Magnetization direction of a semi-infinite heisenberg ferromagnet with perpendicular surface anisotropy(2)

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Magnetization Direction of a Semi-infinite Heisenberg Ferromagnet with Perpendicular Surface Anisotropy II

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Abstract

The surface phase transition of a semi-infinite Heisenberg ferromagnet with perpendicular surface anisotropy is studied by the equation of motion method in the limit of low temperature and weak anisotropy. The expression for the critical surface anisotropy giving the boundary between in-plane ordering and canted-spin states is found from the instability of the surface mode.

§ 1. Introduction

In the recent experiments [1] - [4] , domonant perpendicular anisotropy has been found at the surfaces of magnetic films and semi-infinite magnets, or at the interfaces of multilayers, and the spin reorientation phenomena caused by the temperature or the external field have been investigated extensively. In general, the preferred direction of magnetization in such geometries is parallel to the surface because of a shape anisotropy. The surfaces or interfaces, however, can have perpendicular anisotropy in consequence of the reduced symmetry [5] , so that there occurs an interplay of the perpendicular anisotropy and the shape anisotropy. Theoretical investigations taking into account such an interplay have been performed for magnetic films

[6] and semi-infinite magnets [7] - [9] in the low-temperature region. For ultrathin films and no external field the direction of spins is found to be strictly perpendicular to the surface, whereas it lies strictly in-plane for thicker films. For semi-infinite magnets, which may be considered as films with infinite thickness, the ground-state spin orientation is found to be either in-plane or canted depending on the strength of the surface anisotropy.

In a previous paper [9] (hereafter referred to as I) we have determined the phase diagram of a semi-infinite Heisenberg ferromagnet having perpendicular anisotropy of the form $-D_s(S^z)^2$ ($D_s>0$) in the surface and easy-plane anisotropy of the form $-D_b(S^z)^2$ ($D_b<0$) in the bulk by using the conventional molecular-field method. It was shown that, in the temperature T vs. D_s plane, the phase below the bulk transition temperature T_c^b consists of two distinct ordered phases, i.e., in-plane ordering and canted-spin phases, while there exists a perpendicular ordering phase above T_c^b when the surface anisotropy D_s is larger than a certain critical value.

At the surface of an ordered state there may be localized surface excitaions in addition to the bulk spin waves. The surface excitaions in an exchange-coupled ferromagnet has been studied by De Wames and Walfram [10] , and their study has been extended by Gopalan and Cottam [11] to include single-ion anisotropy. The surface mode of one ordered state would become unstable at the boundary between other phases, if there exist several ordered states in a phase diagram. Therefore, instead of calculating the free energy, the phase boundary between two distinct phases can also be determined from the instability of the surface mode.

In this paper we deal with the same model as that studied in I, but confine ourselves to the case with weak single-ion anisotropy and zero temperature. The system then undergoes a second-order phase transition between in-plane ordering and canted-spin states. We first obtain surface excitaions in the in-plane ordering state by the equation of motion method, and then discuss the relation between the instability of the surface mode and the phase transitions.

§ 2. Equation of Motion

The model studied in I is an exchange-coupled spin-1 semi-infinite ferromagnet

with perpendicular surface anisotropy of single-ion type. The lattice structure is assumed to be simple cubic, and the xy plane is taken to lie in the surface layer and the z axis is taken normal to this surface. The Hamiltonian is

$$H=-J\sum_{\langle lj,l'j'\rangle}\mathbf{S}_{lj}\cdot\mathbf{S}_{l'j'}-\sum_{lj}D_l(S^z_{lj})^2, \tag{1}$$

where J denotes the nearest-neighbor ferromagnetic exchange constant (hereafter we shall use units of J), and l the layer index; $l=1$ is the surface layer, $l=2,3,\cdots$the inner layers, and j denotes lattice points in xy plane. The perpendicular surface anisotropy is represented by taking $D_1(\equiv D_s)$ to be positive, while we take $D_l(\equiv D_b)$ to be negative for the bulk. The bulk spins, therefore, tend to lie in xy plane, while the surface spins orient preferentially to the z direction.

