Quantum corrections to the spin-correlation function and the spin-stiffness constant in a two-dimensional Heisenberg antiferromagnet at zero temperature

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Quantum corrections to the longitudinal spin-correlation function and the spin-stiffness constant are calculated up to $1/(2S)^2$ in a two-dimensional Heisenberg antiferromagnet at zero temperature by using the Holstein-Primakoff transformation. The equal-time longitudinal spin-correlation function is found to compensate almost entirely the reduction caused by the second-order correction in the transverse spin-correlation function, making the spherically averaged correlation function very close to the value given by linear spin-wave theory. In the spin-stiffness constant, a partial cancellation is found between the "paramagnetic" and "diamagnetic" terms, leading to a small second-order correction.

I. INTRODUCTION

The discovery of high-temperature superconductors has greatly increased the theoretical interest in the physics of quantum antiferromagnets, since undoped compounds are known to be well described by the spin-$\frac{1}{2}$ Heisenberg model.[1] It is now widely accepted that the spin-$\frac{1}{2}$ Heisenberg antiferromagnet exhibits Néel long-range order at zero temperature in two dimensions, although the quantum fluctuation considerably reduces the order parameter.[2-10]

One way to attack systematically the problem of such a large quantum fluctuation is to use an expansion with respect to the power of $1/2S$, where S is the length of spins, from the classical limit. The Holstein-Primakoff transformation[11] is useful to carry out this expansion. The leading order of the expansion leads to linear spin-wave (LSW) theory.[12] The first-order correction to LSW theory was studied by Oguchi several decades ago.[13] The perpendicular susceptibility was calculated to order $1/(2S)^2$ in three dimensions (3D) by Itoh and Kanamori for studying its temperature dependence.[14] The damping of spin waves has been studied in three dimensions by several authors.[15,16] Recently, we have calculated the quantum corrections to the spin-wave velocity, the sublattice magnetization, and the perpendicular susceptibility, up to terms of order $1/(2S)^2$, at zero temperature for $D=2$.[17] The second-order corrections to these quantities were not so large, indicating that the $1/2S$ expansion works well. We have also calculated the second-order correction to the dynamical transverse spin-correlation function (TSCF) whose spectral function is found to be strongly modified, showing the sideband structure of the three-magnon excitations. The equal-time TSCF is smaller compared to the value given by LSW theory.

On the other hand, we did not calculate the longitudinal spin-correlation function (LSCF) in Ref. 17. Thus it is quite natural to ask how the LSCF behaves within the $1/2S$ expansion. The purpose of this paper is to answer this question along the same line as in Ref. 17. Since the leading term in the LSCF is one order higher than the TSCF with respect to $1/2S$, accounting for the first-order correction caused by spin-wave interactions is sufficient for our purpose. We find that the spectral function is composed of the continuum of two-magnon excitations as a function of energy. The second-order correction does not give rise to sideband structure in the spectral function, in contrast to the case of the TSCF. The interesting finding is that the equal-time LSCF compensates almost entirely the reduction caused by the second-order correction in the TSCF, for $S=\frac{1}{2}$.

In Ref. 17 we have evaluated the spin-stiffness constant ρ_s by using a hydrodynamic relation $\rho_s=c^2\chi_\perp$, where c is the spin-wave velocity and $\chi_\perp$ is the perpendicular susceptibility. In this paper we formulate ρ_s in terms of the response to the twist of the order parameter and apply the $1/2S$ expansion. (Such attempt to calculate ρ_s directly has been done by Singh and Huse, who used the expansion method introducing the Ising anisotropy.[18]) The treatment of the response to the twist naturally leads to the presence of two kinds of contributions to ρ_s, which may be called "paramagnetic" and "diamagnetic," by analogy with the electrical conductivity.[19] We find that a partial cancellation is occurring between the two terms of the order of $1/(2S)^2$, which makes the remaining correction small.

In Sec. II the Hamiltonian is described in the Holstein-Primakoff formalism. In Sec. III the longitudinal spin-correlation function is calculated. In Sec. IV the spin-stiffness constant is calculated. Section V is devoted to the concluding remarks.

II. HAMILTONIAN

The antiferromagnetic Heisenberg model is described by a Hamiltonian

$$H=J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j\ , \tag{2.1}$$

where $\langle i,j\rangle$ indicates a sum over pairs of nearest neighbors. We consider a square lattice with N spins. In the following we use the same notation as in Ref. 17.

