Spin waves of two-sublattice Heisenberg ferrimagnets

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The method of the retarded-Green's-function equation of motion is applied to investigate the spin-wave spectrum and other properties of two-sublattice Heisenberg ferrimagnets. The algebraic procedure is greatly simplified by introducing the matrix equation for the ferrimagnet for both NaCl and CsCl structures. We find that the spin-wave spectrum breaks into acoustical and optical branches as expected. The mean spin values of individual sublattices are calculated numerically for different single-particle spin values. It is seen that in the special case of an antiferromagnet, our results agree completely with existing work.

I. INTRODUCTION

While there has been a great deal of work on spin waves of ferromagnets and antiferromagnets,[1-6] relatively little attention has been paid to ferrimagnets.[7-11] Perhaps this is because ferrimagnets generally possess rather complicated lattice structures and hence are difficult to handle. From the point of view of practical applications, however, many of the important magnetic materials are ferrimagnetic. Yttrium iron garnet is just one example. It is, therefore, of interest to study the properties of spin waves in ferrimagnets.

Ferrimagnets differ from ferromagnets in that the macroscopic magnetization is the result of the sum of magnetization vectors of all individual sublattices. Unlike antiferromagnets in which the magnetization of individual sublattices cancel out mutually, the individual sublattice magnetization vectors do not offset each other in ferrimagnets. This means that the sublattices in an antiferromagnet are equivalent magnetically, and this equivalence does not hold in ferrimagnets. It is the multilattice structure and the nonequivalence of the sublattices that make the ferrimagnets more difficult to deal with theoretically.

In order to retain the basic features of ferrimagnets and still keep the mathematical description to the simplest level, we consider in this paper a two-lattice Heisenberg ferrimagnet model. Consider two different kinds of magnetic ions a and b. They may form either NaCl structure in which the sublattices are face centered cubic (fcc), or CsCl structure, in which the sublattices are simple cubic (sc). Let the mean value of these a-sublattice spin and b-sublattice spin be $\langle S^z\rangle_a$ and $\langle S^z\rangle_b$, respectively. These mean values are in general different for different sublattices, namely $|\langle S^z\rangle_a| \neq |\langle S^z\rangle_b|$.

For two-sublattice antiferromagnets, it has been shown that the two branches of bulk spin waves are degenerate in energy.[12] Since the two sublattices are not equivalent in ferrimagnets, the two branches of bulk spin waves are not degenerate in energy.[13] They break into optical and acoustical branches.

We apply the method of retarded Green's functions in this paper to study ferrimagnetism. It has been applied to treat ferromagnetism[14-16] and antiferromagnetism.[12,17] It has also been used by various authors[18-21] in their discussions of surface or interface spin waves in ferromagnetic structures. Because of the nonequivalent sublattices, direct application of the method to ferrimagnetic structures leads to equations of motion that require extraordinary complicated algebra to solve. Instead, we express the two-sublattice Green's functions in terms of a 2×2 matrix and find the equation of motion it satisfies. The algebraic procedure of solution is then greatly simplified. As a matter of fact, the algebra for solving equations of motion of the multisublattice ferrimagnet becomes formally the same as that of the ferromagnet. The method introduced here is particularly useful in the treatment of surface spin waves of ferrimagnets.[22]

We remark that part of the effect of many-body interactions is already included in the Green's-function treatment,[14,17,15,16] although it is not easy to specify which part because of the difficulties involved in the treatment of decoupling procedures. In the present case of two-sublattice system, the mean values $\langle S^z\rangle_a$ and $\langle S^z\rangle_b$ calculated from the equations of motion are never equal to their corresponding single-particle values S_a and S_b. That is, we always find $\langle S^z\rangle_a \neq S_a$ and $\langle S^z\rangle_b \neq S_b$, even when $T=0$. This means that particles occupying negative energy states have been included in our consideration.

In Sec. II we derive the equations of motion for the retarded Green's function, and a matrix method is introduced to solve the equations for the Green's functions for both NaCl and CsCl cases in Sec. III. From the Green's functions obtained in Sec. III, we calculate the mean values $\langle S^z\rangle_a$ and $\langle S^z\rangle_b$. The results for both structures are presented and discussed in Sec. IV.