For zero temperature the system described by the Hamiltonian (1) is in an in-plane ordering state if D_s is smaller than a certain critical value D_{s1}^c [9] . In this section we ask for the equation of motion of spins in this state. Since the direction of spins in the in-plane ordering state lies in xy plane, it is convenient to rotate the coordinate axes by angle $\pi/2$ about y axis such that the yz plane is parallel and the x axis is mormal to the surface. The Hamiltonian (1) may then be re-expressed as

$$H=-J\sum_{\langle lj,l'j'\rangle}\mathbf{S}_{lj}\cdot\mathbf{S}_{l'j'}-\sum_{lj}D_l(S^x_{lj})^2. \tag{2}$$

The quantization axis is then taken to be the z axis which lies parallel to the surface layer, and the corresponding averages of spins can be expressed as $<S^z_{lj}>(\equiv\tau_l)$. For ferromagnets of easy-axis type at absolute zero the value of τ_l is equal to its saturated value S. In our system, however, the bulk τ_l is not fully saturated even at absolute zero due to the easy-plane single-ion anisotropy D_b [12] . However, if we confine ourselves to the system with weak single-ion anisotropy, the approximation of τ_l by its saturated value S is found to be valid(see Appendix A).

The equation of motion for the operator $S^+_{lj}(\equiv S^x_{lj}+iS^y_{lj})$ in units of $\hbar$ is given by

$$i\frac{d}{dt}S^+_{lj}(t)=[S^+_{lj}(t),H]\ , \tag{3}$$

where $S^+_{lj}(t)$ is the Heisenberg representation of the operator S^+_{lj} and [,] means the comutator. The right hand side of Eq.(3) consists of a sum of the products of two

spin operators. Under the random-phase approximation the time derivative of $S^{+}_{lj}(t)$ couples to three types of spin operators; S^{+}, $S^{z}S^{+}+S^{+}S^{z}$, and $S^{z}S^{-}+S^{-}S^{z}$, where $S^{-}(\equiv S^{x}-iS^{y})$. The combination with the latter two are caused by the single-ion part in Eq. (2), and they can be replaced by a single operator as follows if we restrict in the subspace spanned by the lowest two states $|S>$ and $|S-1>$;

$$\begin{cases} S^{z}S^{+}+S^{+}S^{z}\rightarrow(2S-1)S^{+}, \\ S^{z}S^{-}+S^{-}S^{z}\rightarrow(2S-1)S^{-}. \end{cases} \tag{4}$$

These replacements are valid only in the limit of low temperature and small anisotropy [13]. The time derivative of $S^{+}_{lj}(t)$then couples only to S^{+} and S^{-}, hence we ask for the equation of motion for $S^{-}_{lj}(t)$, which is the Hermitian adjoint of Eq.(3).

Introducing the Fourier transform of $S^{+}_{lj}(t)$ and $S^{-}_{lj}(t)$ with respect to time,

$$S^{\pm}_{lj}(t)=\int_{-\infty}^{\infty}e^{-i\omega t}S^{\pm}_{lj}(\omega)\,d\omega, \tag{5}$$

and then the two-dimensional Fourier transform utilizing the invariance under the translation parallel to the surface,

$$S^{\pm}_{lj}(\omega)=\frac{1}{\sqrt{N_{\parallel}}}\sum_{k_{\parallel}}e^{ik_{\parallel}\cdot j}S^{\pm}_{l}(k_{\parallel},\omega), \tag{6}$$

where $N_{\parallel}$ is the number of atoms in a layer parallel to the surface and $k_{\parallel}=(k_y,k_z)$, we have the coupled equation of motion for S^{+} and S^{-},