We use the Holstein-Primakoff transformation for spin operators[11] given by

$$S_i^z=S-a_i^\dagger a_i\ , \tag{2.2}$$

$$S_i^+=(S_i^-)^\dagger=\sqrt{2S}f_i(S)a_i\ , \tag{2.3}$$

$$S_j^z=-S+b_j^\dagger b_j\ , \tag{2.4}$$

$$S_j^+=(S_j^-)^\dagger=\sqrt{2S}b_j^\dagger f_j(S)\ , \tag{2.5}$$

with

$$f_l(S)=\left[1-\frac{n_l}{2S}\right]^{1/2}=1-\frac{1}{2}\frac{n_l}{2S}-\frac{1}{8}\left[\frac{n_l}{2S}\right]^2+\cdots\ . \tag{2.6}$$

The indices i and j refer to sites on the a (up) and b (down) sublattices, respectively, with $n_l=a_i^\dagger a_i(l=i)$ or $n_l=b_j^\dagger b_j(l=j)$. The a_i and b_j are boson annihilation operators, whose Fourier transforms are defined as

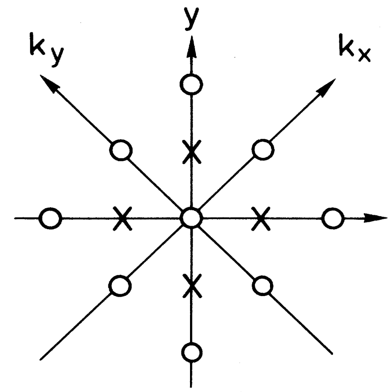

FIG. 1. Coordinate frames used in this paper. The momentum axes are tilted $\pi/4$ from the conventional crystal axes. The open circles and crosses represent the spins in the a and b sublattices, respectively.

$$a_{\mathbf{k}}=\left[\frac{2}{N}\right]^{1/2}\sum_i a_i\exp(-i\mathbf{k}\cdot\mathbf{r}_i)\ ,\quad b_{\mathbf{k}}=\left[\frac{2}{N}\right]^{1/2}\sum_j b_j\exp(-i\mathbf{k}\cdot\mathbf{r}_j)\ . \tag{2.7}$$

Then we introduce the Bogoliubov transformation defined by

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

$$b_{-\mathbf{k}}=m_{\mathbf{k}}\alpha_{\mathbf{k}}^\dagger+l_{\mathbf{k}}\beta_{-\mathbf{k}}\ , \tag{2.9}$$

with

$$l_{\mathbf{k}}=\left[\frac{(1+\varepsilon_{\mathbf{k}})}{2\varepsilon_{\mathbf{k}}}\right]^{1/2},\quad m_{\mathbf{k}}=-\left[\frac{(1-\varepsilon_{\mathbf{k}})}{2\varepsilon_{\mathbf{k}}}\right]^{1/2}\equiv-x_{\mathbf{k}}l_{\mathbf{k}}\ , \tag{2.10}$$

$$\varepsilon_{\mathbf{k}}=(1-\gamma_{\mathbf{k}}^2)^{1/2}\ ,\quad \gamma_{\mathbf{k}}=\cos(k_x/2)\cos(k_y/2)\ , \tag{2.11}$$

where k_x,k_y are in units of $1/(\sqrt{2}a)$, with a being the nearest-neighbor distance (see Fig. 1). Hereafter, we call the quasiparticles described by $\alpha_{\mathbf{k}},\beta_{\mathbf{k}}$ "magnons." In this magnon language the Hamiltonian is expressed as

$$H=H_0+H_1+\cdots\ , \tag{2.12}$$

$$H_0=JSz\sum_{\mathbf{k}}(\varepsilon_{\mathbf{k}}-1)+JSz\sum_{\mathbf{k}}\varepsilon_{\mathbf{k}}(\alpha_{\mathbf{k}}^\dagger\alpha_{\mathbf{k}}+\beta_{\mathbf{k}}^\dagger\beta_{\mathbf{k}})\ , \tag{2.13}$$

