$1/S$ expansion for thermodynamic quantities in a two-dimensional Heisenberg antiferromagnet at zero temperature

Jun-ichi Igarashi
Department of Physics, Faculty of Science, Osaka University, Toyonaka, Osaka 560, Japan
(Received 23 January 1992)

We calculate the spin-wave dispersion, the perpendicular susceptibility, the spin-stiffness constant, and the sublattice magnetization of a two-dimensional Heisenberg antiferromagnet at $T=0$, to order $1/(2S)^2$, treating carefully the umklapp processes. Our numerical estimates for the thermodynamic quantities are in good agreement with series-expansion estimates, and satisfy the hydrodynamic relation very accurately.

I. INTRODUCTION

A great deal of theoretical interest in the physics of quantum antiferromagnets has been raised after the discovery of high-temperature superconductors (HTSC), since the undoped mother materials like La_2CuO_4 are described by a square-lattice spin-$\frac{1}{2}$ antiferromagnetic Heisenberg Hamiltonian,

$$H=J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j\ , \tag{1.1}$$

where $\langle i,j\rangle$ indicates a sum over pairs of nearest neighbors. The quantum fluctuation is expected to be large due to the smallness of the spin $S=\frac{1}{2}$ and the low dimension $D=2$. At the beginning of the discovery of HTSC, there was a controversy whether large quantum fluctuation destroys the antiferromagnetic long-range order or not, but it is now widely accepted that the Heisenberg antiferromagnetic exhibits the Néel long-range order at $T=0$ even for $S=\frac{1}{2}$ in square lattice.[1-3]

The presence of the Néel long-range order suggests that the spin-wave expansion ($1/S$ expansion) makes sense. Actually many authors, evaluating several thermodynamic quantities by various methods such as series expansion,[4] Monte Carlo[5-8] and others,[9-13] have reported that the linear spin-wave (LSW) theory,[14,15] leading order of the $1/S$ expansion, gives good results. This fact indicates that higher-order terms are small. Recently Igarashi and Watabe (IW)[16] have made the $1/S$ expansion on the basis of the Holstein-Primakoff (HP) formalism,[17] and have reported the small corrections of order $1/(2S)^2$ for the spin-wave velocity c, the perpendicular susceptibility $\chi_\perp$, the spin-stiffness constant ρ_s, and the sublattice magnetization M. Also Castilla and Chakravarty (CC)[18] have reported a very small values of order $1/(2S)^2$ for the sublattice magnetization on the basis of the Dyson-Maleev formalism.

In the higher-order terms, the umklapp processes may have important contributions, but these processes were not correctly taken into account by IW. Treating carefully the umklapp processes, we develop IW's idea to calculate thermodynamic quantities in the $1/S$ expansion. We find that the values of order $1/(2S)^2$ for c, $\chi_\perp$, ρ_s, and M are improved from IW's, in good agreement with series-expansion estimates.[4] It is also found that our values are satisfying the hydrodynamic relation, $c=(\rho_s/\chi_\perp)^{1/2}$, within a very small numerical error, indicating that our estimates are quite accurate.

In Sec. II we express the Hamiltonian in a symmetric parametrization. We calculate the spin-wave dispersion in Sec. III, the perpendicular susceptibility in Sec. IV, the spin-stiffness constant in Sec. V, and the sublattice magnetization in Sec. VI. Section VII is devoted to the concluding remarks.

II. HAMILTONIAN

We express the spin operators in terms of boson annihilation operators a_i and b_j (and their Hermite conjugates) using the HP transformation:

$$S_i^z=S-a_i^\dagger a_i\ , \tag{2.1}$$

$$S_i^+=(S_i^-)^\dagger=\sqrt{2S}f_i(S)a_i\ , \tag{2.2}$$

$$S_j^z=-S+b_j^\dagger b_j\ , \tag{2.3}$$

$$S_j^+=(S_j^-)^\dagger=\sqrt{2S}b_j^\dagger f_j(S)\ , \tag{2.4}$$

with

$$f_l(S)=\left[1-\frac{n_l}{2S}\right]^{1/2}=1-\frac{1}{2}\frac{n_l}{2S}-\frac{1}{8}\left[\frac{n_l}{2S}\right]^2+\cdots\ , \tag{2.5}$$

where the indices i and j refer to sites on the a ("up") and b ("down") sublattices, respectively, and $n_l=a_l^\dagger a_l$ or $b_l^\dagger b_l$. We will consider in the following a square lattice. The Fourier transforms of the boson operators are defined by

$$a_i=\left[\frac{2}{N}\right]^{1/2}\sum_{\mathbf{k}}a_{\mathbf{k}}\exp(i\mathbf{k}\mathbf{r}_i)\ ,\qquad b_j=\left[\frac{2}{N}\right]^{1/2}\sum_{\mathbf{k}}b_{\mathbf{k}}\exp(i\mathbf{k}\mathbf{r}_j)\ , \tag{2.6}$$

where the momentum $\mathbf{k}$ is defined in the first Brillouin zone (BZ), that is, $-\pi<k_x\le\pi$, $-\pi<k_y\le\pi$ in units of

$1/(\sqrt{2}a)$ with a being the nearest-neighbor distance. Substituting Eqs. (2.1)–(2.6) into Eq. (1.1), and performing the Bogoliubov transformation,

$$a_{\mathbf{k}}^{\dagger}=l_{\mathbf{k}}\alpha_{\mathbf{k}}^{\dagger}+m_{\mathbf{k}}\beta_{-\mathbf{k}} , \tag{2.7}$$

$$b_{-\mathbf{k}}=m_{\mathbf{k}}\alpha_{\mathbf{k}}^{\dagger}+l_{\mathbf{k}}\beta_{-\mathbf{k}} , \tag{2.8}$$

with

$$l_{\mathbf{k}}=\left[\frac{1+\epsilon_{\mathbf{k}}}{2\epsilon_{\mathbf{k}}}\right]^{1/2} ,m_{k}=-\left[\frac{1-\epsilon_{\mathbf{k}}}{2\epsilon_{\mathbf{k}}}\right]^{1/2}\equiv -x_{\mathbf{k}}l_{\mathbf{k}} , \tag{2.9}$$

$$\epsilon_{\mathbf{k}}=(1-\gamma_{\mathbf{k}}^{2})^{1/2} , \quad \gamma_{\mathbf{k}}=\cos(k_x/2)\cos(k_y/2) , \tag{2.10}$$

we find

$$H=H_0+H_1+H_2+\cdots , \tag{2.11}$$

$$H_0=JSz\sum_{\mathbf{k}}(\epsilon_{\mathbf{k}}-1)+JSz\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}(\alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}}+\beta_{\mathbf{k}}^{\dagger}\beta_{\mathbf{k}}) , \tag{2.12}$$

$$\begin{aligned} H_1=\frac{JSz}{2S}A\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}(\alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}}+\beta_{\mathbf{k}}^{\dagger}\beta_{\mathbf{k}}) &+\frac{-JSz}{2SN}\sum_{1234}\delta_G(1+2-3-4)l_1l_2l_3l_4 \\ &\times[\alpha_1^{\dagger}\alpha_2^{\dagger}\alpha_3\alpha_4B_{1234}^{(1)}+\beta_{-3}^{\dagger}\beta_{-4}^{\dagger}\beta_{-1}\beta_{-2}B_{1234}^{(2)}+4\alpha_1^{\dagger}\beta_{-4}^{\dagger}\beta_{-2}\alpha_3B_{1234}^{(3)} \\ &+(2\alpha_1^{\dagger}\beta_{-2}\alpha_3\alpha_4B_{1234}^{(4)}+2\beta_{-4}^{\dagger}\beta_{-1}\beta_{-2}\alpha_3B_{1234}^{(5)}+\alpha_1^{\dagger}\alpha_2^{\dagger}\beta_{-3}^{\dagger}\beta_{-4}^{\dagger}B_{1234}^{(6)}+\text{H.c.})] , \end{aligned} \tag{2.13}$$

$$H_2=\frac{JSz}{(2S)^2}\sum_{\mathbf{k}}C_1(\mathbf{k})(\alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}}+\beta_{\mathbf{k}}^{\dagger}\beta_{\mathbf{k}})+C_2(\mathbf{k})(\alpha_{\mathbf{k}}^{\dagger}\beta_{\mathbf{k}}^{\dagger}+\beta_{-\mathbf{k}}\alpha_{\mathbf{k}})+\cdots , \tag{2.14}$$