II. EQUATIONS OF MOTION

With nearest-neighbor exchange interactions we write the Heisenberg model Hamiltonian for a two-sublattice ferrimagnet as[13]

$$H=\sum_{\langle a,b\rangle} J\mathbf{S}_a\cdot\mathbf{S}_b \ , \tag{1}$$

where $\sum_{\langle a,b\rangle}$ means the summation over each pair of nearest neighbors only once. The vector **a** stands for the lattice vector of the a sublattice and **b** lattice vector of the b sublattice. $\mathbf{S}_a$ ($\mathbf{S}_b$) is the spin vector located at the lattice point **a** (**b**). J is the nearest-neighbor exchange integral. We note that the nearest neighbors of a spin on the a sublattice are all b spins and vice versa. No anisotropic interaction nor external field is considered in (1).

We consider two types of lattice structures: the simple cubic and body-centered cubic. Because of the two-sublattice nature, sc actually means NaCl structure in which the Bravais lattice is fcc. On the other hand, bcc is actually CsCl structure with sc Bravais lattice. As we shall see later, the spin-wave energy spectra are different for different lattice structures.

Define the spin operators

$$S_a^{\pm}=S_a^x\pm iS_a^y \text{ and } S_b^{\pm}=S_b^x\pm iS_b^y \ . \tag{2}$$

Following the random-phase-approximation (RPA) decoupling procedure[15,16] for the chain of equations of motion, we find in the energy representation, the equation of motion for the operator $\mathbf{S}_a$ in the a sublattice

$$E\langle\langle S_a^+;S_{a'}^-\rangle\rangle=2\langle S_a^z\rangle\delta_{a,a'}+J\langle S_a^z\rangle\sum_{\delta}\langle\langle S_{a+\delta}^+;S_{a'}^-\rangle\rangle$$

$$-J\sum_{\delta}\langle S_{a+\delta}^z\rangle\langle\langle S_a^+;S_{a'}^-\rangle\rangle \ , \tag{3a}$$

where δ denotes the relative position vector between two nearest neighbors and $\sum_\delta$ represents the sum over such nearest neighbors. It should be pointed out that $\mathbf{S}_{a+\delta}$ is always a b spin in the b sublattice. The equation of motion for $\mathbf{S}_b$ is

$$E\langle\langle S_b^+;S_{a'}^F\rangle\rangle=J\langle S_b^z\rangle\sum_{\delta}\langle\langle S_{b+\delta}^+;S_{a'}^-\rangle\rangle$$

$$-J\sum_{\delta}\langle S_{b+\delta}^z\rangle\langle\langle S_b^+;S_{a'}^-\rangle\rangle \ , \tag{3b}$$

where $\mathbf{S}_{b+\delta}$ is an a spin in the a sublattice. In a similar fashion, we can write down two more equations

$$E\langle\langle S_b^+;S_{b'}^-\rangle\rangle=2\langle S_b^z\rangle\delta_{b,b'}+J\langle S_b^z\rangle\sum_{\delta}\langle\langle S_{b+\delta}^+;S_{b'}^-\rangle\rangle$$

$$-J\sum_{\delta}\langle S_{b+\delta}^z\rangle\langle\langle S_b^+;S_{b'}^-\rangle\rangle \ , \tag{4a}$$

$$E\langle\langle S_a^+;S_{b'}^-\rangle\rangle=J\langle S_a^z\rangle\sum_{\delta}\langle\langle S_{a+\delta}^+;S_{b'}^-\rangle\rangle$$

$$-J\sum_{\delta}\langle S_{a+\delta}^z\rangle\langle\langle S_a^+;S_{b'}^-\rangle\rangle \ . \tag{4b}$$

Because of the translational symmetry, the thermal expectation value of the spin is uniform on each lattice. Thus we have

$$\langle S_a^z\rangle=\langle S^z\rangle_a$$

$$=\text{constant for every point } \mathbf{a} \text{ on } a \text{ sublattice}$$

and

$$\langle S_b^z\rangle=\langle S^z\rangle_b$$

$$=\text{constant for every point } \mathbf{b} \text{ on } b \text{ sublattice}$$