$$\begin{aligned}H_1=&\frac{JSz}{2S}A\sum_{\mathbf{k}}\varepsilon_{\mathbf{k}}(\alpha_{\mathbf{k}}^\dagger\alpha_{\mathbf{k}}+\beta_{\mathbf{k}}^\dagger\beta_{\mathbf{k}})\\&+\frac{-JSz}{2SN}\sum_{1234}\delta(1+2-3-4)l_1l_2l_3l_4\\&\times[\alpha_1^\dagger\alpha_2^\dagger\alpha_3\alpha_4B_{1234}^{(1)}+\beta_{-3}^\dagger\beta_{-4}^\dagger\beta_{-1}\beta_{-2}B_{1234}^{(2)}+4\alpha_1^\dagger\beta_{-4}^\dagger\beta_{-2}\alpha_3B_{1234}^{(3)}\\&+(2\alpha_1^\dagger\beta_{-2}\alpha_3\alpha_4B_{1234}^{(4)}+2\beta_{-4}^\dagger\beta_{-1}\beta_{-2}\alpha_3B_{1234}^{(5)}+\alpha_1^\dagger\alpha_2^\dagger\beta_{-3}^\dagger\beta_{-4}^\dagger B_{1234}^{(6)}+\text{H.c.})]\ ,\end{aligned} \tag{2.14}$$

where

$$A=\frac{2}{N}\sum_{\mathbf{k}}(1-\varepsilon_{\mathbf{k}})=0.158\ , \tag{2.15}$$

$$B^{(3)}_{1234}=\gamma_{2-4}+\gamma_{1-3}x_1x_2x_3x_4+\gamma_{1-4}x_1x_2+\gamma_{1-4}x_3x_4 -\tfrac{1}{2}(\gamma_1x_3+\gamma_2x_4+\gamma_3x_1+\gamma_4x_2+\gamma_1x_1x_2x_4+\gamma_2x_1x_2x_3+\gamma_3x_2x_3x_4+\gamma_4x_1x_3x_4)\ , \tag{2.16}$$

$$B^{(6)}_{1234}=\gamma_{2-4}x_2x_3+\gamma_{2-4}x_1x_4+\gamma_{2-3}x_2x_4+\gamma_{2-3}x_1x_3 -\tfrac{1}{2}(\gamma_1x_1x_3x_4+\gamma_2x_2x_3x_4+\gamma_3x_1x_2x_3+\gamma_4x_1x_2x_4+\gamma_1x_2+\gamma_2x_1+\gamma_3x_4+\gamma_4x_3)\ . \tag{2.17}$$

The explicit expressions for $B^{(1)}$, $B^{(2)}$, $B^{(4)}$, and $B^{(5)}$ are omitted here, since they are not used in the following calculation (see Ref. 17 for these expressions). We use 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 H_0 gives the spin-wave energy in the zeroth order (LSW theory). The H_1 describes the perturbation in the first order of $1/2S$; the first term arises from setting the second term representing the spin-wave interaction in normal product form.

III. LONGITUDINAL SPIN-CORRELATION FUNCTIONS

We concentrate our attention to the LSCF, since the TSCF has already been studied in detail in Ref. 17. In this section the energy and frequency are measured in units of JSz.

For the "staggered" and "total" spins,

$$Q^z(\mathbf{k})=S^z_a(\mathbf{k})-S^z_b(\mathbf{k})\ , \tag{3.1}$$

$$S^z(\mathbf{k})=S^z_a(\mathbf{k})+S^z_b(\mathbf{k})\ , \tag{3.2}$$

where

$$S^z_{a(b)}(\mathbf{k})=\left[\frac{2}{N}\right]^{1/2}\sum_{i(j)}S^z_{i(j)}\exp(-i\mathbf{k}\cdot\mathbf{r}_{i(j)})\ , \tag{3.3}$$

and the LSCF is defined by

$$P^{zz}_Q(\mathbf{k},t)=\langle[Q^z(\mathbf{k},t)-\langle Q^z(\mathbf{k})\rangle][Q^z(-\mathbf{k},0)-\langle Q^z(-\mathbf{k})\rangle]\rangle\ , \tag{3.4}$$

$$P^{zz}_S(\mathbf{k},t)=\langle S^z(\mathbf{k},t)S^z(-\mathbf{k},0)\rangle\ , \tag{3.5}$$

where $\langle\cdots\rangle$ denotes the average over the ground state.

