} - \langle a^{\dagger}_{\vec{m}} a_{\vec{g}} \rangle - 2\langle a^{\dagger}_{\vec{g}} a_{\vec{g}} a^{\dagger}_{\vec{m}} a_{\vec{m}} \rangle \; . \quad (3.13)$$

We also get the same information as contained in Eqs. (3.12) and (3.13), for $\vec{f} = \vec{g}$.

Combining Eqs. (3.5), (3.12), and (3.13), and putting $\mu_{mg} = \langle a^{\dagger}_{\vec{m}} a_{\vec{g}} \rangle$, we find

$$f_0 = \frac{A_3 - A_1 A_4}{A_3 - A_1 A_2} \text{ and } f_2 = \frac{A_4 - A_2}{A_3 - A_1 A_2} \; , \quad (3.14)$$

with

$$A_1 = \frac{2\mu_{mg}(1 - \bar{n} - \mu_{mg})}{\mu_{mg} - \bar{n}} \; ,$$
$$A_2 = \mu_{gm}(1 - 2\mu_{gm}) - \bar{n}(1 - 2\bar{n}) \; ,$$
$$A_3 = 2\mu_{gm}(1 - \bar{n} - \mu_{gm}) \; , \quad (3.15)$$
$$A_4 = \mu_{gm} - \bar{n} 2\langle n_m n_g \rangle \; .$$

Equations (3.5)–(3.15) can be used to determine the decoupling parameters. We find that the decoupling parameters are the functions of n, μ_{gm}, and $\langle n_g n_m \rangle$. Owing to the assumed translational invariance, $\mu_{gm} = \mu_{mg}$ and μ_{mg} and $\langle n_m n_g \rangle$ depend on $\vec{g} - \vec{m}$ only. The average value of n remained the same throughout. The present decoupling approximation reduces to the previous decoupling schemes by suitable choice of the decoupling parameters as shown in Table I.

IV. SOLUTION OF THE EQUATION OF MOTION

Introducing the present decoupling scheme, the equations of motion of the following Green's functions become

TABLE I. Decoupling parameters for $G^{\pm}_{\vec{g}\,\vec{g}\,\vec{m}\,\vec{f}}(E)$ in various first-order Green's-function theories for $S = \frac{1}{2}$.

Theory	Heisenberg ferromagnets Coefficient of $\langle a^{\dagger}_{g} a_{\vec{g}} \rangle \langle\langle a_{\vec{m}}, a^{\dagger}_{\vec{f}} \rangle\rangle_E$	Coefficient of $\langle a^{\dagger}_{\vec{g}} a_{\vec{g}} \rangle \langle\langle a_{\vec{m}}, a^{\dagger}_{\vec{f}} \rangle\rangle_E$	Coefficient of $\langle a^{\dagger}_{\vec{g}} a_{\vec{g}} \rangle \langle\langle a_{\vec{m}}, a^{\dagger}_{\vec{f}} \rangle\rangle_E$	Additional term
RPA	1	0	0	0
Oguchi and Honma (HF approximation)	1	0	1	0
Katsura and Horiguchi (KH)	1	1	0	0
Callen	1	0	$\sigma = (1 - 2\bar{n})$	0
Present work	$f_0(\sigma, \mu_{mg})$	$f_1(\sigma, \mu_{mg})$	$f_2(\sigma, \mu_{mg})$	$\rho(\vec{g}, \vec{m}, \vec{f})$

$$[E - zJ_{||}(1-2f_0\bar{n}) - g\mu_B H]G^{+}_{\vec{g}\vec{f}}(E)$$
$$= (2\pi)^{-1}\delta_{\vec{g}\vec{f}}(1-2\bar{n}) + 2(2\pi)^{-1}\langle a^{\dagger}_{\vec{f}} a_{\vec{g}}\rangle - (1-2f_0\bar{n})\sum_{\vec{m}} J_{\perp}(\vec{g}-\vec{m})G^{+}_{\vec{m}\vec{f}}(E)$$
$$+2f_1\left[\sum_{\vec{m}} J_{\perp}(\vec{g}-\vec{m})\langle a^{\dagger}_{\vec{g}} a_{\vec{m}}\rangle G^{-}_{\vec{g}\vec{f}}(E) - \sum_{\vec{m}} J_{||}(\vec{g}-\vec{m})\langle a^{\dagger}_{\vec{m}} a_{\vec{g}}\rangle G^{-}_{\vec{m}\vec{f}}(E)\right]$$
$$+2f_2\left[\sum_{\vec{m}} J_{\perp}(g-m)\langle a^{\dagger}_{\vec{g}} a_{\vec{m}}\rangle G^{+}_{\vec{g}\vec{f}}(E) - \sum_{\vec{m}} J_{||}(\vec{g}-\vec{m})\langle a^{\dagger}_{\vec{m}} a_{\vec{g}}\rangle G^{+}_{\vec{m}\vec{f}}(E)\right]$$
$$+2\left[\sum_{\vec{m}} J_{\perp}(\vec{g}-\vec{m})\rho(\vec{g},\vec{m},\vec{f}) - \sum_{\vec{m}} J_{||}(\vec{g}-\vec{m})\rho(\vec{m},\vec{g},\vec{f})\right], \quad (4.1)$$

$$[E - zJ_{||}(1-2f_0\bar{n}) - g\mu_B H]G^{-}_{gf}(E)$$
$$= (2\pi)^{-1}\delta_{gf}(1-2\bar{n}) - (1-2f_0\bar{n})\sum_{\vec{m}} J_{\perp}(\vec{g}-\vec{m})G^{-}_{\vec{m}\vec{f}}(E)$$
$$+2f_1\left[\sum_{\vec{m}} J_{\perp}(\vec{g}-\vec{m})\langle a^{\dagger}_{\vec{g}} a_{\vec{m}}\rangle G^{+}_{\vec{g}\vec{f}}(E) - \sum_{\vec{m}} J_{||}(\vec{g}-\vec{m})\langle a^{\dagger}_{m} a_{g}\rangle G^{+}_{\vec{m}\vec{f}}(E)\right]$$
$$+2f_2\left[\sum_{\vec{m}} J_{\perp}(\vec{g}-\vec{m})\langle a^{\dagger}_{\vec{g}} a_{\vec{m}}\rangle G^{-}_{\vec{g}\vec{f}}(E) - \sum_{m} J_{||}(\vec{g}-\vec{m})\langle a^{\dagger}_{\vec{m}} a_{\vec{g}}\rangle G^{-}_{\vec{m}\vec{f}}(E)\right]$$
$$+2\left[\sum_{\vec{m}} J_{\perp}(\vec{g}-\vec{m})\rho(\vec{g},\vec{m},\vec{f}) - \sum_{\vec{m}} J_{||}(\vec{g}-\vec{m})\rho(\vec{m},\vec{g},\vec{f})\right]. \quad (4.2)$$