$$\begin{cases} (\omega-a_l)S^{+}_{l}+S^{+}_{l-1}+S^{+}_{l+1}+c_lS^{-}_{l}=0 \\ (-\omega-a_l)S^{-}_{l}+S^{-}_{l-1}+S^{-}_{l+1}+c_lS^{+}_{l}=0, \end{cases} \tag{7}$$

where

$$\begin{cases} a_1=5-\frac{1}{2}D_s-4\gamma_{k_{\parallel}}\equiv a_s \\ c_1=\frac{1}{2}D_s\equiv c_s \\ a_l=6-\frac{1}{2}D_b-4\gamma_{k_{\parallel}}\equiv a_b \\ c_l=\frac{1}{2}D_b\equiv c_b, \qquad l=2,3,\cdots \end{cases} \tag{8}$$

with $\gamma_{k_{\parallel}}=(\cos k_y+\cos k_z)/2$, and S^{+}_{0} and S^{-}_{0} vanish due to the boundary condition at the surface. We have written $S^{\pm}_{l}(k_{\parallel},\omega)$ as $S^{\pm}_{l}$ for brevity. The coupled equation (7)

can be rewritten more compactly as

$$\begin{cases} (\omega \mathbf{I}-\mathbf{A})\mathbf{S}^{+}=\mathbf{C}\mathbf{S}^{-} \\ (-\omega \mathbf{I}-\mathbf{A})\mathbf{S}^{-}=\mathbf{C}\mathbf{S}^{+}, \end{cases} \tag{9}$$

where $\mathbf{I}$ denotes the unit matrix, and $\mathbf{A}$ is an $\infty\times\infty$ tri-diagonal matrix having diagonal elements a_s, a_b, $\cdots$ and sub-diagonal elements -1, and $\mathbf{C}$ is an $\infty\times\infty$ diagonal matrix with elements $-c_s, -c_b, \cdots$ and $\mathbf{S}^{+}$ and $\mathbf{S}^{-}$ are respectively infinite column matrices with elements S_l^{+} and S_l^{-} $(l=1,2,\cdots)$.

§ 3. Critical Surface Anisotropy D_{s1}^{c}

From the equation (9) we can determine the critical surface anisotropy D_{s1}^{c} over which spin canting appears near the surface. Setting $k_{\parallel}=0$ in Eq.(8) and $\omega=0$ in Eq. (9), we have two conditions;

$$\det(\mathbf{A}+\mathbf{C})=0, \tag{10}$$

and

$$\det(\mathbf{A}-\mathbf{C})=0. \tag{11}$$

The explicit form of Eq.(10) is

$$\begin{vmatrix} c_s-a_s & 1 & & & \\ 1 & c_b-a_b & 1 & & \\ & 1 & c_b-a_b & 1 & \\ & & & \ddots & \ddots \end{vmatrix} =0 \tag{12}$$

The properties of the determinant of this form, which appears frequently in the study of surface problem, has been discussed in detail by Selzer and Majlis [14]. Following them, if we call the above determinant as D_N, and D_{N-p} as the determinant obtained from D_N by deleting the first p rows and columns, we get recurrence relations,

$$\begin{cases} D_N=(c_s-a_s)D_{N-1}-D_{N-2} \\ D_{N-p}=(c_b-a_b)D_{N-p-1}-D_{N-p-2}, \qquad \text{for } p\geq 1. \end{cases} \tag{13}$$

The second relations in Eq.(13) yields

$$\frac{D_{N-p-1}}{D_{N-p}}=\frac{1}{c_b-a_b-\dfrac{D_{N-p-2}}{D_{N-p-1}}}. \tag{14}$$