We now introduce the two-dimensional Fourier transform

$$\langle\langle S_a^+;S_{a'}^-\rangle\rangle=\frac{1}{N_0}\sum_{\kappa}2\langle S^z\rangle_a g_{aa}(\kappa,E;m,n)e^{i\kappa\cdot(\mathbf{a}-\mathbf{a}')} \ , \tag{5a}$$

$$\langle\langle S_b^+;S_{a'}^-\rangle\rangle=\frac{1}{N_0}\sum_{\kappa}2\langle S^z\rangle_a g_{ba}(\kappa,E;m,n)e^{i\kappa\cdot(\mathbf{b}-\mathbf{a}')} \ , \tag{5b}$$

$$\langle\langle S_a^+;S_{b'}^-\rangle\rangle=\frac{1}{N_0}\sum_{\kappa}2\langle S^z\rangle_b g_{ab}(\kappa,E;m,n)e^{i\kappa\cdot(\mathbf{a}-\mathbf{b}')} \ , \tag{5c}$$

$$\langle\langle S_b^+;S_{b'}^-\rangle\rangle=\frac{1}{N_0}\sum_{\kappa}2\langle S^z\rangle_b g_{bb}(\kappa,E;m,n)e^{i\kappa\cdot(\mathbf{b}-\mathbf{b}')} \ , \tag{5d}$$

where N_0 is the total number of unit cells in each layer and the g's are Green's functions expressed in the Bloch-Wannier representation in which the Bloch function is used in the xy plane and the Wannier function is used in the z direction. κ is a two-dimensional wave vector defined by $\mathbf{k}=(\kappa,q)=(k_x,k_y,q)$. m represents the z component of **a** or **b**, and n stands for the z component of **a'** or **b'**. The factors $2\langle S^z\rangle_a$ and $2\langle S^z\rangle_b$ are introduced for convenience, and the purpose of doing so will become clear after equations of motion for the Green's functions are derived.

In terms of the Green's functions defined by (5), Eqs. (3) and (4) take the form for NaCl structure

$$(E+6J\langle S^z\rangle_b)g_{aa}(\kappa,E;m,n)=\delta_{mn}+4J\langle S^z\rangle_a\xi(\kappa)g_{ba}(\kappa,E;m,n)+J\langle S^z\rangle_a[g_{ba}(\kappa,E;m+1,n)+g_{ba}(\kappa,E;m-1,n)]\ , \tag{6a}$$

$$(E+6J\langle S^z\rangle_a)g_{ba}(\kappa,E;m,n)=4J\langle S^z\rangle_b\xi(\kappa)g_{aa}(\kappa,E;m,n)+J\langle S^z\rangle_b[g_{aa}(\kappa,E;m+1,n)+g_{aa}(\kappa,E;m-1,n)]\ , \tag{6b}$$

$$(E+6J\langle S^z\rangle_b)g_{ab}(\kappa,E;m,n)=4J\langle S^z\rangle_a\xi(\kappa)g_{bb}(\kappa,E;m,n)+J\langle S^z\rangle_a[g_{bb}(\kappa,E;m+1,n)+g_{bb}(\kappa,E;m-1,n)]\ , \tag{6c}$$

$$(E+6J\langle S^z\rangle_a)g_{bb}(\kappa,E;m,n)=\delta_{mn}+4J\langle S^z\rangle_b\xi(\kappa)g_{ab}(\kappa,E;m,n)+J\langle S^z\rangle_b[g_{ab}(\kappa,E;m+1,n)+g_{ab}(\kappa,E;m-1,n)]\ , \tag{6d}$$

where we have defined $\xi(\kappa)=\frac{1}{2}(\cos k_x d+\cos k_y d)$ and d the distance between the nearest-neighbor spins S_a and S_b. Before we write down the equations for CsCl structure, we must remember that a spins and b spins form alternative layers. In fact, it may be regarded as the simplest idealized superlattice. If we denote the distance between neighboring layers by d, then each sublattice has a period $2d$ along the z direction. Thus, we label the layers of a sublattice by integers $0,\pm1,\pm2,\ldots$ and the b sublattice by half-integers $\pm1/2,\pm3/2,\ldots$. The equations of motion for the Green's functions are then