where

$$A=\frac{2}{N}\sum_{\mathbf{k}}(1-\epsilon_{\mathbf{k}})=0.1579 , \tag{2.15}$$

$$\begin{aligned} B_{1234}^{(1)}=&\gamma_{1-4}x_1x_4+\gamma_{1-3}x_1x_3+\gamma_{2-4}x_2x_4+\gamma_{2-3}x_2x_3 \\ &-\tfrac{1}{2}(\gamma_1x_1+\gamma_2x_2+\gamma_3x_3+\gamma_4x_4+\gamma_{2-3-4}x_2x_3x_4+\gamma_{1-3-4}x_1x_3x_4+\gamma_{4-2-1}x_1x_2x_4+\gamma_{3-2-1}x_1x_2x_3) , \end{aligned} \tag{2.16}$$

$$\begin{aligned} B_{1234}^{(2)}=&\gamma_{2-4}x_1x_3+\gamma_{1-4}x_2x_3+\gamma_{2-3}x_1x_4+\gamma_{1-3}x_2x_4 \\ &-\tfrac{1}{2}(\gamma_2x_1x_3x_4+\gamma_1x_2x_3x_4+\gamma_4x_1x_2x_3+\gamma_3x_1x_2x_4+\gamma_{2-3-4}x_1+\gamma_{1-3-4}x_2+\gamma_{4-2-1}x_3+\gamma_{3-2-1}x_4) , \end{aligned} \tag{2.17}$$

$$\begin{aligned} B_{1234}^{(3)}=&\gamma_{2-4}+\gamma_{1-3}x_1x_2x_3x_4+\gamma_{1-4}x_1x_2+\gamma_{2-3}x_3x_4 \\ &-\tfrac{1}{2}(\gamma_2x_4+\gamma_1x_1x_2x_4+\gamma_{2-3-4}x_3+\gamma_{1-3-4}x_1x_2x_3+\gamma_4x_2+\gamma_3x_2x_3x_4+\gamma_{4-2-1}x_1+\gamma_{3-2-1}x_1x_3x_4) , \end{aligned} \tag{2.18}$$

$$\begin{aligned} B_{1234}^{(4)}=&-\gamma_{2-4}x_4-\gamma_{1-4}x_1x_2x_4-\gamma_{2-3}x_3-\gamma_{1-3}x_1x_2x_3 \\ &+\tfrac{1}{2}(\gamma_2+\gamma_1x_1x_2+\gamma_3x_2x_3+\gamma_4x_2x_4+\gamma_{2-3-4}x_3x_4+\gamma_{1-3-4}x_1x_2x_3x_4+\gamma_{3-2-1}x_1x_3+\gamma_{4-2-1}x_1x_4) , \end{aligned} \tag{2.19}$$

$$\begin{aligned} B_{1234}^{(5)}=&-\gamma_{2-4}x_1-\gamma_{2-3}x_1x_3x_4-\gamma_{1-4}x_2-\gamma_{1-3}x_2x_3x_4 \\ &+\tfrac{1}{2}(\gamma_2x_1x_4+\gamma_1x_2x_4+\gamma_4x_1x_2+\gamma_3x_1x_2x_3x_4+\gamma_{2-3-4}x_1x_3+\gamma_{1-3-4}x_2x_3+\gamma_{4-2-1}+\gamma_{3-2-1}x_3x_4) , \end{aligned} \tag{2.20}$$

$$\begin{aligned} B_{1234}^{(6)}=&\gamma_{2-4}x_2x_3+\gamma_{2-3}x_2x_4+\gamma_{1-3}x_1x_4+\gamma_{1-4}x_1x_3 \\ &-\tfrac{1}{2}(\gamma_2x_2x_3x_4+\gamma_3x_4+\gamma_{2-3-4}x_2+\gamma_{3-2-1}x_1x_2x_4+\gamma_1x_1x_3x_4+\gamma_4x_3+\gamma_{1-3-4}x_1+\gamma_{4-2-1}x_1x_2x_3) , \end{aligned} \tag{2.21}$$

$$C_1(\mathbf{k})=\frac{1}{2}\left[\frac{2}{N}\right]^2\sum_{12}l_{\mathbf{k}}^2l_1^2l_2^2\times(-6\gamma_{2-1-\mathbf{k}}x_{\mathbf{k}}x_1x_2+\gamma_2x_1^2x_2+\gamma_2x_{\mathbf{k}}^2x_1^2x_2+2\gamma_{\mathbf{k}}x_{\mathbf{k}}x_1^2+\gamma_1x_{\mathbf{k}}^2x_1+\gamma_2x_2) , \tag{2.22}$$

$$C_2(\mathbf{k})=\frac{1}{2}\left[\frac{2}{N}\right]^2\sum_{12}l_{\mathbf{k}}^2l_1^2l_2^2\times(3\gamma_{2-1-\mathbf{k}}x_1x_2+3\gamma_{2-1-\mathbf{k}}x_{\mathbf{k}}^2x_1x_2-2\gamma_1x_{\mathbf{k}}x_1x_2^2-2\gamma_2x_{\mathbf{k}}x_2-\gamma_{\mathbf{k}}x_2^2-\gamma_{\mathbf{k}}x_{\mathbf{k}}^2x_2^2) . \tag{2.23}$$

The part H_0 represents the spin-wave energy in the LSW theory. The part H_1 represents the energy of order $1/2S$; the first term in Eq. (2.13) comes out through the process of setting the products of four boson operators in a normal product form.[19] We have used the abbreviations $a_1=a_{\mathbf{k}_1}, b_{-2}=b_{-\mathbf{k}_2}$, $\gamma_{1-2}=\gamma_{\mathbf{k}_1-\mathbf{k}_2}$, etc. The Kronecker delta $\delta_G(1+2-3-4)$ represents the conservation of momenta within a reciprocal lattice vector $\mathbf{G}$. The vertex functions $B^{(i)}_{1234}$'s are given in a symmetric parametrization.[20] It is important to notice that $\gamma_{2-4}\neq\gamma_{1-3}$ if $\mathbf{G}\neq 0$ for $\delta_G(1+2-3-4)$ *because of a possible sign change in* $\gamma_{\mathbf{k}}$ *with* $\mathbf{k}\to\mathbf{k}+\mathbf{G}(\gamma_{\mathbf{k}+\mathbf{G}}=\pm\gamma_{\mathbf{k}})$. The expressions for the vertex functions by IW may be incorrect, since this type of sign change is disregarded. The part H_2 represents the energy of order $1/(2S)^2$, which comes out through the process of setting the products of six boson operators in a normal product form.

III. SPIN-WAVE DISPERSION

We define the Green's functions at zero temperature:[20]

$$G_{\alpha\alpha}(\mathbf{k},t)=-i\langle T(\alpha_{\mathbf{k}}(t)\alpha^\dagger_{\mathbf{k}}(0))\rangle , \tag{3.1}$$

$$G_{\alpha\beta}(\mathbf{k},t)=-i\langle T(\alpha_{\mathbf{k}}(t)\beta_{-\mathbf{k}}(0))\rangle , \tag{3.2}$$

$$G_{\beta\alpha}(\mathbf{k},t)=-i\langle T(\beta^\dagger_{-\mathbf{k}}(t)\alpha^\dagger_{\mathbf{k}}(0))\rangle , \tag{3.3}$$

$$G_{\beta\beta}(\mathbf{k},t)=-i\langle T(\beta^\dagger_{-\mathbf{k}}(t)\beta_{-\mathbf{k}}(0))\rangle , \tag{3.4}$$

where $\langle \cdots \rangle$ denotes the average over the ground state, and T is the time-ordering operator. The Fourier-transformed unperturbed propagators are given by

$$G^0_{\alpha\alpha}(\mathbf{k},\omega)=[\omega-\epsilon_{\mathbf{k}}+i\delta]^{-1} , \tag{3.5}$$

$$G^0_{\alpha\beta}(\mathbf{k},\omega)=G^0_{\beta\alpha}(\mathbf{k},\omega)=0 , \tag{3.6}$$

$$G^0_{\beta\beta}(\mathbf{k},\omega)=[-\omega-\epsilon_{\mathbf{k}}+i\delta]^{-1} , \tag{3.7}$$

with $\delta\to 0^+$. The self-energy is defined by the Dyson equation:

$$G_{\mu\nu}(\mathbf{k},\omega)=G^0_{\mu\nu}(\mathbf{k},\omega)+\sum_{\mu'\nu'}G^0_{\mu\mu'}(\mathbf{k},\omega)\Sigma_{\mu'\nu'}(\mathbf{k},\omega)G_{\nu'\nu}(\mathbf{k},\omega) . \tag{3.8}$$