Defining the ratio in the limit $N\to\infty$ as

$$\epsilon=\lim_{N\to\infty}\frac{D_{N-p-1}}{D_{N-p}}, \tag{15}$$

we have from Eq.(14),

$$\epsilon=\frac{1}{c_b-a_b-\epsilon}. \tag{16}$$

On the other hand, by setting $D_N=0$ and taking the limit $N\to\infty$ in the first relation in Eq.(13), we have $\epsilon=c_s-a_s$. By substituting this into Eq.(16) and solving for D_s, we get the critical surface anisotropy

$$D_{s1}^{c}=\frac{1}{2}\{\sqrt{D_b(D_b-4)}+D_b\}. \tag{17}$$

As shown in Appendix A, the same expression can be derived from the molecular-field approach in I in the limit of small $|D|$. In a similar way as above we find that Eq. (11) is identically satisfied, which implies that in our system an uniform rotation of spins in a plane parallel to the surface shows no energy gap.

§ 4. Surface Mode

In this section we calculate surface excitations in the in-plane ordering state following Gopalan and Cottam [11]. Solving Eq.(9) simultaneously, we obtain

$$[(-\omega\mathbf{I}-\mathbf{A})\mathbf{C}^{-1}(\omega\mathbf{I}-\mathbf{A})-\mathbf{C}]\,\mathbf{S}^{+}=0, \tag{18}$$

and

$$[(\omega\mathbf{I}-\mathbf{A})\mathbf{C}^{-1}(-\omega\mathbf{I}-\mathbf{A})-\mathbf{C}]\ \mathbf{S}^{-}=0. \tag{19}$$

Since Eq.(19) is the same as Eq.(18) by changing the sign of ω, we use Eq.(18) in the following. If we define $\mathbf{A}_0$ as the tri-diagonal matrix having diagonal elements a_b and sub-diagonal elements -1, and decompose $\mathbf{A}$ into $\mathbf{A}_0$ and $\mathbf{V}$, $\mathbf{V}\equiv\mathbf{A}-\mathbf{A}_0$, Eq.(18) can be rewritten as

$$[(-\omega\mathbf{I}-\mathbf{A}_0)\mathbf{C}^{-}(\omega\mathbf{I}-\mathbf{A}_0)-\mathbf{V}\mathbf{C}^{-1}(\omega\mathbf{I}-\mathbf{A}_0)-(-\omega\mathbf{I}-\mathbf{A}_0)\mathbf{C}^{-1}\mathbf{V}+\mathbf{V}\mathbf{C}^{-1}\mathbf{V}-\mathbf{C}]\ \mathbf{S}^{+}=0. \tag{20}$$

Furthere introducing the tri-diagonal matrices $\mathbf{A}_1$ and $\mathbf{A}_2$ defined as $\mathbf{A}_0$ but with diagonal elements $a_b+\sqrt{\omega^2+c_b^2}$ and $a_b-\sqrt{\omega^2+c_b^2}$, respectively, we can simplify Eq. (20) to

$$(\mathbf{A}_1\mathbf{A}_2+\mathbf{U})\mathbf{S}^{+}=0, \tag{21}$$

or equivalently

$$(\mathbf{I}+\mathbf{A}_2^{-1}\mathbf{A}_1^{-1}\mathbf{U})\mathbf{S}^{+}=0, \tag{22}$$

where $\mathbf{U}$ is an $\infty\times\infty$ matrix with only the first 2×2 nonzero elements, U_{11}, U_{12}, U_{21}, and U_{22}. The surface mode can be obtained by requiring the determinant of Eq.(22) to vanish,

$$\det(\mathbf{I}+\mathbf{A}_2^{-1}\mathbf{A}_1^{-1}\mathbf{U})=0. \tag{23}$$

Since the matrix elements of inverse of $\mathbf{A}_1$ and $\mathbf{A}_2$ are constructed [10,11] by introducing the complex variables x_1 and x_2 defined by

$$\begin{cases} x_1+x_1^{-1}=a_b+\sqrt{\omega^2+c_b^2} \\ x_2+x_2^{-1}=a_b-\sqrt{\omega^2+c_b^2}, \end{cases} \tag{24}$$

we can reduce Eq.(23) to a simple algebraic equation for unknowns x_1 and x_2.