Here we consider the relative magnetization σ of the lattice which can be given by

$$\sigma = \langle S^z\rangle/S = \langle 2S^z\rangle = 1 - 2\langle a^{\dagger}a\rangle = 1 - 2\bar{n}\ . \quad (4.3)$$

The last term in Eqs. (4.1) and (4.2) can be written as

$$\sum_{\vec{m}} [J_{\perp}(\vec{g}-\vec{m}) - J_{||}(\vec{g}-\vec{m})]\rho(\vec{g},\vec{m},\vec{f}) = \frac{1}{2\pi}\beta(\vec{g},\vec{f})\ . \quad (4.4)$$

It depends only on the positions of the two lattice sites $\vec{g}$ and $\vec{f}$. We assume as usual the spatial Fourier transform; by making use of the translational invariance we have

$$G^{\pm}(E) = \frac{1}{N}\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{g}-\vec{f})}G^{\pm}(\vec{k},E)\ ,$$
$$\langle a^{\dagger}_{\vec{f}} a_{\vec{g}}\rangle = \frac{1}{N}\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{g}-\vec{f})}n(\vec{k})\ ,$$
$$\delta_{gf} = \frac{1}{N}\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{g}-\vec{f})}\ , \quad (4.5)$$
$$J_{\perp,||}(\vec{g}-\vec{f}) = \frac{1}{N}\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{g}-\vec{f})}J_{\perp,||}(\vec{k})\ ,$$
$$\beta(\vec{g},\vec{f}) = \frac{1}{N}\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{g}-\vec{f})}\beta(\vec{k})\ .$$

We also put

$$J_{\perp,||}(\vec{k}) = J_{\perp,||}z\gamma(\vec{k}), \quad \gamma(\vec{k}) = \frac{1}{Z}\sum_{\vec{\Delta}} e^{i\vec{k}\cdot\vec{\Delta}}\ . \quad (4.6)$$

The periodic boundary condition is used and hence the reciprocal-lattice sums are restricted to the first Brillouin zone.

The Fourier-transformed equations of motion are

$$\begin{bmatrix} E-E(\vec{k})-f_2Q(\vec{k}) & -f_1Q(\vec{k}) \\ -f_1Q(\vec{k}) & E-E(\vec{k})-f_2Q(\vec{k}) \end{bmatrix} \begin{bmatrix} G^+(\vec{k},E) \\ G^-(\vec{k},E) \end{bmatrix} = (2\pi)^{-1} \begin{bmatrix} \sigma+\beta(\vec{k})+2n(\vec{k}) \\ \sigma+\beta(\vec{k}) \end{bmatrix}, \tag{4.7}$$

where

$$E(\vec{k}) = g\mu_B H + z(1-2f_0\bar{n})[J_{\parallel} - J_{\perp}\gamma(\vec{k})] \tag{4.8}$$

and

$$Q(\vec{k}) = \frac{2}{N} z \sum_{\vec{q}} [J_{\perp}\gamma(\vec{k}) - J_{\parallel}\gamma(\vec{q}-\vec{k}) n(\vec{q})] .$$

We solve Eqs. (4.7) for $G^+(\vec{k},E)$, and we get

$$\begin{bmatrix} G^+(\vec{k},E) \\ G^-(\vec{k},E) \end{bmatrix} = \frac{1}{2\pi} \begin{bmatrix} \dfrac{1}{E_-} & \dfrac{1}{E_+} \\ -\dfrac{1}{E_-} & \dfrac{1}{E_+} \end{bmatrix} \begin{bmatrix} n(\vec{k}) \\ n(\vec{k})+\beta(\vec{k})+\sigma \end{bmatrix}, \tag{4.9}$$

where

$$E_{\pm} = E - E(\vec{k}) - f_{\pm}Q(\vec{k}) ,$$

and

$$f_{\pm} = f_2 \pm f_1 . \tag{4.10}$$

Knowing the Green's functions $G^{\pm}(\vec{k},E)$ from (4.9), we determine the equal-time correlation function $\langle a_f^\dagger a_g \rangle^{\pm}$ by using Eq. (2.8) and putting $t=t'$ as

$$\langle a_{\vec{f}}^\dagger a_{\vec{g}} \rangle^+ = \frac{1}{N} \sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{g}-\vec{f})} n^+(\vec{k})$$

$$= \frac{1}{N} \sum_{\vec{k}} \left[\frac{n^+(\vec{k})}{1+\exp\{\beta[E(\vec{k})+f_0Q(\vec{k})]\}} + \frac{n(\vec{k})+\beta(\vec{k})+\sigma}{1+\exp\{\beta[E(\vec{k})+f_+Q(\vec{k})]\}} \right] e^{i\vec{k}\cdot(\vec{g}-\vec{f})} \tag{4.11}$$

and

$$\langle a_{\vec{f}}^\dagger a_{\vec{g}} \rangle^- = \frac{1}{N} \sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{g}-\vec{f})} n^-(\vec{k})$$

$$= \frac{1}{N} \sum_{\vec{k}} \left[\frac{-n^-(\vec{k})}{\exp\{\beta[E(\vec{k})+f_-Q(\vec{k})]\}-1} + \frac{n^-(\vec{k})+\beta(\vec{k})+\sigma}{\exp\{\beta[E(\vec{k})+f_+Q(\vec{k})]\}-1} \right] e^{i\vec{k}\cdot(\vec{g}-\vec{f})} . \tag{4.12}$$

We have made use of the identity

$$\lim_{\epsilon\to 0^+} \left[\frac{1}{\omega-E+i\epsilon} - \frac{1}{\omega-E-i\epsilon} \right] = -2\pi i \delta(\omega-E) . \tag{4.13}$$