$$(E+8J\langle S^z\rangle_b)g_{aa}(\kappa,E;m,n)=\delta_{mn}+4J\langle S^z\rangle_a\eta(\kappa)[g_{ba}(\kappa,E;m+\tfrac{1}{2},n)+g_{ba}(\kappa,E;m-\tfrac{1}{2},n)]\ , \tag{7a}$$

$$(E+8J\langle S^z\rangle_a)g_{ba}(\kappa,E;m',n)=4J\langle S^z\rangle_b\eta(\kappa)[g_{aa}(\kappa,E;m'+\tfrac{1}{2},n)+g_{aa}(\kappa,E;m'-\tfrac{1}{2},n)]\ , \tag{7b}$$

$$(E+8J\langle S^z\rangle_b)g_{ab}(\kappa,E;m,n')=4J\langle S^z\rangle_a\eta(\kappa)[g_{bb}(\kappa,E;m+\tfrac{1}{2},n')+g_{bb}(\kappa,E;m-\tfrac{1}{2},n')]\ , \tag{7c}$$

$$(E+8J\langle S^z\rangle_a)g_{bb}(\kappa,E;m',n')=\delta_{m'n'}+4J\langle S^z\rangle_b\eta(\kappa)[g_{ab}(\kappa,E;m'+\tfrac{1}{2},n')+g_{ab}(\kappa,E;m'-\tfrac{1}{2},n')]\ , \tag{7d}$$

where m,n are integers and m',n' are half-integers. We have also defined the function $\eta(\kappa)=\cos k_x d\cos k_y d$.

III. METHOD OF SOLUTION

The bulk magnetic properties and spin-wave spectra of ferrimagnets can be calculated from the Green's functions which we proceed to find by solving Eqs. (6) and (7). We first define the matrix Green's function

$$\bar{g}(\kappa,\mathbf{E};m,n)=\begin{bmatrix} g_{aa}(\kappa,E;m,n) & g_{ab}(\kappa,E;m,n)\\ g_{ba}(\kappa,E;m,n) & g_{bb}(\kappa,E;m,n)\end{bmatrix}. \tag{8}$$

The system of coupled equations (6) can then be written in the form of matrix equation

$$(E\mathbf{1}-D)\bar{g}(\kappa,E;m,n) -F[\bar{g}(\kappa,E;m+1,n)+\bar{g}(\kappa,E;m-1,n)]=\delta_{mn}\mathbf{1}\ , \tag{9}$$

where we have also defined the 2×2 unit matrix $\mathbf{1}$ and

$$D=\begin{bmatrix} -6J\langle S^z\rangle_b & 4J\langle S^z\rangle_a\xi(\kappa)\\ 4J\langle S^z\rangle_b\xi(\kappa) & -6J\langle S^z\rangle_a\end{bmatrix}, \tag{9a}$$

$$F=\begin{bmatrix} 0 & J\langle S^z\rangle_a\\ J\langle S^z\rangle_b & 0\end{bmatrix}. \tag{9b}$$

In a similar fashion, we have from (7) the matrix equation for CsCl structure,

$$(E\mathbf{1}-D')\bar{g}(\kappa,E;m,n)-F_1\bar{g}(\kappa,E;m+1,n) -F_2\bar{g}(\kappa,\mathbf{E};m-1,n)=\delta_{mn}\mathbf{1}\ , \tag{10}$$

where the matrices D', F_1, and F_2 are defined by

$$D'=\begin{bmatrix} -8J\langle S^z\rangle_b & 4J\langle S^z\rangle_a\eta(\kappa)\\ 4J\langle S^z\rangle_b\eta(\kappa) & -8J\langle S^z\rangle_a\end{bmatrix}, \tag{10a}$$

$$F_1=\begin{bmatrix} 0 & 4J\langle S^z\rangle_a\eta(\kappa)\\ 0 & 0\end{bmatrix}, \tag{10b}$$

$$F_2=\begin{bmatrix} 0 & 0\\ 4J\langle S^z\rangle_b\eta(\kappa) & 0\end{bmatrix}. \tag{10c}$$