The bulk spin-wave corresponds to $|x_1|=|x_2|=1$, or equivalently x_1 or x_2 equals $\exp(ik_x)$, and is given by

$$\omega_b=\sqrt{6(1-\gamma_k)\ \{6(1-\gamma_k)-D_b\}} \tag{25}$$

with $\gamma_k=(\cos k_x+\cos k_y+\cos k_z)/3$, whereas the localized surface mode requiring

$|x_1|<1$ and $|x_2|<1$ is given by

$$\omega_s=\sqrt{\{(x_a+\frac{1}{x_a})-a_b\}^2-c_b^2}, \tag{26}$$

where $\alpha=1$ or 2. In Appendix B, we develop the equation of motion method valid for any magnitude of the single-ion anisotropy and show that the bulk spectrum (25) corresponds to the limiting case of small $|D_b|$ of the bulk spectrum obtained there. The complex variables x_1 and x_2 are the roots of the quadratic equation

$$x^2-\frac{2\,a_b y}{1+y}x+y=0, \tag{27}$$

where $y(\equiv x_1x_2)$ is a root of the cubic equation

$$\{c_b^2(1-\nu)^2-\delta^2\}y^3+\{2\,c_b^2(1-\nu)-2\,a_b\delta-1\}y^2+\{2\,a_b\delta+\delta^2+c_b^2(1-\nu^2)\}y+1=0, \tag{28}$$

where $\nu=D_s/D_b$ and $\delta=(D_b-D_s)/2-1$.

The surface spectra are illustrated in Fig.1 for $D_b=-1$ and for $D_s=0.1, 0.6, 1.0$, and 2.0. The shaded area in the figure represents the bulk spectrum according to Eq. (25). We find a single surface mode below the bulk spectrum, but it vanishes at the finite value of $k_\parallel$ if the surface anisotropy exceeds the critical value $D_{s1}^c=0.618$.

The expression for the critical value D_{s1}^c as a function of D_b is obtained by setting $k_\parallel=0$ in the above equations. Then, Eq.(28) reduces to

$$(D_b-D_s-1)y^3+(D_b^2-D_bD_s-3\,D_b+2\,D_s+3)y^2+(2\,D_b-D_s-3)y+1=0, \tag{29}$$

which yields three distinct roots,

$$\begin{cases} y^{\pm}=1-\dfrac{1}{2}\{D_b\pm\sqrt{D_b(D_b-4)}\} \\ y_s=\dfrac{1}{D_s-D_b+1} \end{cases} \tag{30}$$

Among them y^- is unphysical because $|x_a|>1$, and y^+ leads to the uniformly rotating mode in a plane as discussed in § 3. The solution y_s can lead to the instability of the surface mode at $k_\parallel=0$ because it is dependent on D_s, and substituting into Eqs.(27) and (26), we find