A superscript + or − on $n(\vec{k})$ denotes whether it has been calculated by using G^+ or G^-, respectively. We can simplify Eqs. (4.11) and (4.12) to get $n^{\pm}(\vec{k})$ as

$$n^+(\vec{k}) = [\sigma+\beta(\vec{k})] \frac{\exp\{\beta[E(\vec{k})+f_-Q(\vec{k})]\}+1}{\exp\{2\beta[E(\vec{k})+f_2Q(\vec{k})]\}-1} , \tag{4.14}$$

$$n^-(\vec{k})=[\sigma+\beta(\vec{k})]\frac{\exp\{\beta[E(\vec{k})+f_-Q(\vec{k})]\}-1}{1-2\exp\{\beta[E(\vec{k})+f_-Q(\vec{k})]\}+\exp\{2\beta[E(\vec{k})+f_2Q(\vec{k})]\}} . \tag{4.15}$$

We can now determine the magnetization σ from

$$\sigma=1-2\bar{n}=1-\frac{2}{N}\sum_{\vec{k}} n(\vec{k}) . \tag{4.16}$$

By substituting the expressions (4.14) and (4.15) in Eq. (4.16), we get

$$\frac{1}{\sigma^+}=\frac{1}{N}\sum_{\vec{k}}\frac{1+\exp\{2\beta[E(\vec{k})+f_2Q(\vec{k})]\}+2\exp\{\beta[E(\vec{k})+f_-Q(\vec{k})]\}}{\exp\{2\beta[E(\vec{k})+f_2Q(\vec{k})]\}-1}\frac{1}{D_1} , \tag{4.17}$$

$$D_1=1-\frac{2}{N}\sum_{\vec{k}}\beta(\vec{k})\frac{\exp\{-\beta[E(\vec{k})+f_2Q(\vec{k})]\}+\exp[-f_1Q(\vec{k})]}{2\sinh\{\beta[E(\vec{k})+f_2Q(\vec{k})]\}} , \tag{4.18}$$

$$\frac{1}{\sigma^-}=\frac{1}{N}\sum_{\vec{k}}\frac{\exp\{2\beta[E(\vec{k})+f_2Q(\vec{k})]\}-1}{1-2\exp\{\beta[E(\vec{k})+f_-Q(\vec{k})]\}+\exp\{2\beta[E(\vec{k})+f_2Q(\vec{k})]\}}\frac{1}{D_2} , \tag{4.19}$$

$$D_2=1-\frac{2}{N}\sum_{\vec{k}}\beta(\vec{k})\frac{\exp[-\beta f_1Q(\vec{k})]-\exp\{-\beta[E(\vec{k})+f_2Q(\vec{k})]\}}{2\cosh\{\beta[E(\vec{k})+f_2Q(\vec{k})]\}-2\exp[-\beta f_1Q(\vec{k})]} . \tag{4.20}$$

The expression for $Q(\vec{k})$ can also be simplified as

$$Q(\vec{k})=zp[J_\perp-J_{\parallel}\gamma(\vec{k})] , \tag{4.21}$$

where

$$p=\frac{2}{N}\sum_{\vec{k}}\gamma(\vec{k})n(\vec{k}) . \tag{4.22}$$

Substituting for $n(\vec{k})$ in Eq. (4.22), we get

$$p^+=\frac{1}{N}\sum_{\vec{k}}\gamma(\vec{k})[\beta(\vec{k})+\sigma^+]\frac{\exp\{\beta[E(\vec{k})+f_-Q(\vec{k})]\}+1}{\exp\{2\beta[E(\vec{k})+f_2Q(\vec{k})]\}-1} , \tag{4.23}$$

$$p^-=\frac{1}{N}\sum_{\vec{k}}\gamma(\vec{k})[\beta(\vec{k})+\sigma]\frac{\exp\{\beta[E(\vec{k})+f_-Q(\vec{k})]\}-1}{1-2\exp\{\beta[E(\vec{k})+f_-Q(\vec{k})]\}\exp\{2\beta[E(\vec{k})+f_2Q(\vec{k})]\}} . \tag{4.24}$$

We have thus obtained the coupled equations from which we can determine the magnetization, Curie temperature, and the zero-field susceptibility, etc.

It may be remarked here that the results contained in Eqs. (4.17)–(4.24) reduced to the well-known results of earlier theories when we take appropriate values of f_0, f_1, and f_2 from Table I.

For example, we consider Eqs. (4.17) and (4.18), and Table I, to substitute the different values of (f_0,f_1,f_2) for different decoupling parameters to get the previous decoupling schemes. We find that

$$\left[\frac{1}{\sigma}\right]_{\text{RPA}}=\frac{1}{N}\sum_{\vec{k}}\frac{1+\exp[-2\beta E(\vec{k})]+2\exp[-\beta E(\vec{k})]}{1-\exp[-2\beta E(\vec{k})]} \tag{4.25a}$$

with

$$E(\vec{k})=g\mu_BH+z\sigma[J_{\parallel}-J_\perp\gamma(\vec{k})] , \tag{4.25b}$$

$$\left[\frac{1}{\sigma}\right]_{\text{HFA}}=\frac{1}{N}\sum_{\vec{k}}\frac{1+\exp\{-2\beta[E(\vec{k})+f_2Q(\vec{k})]\}+2\exp\{-\beta[E(\vec{k})+f_2Q(\vec{k})]\}}{1-\exp\{-2\beta[E(\vec{k})+f_2Q(\vec{k})]\}}$$

with $E(\vec{k})$ the same as in (4.25b), and

$$Q(\vec{k})=\frac{2}{N}\sum_{\vec{k}} z\{[J_\perp\gamma(\vec{k})-J_{\parallel}\gamma(\vec{q}-\vec{k})]n(\vec{q})\}\ ,$$
$$\langle a_f^\dagger a_g\rangle=\frac{1}{N}\sum_{\vec{q}}\exp[i\vec{q}\cdot(\vec{g}-\vec{f})]n(\vec{q})\ , \tag{4.26}$$

$$\left[\frac{1}{\sigma}\right]_{\mathrm{KH}}=\frac{1}{N}\sum_{\vec{k}}\frac{1+\exp\{-2\beta[E(\vec{k})]\}+2\exp\{-\beta[E(\vec{k})+Q(\vec{k})]\}}{1-\exp[-2\beta E(\vec{k})]}\ , \tag{4.27}$$

where $E(\vec{k})$ and $Q(\vec{k})$ are the same as described by Eqs. (4.25b) and (4.26), and KH stands for Katsura and Horiguchi.