Equations (9) and (10) are written down for a particular layer m. For the bulk ferrimagnetic crystal, we combine equations for all layers together and obtain the supermatrix equation. This is, for CsCl structure,

$$\begin{bmatrix} \ddots & \vdots & & & & & \\ \cdots & E\mathbb{1}-D' & -F_2 & & & & \\ & -F_1 & E\mathbb{1}-D' & -F_2 & & & \\ & & -F_1 & E\mathbb{1}-D' & -F_2 & & \\ & & & -F_1 & E\mathbb{1}-D' & -F_2 & \\ & & & & -F_1 & E\mathbb{1}-D' & \cdots \\ & & & & & \vdots & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ \bar{g}(\kappa,E;2,n) \\ \bar{g}(\kappa,E;1,n) \\ \bar{g}(\kappa,E;0,n) \\ \bar{g}(\kappa,E;-1,n) \\ \bar{g}(\kappa,E;-2,n) \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ \delta_{2n} \\ \delta_{1n} \\ \delta_{0n} \\ \delta_{-1n} \\ \delta_{-2n} \\ \vdots \end{bmatrix} \tag{11}$$

Every matrix element in this equation is itself a 2×2 matrix, and every row represents the equation of motion for one layer of the crystal. When we set $D'=D$, and $F_1=F_2=F$, Eq. (11) becomes the equation for the NaCl structure. Equation (11) is not difficult to solve because its coefficient matrix is a tridiagonal one, and all the matrix elements along any of the diagonals are the same. The easiest way is to introduce the z-component Fourier transform

$$\bar{g}(\kappa,E;m,n)=\frac{1}{N_z}\sum_q \bar{g}(\kappa,E;q)e^{iqa_0(m-n)}, \tag{12}$$

where N_z is the total number of unit cells in the z direction, a_0 is the period in the z direction. For the case of the NaCl structure, $a_0=d$, and for CsCl, $a_0=2d$. Substituting (12) in (9) and (10), and remembering the relation

$$\delta_{mn}=\frac{1}{N_z}\sum_q e^{iqa_0(m-n)} \tag{12a}$$

we find for the NaCl structure

$$\begin{bmatrix} E+6J\langle S^z\rangle_b & -J\langle S^z\rangle_a[4\xi(\kappa)+2\cos qd] \\ -J\langle S^z\rangle_b[4\xi(\kappa)+2\cos qd] & E+6J\langle S^z\rangle_a \end{bmatrix} \begin{bmatrix} g_{aa}(\kappa,E;q) & g_{ab}(\kappa,E;q) \\ g_{ba}(\kappa,E;q) & g_{bb}(\kappa,E;q) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{13}$$

and for the CsCl structure

$$\begin{bmatrix} E+8J\langle S^z\rangle_b & -4J\langle S^z\rangle_a\eta(\kappa)(1+e^{\cdot} \\ -4J\langle S^z\rangle_b\eta(\kappa)(1+e^{-2iqd}) & E+8J\langle S^z\rangle_a \end{bmatrix} \begin{bmatrix} g_{aa}(\kappa,E;q) & g_{ab}(\kappa,E;q) \\ g_{ba}(\kappa E;q) & g_{bb}(\kappa,E;q) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{14}$$

Equations (13) and (14) can be solved simply by finding the inverse of the coefficient matrix. Thus, we find from (13) the solution for the NaCl structure

$$\begin{bmatrix} g_{aa}(\kappa,E;q) & g_{ab}(\kappa,E;q) \\ g_{ba}(\kappa,E;q) & g_{bb}(\kappa,E;q) \end{bmatrix} = \frac{1}{[E-E_+(\mathbf{k})][E-E_-(\mathbf{k})]} \begin{bmatrix} E+6J\langle S^z\rangle_a & 6J\langle S^z\rangle_a\gamma_1(\mathbf{k}) \\ -6\alpha J\langle S^z\rangle_a\gamma_1(\mathbf{k}) & E-6\alpha J\langle S^z\rangle_a \end{bmatrix}, \tag{15}$$

where we have defined

$$E_\pm(\mathbf{k})=-3J\langle S^z\rangle_a(1-\alpha)\pm 3J\langle S^z\rangle_a[(1+\alpha)^2-4\alpha\gamma_1^2(\mathbf{k})]^{1/2}, \tag{16}$$

$$\gamma_1(\mathbf{k})=\tfrac{1}{3}(\cos k_x d+\cos k_y d+\cos qd). \tag{17}$$

The mean values $\langle S^z\rangle_a$ and $\langle S^z\rangle_b$ are independent quantities. We introduce a parameter $\alpha=-\langle S^z\rangle_b/\langle S^z\rangle_a$ for convenience. The minus sign reflects the fact that the spins are opposite in a sublattice and b sublattice. In the following we shall assume $\alpha\le 1$ without loss of generality.