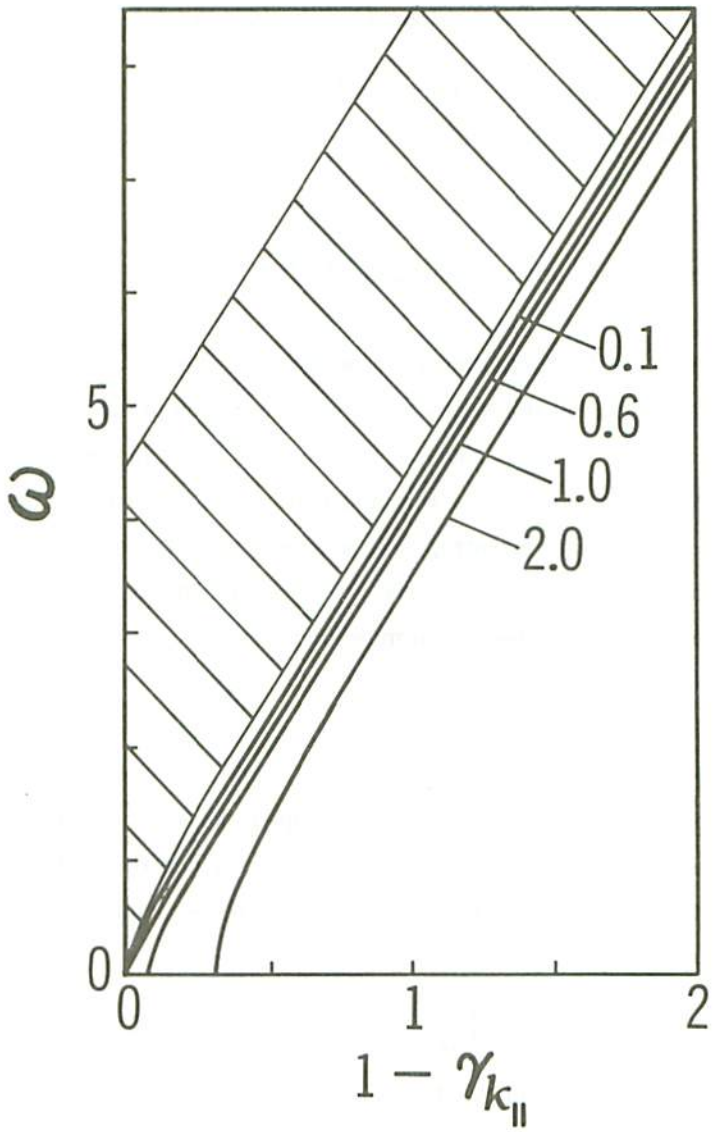

Fig. 1
Illustration of the localized surface modes for $D_b=-1$ and $D_s=0.1, 0.6, 1.0$, and 2.0. The shaded area represents the bulk spin-wave spectrum. The critical anisotropy D_{s1}^{c} is 0.618.

$$\omega_s(k_{\parallel}=0)=\frac{|\,D_s^2-D_bD_s+D_b\,|}{(D_s-D_b+2)\sqrt{D_s-D_b+1}}\,i \tag{31}$$

for $D_s \geq D_{s1}^c$(The case $D_s<D_{s1}^c$is unphysical because $|\,x_\alpha\,|>1$). Therefore, the surface mode with $k_{\parallel}=0$ vanishes at

$$D_{s1}^c=\frac{1}{2}\{\sqrt{D_b(D_b-4)}+D_b\}\ , \tag{32}$$

which coinsides with the critical value given by Eq.(17) in § 3, but it becomes imaginary if $D_s>D_{s1}^c$.

In conclusion, we have examined the behavior of the surface excitations in the system with perpendicular anisotropy by using the equation of motion method. At low temperatures and for weak anisotropy, we have obtained, in the in-plane ordering state, a single surface mode below the bulk continuum. The surface mode becomes imaginary when the surface anisotropy exceeds the critical value given by Eq.(32), so that a new ordered state will appear. These results are consistent with those obtained in I, where we have used conventional molecular-field theory.

Appendix A

In the molecular-field approximation developed in I, the analytic form to determine the phase boundary between the in-plane ordering and the canted-spin states is given by a set of homogeneous equations in μ_l, μ_l the perpendicular components of spins,

$$\mu_l+2\left[\frac{K_l^2}{X_l}\left\{\frac{P_{l3}^0}{(\lambda_{l3}^0)^2}-\frac{P_{l1}^0}{(\lambda_{l1}^0)^2}\right\}+\frac{D_l}{K_l^2}P_{l2}^0\right]E_l=0, \tag{A.1}$$

where $K_l=4\,\tau_l+\tau_{l-1}+\tau_{l+1}$ and $E_l=4\,\mu_l+\mu_{l-1}+\mu_{l+1}$, and