Expanding the self-energy in powers of $1/2S$,

$$\Sigma_{\mu\nu}(\mathbf{k},\omega)=\frac{1}{2S}\Sigma^{(1)}_{\mu\nu}(\mathbf{k},\omega)+\frac{1}{(2S)^2}\Sigma^{(2)}_{\mu\nu}(\mathbf{k},\omega)+\cdots , \tag{3.9}$$

and performing the second-order perturbation, we obtain

$$\Sigma^{(1)}_{\alpha\alpha}(\mathbf{k},\omega)=\Sigma^{(1)}_{\beta\beta}(\mathbf{k},\omega)=A\epsilon_k , \quad \Sigma^{(1)}_{\alpha\beta}(\mathbf{k},\omega)=\Sigma^{(1)}_{\beta\alpha}(\mathbf{k},\omega)=0 , \tag{3.10}$$

$$\Sigma^{(2)}_{\alpha\alpha}(\mathbf{k},\omega)=\Sigma^{(2)}_{\beta\beta}(-\mathbf{k},-\omega)=C_1(\mathbf{k})+\left[\frac{2}{N}\right]^2\sum_{\mathbf{pq}}2l^2_{\mathbf{k}}l^2_{\mathbf{p}}l^2_{\mathbf{q}}l^2_{\mathbf{k+p-q}}\left[\frac{|B^{(4)}_{\mathbf{k,p,q,[k+p-q]}}|^2}{\omega-\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{q}}-\epsilon_{\mathbf{k+p-q}}+i\delta}-\frac{|B^{(6)}_{\mathbf{k,p,q,[k+p-q]}}|^2}{\omega+\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{k+p-q}}-i\delta}\right] , \tag{3.11}$$

$$\Sigma^{(2)}_{\alpha\beta}(\mathbf{k},\omega)=\Sigma^{(2)}_{\beta\alpha}(-\mathbf{k},-\omega)=C_2(\mathbf{k})+\left[\frac{2}{N}\right]^2\sum_{\mathbf{pq}}2l^2_{\mathbf{k}}l^2_{\mathbf{p}}l^2_{\mathbf{q}}l^2_{\mathbf{k+p-q}}\mathrm{sgn}(\gamma_{\mathbf{G}})B^{(4)}_{\mathbf{k,p,q,[k+p-q]}}\times B^{(6)}_{\mathbf{k,p,q,[k+p-q]}}\frac{2(\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{k+p-q}})}{\omega^2-(\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{k+p-q}})^2+i\delta} . \tag{3.12}$$

Here $[\mathbf{k+p-q}]$ stands for the momentum $\mathbf{k+p-q}$ reduced in the first BZ by a reciprocal lattice vector $\mathbf{G}$, that is $[\mathbf{k+p-q}]=\mathbf{k+p-q-G}$, and $\mathrm{sgn}(\gamma_{\mathbf{G}})$ denotes the sign of $\gamma_{\mathbf{G}}$. Note that $\epsilon_{\mathbf{k+p-q}}=\epsilon_{[\mathbf{k+p-q}]}$ and $l_{\mathbf{k+p-q}}=l_{[\mathbf{k+p-q}]}$. The last terms in Eqs. (3.11) and (3.12) correspond to the diagrams shown in Fig. 1, where we have used the relations,

$$\begin{aligned}B^{(5)}_{[\mathbf{k+p-q}],\mathbf{q},\mathbf{p},\mathbf{k}}&=\mathrm{sgn}(\gamma_{\mathbf{G}})B^{(4)}_{\mathbf{k,p,q,[k+p-q]}},\\ B^{(6)}_{\mathbf{q},[\mathbf{k+p-q}],\mathbf{k},\mathbf{p}}&=\mathrm{sgn}(\gamma_{\mathbf{G}})B^{(6)}_{\mathbf{k,p,q,[k+p-q]}} .\end{aligned} \tag{3.13}$$

Now we discuss the behavior of $\Sigma^{(2)}_{\mu\nu}(\mathbf{k},\omega=0)$ for small $\mathbf{k}$. The vertex functions are expanded as

$$B^{(4)}_{\mathbf{k,p,q,[k+p-q]}}=t_{\mathbf{p,q}}+\mathrm{sgn}(\gamma_{\mathbf{G}})s_{\mathbf{p,q}}-t_{\mathbf{p,q}}\epsilon_{\mathbf{k}}+X^{(4)}(\mathbf{k}\cdot\nabla_{\mathbf{p}}\epsilon_{\mathbf{p}},\cdots)+\cdots , \tag{3.14}$$

$$B^{(6)}_{\mathbf{k,p,q,[k+p-q]}}=-\mathrm{sgn}(\gamma_{\mathbf{G}})t_{\mathbf{p,q}}-s_{\mathbf{p,q}}+s_{\mathbf{p,q}}\epsilon_k+X^{(6)}(\mathbf{k}\cdot\nabla_{\mathbf{p}}\epsilon_{\mathbf{p}},\cdots)+\cdots , \tag{3.15}$$

with

$$s_{\mathbf{p,q}}=-\gamma_{\mathbf{q}}x_{\mathbf{p-q}}-\mathrm{sgn}(\gamma_{\mathbf{G}})\gamma_{\mathbf{p-q}}x_{\mathbf{q}}+\tfrac{1}{2}\{x_{\mathbf{q}}x_{\mathbf{p-q}}+\mathrm{sgn}(\gamma_{\mathbf{G}})\gamma_{\mathbf{q}}x_{\mathbf{p}}x_{\mathbf{q}}+\gamma_{\mathbf{p-q}}x_{\mathbf{p}}x_{\mathbf{p-q}}+\mathrm{sgn}(\gamma_{\mathbf{G}})\gamma_{\mathbf{p}}\} , \tag{3.16}$$

$$t_{\mathbf{p,q}}=-\mathrm{sgn}(\gamma_{\mathbf{G}})\gamma_{\mathbf{p-q}}x_{\mathbf{p}}x_{\mathbf{p-q}}-\gamma_{\mathbf{q}}x_{\mathbf{p}}x_{\mathbf{q}}+\tfrac{1}{2}\{\mathrm{sgn}(\gamma_{\mathbf{G}})\gamma_{\mathbf{q}}x_{\mathbf{p-q}}+\gamma_{\mathbf{p-q}}x_{\mathbf{q}}+\mathrm{sgn}(\gamma_{\mathbf{G}})\gamma_{\mathbf{p}}x_{\mathbf{p}}x_{\mathbf{q}}x_{\mathbf{p-q}}+x_{\mathbf{p}}\} , \tag{3.17}$$

where $\mathbf{G}=\mathbf{p-q}-[\mathbf{p-q}]$, and $X^{(4)}$ and $X^{(6)}$ are linear functions of $\mathbf{k}\cdot\nabla_{\mathbf{p}}\gamma_{\mathbf{p}}$, $\mathbf{k}\cdot\nabla_{\mathbf{q}}\gamma_{\mathbf{q}}$, and $\mathbf{k}\cdot\nabla_{\mathbf{p-q}}\gamma_{\mathbf{p-q}}$. Note that $x_{\mathbf{p-q}}=x_{[\mathbf{p-q}]}$. Also $C_1(\mathbf{k})$ and $C_2(\mathbf{k})$ are expanded as

$$C_1(\mathbf{k})=c_0\epsilon_{\mathbf{k}}^{-1}+c_1\epsilon_{\mathbf{k}}+\cdots , \tag{3.18}$$

$$C_2(\mathbf{k})=-c_0\epsilon_{\mathbf{k}}^{-1}+c'_1\epsilon_{\mathbf{k}}+\cdots , \tag{3.19}$$