The bulk spin wave has two branches with spectra determined by (16). $E_+(\mathbf{k})=0$ when $\gamma_1(\mathbf{k})=1$, and hence represents the acoustic branch while E_- represents the optical branch because it remains finite when $\gamma_1(\mathbf{k})=1$. In general, $E_+(\mathbf{k})\ge 0$ and $E_-(\mathbf{k})\le 0$. The negative energy is understood in the following manner. As elementary excitations, we consider the magnon vacuum as the ground state. Therefore magnons excited out of the filled sea constitute the acoustic branch with energy E_+ and the optical branch with energy E_-.

Since both $\langle S^z\rangle_a$ and $\langle S^z\rangle_b$ depend on temperature, the parameter α is, in general, a function of temperature. Therefore the spin-wave spectra for ferrimagnets, even expressed in the unit of $J\langle S^z\rangle_a$, depend on temperature. This is in contrast to the antiferromagnets for which $\alpha=1$, and the spin-wave spectra of both branches are independent of temperature when expressed in the same unit.

Similarly, we find from (14) the Green's functions for the CsCl structure

$$\begin{bmatrix} g_{aa}(\kappa,E;q) & g_{ab}(\kappa,E;q) \\ g_{ba}(\kappa,E;q) & g_{bb}(\kappa,E;q) \end{bmatrix} = \frac{1}{[E-E_+(\mathbf{k})][E-E_-(\mathbf{k})]} \begin{bmatrix} E+8J\langle S^z\rangle_a & 8J\langle S^z\rangle_a\gamma_2(\mathbf{k})e^{-iqd} \\ -8\alpha J\langle S^z\rangle_a\gamma_2(\mathbf{k})e^{-iqd} & E-8\alpha J\langle S^z\rangle_a \end{bmatrix}, \tag{18}$$

where the spin-wave spectra are given by

$$E_{\pm}(\mathbf{k})=-4J\langle S^z\rangle_a(1-\alpha)\pm 4J\langle S^z\rangle_a[(1+\alpha)^2-4\alpha\gamma_2(\mathbf{k})]^{1/2} \tag{19}$$

and

$$\gamma_2(\mathbf{k})=\cos k_x d\,\cos k_y d\,\cos qd\ .$$

Substituting (15) or (18) in (12) and then back in (5), we find the retarded Green's functions in Wannier representation. For instance,

$$\langle\langle S_{\mathbf{a}}^{+};S_{\mathbf{a}'}^{-}\rangle\rangle=\frac{1}{N_0N_z}\sum_{\kappa}\sum_{q}\frac{2\langle S^z\rangle_a(E+6J\langle S^z\rangle_a)}{[E-E_+(\mathbf{k})][E-E_-(\mathbf{k})]}e^{i\mathbf{k}\cdot(\mathbf{a}-\mathbf{a}')}\ , \tag{20a}$$

$$\langle\langle S_{\mathbf{b}}^{+};S_{\mathbf{b}'}^{-}\rangle\rangle=\frac{1}{N_0N_z}\sum_{\kappa}\sum_{q}\frac{2\langle S^z\rangle_b(E-6\alpha J\langle S^z\rangle_a)}{[E-E_+(\mathbf{k})][E-E_-(\mathbf{k})]}e^{i\mathbf{k}\cdot(\mathbf{b}-\mathbf{b}')}\ . \tag{20b}$$