$$P^0{}_{li}=\frac{\exp(-\beta\lambda^0{}_{li})}{\sum_{j=1}^{3}\exp(-\beta\lambda_{lj}^0)}, \qquad i=1,2,3, \tag{A.2}$$

with $\lambda_{l1}^0=\frac{1}{2}(D_l-X_l)$, $\lambda_{l2}^0=0$, $\lambda_{l3}^0=\frac{1}{2}(D_l+X_l)$, and $X_l=\sqrt{D_l^2+4K_l^2}$. In-plane components of spins τ_l are given by

$$\tau_l = \frac{4\,K_l \sinh(\frac{\beta X_l}{2})}{X_l\,\{2\cosh(\frac{\beta X_l}{2}) + \exp(\frac{\beta D_l}{2})\}}\,. \tag{A.3}$$

If we expand these expressions in powers of $|\,D_l\,|$ retaining the lowest order, we have at $T=0(\beta\to\infty)$

$$\tau_l = (1+\frac{D_l^2}{8\,K_l^2})^{-1} \approx 1 \tag{A.4}$$

from Eq.(A.3), and

$$(4-K_l+D_l)\mu_l + \mu_{l-1} + \mu_{l+1} = 0 \tag{A.5}$$

from Eq.(A.1). The martix form of Eq.(A.5) coincides with Eq.(12) in § 3.

Appendix B

In order to check the decoupling approximation given in § 3 for $S^zS^+ + S^+S^z(\equiv \tilde{S}^+)$ and $S^zS^- + S^-S^z(\equiv \tilde{S}^-)$, in this appendix we start from the equations of motions without decoupling. The equaton of motion for S_l^+ is given by

$$\omega S_l^+ = (K_l - 4\,\tau_l\gamma_{k_\parallel})\,S_l^+ - \tau_l S_{l-1}^+ - \tau_l S_{l+1}^+ - \frac{1}{2}D_l\tilde{S}_l^+ - \frac{1}{2}D_l\tilde{S}_l^-, \tag{B.1}$$

thus couples to $\tilde{S}^+$ and $\tilde{S}^-$. The equation of motion for $\tilde{S}^+$ is given by

$$\omega\,\tilde{S}_l^+ = (K_l\tilde{S}_l^+ - (4\,Z_l\gamma_{k_\parallel} + \frac{1}{2}D_l)S_l^+ - Z_lS_{l-1}^+ - Z_lS_{l+1}^+ - \frac{1}{2}D_lS_l^-, \tag{B.2}$$

where $Z_l \equiv 3<(S_{lj}^z)^2> -2$. Therefore, we need to calculate the equations of motions for S^- and $\tilde{S}^-$, which are the Hermitian adjoint of Eqs.(B.1) and (B.2), respectively.

At $T=0(\beta\to\infty)$, and small $|\,D_l\,|$, we can approximate $\tau_l \approx 1$ and $Z_l \approx 1$. We here consider the bulk spin-wave spectrum. Taking the Fourier transform with respect to l, we have a seqular equation to determine the bulk spin-wave spectrum,

$$\begin{pmatrix} \omega-a & 0 & \frac{1}{2}D_b & \frac{1}{2}D_b \\ 0 & -\omega-a & \frac{1}{2}D_b & \frac{1}{2}D_b \\ b & -\frac{1}{2}D_b & \omega-6 & 0 \\ -\frac{1}{2}D_b & b & 0 & -\omega-6 \end{pmatrix} \begin{pmatrix} S_k^+ \\ S_k^- \\ \tilde{S}_k^+ \\ \tilde{S}_k^- \end{pmatrix} = 0, \qquad (B.3)$$

where $a=6(1-\gamma_k)$ and $b=6\gamma_k+D_b/2$ with $\gamma_k=(\cos k_x+\cos k_y+\cos k_z)/3$. By equating the coefficient matrix in Eq.(B.3) to zero, and retaining the lowest order in $|D_l|$, we can derive the same bulk spin-wave spectrum as shown in Eq.(25) in § 4.

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