where

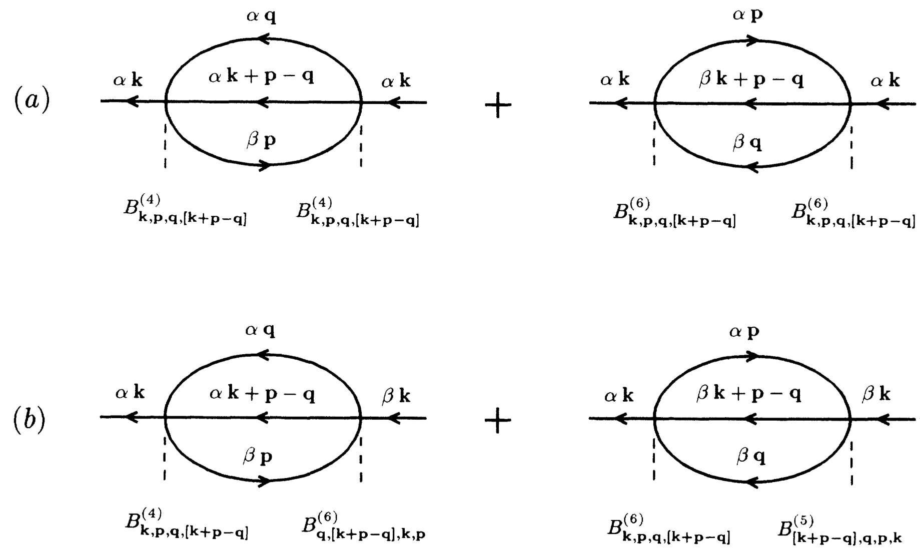

FIG. 1. Diagrams for the self-energy in the second-order perturbation: (a) $\Sigma^{(2)}_{\alpha\alpha}(\mathbf{k},\omega)$; (b) $\Sigma^{(2)}_{\alpha\beta}(\mathbf{k},\omega)$. The solid lines represent the unperturbed Green's functions $G^0_{\mu\mu}(\mathbf{k},\omega)$. Momentum $[\mathbf{k}+\mathbf{p}-\mathbf{q}]$ in the vertex functions stands for the reduced value of $\mathbf{k}+\mathbf{p}-\mathbf{q}$ in the 1st BZ. The arrows for $G^0_{\beta\beta}(\mathbf{k},\omega)$ run in the opposite directions to the conventional ones due to our definition.

$$c_0=\frac{1}{2}\left[\frac{2}{N}\right]^2\sum_{\mathbf{pq}} l_{\mathbf{p}}^2 l_{\mathbf{q}}^2\{-3\gamma_{\mathbf{p-q}}x_{\mathbf{p}}x_{\mathbf{q}}+x_{\mathbf{p}}^2+\gamma_{\mathbf{p}}x_{\mathbf{p}}x_{\mathbf{q}}^2+\gamma_{\mathbf{q}}x_{\mathbf{q}}\}\ , \quad (3.20)$$

$$c_1=\frac{1}{2}\left[\frac{2}{N}\right]^2\sum_{\mathbf{pq}} l_{\mathbf{p}}^2 l_{\mathbf{q}}^2\{3\gamma_{\mathbf{p-q}}x_{\mathbf{p}}x_{\mathbf{q}}-x_{\mathbf{p}}^2\}\ , \quad (3.21)$$

$$c_1'=\frac{1}{2}\left[\frac{2}{N}\right]^2\sum_{\mathbf{qq}} l_{\mathbf{p}}^2 l_{\mathbf{q}}^2\{-\tfrac{3}{2}\gamma_{\mathbf{p-q}}x_{\mathbf{p}}x_{\mathbf{q}}+\tfrac{1}{2}x_{\mathbf{p}}^2+\tfrac{1}{2}\gamma_{\mathbf{p}}x_{\mathbf{p}}x_{\mathbf{q}}^2+\tfrac{1}{2}\gamma_{\mathbf{q}}x_{\mathbf{q}}\}\ . \quad (3.22)$$

Substituting Eqs. (3.14)–(3.22) into Eq. (3.11), we have

$$\Sigma^{(1)}_{\alpha\alpha}(\mathbf{k},0)=\frac{1}{\epsilon_{\mathbf{k}}}\left[c_0+\left[\frac{2}{N}\right]^2\sum_{\mathbf{p,q}} l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{p-q}}^2\frac{-2(t_{\mathbf{p,q}}+\mathrm{sgn}(\gamma_G)s_{\mathbf{p,q}})^2}{\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{p-q}}}\right]+v_2\epsilon_{\mathbf{k}}\ , \quad (3.23)$$

where v_2 is a certain numerical constant. Substituting the relation,

$$t_{\mathbf{p,q}}+\mathrm{sgn}(\gamma_G)s_{\mathbf{p,q}} =\tfrac{1}{2}(\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{p-q}})\{x_{\mathbf{p}}-\mathrm{sgn}(\gamma_G)x_{\mathbf{q}}x_{\mathbf{p-q}}\}\ , \quad (3.24)$$

into Eq. (3.23), with the help of the relations

$$\sum_{\mathbf{pq}} l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{p-q}}^2\mathrm{sgn}(\gamma_G)\epsilon_{\mathbf{p}}x_{\mathbf{p}}x_{\mathbf{q}}x_{\mathbf{p-q}} =\sum_{\mathbf{pq}} l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{p-q}}^2\mathrm{sgn}(\gamma_G)\epsilon_{\mathbf{p-q}}x_{\mathbf{p}}x_{\mathbf{q}}x_{\mathbf{p-q}}$$

and

$$l_{\mathbf{p-q}}^2\mathrm{sgn}(\gamma_G)\epsilon_{\mathbf{p-q}}x_{\mathbf{p-q}}=\gamma_{\mathbf{p-q}}/2\ ,$$

we find that the first term of Eq. (3.23) vanishes. Thus we find that $\Sigma^{(2)}_{\alpha\alpha}(\mathbf{k}\to 0,0)=0$, which the rotational invariance of the Hamiltonian is demanding. We can similarly prove that $\Sigma^{(2)}_{\alpha\beta}(\mathbf{k}\to 0,0)=0$.

The quasiparticle energy $\tilde{\epsilon}_{\mathbf{k}}$ for spin-wave excitation up to order $1/(2S)^2$ may be given by

$$\tilde{\epsilon}_{\mathbf{k}}=\epsilon_{\mathbf{k}}+\frac{1}{2S}A\epsilon_{\mathbf{k}}+\frac{1}{(2S)^2}\Sigma^{(2)}_{\alpha\alpha}(\mathbf{k},\epsilon_{\mathbf{k}})\ . \quad (3.25)$$

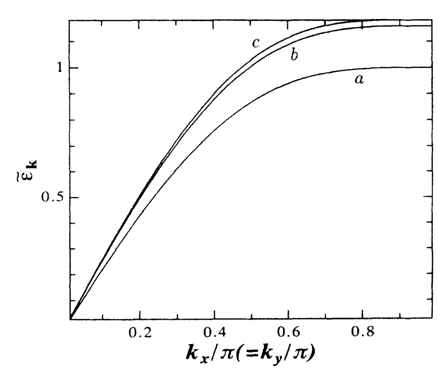

FIG. 2. Spin-wave dispersion relation $\tilde{\epsilon}_{\mathbf{k}}$ for $k_x=k_y$. Curve *a* represents the linear spin-wave value $\epsilon_{\mathbf{k}}$. Curves *b* and *c* represent the values up to order $1/(2S)$ and $1/(2S)^2$, respectively. The energy is measured in units of *JSz*.

To evaluate Eq. (3.25), we sum up 6400 points of **p** and **q** in the 1st BZ for $\Sigma^{(2)}_{\alpha\alpha}(\mathbf{k},\epsilon_{\mathbf{k}})$ given by Eq. (3.11). Figure 2 shows the spin-wave dispersion thus evaluated. The second-order correction is positive. The spin-wave velocity is estimated from $\Sigma^{(2)}_{\alpha\alpha}(\mathbf{k},\epsilon_{\mathbf{k}})/\epsilon_{\mathbf{k}}$ for $k_x=k_y=\pi/N_L$ with $N_L=40,80,160$, and by extrapolating the values to $N_L\to\infty$.[21] [For $\Sigma^{(2)}_{\alpha\alpha}(\mathbf{k},\epsilon_{\mathbf{k}})$, we sum up N_L^2 points of **p** and **q** in the 1st BZ.] The renormalization factor of the spin-wave velocity is given by

$$Z_c\equiv\lim_{\mathbf{k}\to 0}\tilde{\epsilon}_{\mathbf{k}}/\xi_{\mathbf{k}}=1+\frac{0.1579}{2S}+\frac{0.0215(\pm 0.0002)}{(2S)^2}, \quad (3.26)$$

which yields $Z_c=1.1794$ for $S=\frac{1}{2}$. Here the lowest bound 0.0213 of order $1/(2S)^2$ is the value at $N_L=160$.