We first express the staggered and total spins in the magnon picture by applying the Bogoliubov transformation, Eqs. (2.8) and (2.9) to Eqs. (2.2) and (2.4). The results are

$$Q^z(\mathbf{k})=R_+(\mathbf{k})+2(S-\Delta S)\left[\frac{N}{2}\right]^{1/2}\delta(\mathbf{k})\ , \tag{3.6}$$

$$S^z(\mathbf{k})=R_-(\mathbf{k})\ , \tag{3.7}$$

where

$$R_\pm(\mathbf{k})=-\left[\frac{2}{N}\right]^{1/2}\sum_{\mathbf{p}}[(l_{\mathbf{p}}l_{\mathbf{p}+\mathbf{k}}\pm m_{\mathbf{p}}m_{\mathbf{p}+\mathbf{k}})(\alpha^\dagger_{\mathbf{p}}\alpha_{\mathbf{p}+\mathbf{k}}\pm\beta^\dagger_{-\mathbf{p}-\mathbf{k}}\beta_{-\mathbf{p}})+(l_{\mathbf{p}}m_{\mathbf{p}+\mathbf{k}}\pm m_{\mathbf{p}}l_{\mathbf{p}+\mathbf{k}})(\alpha^\dagger_{\mathbf{p}}\beta^\dagger_{-\mathbf{p}-\mathbf{k}}\pm\beta_{-\mathbf{p}}\alpha_{\mathbf{p}+\mathbf{k}})]\ . \tag{3.8}$$

The ΔS in Eq. (3.6) represents the well-known reduction factor of magnetization,

$$\Delta S\equiv\frac{2}{N}\sum_{\mathbf{k}}m^2_{\mathbf{k}}=0.197\ . \tag{3.9}$$

This arises from setting the rest of the terms into normal product form. Next, we introduce the two-particle Green function in a matrix form:

$$[W(\mathbf{k},t)]_{1\mathbf{p},1\mathbf{p}'}=-i\langle T[\beta_{-\mathbf{p}}(t)\alpha_{\mathbf{p}+\mathbf{k}}(t)\alpha^\dagger_{\mathbf{p}'+\mathbf{k}}(0)\beta^\dagger_{-\mathbf{p}'}(0)]\rangle\ , \tag{3.10}$$

$$[W(\mathbf{k},t)]_{1\mathbf{p},2\mathbf{p}'}=-i\langle T[\beta_{-\mathbf{p}}(t)\alpha_{\mathbf{p}+\mathbf{k}}(t)\beta_{-\mathbf{p}'-\mathbf{k}}(0)\alpha_{\mathbf{p}'}(0)]\rangle\ , \tag{3.11}$$

$$[W(\mathbf{k},t)]_{2\mathbf{p},1\mathbf{p}'}=-i\langle T[\alpha^\dagger_{\mathbf{p}}(t)\beta^\dagger_{-\mathbf{p}-\mathbf{k}}(t)\alpha^\dagger_{\mathbf{p}'+\mathbf{k}}(0)\beta^\dagger_{-\mathbf{p}'}(0)]\rangle\ , \tag{3.12}$$

$$[W(\mathbf{k},t)]_{2\mathbf{p},2\mathbf{p}'}=-i\langle T[\alpha^\dagger_{\mathbf{p}}(t)\beta^\dagger_{-\mathbf{p}-\mathbf{k}}(t)\beta_{-\mathbf{p}'-\mathbf{k}}(0)\alpha_{\mathbf{p}'}(0)]\rangle\ , \tag{3.13}$$

where T is the time-ordering operator. Then the spectral function of the correlation function is related to the temporal Fourier transform of the Green function (for $\omega>0$) as follows:

$$P_Q^{zz}(\mathbf{k},\omega)=\frac{2}{N}\sum_{\mathbf{p},\mathbf{p}'}(l_{\mathbf{p}}m_{\mathbf{p}+\mathbf{k}}+m_{\mathbf{p}}l_{\mathbf{p}+\mathbf{k}})(l_{\mathbf{p}'+\mathbf{k}}m_{\mathbf{p}'}+m_{\mathbf{p}'+\mathbf{k}}l_{\mathbf{p}'})$$
$$\times\left[\frac{-1}{\pi}\right]\mathrm{Im}\{[W(\mathbf{k},\omega)]_{1\mathbf{p},1\mathbf{p}'}+[W(\mathbf{k},\omega)]_{1\mathbf{p},2\mathbf{p}'}+[W(\mathbf{k},\omega)]_{2\mathbf{p},1\mathbf{p}'}+[W(\mathbf{k},\omega)]_{2\mathbf{p},2\mathbf{p}'}\}\ , \qquad (3.14)$$