IV. RESULTS AND DISCUSSIONS

We now attempt to calculate the mean values $\langle S^z\rangle_a$ and $\langle S^z\rangle_b$ from the Green's functions by means of a method that has been used in Refs. 14 and 15. We first introduce the auxiliary functions $\Phi_a(T)$ and $\Phi_b(T)$ defined by

$$\Phi_a(T)=\frac{i}{2\pi N_0N_z}\int_{-\infty}^{\infty}\frac{dE}{e^{\beta E}-1}\sum_{\kappa}\sum_{q}[g_{aa}(\kappa,E+i0^+;q)-g_{aa}(\kappa,E-i0^+;q)]\ , \tag{21a}$$

$$\Phi_b(T)=\frac{i}{2\pi N_0N_z}\int_{-\infty}^{\infty}\frac{dE}{e^{\beta E}-1}\sum_{\kappa}\sum_{q}[g_{bb}(\kappa,E+i0^+;q)-g_{bb}(\kappa,E-i0^+;q)]\ , \tag{21b}$$

where $\beta=1/k_BT$ with the Boltzman constant k_B. The purpose of introducing these auxiliary functions can be made clear from the following example. If $S_a=S_b=\frac{1}{2}$, then we find from (20) with the aid of the fluctuation-dispersion theorem[15,16]

$$\langle S_{\mathbf{a}}^{-}S_{\mathbf{a}}^{+}\rangle=2\langle S^z\rangle_a\Phi_a(T)\ , \tag{22a}$$

$$\langle S_{\mathbf{b}}^{-}S_{\mathbf{b}}^{+}\rangle=2\langle S^z\rangle_b\Phi_b(T)\ . \tag{22b}$$

But since $\langle S_a^-S_a^+\rangle=\frac{1}{2}-\langle S^z\rangle_a$, $\langle S_b^-S_b^+\rangle=\frac{1}{2}-\langle S^z\rangle_b$ for spin $\frac{1}{2}$, we obtain immediately that

$$\langle S^z\rangle_a=\tfrac{1}{2}[1+\Phi_a(T)]^{-1}\ , \tag{23a}$$

$$\langle S^z\rangle_b=\tfrac{1}{2}[1+\Phi_b(T)]^{-1}\ . \tag{23b}$$

For general spin values, it has been shown in Refs. 14 and 15 that

$$\langle S^z\rangle_a=\frac{[S_a-\Phi_a(T)][1+\Phi_a(T)]^{2S_a+1}+[S_a+1+\Phi_a(T)][\Phi_a(T)]^{2S_a+1}}{[1+\Phi_a(T)]^{2S_a+1}-[\Phi_a(T)]^{2S_a+1}}\ , \tag{24a}$$

$$\langle S^z\rangle_b=\frac{[S_b-\Phi_b(T)][1+\Phi_b(T)]^{2S_a+1}+[S_b+1+\Phi_b(T)][\Phi_b(T)]^{2S_b+1}}{[1+\Phi_b(T)]^{2S_b+1}-[\Phi_b(T)]^{2S_b+1}}\ . \tag{24b}$$

However, the function Φ involves the Green's functions which depend upon $\langle S^z\rangle_a$ and α; Eqs. (24) must be solved self-consistently.

For simplicity, we consider the ground state ($T=0$) only. The factor $(e^{\beta E}-1)^{-1}$ is zero for $E>0$ and is -1 for $E<0$. The auxiliary functions for the NaCl structure are then from (21) and (15)

$$\Phi_a(0)=-\int_{-\infty}^{0}\frac{dE}{N_0N_z}\sum_{\mathbf{k}}\frac{\{[E_+(\mathbf{k})+6J\langle S^z\rangle_a]\delta(E-E_+(\mathbf{k}))-[E_-(\mathbf{k})+6J\langle S^z\rangle_a]\delta(E-E_-(\mathbf{k}))\}}{[E_+(\mathbf{k})-E_-(\mathbf{k})]}$$

$$=\frac{1}{N_0N_z}\sum_{\mathbf{k}}\{[E_-(\mathbf{k})+6J\langle S^z\rangle_a]/[E_+(\mathbf{k})-E_-(\mathbf{k})]\ , \tag{25a}$$

$$\Phi_b(0)=-\int_{-\infty}^{0}\frac{dE}{N_0N_z}\sum_{\mathbf{k}}\frac{\{[E_+(\mathbf{k})-6\alpha J\langle S^z\rangle_a]\delta(E-E_+(\mathbf{k}))-[E_-(\mathbf{k})-6\alpha J\langle S^z\rangle_a]\delta(E-E_-(\mathbf{k}))\}}{[E_+(\mathbf{k})-E_-(\mathbf{k})]}$$

$$=\frac{1}{N_0N_z}\sum_{\mathbf{k}}[E_-(\mathbf{k})-6\alpha J\langle S^z\rangle_a]/[E_+(\mathbf{k})-E_-(\mathbf{k})]\ . \tag{25b}$$