IV. PERPENDICULAR SUSCEPTIBILITY

According to the linear-response theory, we may express the perpendicular susceptibility in terms of the Green's functions:

$$\chi_\perp=\frac{-N(g\mu_B)^2}{4}\lim_{\mathbf{k}\to 0}-i\int_{-\infty}^{\infty}dt\langle T[(S_a^+(\mathbf{k},t)+S_b^+(\mathbf{k},t))(S_a^-(\mathbf{k},0)+S_b^-(\mathbf{k},0))]\rangle\ , \quad (4.1)$$

where

$$S_a^+(\mathbf{k})=[S_a^-(\mathbf{k})]^\dagger=\left[\frac{2}{N}\right]^{1/2}\sum_i S_i^+\exp(-i\mathbf{k}\mathbf{r}_i)\ , \quad (4.2)$$

$$S_b^+(\mathbf{k})=[S_b^-(\mathbf{k})]^\dagger=\left[\frac{2}{N}\right]^{1/2}\sum_j S_j^+\exp(-i\mathbf{k}\mathbf{r}_j)\ . \quad (4.3)$$

Introducing the operators,

$$Y_\alpha^+(\mathbf{k})=[Y_\alpha^-(\mathbf{k})]^\dagger=[l_{\mathbf{k}}S_a^+(\mathbf{k})-m_{\mathbf{k}}S_b^+(\mathbf{k})]/(2S)^{1/2}\ , \quad (4.4)$$

$$Y_\beta^+(\mathbf{k})=[Y_\beta^-(\mathbf{k})]^\dagger=[-m_{\mathbf{k}}S_a^+(\mathbf{k})+l_{\mathbf{k}}S_b^+(\mathbf{k})]/(2S)^{1/2}\ , \quad (4.5)$$

and the associated Green's functions,

$$F_{\mu\nu}(\mathbf{k},\omega)=-i\int_{-\infty}^{\infty}dt\ e^{i\omega t}\langle T[Y_\mu^+(\mathbf{k},t)Y_\nu^-(\mathbf{k},0)]\rangle\ , \quad (4.6)$$

we may rewrite $\chi_\perp$ as

$$\chi_\perp=\frac{-N(g\mu_B)^2}{4JSz}\lim_{\mathbf{k}\to 0}2S(l_{\mathbf{k}}+m_{\mathbf{k}})^2\times[F_{\alpha\alpha}(\mathbf{k},\omega=0)+F_{\alpha\beta}(\mathbf{k},\omega=0)+F_{\beta\alpha}(\mathbf{k},\omega=0)+F_{\beta\beta}(\mathbf{k},\omega=0)]\ , \quad (4.7)$$

where the energy is measured in units of JSz.

We perform the HP transformation and the Bogoliubov transformation for the spin operators defined by Eqs. (4.4) and (4.5), so that

$$Y_\alpha^+(\mathbf{k})=D\alpha_{\mathbf{k}}-\frac{1}{2S}\frac{1}{N}\sum_{234}\delta_G(\mathbf{k}+2-3-4)l_{\mathbf{k}}l_2l_3l_4(M^{(1)}_{\mathbf{k}234}\beta_{-2}\alpha_3\alpha_4+M^{(2)}_{\mathbf{k}234}\alpha_2^\dagger\beta_{-3}^\dagger\beta_{-4}^\dagger+\cdots)\ , \quad (4.8)$$

$$Y_\beta^+(\mathbf{k})=D\beta_{-\mathbf{k}}^\dagger-\frac{1}{2S}\frac{1}{N}\sum_{234}\delta_G(\mathbf{k}+2-3-4)l_{\mathbf{k}}l_2l_3l_4\mathrm{sgn}(\gamma_G)(M^{(2)}_{\mathbf{k}234}\beta_{-2}\alpha_3\alpha_4+M^{(1)}_{\mathbf{k}234}\alpha_2^\dagger\beta_{-3}^\dagger\beta_{-4}^\dagger+\cdots)\ . \quad (4.9)$$

Here the "spin reduction" factor D is given by

$$D=1-\frac{\Delta S}{2S}-\frac{1}{4}\frac{\Delta S(1+3\Delta S)}{(2S)^2}\ , \quad (4.10)$$

with

$$\Delta S=(1/N)\sum_{\mathbf{q}}(\epsilon_{\mathbf{q}}^{-1}-1)=0.196\,60\ . \quad (4.11)$$

The first-order term in Eq. (4.10) arises from the process of setting the products of four boson operators in the normal product form, while the second-order term arises from the process of setting the products of six boson operators in the normal product form. The "nonlinear" matrix elements $M^{(i)}$ are given by

$$M^{(1)}_{\mathbf{k}234}=-x_2+\mathrm{sgn}(\gamma_G)x_{\mathbf{k}}x_3x_4\ , \quad (4.12)$$

$$M^{(2)}_{\mathbf{k}234}=x_3x_4-\mathrm{sgn}(\gamma_G)x_{\mathbf{k}}x_2\ , \quad (4.13)$$

with $\mathbf{G}=\mathbf{k}+2-3-4$.

Substituting Eqs. (4.8) and (4.9) into Eq. (4.6), and performing the second-order perturbation (the corresponding diagrams are shown in Fig. 3), we find

$$F_{\mu\nu}(\mathbf{k},\omega)=D^2G_{\mu\nu}(\mathbf{k},\omega),+I_{\mu\nu}(\mathbf{k},\omega)G^0_{\nu\nu}(\mathbf{k},\omega)+G^0_{\mu\mu}(\mathbf{k},\omega)\tilde{I}_{\mu\nu}(\mathbf{k},\omega)+J_{\mu\nu}(\mathbf{k},\omega)\ , \tag{4.14}$$

where

$$I_{\alpha\alpha}(\mathbf{k},\omega)=\tilde{I}_{\alpha\alpha}(\mathbf{k},\omega)=\frac{1}{(2S)^2}\left[\frac{2}{N}\right]^2\sum_{\mathbf{pq}} l_{\mathbf{k}}^2 l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{k+p-q}}^2\left[\frac{M^{(1)}_{\mathbf{k,p,q,[k+p-q]}}B^{(4)}_{\mathbf{k,p,q,[k+p-q]}}}{\omega-\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{q}}-\epsilon_{\mathbf{k+p-q}}+i\delta}-\frac{M^{(2)}_{\mathbf{k,p,q,[k+p-q]}}B^{(6)}_{\mathbf{k,p,q,[k+p-q]}}}{\omega+\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{k+p-q}}-i\delta}\right]\ , \tag{4.15}$$

$$I_{\alpha\beta}(\mathbf{k},\omega)=\tilde{I}_{\beta\alpha}(\mathbf{k},\omega)=\frac{1}{(2S)^2}\left[\frac{2}{N}\right]^2\sum_{\mathbf{pq}} l_{\mathbf{k}}^2 l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{k+p-q}}^2\,\mathrm{sgn}(\gamma_{\mathbf{G}})\left[\frac{M^{(1)}_{\mathbf{k,p,q,[k+p-q]}}B^{(6)}_{\mathbf{k,p,q,[k+p-q]}}}{\omega-\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{q}}-\epsilon_{\mathbf{k+p-q}}+i\delta}-\frac{M^{(2)}_{\mathbf{k,p,q,[k+p-q]}}B^{(4)}_{\mathbf{k,p,q,[k+p-q]}}}{\omega+\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{k+p-q}}-i\delta}\right]\ , \tag{4.16}$$