V. THERMODYNAMIC PROPERTIES

We calculate the thermodynamic properties of the anisotropic Heisenberg ferromagnet from $G^+(\vec{k},E)$ and restrict the calculations to $\beta(\vec{k})=0$. Our aim is to compare our present results for the Curie temperature with those obtained by using RPA- and HE-decoupling schemes; we therefore consider at this stage the results for $G^+(\vec{k},E)$ and $\beta(\vec{k})=0$. For different values of the various decoupling parameters, we can obtain different decoupling schemes only when $\beta(\vec{k})=0$.

A. Curie temperature

We can determine the Curie temperature by putting $H=0$, and taking the $\sigma\to 0$ limit in Eq. (4.17a), which can be put in the form

$$\frac{1}{\sigma}=\frac{1}{N}\sum_{\vec{k}}\frac{1+\exp\{-2\beta[E(\vec{k})+f_2Q(\vec{k})]\}+2\exp\{-\beta[E(\vec{k})+f_2Q(\vec{k})]\}}{1-\exp\{-2\beta[E(\vec{k})+f_2Q(\vec{k})]\}}\ , \tag{5.1}$$

where

$$E(\vec{k})=z(1-2f_0\bar{n})[J_{\parallel}-J_\perp\gamma(\vec{k})]$$
$$=z[1+f_0(\sigma-1)][J_{\parallel}-J_\perp\gamma(\vec{k})] \tag{5.2}$$

and $Q(\vec{k})$ is given by Eq. (4.21). p is given by

$$\frac{p}{\sigma}=\frac{1}{N}\sum_{\vec{k}}\gamma(\vec{k})\frac{\exp\{\beta[E(\vec{k})+f_2Q(\vec{k})]\}+1}{\exp\{2\beta[E(\vec{k})+f_2Q(\vec{k})]\}-1}\ . \tag{5.3}$$

In taking the limit $\sigma\to 0$ we have

$$\lim_{\sigma\to 0}E(\vec{k})=z(1-f_0)[J_{\parallel}-J_\perp\gamma(\vec{k})]\ , \tag{5.4}$$

$$\lim_{\sigma\to 0}Q(\vec{k})=Q_c(\vec{k})=zp_c[J_\perp-J_{\parallel}\gamma(\vec{k})]\ . \tag{5.5}$$

We shall assume simple polynomial expansions for the three decoupling parameters as

$$\begin{bmatrix}f_0\\f_1\\f_2\end{bmatrix}=\begin{bmatrix}a_0\\b_0\\c_0\end{bmatrix}+\begin{bmatrix}a_1\\b_1\\c_1\end{bmatrix}\sigma+\begin{bmatrix}a_2\\b_2\\c_2\end{bmatrix}\sigma^2+\cdots\ . \tag{5.6}$$

We have in the limit $\sigma\to 0$, where $\mathscr{R}$ stands for the right-hand side of Eq. (5.1),

$$\lim_{\sigma\to 0}\mathscr{R}=\frac{1}{N}\sum_{\vec{k}}\frac{1+\exp[-2z\beta_cJ_1(\vec{k})]+2\exp[-z\beta_cJ_2(\vec{k})]}{1-\exp[-2z\beta_cJ_1(\vec{k})]} \tag{5.7}$$

where

$$J_1(\vec{k})=(1-a_0)[J_{\parallel}-J_{\perp}\gamma(\vec{k})]+c_0p_c[J_{\perp}-J_{\parallel}\gamma(\vec{k})] , \tag{5.8}$$

$$J_2(\vec{k})=(1-a_0)[J_{\parallel}-J_{\perp}\gamma(\vec{k})]+(b_0+c_0)p_c[J_{\perp}-J_{\parallel}\gamma(\vec{k})] , \tag{5.9}$$

$$\beta_c=1/k_BT_c . \tag{5.10}$$

Since the left-hand side of Eq. (5.1) is infinite at the Curie temperature, so the denominator of the right-hand side of Eq. (5.7) should be equal to zero. If $a_0 \neq 0$ and $c_0 \neq 0$, then β_c should be equal to zero in order to make the right-hand side of Eq. (5.7) go to infinity. This corresponds to infinite Curie temperature. We find that the two conditions which are to be satisfied in order to get a finite Curie temperature of the lattice are

$$a_0=1 \text{ and } c_0=0 . \tag{5.11}$$

In the HF approximation, we have $a_0=1$ and $c_0=1$, so we get an infinite Curie temperature. On substituting these conditions in the expression for the magnetization and taking the limit $\sigma \to 0$, we get

$$z\beta_c=\frac{1}{N}\sum_{\vec{k}}\frac{1-\exp\{-z\beta_cp_cb_0[J_{\perp}-J_{\parallel}\gamma(\vec{k})]\}}{(1-a_1)[J_{\parallel}-J_{\perp}\gamma(\vec{k})]+c_1p_c[J_{\perp}-J_{\parallel}\gamma(\vec{k})]} . \tag{5.12}$$

The above equation determines the Curie temperature with the parameter p_c, which can be given by

$$z\beta_cp_c=\frac{1}{N}\sum_{\vec{k}}\gamma(\vec{k})\frac{1+\exp\{-z\beta_cp_cb_0[J_{\perp}-J_{\parallel}\gamma(\vec{k})]\}}{(1-a_1)[J_{\parallel}-J_{\perp}\gamma(\vec{k})]+\sigma_1p_c[J_{\perp}-J_{\parallel}\gamma(\vec{k})]} . \tag{5.13}$$

Equations (5.12) and (5.13) together give the expression for the Curie temperature and they can be reduced to the previous results when we substitute the following values of the different constants (from RPA, CH, and Callen, respectively):

$$\begin{aligned} &a_1=0,\ b_0=0,\ c_1=0 ,\\ &a_1=0,\ b_0=1,\ c_1=0 ,\\ &a_0=0,\ b_0=0,\ c_1=1 . \end{aligned} \tag{5.14}$$

Using Eqs. (5.6) and (5.11) in the present approximation we find

$$a_0=1,\ b_0=1,\ c_1=0 ,$$

and (5.15)

$$a_n+c_n=b_n$$

for any value of n.