TABLE I. Mean spin values of ferrimagnet with NaCl structure at $T=0$. For each set of values of S_a and S_b, we give $\langle S^z\rangle_a$ and, below it, α.

S_a \ S_b	0.5	1.0	1.5	2.0	2.5
0.5	0.433				
	1				
1.0	0.944	0.923			
	0.476	1			
1.5	1.458	1.433	1.422		
	0.316	0.651	1		
2.0	1.967	1.943	1.928	1.922	
	0.238	0.486	0.741	1	
2.5	2.473	2.451	2.436	2.426	2.422
	0.192	0.388	0.589	0.794	1

TABLE II. Mean spin values of ferrimagnet with CsCl structure at $T=0$. For each set of values of S_a and S_b, we give $\langle S^z\rangle_a$ and, below it, α.

S_a \ S_b	0.5	1.0	1.5	2.0	2.5
0.5	0.447				
	1				
1.0	0.958	0.941			
	0.481	1			
1.5	1.468	1.449	1.441		
	0.320	0.655	1		
2.0	1.975	1.957	1.946	1.941	
	0.241	0.489	0.743	1	
2.5	2.479	2.463	2.451	2.444	2.441
	0.194	0.391	0.592	0.796	1

It is observed that terms involving $E_+(\mathbf{k})$ do not contribute to the integral. This reflects the fact that all the negative energy states are filled in the ground state of the system.

Using the explicit expressions (16) and (17), we can solve the coupled equations (25) for $\langle S^z\rangle_a$ and α at $T=0$ with given single-particle spins S_a and S_b. We have made the calculation on a computer for several choices of S_a and S_b. Our results are posted in Table I. Numbers in the first line for each S_a are $\langle S^z\rangle_a$ and in the second line are α. We have computed $S_a \geq S_b$ cases, but results for $S_a < S_b$ can be derived by interchanging the sublattices. It is noted that the special case $S_a = S_b$ or $\alpha = 1$ corresponds to the two-sublattice antiferromagnet. Our results for $\alpha = 1$ agree completely with those given in Refs. 12 and 17. We note further that the computed mean spin values for all cases are smaller than the single-particle spin in contrast with ferromagnets. It is now well known that at $T=0$, the mean spin value in a ferromagnet is the same as the spin quantum number.[16] On the other hand, it has been pointed out[12,17] that $\langle S^z\rangle_a \neq S_a$ in antiferromagnets because of the zero-point vibration of the magnon. In the present case of ferrimagnetism, as we have explained previously, the ground state $T=0$ has all the negative energy states filled by magnons. It is this many-body effect that results in $\langle S^z\rangle_a \neq S_a$.

The above calculation applies as well to the CsCl structure except for the replacement of the coordination number 6 by 8 in (25). We present the results in Table II. Once more we find that when $\alpha = 1$, our calculation yields the same result as those for antiferromagnets obtained in Refs. 12 and 17.

We have discussed the bulk properties of two-sublattice ferrimagnets by means of the Green's-function matrix method. Explicit expressions of the Green's functions are calculated by solving the coupled equations in matrix form. The mean spin values over individual sublattices are calculated self-consistently. The method introduced here can be applied to treat the surface spin waves of ferrimagnets of either the NaCl or CsCl structure.[22] It can also be generalized without difficulty to treat the multisublattice ferrimagnets as well as interface problems. The major advantage is that the resulting equation of motion is formally the same as that of a single-lattice ferromagnet. Since the CsCl structure is a structure of alternating layers of a and b ions, it may be regarded as the simplest superlattice. Therefore our method should be useful in the treatment of magnetic superlattices with or without surface.

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