$$I_{\beta\alpha}(\mathbf{k},\omega)=\tilde{I}_{\alpha\beta}(\mathbf{k},\omega)=\frac{1}{(2S)^2}\left[\frac{2}{N}\right]^2\sum_{\mathbf{pq}} l_{\mathbf{k}}^2 l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{k+p-q}}^2\,\mathrm{sgn}(\gamma_{\mathbf{G}})\left[\frac{M^{(2)}_{\mathbf{k,p,q,[k+p-q]}}B^{(4)}_{\mathbf{k,p,q,[k+p-q]}}}{\omega-\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{q}}-\epsilon_{\mathbf{k+p-q}}+i\delta}-\frac{M^{(1)}_{\mathbf{k,p,q,[k+p-q]}}B^{(6)}_{\mathbf{k,p,q,[k+p-q]}}}{\omega+\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{k+p-q}}-i\delta}\right]\ , \tag{4.17}$$

$$I_{\beta\beta}(\mathbf{k},\omega)=\tilde{I}_{\beta\beta}(\mathbf{k},\omega)=\frac{1}{(2S)^2}\left[\frac{2}{N}\right]^2\sum_{\mathbf{pq}} l_{\mathbf{k}}^2 l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{k+p-q}}^2\left[\frac{M^{(2)}_{\mathbf{k,p,q,[k+p-q]}}B^{(6)}_{\mathbf{k,p,q,[k+p-q]}}}{\omega-\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{q}}-\epsilon_{\mathbf{k+p-q}}+i\delta}-\frac{M^{(1)}_{\mathbf{k,p,q,[k+p-q]}}B^{(4)}_{\mathbf{k,p,q,[k+p-q]}}}{\omega+\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{k+p-q}}-i\delta}\right]\ , \tag{4.18}$$

$$J_{\alpha\alpha}(\mathbf{k},\omega)=\frac{1}{(2S)^2}\frac{1}{2}\left[\frac{2}{N}\right]^2\sum_{\mathbf{pq}} l_{\mathbf{k}}^2 l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{k+p-q}}^2\left[\frac{|M^{(1)}_{\mathbf{k,p,q,[k+p-q]}}|^2}{\omega-\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{q}}-\epsilon_{\mathbf{k+p-q}}+i\delta}-\frac{|M^{(2)}_{\mathbf{k,p,q,[k+p-q]}}|^2}{\omega+\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{k+p-q}}-i\delta}\right]\ , \tag{4.19}$$

$$J_{\alpha\beta}(\mathbf{k},\omega)=\frac{1}{(2S)^2}\frac{1}{2}\left[\frac{2}{N}\right]^2\sum_{\mathbf{pq}} l_{\mathbf{k}}^2 l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{k+p-q}}^2\,\mathrm{sgn}(\gamma_{\mathbf{G}})M^{(1)}_{\mathbf{k,p,q,[k+p-q]}}M^{(2)}_{\mathbf{k,p,q,[k+p-q]}}\frac{2(\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{k+p-q}})}{\omega^2-(\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{k+p-q}})^2+i\delta}\ , \tag{4.20}$$

$$J_{\beta\alpha}(\mathbf{k},\omega)=J_{\alpha\beta}(\mathbf{k},\omega)\ , \tag{4.21}$$

$$J_{\beta\beta}(\mathbf{k},\omega)=\frac{1}{(2S)^2}\frac{1}{2}\left[\frac{2}{N}\right]^2\sum_{\mathbf{pq}} l_{\mathbf{k}}^2 l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{k+p-q}}^2\left[\frac{|M^{(2)}_{\mathbf{k,p,q,[k+p-q]}}|^2}{\omega-\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{q}}-\epsilon_{\mathbf{k+p-q}}+i\delta}-\frac{|M^{(1)}_{\mathbf{k,p,q,[k+p-q]}}|^2}{\omega+\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{k+p-q}}-i\delta}\right]\ , \tag{4.22}$$

with $\mathbf{G}=\mathbf{k}+\mathbf{p}-\mathbf{q}-[\mathbf{k}+\mathbf{p}-\mathbf{q}]$. Using Eqs. (4.14)–(4.22), we may express $F_{\mu\nu}(\mathbf{k},\omega=0)$'s for small $\mathbf{k}$ in the following form:

$$F_{\alpha\alpha}(\mathbf{k},0)=F_{\beta\beta}(\mathbf{k},0)\simeq-\frac{1}{\epsilon_{\mathbf{k}}}\left[D^2\left[1-\frac{A}{2S}+\frac{A^2}{(2S)^2}\right]+\frac{1}{(2S)^2}(-\sigma_{\alpha\alpha}+2i_{\alpha\alpha}-j_{\alpha\alpha})\right]\ , \tag{4.23}$$

$$F_{\alpha\beta}(\mathbf{k},0)=F_{\beta\alpha}(\mathbf{k},0)\simeq-\frac{1}{\epsilon_{\mathbf{k}}}\frac{1}{(2S)^2}(-\sigma_{\alpha\beta}+2i_{\alpha\beta}-j_{\alpha\beta})\ , \tag{4.24}$$

where

$$\sigma_{\mu\nu}\equiv\lim_{\mathbf{k}\to 0}\frac{1}{\epsilon_{\mathbf{k}}}\Sigma^{(2)}_{\mu\nu}(\mathbf{k},0)\ , \tag{4.25}$$

$$\frac{1}{(2S)^2}i_{\mu\nu}\equiv\lim_{\mathbf{k}\to 0}I_{\mu\nu}(\mathbf{k},0)\ , \tag{4.26}$$

$$\frac{1}{(2S)^2}j_{\mu\nu}\equiv\lim_{\mathbf{k}\to 0}\epsilon_{\mathbf{k}}J_{\mu\nu}(\mathbf{k},0)\ . \tag{4.27}$$

Since $(l_{\mathbf{k}}+m_{\mathbf{k}})^2 \sim \epsilon_{\mathbf{k}}/2$, the substitution of Eqs. (4.23) and (4.24) into Eq. (4.7) yields

$$\chi_\perp = \frac{N(g\mu_B)^2}{2Jz}\left\{1-\frac{1}{2S}(2\Delta S + A) + \frac{1}{(2S)^2}\left[-\frac{\Delta S}{2}-\frac{(\Delta S)^2}{2}+2A\,\Delta S + A^2 - \sigma_{\alpha\alpha}-\sigma_{\alpha\beta}+2i_{\alpha\alpha}+2i_{\alpha\beta}-j_{\alpha\alpha}-j_{\alpha\beta}\right]\right\}. \tag{4.28}$$

The term of order $1/(2S)$ is identical to Oguchi's.[19] In the terms of order $1/(2S)^2$, $\sigma_{\alpha\alpha}+\sigma_{\alpha\beta}$ may be expressed as

$$\sigma_{\alpha\alpha}+\sigma_{\alpha\beta}=c_1+c_1'-\left[\frac{2}{N}\right]^2\sum_{\mathbf{pq}} l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{p-q}}^2\frac{\{-t_{\mathbf{p,q}}+\mathrm{sgn}(\gamma_{\mathbf{G}})s_{\mathbf{p,q}}\}^2}{\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{p-q}}}, \tag{4.29}$$

with $\mathbf{G}=\mathbf{p}-\mathbf{q}-[\mathbf{p}-\mathbf{q}]$, where c_1, c_1', $s_{\mathbf{p,q}}$, and $t_{\mathbf{p,q}}$ are defined by Eqs. (3.21), (3.22), (3.16), and (3.17), respectively. In deriving Eq. (4.29), we have used the relation, $X^{(4)}+\mathrm{sgn}(\gamma_{\mathbf{G}})X^{(6)}=0$. Also $i_{\alpha\alpha}+i_{\alpha\beta}$ and $j_{\alpha\alpha}+j_{\alpha\beta}$ may be expressed as

$$i_{\alpha\alpha}+i_{\alpha\beta}=\left[\frac{2}{N}\right]^2\sum_{\mathbf{pq}} l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{p-q}}^2\frac{(x_{\mathbf{p}}-\mathrm{sgn}(\gamma_{\mathbf{G}})x_{\mathbf{q}}x_{\mathbf{p-q}})(-t_{\mathbf{p,q}}+\mathrm{sgn}(\gamma_{\mathbf{G}})s_{\mathbf{p,q}})}{\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{p-q}}}, \tag{4.30}$$

$$j_{\alpha\alpha}+j_{\alpha\beta}=-\left[\frac{2}{N}\right]^2\sum_{\mathbf{pq}} l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{p-q}}^2\frac{(x_{\mathbf{p}}-\mathrm{sgn}(\gamma_{\mathbf{G}})x_{\mathbf{q}}x_{\mathbf{p-q}})^2}{\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{p-q}}}. \tag{4.31}$$