B. Low-temperature expansion of magnetization

We consider the case of simple cubic lattice with a lattice constant equal to a and the nearest-neighbor number $z=6$. For a simple cubic lattice

$$\gamma(\vec{k})=\tfrac{1}{3}(\cos k_xa+\cos k_ya+\cos k_za) , \tag{5.16}$$

where (k_x,k_y,k_z) are the components of the vector $\vec{k}$. In the limit $N\to\infty$, the sums over $\vec{k}$ can be replaced by the integrals given as follows:

$$\frac{1}{N}\sum_{\vec{k}}\to\frac{\Omega}{(2\pi)^3}\int_{-\pi/a}^{\pi/a}dk_x\int_{-\pi/a}^{\pi/a}dk_y\int_{-\pi/a}^{\pi/a}dk_z , \tag{5.17}$$

where Ω is the volume of a unit cell. In our case $\Omega=a^3$. The vector $\vec{k}$ is restricted to be inside the first Brillouin zone, and hence the limits of integrations are $-\pi/a$ to $+\pi/a$.

The expressions for the spontaneous magnetization σ and the parameter p are obtained as

$$\frac{1}{\sigma}=1+\frac{2a^3}{(2\pi)^3}\int_{-\pi/a}^{\pi/a}dk_x\int_{-\pi/a}^{\pi/a}dk_y\int_{-\pi/a}^{\pi/a}dk_z\frac{n(\vec{k})}{\sigma} , \tag{5.18}$$

$$\frac{p}{\sigma}=\frac{2a^3}{(2\pi)^3}\int_{-\pi/a}^{\pi/a}dk_x\int_{-\pi/a}^{\pi/a}dk_y\int_{-\pi/a}^{\pi/a}dk_z\gamma(\vec{k})\frac{n(\vec{k})}{\sigma} , \tag{5.19}$$

with

$$n(\vec{k})=\frac{1+\exp\{-\beta[E(\vec{k})+f_+Q(\vec{k})]\}}{1-\exp\{-2\beta[E(\vec{k})+f_2Q(\vec{k})]\}}\ , \tag{5.20}$$

with $E(\vec{k})$ given by Eq. (5.2) and $Q(\vec{k})$ given by Eq. (4.21). Since we are interested in the low-temperature expansion of the magnetization, we expand the integrand of Eq. (5.17), i.e., $[n(\vec{k})/\sigma]$, by powers of $e^{-\beta E(\vec{k})}$. The result is

$$\frac{n(\vec{k})}{\sigma}=\sum_{r=0}^{\infty}(\exp\{-(2r+1)\beta[E(\vec{K})+f_2Q(\vec{k})]-\beta f_1Q(\vec{k})\}+\exp\{-2(r+1)\beta[E(\vec{k})+f_2Q(\vec{k})]\})\ . \tag{5.21}$$

We can simplify the curly brackets as

$$\begin{aligned}(2r+1)\beta[E(\vec{k})+f_2Q(\vec{k})]+f_1Q(\vec{k})=&zJ\beta\{p\phi[(2r+1)f_2+f_1]+(2r+1)[1+f_0(\sigma-1)]\}\\&-zJ\beta\gamma(\vec{k})\{p[(2r+1)f_2+f_1]+(2r+1)\phi[1+f_0(\sigma-1)]\}\end{aligned} \tag{5.22}$$

and

$$\begin{aligned}2(r+1)\beta[E(\vec{k})+f_2Q(\vec{k})]=&2zJ\beta(r+1)\{p\phi f_2+[1+f_0(\sigma-1)]\}\\&-2zJ\beta(r+1)\gamma(\vec{k})\{pf_2+\phi[1+f_0(\sigma-1)]\}\ .\end{aligned} \tag{5.23}$$

We put $J_\perp/J_{||}=\phi$, the interaction anisotropy parameter, and $J_{||}=J$. We also substitute

$$\begin{aligned}&A_r=zJ\beta\{p\phi[(2r+1)f_2+f_1]+(2r+1)[1+f_0(\sigma-1)]\}\ ,\\&B_r=\tfrac{1}{3}zJ\beta\{p[(2r+1)f_2+f_1]+(2r+1)\phi[1+f_0(\sigma-1)]\}\ ,\\&C_r=2zJ\beta(r+1)\{p\phi f_2+[1+f_0(\sigma-1)]\}\ ,\\&D_r=\tfrac{2}{3}zJ\beta(r+1)\{pf_2+\phi[1+f_0(\sigma-1)]\}\ .\end{aligned} \tag{5.24}$$

Equation (5.20) is now written as

$$\frac{n(\vec{k})}{\sigma}=\sum_{r=0}^{\infty}\{\exp[-A_r+3B_r\gamma(\vec{k})]+\exp[-C_r+3D_r\gamma(\vec{k})]\}\ . \tag{5.25}$$

Let us consider an integral of the type

$$I_1=\frac{a^3}{(2\pi)^3}\int_{-\pi/a}^{\pi/a}dk_x\int_{-\pi/a}^{\pi/a}dk_y\int_{-\pi/a}^{\pi/a}dk_z e^{3B_r\gamma(\vec{k})}\ , \tag{5.26}$$

with $\gamma(\vec{k})$ given by Eq. (5.16). Equation (5.25) reduces to

$$I_1=\frac{1}{\pi}\left[\int_0^\pi e^{B_r\cos\theta}d\theta\right]^3=I_0^3(B_r)\ , \tag{5.27}$$

where $I_0(x)$ is the modified Bessel function of the zeroth order. We assume

$$I_2=\frac{a^3}{(2\pi)^3}\int_{-\pi/a}^{\pi/a}dk_x\int_{-\pi/a}^{\pi/a}dk_y\int_{-\pi/a}^{\pi/a}dk_z\gamma(\vec{k})e^{3B_r\gamma(\vec{k})}\ . \tag{5.28}$$

It can be reduced to

$$I_2=\frac{1}{\pi^3}\left[\int_0^\pi\cos\theta_1 e^{B_r\cos\theta_1}d\theta_1\right]\left[\int_0^\pi e^{B\cos\theta_2}d\theta_2\right]^2=I_1(B_r)I_0^2(B_r)\ , \tag{5.29}$$

where $I_1(x)$ is the modified first-order Bessel function.