Combining Eqs. (4.29)–(4.31), we finally find

$$-\sigma_{\alpha\alpha}-\sigma_{\alpha\beta}+2i_{\alpha\alpha}+2i_{\alpha\beta}-j_{\alpha\alpha}-j_{\alpha\beta}=-\frac{1}{16}\{(4\Delta S+A)(4\Delta S+3A)+2A\} + \left[\frac{2}{N}\right]^2\sum_{\mathbf{pq}} l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{p-q}}^2\frac{\{-t_{\mathbf{p,q}}+\mathrm{sgn}(\gamma_{\mathbf{G}})s_{\mathbf{p,q}}+x_{\mathbf{p}}-\mathrm{sgn}(\gamma_{\mathbf{G}})x_{\mathbf{q}}x_{\mathbf{p-q}}\}^2}{\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{p-q}}}. \tag{4.32}$$

Itoh and Kanamori[22] have given a similar expression of order $1/(2S)^2$ in a different context. To evaluate Eq. (4.32), we sum up $N_L^2/8$ points of $\mathbf{p}$ in the 1/8 part of the 1st BZ and N_L^2 points of $\mathbf{q}$ in the first BZ, with

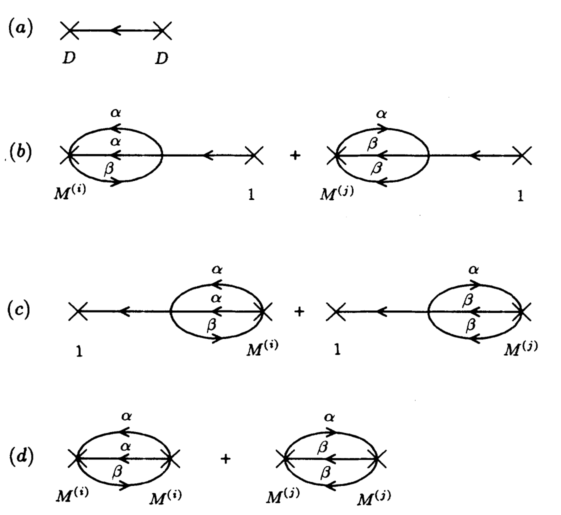

FIG. 3. Diagrams for $F_{\mu\nu}(\mathbf{k},\omega)$: (a) $D^2G_{\mu\nu}(\mathbf{k},\omega)$; (b) $I_{\mu\nu}(\mathbf{k},\omega)G^0_{\nu\nu}(\mathbf{k},\omega)$; (c) $G^0_{\mu\mu}(\mathbf{k},\omega)\tilde{I}_{\mu\nu}(\mathbf{k},\omega)$; (d) $J_{\mu\nu}(\mathbf{k},\omega)$. The solid line for (a) represents the Green's function including the self-energy correction, while the solid lines for (b)–(d) represent the unperturbed ones. The crosses for (a) represent D, while the crosses for (b)–(d) represent 1 or $M^{(1)}_{\mathbf{k,p,q,[k+p-q]}}$ or $M^{(2)}_{\mathbf{k,p,q,[k+p-q]}}$ [$\mathrm{sgn}(\gamma_{\mathbf{G}})$ is omitted].

$N_L=160,320,480$, and extrapolate the values to $N_L\to\infty$.[21] The renormalization factor for $\chi_\perp$ is given by

$$Z_\chi \equiv \frac{\chi_\perp(2Jz)}{N(g\mu_B)^2}=1-\frac{0.551}{2S}+\frac{0.065(\pm 0.001)}{(2S)^2}, \tag{4.33}$$

which yields $Z_\chi=0.514$ for $S=1/2$. Here the lowest bound 0.064 of order $1/(2S)^2$ is the value at $N_L=480$.

V. SPIN-STIFFNESS CONSTANT

Let the order parameter be twisted by an angle θ per lattice constant along one of the crystal axes (denoted as y), which points to the direction tilting $\pi/4$ relative to the axes of momentum. The twist of the order parameter is conveniently handled by introducing the local coordinate frame for spin variables such that the spins are aligned in the $\pm z$ directions.[4] In this coordinate frame the Hamiltonian may be expressed as

$$H=J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j+J\theta\sum_{l}(S_l^xS_{l+\mathbf{b}}^z-S_l^zS_{l+\mathbf{b}}^x) -J\tfrac{1}{2}\theta^2\sum_{l}(S_l^xS_{l+\mathbf{b}}^x+S_l^zS_{l+\mathbf{b}}^z)+O(\theta), \tag{5.1}$$

where l runs over all lattice sites, and $l+\mathbf{b}$ indicates the nearest neighbor to the lth site in the positive y direction. The stiffness constant ρ_s is defined by the coefficient for an increase of the ground-state energy due to such twist: $\Delta E=(N/2)\rho_s\theta^2+\cdots$.

Applying the HP transformation and the Bogoliubov transformation to the second term of Eq. (5.1), we find

$$J\theta \sum_l (S_l^x S_{l+b}^z - S_l^z S_{l+b}^x) = -J\theta \tfrac{1}{2}\sqrt{2S} \left[\frac{2}{N} \right]^{1/2} \sum_{123} \delta_G(1-2+3) l_1 l_2 l_3 \times (W_{123}^{(1)} \alpha_1^\dagger \beta_{-2}^\dagger \alpha_3^\dagger + W_{123}^{(2)} \beta_{-1}^\dagger \alpha_2^\dagger \beta_{-3}^\dagger + \text{H.c.}) + \cdots , \quad (5.2)$$

where the vertex functions are given in a symmetric parametrization by

$$W_{123}^{(1)} = -\tfrac{1}{2}(\eta_3 x_2 x_3 + \eta_1 x_1 x_2 + \eta_{2-3} x_3 + \eta_{2-1} x_1) , \quad (5.3)$$

$$W_{123}^{(2)} = -\tfrac{1}{2}(\eta_{2-3} x_1 x_2 + \eta_{2-1} x_2 x_3 + \eta_3 x_1 + \eta_1 x_3) , \quad (5.4)$$

with

$$\eta_{\mathbf{k}} = -2i \sin \left[\frac{k_x + k_y}{2} \right] . \quad (5.5)$$

The second-order perturbation with respect to Eq. (5.2) gives rise to a change of the ground-state energy of order θ^2, which may lead to an expression of the spin-stiffness constant as

$$\rho_s^{\text{para}} = -\frac{J}{z} \left[\frac{2}{N} \right]^2 \sum_{\mathbf{pq}} l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{p+q}}^2 \frac{|W_{\mathbf{p},[\mathbf{p+q}],\mathbf{q}}^{(1)}|^2 + |W_{\mathbf{p},[\mathbf{p+q}],\mathbf{q}}^{(2)}|^2}{\epsilon_{\mathbf{p}} + \epsilon_{\mathbf{q}} + \epsilon_{\mathbf{p+q}}} . \quad (5.6)$$

The third term of Eq. (5.1) averaged over the ground state gives rise to another change of the energy of order θ^2. Applying the HP transformation and the Bogoliubov transformation to the third term of Eq. (5.1), we find

$$\rho_s^{\text{dia}} = JS^2 \left\{ 1 - \frac{1}{2S}(2\Delta S - A) + \frac{1}{(2S)^2}[4(\Delta S)^2 + 2(\Delta S)A + A^2] \right\} . \quad (5.7)$$

The total spin-stiffness constant ρ_s is the sum of ρ_s^{para} and ρ_s^{dia}. To evaluate Eq. (5.6), we sum up $N_L^2/2$ points of $\mathbf{p}$ in the $\frac{1}{2}$ part of the first BZ and N_L^2 points of $\mathbf{q}$ in the first BZ, with $N_L = 80, 160, 320$, and extrapolate the values to $N_L \to \infty$.[21] The renormalization factor for ρ_s is given by

$$Z_\rho \equiv \rho_s/(JS^2) = 1 - \frac{0.235}{2S} - \frac{0.041(\pm 0.003)}{(2S)^2} , \quad (5.8)$$

which yields $Z_\rho = 0.724$ for $S = \frac{1}{2}$. Here the lowest bound 0.038 of order $1/(2S)^2$ is the value at $N_L = 320$.