We can write down Eqs. (5.18) and (5.19) as

$$\frac{1}{\sigma}=1+2\sum_{r=0}^{\infty}e^{-A_r}I_0^3(B_r)+2\sum_{r=0}^{\infty}e^{-C_r}I_0^3(D_r)\ , \tag{5.30}$$

$$\frac{p}{\sigma}=2\sum_{r=0}^{\infty}e^{-A_r}I_1(B_r)I_0^2(B_r)+2\sum_{r=0}^{\infty}e^{-C_r}I_1(D_r)I_0^2(D_r)\ . \tag{5.31}$$

The asymptotic expansions can be obtained as

$$\frac{1}{\sigma}=1+\frac{2}{(2\pi)^{3/2}}[m_1(\tfrac{1}{3}zJ\beta)^{-3/2}+\tfrac{3}{8}m_2(\tfrac{1}{3}zJ\beta)^{-5/2}+m_3p(\tfrac{1}{3}zJ\beta)^{-3/2}+\tfrac{3}{8}m_4(\tfrac{1}{3}zJ\beta)^{-5/2}p + \tfrac{33}{128}m_5(\tfrac{1}{3}zJ\beta)^{-7/2}+O(\beta^{-9/2})] , \quad (5.32)$$

$$\frac{p}{\sigma}=\frac{2}{(2\pi)^{3/2}}[m_1(\tfrac{1}{3}zJ\beta)^{-3/2}-\tfrac{1}{8}m_2(\tfrac{1}{3}zJ\beta)^{-5/2}+m_3p(\tfrac{1}{3}zJ\beta)^{-3/2}-\tfrac{1}{8}m_4^4p(\tfrac{1}{3}zJ\beta)^{-5/2} - \tfrac{7}{128}m_5(\tfrac{1}{3}zJ\beta)^{-7/2}+O(\beta^{-9/2})] , \quad (5.33)$$

where

$$m_1=[1+f_0(\sigma-1)]^{-3/2}\xi(\tfrac{3}{2}) ,$$
$$m_2=[1+f_0(\sigma-1)]^{-5/2}\xi(\tfrac{5}{2}) ,$$
$$m_3=-\tfrac{3}{2}[1+f_0(\sigma-1)]^{-5/2}\times[\xi(\tfrac{3}{2})f_2+\xi(\tfrac{5}{2},\tfrac{1}{2})f_1 2^{-5/2}] , \quad (5.34)$$
$$m_4=-\tfrac{5}{2}[1+f_0(\sigma-1)]^{-7/2}\times[\xi(\tfrac{7}{2})f_2+\xi(\tfrac{7}{2},\tfrac{1}{2})f_1 2^{-5/2}] ,$$
$$m_5=[1+f_0(\sigma-1)]^{-7/2}\xi(\tfrac{7}{2}) .$$

The leading term in σ is $O(1)$ and in p/σ is $O(\beta^{-3/2})$. Making use of this in collecting the terms in increasing negative powers of β, we get a value equal to

$$1+a\beta^{-3/2}+b\beta^{-5/2}+c\beta^{-3}+d\beta^{-7/2} +e\beta^{-4}+O(\beta^{-9/2}) , \quad (5.35)$$

where

$$a=\frac{2}{(2\pi)^{3/2}}(\tfrac{1}{3}zJ)^{-3/2}\xi(\tfrac{3}{2}) ,$$
$$b=\frac{3}{4(2\pi)^{3/2}}(\tfrac{1}{3}zJ)^{-5/2}\xi(\tfrac{5}{2}) ,$$
$$c=\frac{6}{(2\pi)^{3}}(\tfrac{1}{3}zJ)^{-3}[\xi(\tfrac{3}{2})f_2+\xi(\tfrac{5}{2},\tfrac{1}{2})f_1 2^{-5/2} -5\xi(\tfrac{3}{2})\xi(\tfrac{5}{2})f_2 +\xi(\tfrac{7}{2},\tfrac{1}{2})f_1 2^{-5/2}] , \quad (5.36)$$
$$d=[33/64(2\pi)^{3/2}](\tfrac{1}{3}zJ)^{-7/2}\xi(\tfrac{7}{2}) ,$$
$$e=[3/4(2\pi)^{3}](\tfrac{1}{3}zJ)^{-4}\times\{\xi(\tfrac{5}{2})[\xi(\tfrac{3}{2})f_2+\xi(\tfrac{5}{2},\tfrac{1}{2})f_1 2^{-5/2}] -5\xi(\tfrac{3}{2})[\xi(\tfrac{5}{2})f_2+\xi(\tfrac{7}{2},\tfrac{1}{2})f_1 2^{-5/2}]\} .$$

The expression for the spontaneous magnetization becomes equal to

$$1-a\beta^{-3/2}-b\beta^{-5/2}-(c-a^2)\beta^{-3}-d\beta^{-7/2} -(e-2ab)\beta^{-4}+O(\beta^{-1/2}) . \quad (5.37)$$

Here in Eq. (5.36), $f_1=\sum_n b_n$ and $f_2=\sum_n c_n$, i.e., the values of decoupling parameters when $\sigma=1$. We are interested in the coefficients of β^{-3} and β^{-4}. The other terms are standard ones. The coefficient of β^{-3} is

$$\frac{2}{(2\pi)^3}(\tfrac{1}{3}zJ)^{-3}\epsilon(\tfrac{3}{2})[(2+3f_2)\epsilon(\tfrac{3}{2}) +2^{-5/2}f_1\xi(\tfrac{5}{2},\tfrac{1}{2})] , \quad (5.38)$$

while the coefficient of β^{-4} is

$$\frac{3}{4(2\pi)^3}(\tfrac{1}{3}zJ)^{-4}\{4(1+f_2)\xi(\tfrac{3}{2})\xi(\tfrac{5}{2}) +2^{-5/2}f_1[\xi(\tfrac{5}{2})\xi(\tfrac{7}{2},\tfrac{1}{2})\xi(\tfrac{3}{2}) -\xi(\tfrac{5}{2},\tfrac{1}{2})\xi(\tfrac{5}{2})]\} . \quad (5.39)$$

These coefficients can be compared with the spin-wave-theory results of Dyson,[17] RPA results of Tyablikov,[2] and KH results of Katsura and Horiguchi.[5]

The coefficient of the β^{-3} term is, for RPA, for Dyson, and for KH, respectively,

$$-\frac{2}{(2\pi)^3}(\tfrac{1}{3}zJ)^{-3}\xi(3) , \quad (5.40a)$$
$$\frac{2}{(2\pi)^3}(\tfrac{1}{3}zJ)^{-3}\xi(\tfrac{3}{2})[2\xi(\tfrac{3}{2})+2^{-5/2}\xi(\tfrac{5}{2},\tfrac{1}{2})] .$$

The coefficient of the β^{-4} term is, for Dyson, for KH, and for RPA, respectively,

$$-\frac{3}{4(2\pi)^3}(\tfrac{1}{3}zJ)^{-1}[2(1.68)\xi(\tfrac{5}{2})\xi(\tfrac{3}{2})]\ ,$$

$$\frac{3}{4(2\pi)^3}(\tfrac{1}{3}zJ)^{-4}\{4\xi(\tfrac{5}{2})\xi(\tfrac{3}{2})+2^{-5/2}[\xi(\tfrac{5}{2})\xi(\tfrac{7}{2},\tfrac{1}{2})\xi(\tfrac{3}{2})-\xi(\tfrac{5}{2},\tfrac{1}{2})\xi(\tfrac{5}{2})]\}\ ,$$

$$-\frac{3}{(2\pi)^3}(\tfrac{1}{3}zJ)^{-4}\xi(\tfrac{5}{2})\xi(\tfrac{3}{2})\ . \qquad (5.40b)$$

The coefficients of the β^{-3} term in Eq. (5.38) can be made to agree with Dyson's result if we assume

$$(2+3f_2)/f_1=-0.4252\ . \qquad (5.41)$$

The first-order Green's-function theory cannot give the correct coefficient of the β^{-4} term because for this we have to take into account the spin-spin interactions. For a simple cubic lattice the variation of Curie temperature with the anisotropy parameter ϕ can be obtained as[18] (see Fig. 1)

$$zJ_{\|}\beta_c[(1-a_1)+c_1\phi\theta_c]=\frac{a^3}{(2\pi)^3}\int d^3k\left[\frac{1+\exp\{-zJ_{\|}\beta_c p_c b_0[\phi-\gamma(\vec{k})]\}}{1-\eta\gamma(\vec{k})}\right] \qquad (5.42)$$

and

$$zJ_{\|}\beta_c p_c[(1-a_1)\phi+c_1p_c]=zJ_{\|}\beta_c[(1-a_1)+c_1\phi p_c]-1-\frac{a^3}{(2\pi)^3}\int d^3k\, e^{-zJ_{\|}\beta_c p_c b_0[\phi-\gamma(\vec{k})]}\ , \qquad (5.43)$$

where $z=6$, a is the lattice constant, $\gamma(\vec{k})$ is given by Eq. (5.16), and η is defined as

$$\eta=\frac{(1-a_1)\phi+c_1p_c}{1-a_1+c_1\phi p_c}\ . \qquad (5.44)$$

If we put $a_1=0$, $b_0=0$, and $c_1=0$ in Eq. (5.42) we get

$$zJ_{\|}\beta_c(\mathrm{RPA})=\frac{2a^3}{(2\pi)^3}\int d^3k\frac{1}{1-\phi\gamma(\vec{k})}=2F(\phi)\ . \qquad (5.45)$$

Substituting Eq. (5.44) in Eq. (5.42) we find

$$zJ_{\|}\beta_c[(1-a_1)+c_1\phi p_c]=F(\eta)+\frac{a^3}{(2\pi)^3}\int d^3k\frac{\exp\{-zJ_{\|}\beta_c p_c b_0[\phi-\gamma(\vec{k})]\}}{1-\eta\gamma(\vec{k})}\ . \qquad (5.46)$$

Doing the integration as usual, we finally obtain

$$zJ_{\|}p_c\beta_c[(1-a_1)\phi+c_1p_c]=zJ_{\|}\beta_c[(1-a_1)+c_1\phi p_c)]-1-\exp(-zJ_{\|}\beta_c p_c b_0\phi)[I_0(\tfrac{1}{3}zJ_{\|}\beta_c p_c b_0)]^3\ . \qquad (5.47)$$

Equation (5.47) represents the variation of the Curie temperature with the anisotropy constant ϕ and the different parameters. Equation (5.47) is appreciably modified as compared to results previously calculated by Dalton and Wood.[18]

VI. THERMAL CONDUCTIVITY DUE TO MAGNONS

Recently Kumar[6] has shown that the magnon conductivity gets modified by the spin-wave renormalization. Initially McCollum, Wild, and Callaway[19] have calculated the magnon conductivity as

$$K_m(T)=\frac{k_B^2}{6\pi^2\hbar\gamma}T^2\int_0^{x_m}l_m(x,T)\frac{x^3e^x}{(e^x-1)^2}dx$$

$$=AT^2\int_0^{x_m}l_m(x,T)\frac{x^3e^x}{(e^x-1)^2}dx\ ,$$

where

$$A=k_B^3/6\pi^2\hbar\gamma\ . \qquad (6.1)$$

Here the spin-wave energy is defined as

$$E(\vec{k})=\gamma k^2\ , \qquad (6.2)$$

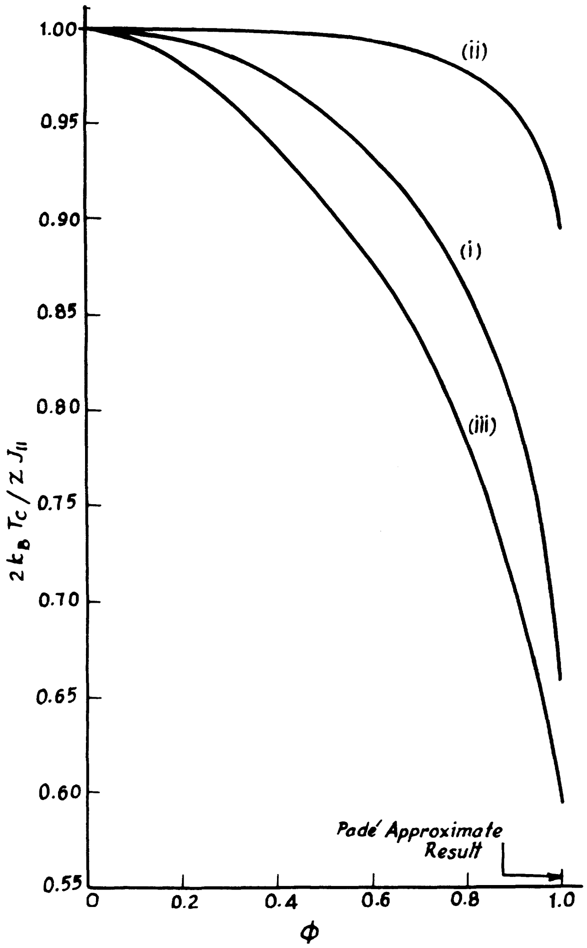

FIG. 1. Plot of $2k_BT_c/zJ_{\parallel}$ vs the anisotropy parameter ϕ $(=J_{\perp}/J_{\parallel})$ for a simple cubic lattice using different decoupling schemes: (i) RPA ($a_0=1$, $a_1=0$, $b_0=0$, $c_0=0$, $C_1=0$); (ii) KH decoupling scheme ($a_0=1$, $a_1=0$, $b_0=1$, $c_0=0$, $c_1=0$); (iii) intermediate decoupling from the present scheme ($a_0=1$, $a_1=\frac{1}{2}$, $b_0=1$, $c_0=0$, $c_1=-\frac{1}{2}$).

where γ entirely depends upon the technique of calculating the spin-wave energy. With the use of Zubarev's double-time Green's functions, γ depends upon the various decoupling parameters. Therefore, the degree of the deviation between theory and experiment will depend upon the inadequacy involved in the different decoupling approximations.