VI. SUBLATTICE MAGNETIZATION

The sublattice magnetization may be expressed as

$$M \equiv S - \langle a_i^\dagger a_i \rangle = S - \frac{2}{N} \sum_k \lim_{\eta \to 0^+} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} i e^{i\omega\eta} \{ l_{\mathbf{k}}^2 G_{\alpha\alpha}(\mathbf{k},\omega) + l_{\mathbf{k}} m_{\mathbf{k}} [G_{\alpha\beta}(\mathbf{k},\omega) + G_{\beta\alpha}(\mathbf{k},\omega)] + m_{\mathbf{k}}^2 G_{\beta\beta}(\mathbf{k},\omega) \} . \quad (6.1)$$

The substitution of Eqs. (3.11) and (3.12) into Eq. (6.1) yields

$$M = S - \Delta S + \frac{1}{(2S)^2} \frac{2}{N} \sum_{\mathbf{k}} \left\{ \frac{l_{\mathbf{k}} m_{\mathbf{k}}}{\epsilon_{\mathbf{k}}} \Sigma_{\alpha\beta}^{(2)}(\mathbf{k}, -\epsilon_{\mathbf{k}}) - \left[\frac{2}{N} \right]^2 \sum_{\mathbf{pq}} 2 l_{\mathbf{k}}^2 l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 l_{\mathbf{k+p-q}}^2 \left[\frac{(l_{\mathbf{k}}^2 + m_{\mathbf{k}}^2)|B_{\mathbf{k},\mathbf{p},\mathbf{q},[\mathbf{k+p-q}]}^{(6)}|^2}{(\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{p}} + \epsilon_{\mathbf{q}} + \epsilon_{\mathbf{k+p-q}})^2} + \frac{2 l_{\mathbf{k}} m_{\mathbf{k}} \operatorname{sgn}(\gamma_G) B_{\mathbf{k},\mathbf{p},\mathbf{q},[\mathbf{k+p-q}]}^{(4)} B_{\mathbf{k},\mathbf{p},\mathbf{q},[\mathbf{k+p-q}]}^{(6)}}{\epsilon_{\mathbf{k}}^2 - (\epsilon_{\mathbf{p}} + \epsilon_{\mathbf{q}} + \epsilon_{\mathbf{k+p-q}})^2} \right] \right\} , \quad (6.2)$$

where $\mathbf{G} = \mathbf{k+p-q} - [\mathbf{k+p-q}]$. To evaluate Eq. (6.2), we sum up N_L^2 points of $\mathbf{p}$ and $\mathbf{q}$ in the first BZ, and $N_L^2/8$ points of $\mathbf{k}$ in the $\frac{1}{8}$ part of the first BZ, with $N_L = 20, 40$. The convergence of order $1/(2S)^2$ with respect to N_L is very good. The sublattice magnetization is given by

$$M = S - 0.19660 + \frac{0.0035}{(2S)^2} , \quad (6.3)$$

which yields $M = 0.3069$ for $S = \frac{1}{2}$. Our value of order $1/(2S)^2$ is different from the value of CC, who have used the Dyson-Maleev formalism. We hope that our value is more reliable in view of the treatment of the umklapp processes.

VII. CONCLUDING REMARKS

Treating the umklapp processes carefully, we have developed IW's idea, and have calculated the spin-wave dispersion, the perpendicular susceptibility, the spin-stiffness constant, and the sublattice magnetization, to order $1/(2S)^2$, using the HP formalism. The calculated values of order $1/(2S)^2$ are not negligible, though small, indicating that the $1/S$ expansion is a useful asymptotic expansion. In Table I, our estimates are listed for $S=1/2$, in comparison with the series-expansion estimates[4] and the Monte Carlo estimates.[5,8] Our values are in good agreement with the series-expansion estimates.[23]

Whether or not our values are satisfying the hydrodynamic relation, $Z_c=(Z_\rho/Z_\chi)^{1/2}$, may be a crucial test for their accuracy. Substituting Eqs. (4.33) and (5.8) into this relation, we find

$$Z_c=1+\frac{0.1580}{2S}+\frac{0.0216}{(2S)^2}\,, \tag{7.1}$$

which is equivalent to Eq. (3.26) within a very small numerical error. Thus we believe that our estimates are quite accurate.

TABLE I. Renormalization factors for the spin-wave velocity Z_c, the perpendicular susceptibility Z_χ, and the spin-stiffness constant Z_ρ, as well as the sublattice magnetization M $[S=\frac{1}{2}]$.

Theory	Z_c	Z_χ	Z_ρ	M
$1/S$ expansion				
this work	1.1794	0.514	0.724	0.3069
CC (Ref. 18)				0.30068
Series expansion (Ref. 4)	1.176[a]	0.52	0.72	0.3025
Monte-Carlo				
TC (Ref. 5)	1.14			0.31
MD (Ref. 8)			0.796	

[a]Value evaluated from the relation $Z_c=(Z_\rho/Z_\chi)^{1/2}$.

ACKNOWLEDGMENTS

We would like to thank H. Akai and K. Hirai for valuable discussions. This work was partially supported by a Grant-in-Aid for Scientific Research from the Japanese Ministry of Education, Science, and Culture.

[1]J. D. Reger and A. P. Young, Phys. Rev. B **37**, 5978 (1988).
[2]Y. Okabe and M. Kikuchi, J. Phys. Soc. Jpn. **57**, 4351 (1988).
[3]S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. Lett. **60**, 1057 (1988); Phys. Rev. B **39**, 2344 (1989).
[4]R. R. P. Singh, Phys. Rev. B **39**, 9760 (1989); R. R. P. Singh and D. A. Huse, *ibid.* **40**, 7247 (1989).
[5]N. Trivedi and D. M. Ceperley, Phys. Rev. B **40**, 2737 (1989).
[6]E. Manousakis and E. Salvador, Phys. Rev. Lett. **60**, 840 (1988); Phys. Rev. B **39**, 575 (1989).
[7]G. Gomez-Santos, J. D. Joannopoulos, and J. W. Negele, Phys. Rev. B **39**, 4435 (1989).
[8]M. S. Makivic and H.-Q. Ding. Phys. Rev. B **43**, 3562 (1991).
[9]P. Horsch and W. von der Linden, Z. Phys. B **72**, 181 (1988).
[10]K. W. Becker, H. Won, and P. Fulde, Z. Phys. B **75**, 335 (1989).
[11]A. Auerbach and D. P. Arovas, Phys. Rev. Lett. **61**, 617 (1988); D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988).
[12]M. Takahashi, Phys. Rev. B **40**, 2494 (1989).
[13]J. Oitmaa and D. D. Betts, Can. J. Phys. **56**, 897 (1978); S. Tang and J. E. Hirsch, Phys. Rev. B **39**, 4548 (1989); M. Gross, E. Sanchez-Velasco, and E. D. Siggia, *ibid.* **40**, 11 328 (1989).
[14]P. W. Anderson, Phys. Rev. **86**, 694 (1952).
[15]R. Kubo, Phys. Rev. **87**, 568 (1952).
[16]J. Igarashi and A. Watabe, Phys. Rev. B **43**, 13 456 (1991); *ibid.* **44**, 5057 (1991).
[17]T. Holstein and H. Primakoff, Phys. Rev. **58**, 1098 (1940).
[18]G. E. Castilla and S. Chakravarty, Phys. Rev. B **43**, 13 687 (1991).
[19]T. Oguchi, Phys. Rev. **117**, 117 (1960).
[20]A. B. Harris, D. Kumar, B. I. Halperin, and P. C. Hohenberg, Phys. Rev. B **3**, 961 (1971).
[21]The values are well fitted by a function $A+B/N_L$.
[22]Y. Itoh and J. Kanamori, J. Phys. Soc. Jpn. **33**, 315 (1972).
[23]The second-order correction to the spin-wave dispersion has recently been calculated by means of the Dyson-Maleev formalism by C. M. Canali, S. M. Girvin, and Mats Wallin, Phys. Rev. B **45**, 10 131 (1992), which has yielded exactly the same result as in the present paper.