We now study the modifications in the magnon conductivity which occur by using the present decoupling scheme. Following Callaway,[20] the magnon conductivity can be expressed as

$$K_m(T)=\frac{1}{(2\pi)^3}\int V_{\vec{k}}^2\tau_m(\vec{k})\cos^2\theta C_m(\vec{k})d^3k\ , \tag{6.3}$$

where

$$V_{\vec{k}}=\frac{dE(\vec{k})}{dk}\ , \tag{6.4}$$

$$C_m(\vec{k})=k_B\left[\frac{E(\vec{k})}{k_BT}\right]^2\frac{e^{E(\vec{k})/k_BT}}{(e^{E(\vec{k})/k_BT}-1)^2}\ , \tag{6.5}$$

$$\tau_m(\vec{k})=l_m(\vec{k})V_k\ . \tag{6.6}$$

In Eq. (6.3), $E(\vec{k})$ is the spin-wave energy which is obtained as

$$E_+(\vec{k})=a-b\gamma(\vec{k})\ , \tag{6.7}$$

with

$$a=(zJ\sigma+f_+zJp\phi)\ ,\qquad b=(zJ\sigma\phi+f_+zJp)\ . \tag{6.8}$$

Equation (6.7) can be further simplified for a simple cubic lattice as

$$E_+(\vec{k})=(\bar{a}-b)+\frac{b}{6}k^2a^2=\alpha_1+\beta_1k^2\ , \tag{6.9}$$

with

$$\alpha_1=(\bar{a}-b)\ ,$$

$$\beta_1=\frac{1}{6}ba^2\ .$$

Following Callaway, we assume

$$\frac{\beta_1k^2}{k_BT}=x\quad\text{and}\quad\frac{\alpha_1}{k_BT}=\delta\ . \tag{6.10}$$

Substituting Eqs. (6.9) and (6.10) into Eqs. (6.3) and (6.4), we get the magnon velocity as

$$V_k=\frac{1}{\hbar}2\beta_1k=\frac{2\beta_1k}{\hbar}\ , \tag{6.11}$$

$$C_m(x)=k_B(x+\delta)^2\frac{e^{x+\delta}}{(e^{x+\delta}-1)^2}\ . \tag{6.12}$$

The magnon conductivity reduces to

$$K_m(T)=A\left[\frac{\gamma}{\beta_1}\right]T^2\int_0^{x_m}l_m(x,T)x(x+\delta)^2\times I(x+\delta)dx\ ,\qquad I(\eta)=\frac{e^{\eta}}{(e^{\eta}-1)^2}\ . \tag{6.13}$$

Equation (6.13) clearly shows that the magnon conductivity depends not only on the two decoupling constants (β_1,α_1) but also on the anisotropy constant. If we assume that the neglect of the parameter δ does not appreciably change the function $I(x)$ the magnon conductivity can be written as

$$K_m(T)=A\left[\frac{\gamma}{\beta_1}\right]T^2\int_0^{x_m} l_m(x,T)x(x+\delta)^2 I(x)dx \ . \tag{6.14}$$

Equation (6.14) can be further simplified as

$$K_m(T)=A\left[\frac{\gamma}{\beta_1}\right]T^2\left[\int_0^{x_m} l_m(x,T)x^3 I(x)dx+2\delta\int_0^{x_m} l_m(x,T)x^2 I(x)dx+\delta^2\int_0^{x_m} l_m(x,T)xI(x)dx\right] . \tag{6.15}$$

We can rewrite Eq. (6.15) as

$$K_m(T)=K_m(T)\left[1+2\delta\frac{I_2(x)}{I_3(x)}+\delta^2\frac{I_1(x)}{I_3(x)}\right] ,$$

where

$$I_n(x)=\int_0^{x_m} l_m(x,T)x^n I(x)dx \ . \tag{6.16}$$

Equation (6.16) represents the magnon conductivity which depends upon the additional decoupling parameters and the anisotropy constant ϕ. We now study the effect of the anisotropy on the magnon conductivity. Equation (6.9) shows that

$$\delta=\frac{\alpha_1}{k_BT}=\frac{1}{k_BT}(zJ\sigma-f_+zJp)(1-\phi)$$
$$=zJ\beta\sigma\left[1-f_+\frac{p}{\sigma}\right](1-\phi) \ . \tag{6.17}$$

Substituting Eqs. (5.6) and (5.33) into Eq. (6.17), we observe that the series expansion corresponding to the term $[f_+(p/\sigma)]$ is obtained depending upon σ and $(\frac{1}{3}zJ\beta)^{-3/2}$. The temperature dependence is same as that of (p/σ). The magnon conductivity has been effectively increased by considering the anisotropy. However, for $\phi=1$, i.e., isotropic systems, we find

$$\delta=0 \ .$$

Therefore,

$$K_m(T)=K_m(T)\left[\frac{\gamma}{\beta_1}\right] . \tag{6.18}$$

It is therefore observed that the magnon conductivity varies with the anisotropy constant. Equation (6.18) shows that the additional decoupling parameters are still important for isotropic systems because of the multiplication factor γ/β_1. We observe that

$$\beta_1=\tfrac{1}{6}ba^2=\tfrac{1}{6}a^2(zJ\sigma\phi+f_+zJp)$$
$$=\tfrac{1}{6}a^2zJ\sigma\left[\phi+f_+\frac{p}{\sigma}\right] . \tag{6.19}$$

There the multiplication factor (γ/β_1) is of the form

$$\frac{\gamma}{\beta_1}=\frac{1}{[\phi+f_+(p/\sigma)]} \ . \tag{6.20}$$

Equation (6.20) is again a series-dependent term and depends upon the different decoupling parameters used in the calculations along with the temperature, as previously suggested by Kumar.[6]

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