$$P_S^{zz}(\mathbf{k},\omega)=\frac{2}{N}\sum_{\mathbf{p},\mathbf{p}'}(l_{\mathbf{p}}m_{\mathbf{p}+\mathbf{k}}-m_{\mathbf{p}}l_{\mathbf{p}+\mathbf{k}})(l_{\mathbf{p}'+\mathbf{k}}m_{\mathbf{p}'}-m_{\mathbf{p}'+\mathbf{k}}l_{\mathbf{p}'})$$
$$\times\left[\frac{-1}{\pi}\right]\mathrm{Im}\{-[W(\mathbf{k},\omega)]_{1\mathbf{p},1\mathbf{p}'}+[W(\mathbf{k},\omega)]_{1\mathbf{p},2\mathbf{p}'}+[W(\mathbf{k},\omega)]_{2\mathbf{p},1\mathbf{p}'}-[W(\mathbf{k},\omega)]_{2\mathbf{p},2\mathbf{p}'}\}\ . \qquad (3.15)$$

Note that the leading-order term in the LSCF is one order higher than that in the TSCF. Thus taking account of the first-order correction by the spin-wave interaction is sufficient to obtain the correction up to $1/(2S)^2$.

The lowest-order (the first order in $1/2S$) arises from the diagram shown in Fig. 2(a). The imaginary part for $\omega>0$ is simply given by

$$\mathrm{Im}[W(\mathbf{k},\omega)]_{1\mathbf{p},1\mathbf{p}}=-\pi\delta(\omega-\varepsilon_{\mathbf{p}+\mathbf{k}}-\varepsilon_{\mathbf{p}})\ , \qquad (3.16)$$

and the other components are zero. The next-order corrections arise from the diagrams shown in Figs. 2(b) and 2(c). The imaginary parts for $\omega>0$ are estimated as

$$\mathrm{Im}[W(\mathbf{k},\omega)]_{1\mathbf{p},1\mathbf{p}'}=-\pi[\delta(\omega-\varepsilon_{\mathbf{p}+\mathbf{k}}-\varepsilon_{\mathbf{p}})-\delta(\omega-\varepsilon_{\mathbf{p}'+\mathbf{k}}-\varepsilon_{\mathbf{p}'})]V_{1\mathbf{p},1\mathbf{p}'}(\mathbf{k})(\varepsilon_{\mathbf{p}+\mathbf{k}}+\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}'+\mathbf{k}}-\varepsilon_{\mathbf{p}'})^{-1}\ , \qquad (3.17)$$

$$\mathrm{Im}[W(\mathbf{k},\omega)]_{1\mathbf{p},2\mathbf{p}'}=\mathrm{Im}[W(\mathbf{k},\omega)]_{2\mathbf{p}',1\mathbf{p}}$$
$$=\pi\delta(\omega-\varepsilon_{\mathbf{p}+\mathbf{k}}-\varepsilon_{\mathbf{p}})V_{1\mathbf{p},2\mathbf{p}'}(\mathbf{k})(\varepsilon_{\mathbf{p}+\mathbf{k}}+\varepsilon_{\mathbf{p}}+\varepsilon_{\mathbf{p}'+\mathbf{k}}+\varepsilon_{\mathbf{p}'})^{-1}\ , \qquad (3.18)$$

where

$$V_{1\mathbf{p},1\mathbf{p}'}(\mathbf{k})=V_{2\mathbf{p},2\mathbf{p}'}(\mathbf{k})=-\frac{1}{N}\frac{1}{2S}4l_{\mathbf{p}+\mathbf{k}}l_{\mathbf{p}'}l_{\mathbf{p}'+\mathbf{k}}l_{\mathbf{p}}B^{(3)}_{\mathbf{p}+\mathbf{k},\mathbf{p}',\mathbf{p}'+\mathbf{k},\mathbf{p}}\ , \qquad (3.19)$$

$$V_{1\mathbf{p},2\mathbf{p}'}(\mathbf{k})=V_{2\mathbf{p},1\mathbf{p}'}(\mathbf{k})=-\frac{1}{N}\frac{1}{2S}4l_{\mathbf{p}+\mathbf{k}}l_{\mathbf{p}'}l_{\mathbf{p}'+\mathbf{k}}l_{\mathbf{p}}B^{(6)}_{\mathbf{p}+\mathbf{k},\mathbf{p}',\mathbf{p}'+\mathbf{k},\mathbf{p}}\ . \qquad (3.20)$$

We have included a factor of 4 in Eq. (3.20) by using the relation, $B^{(6)}_{1234}=B^{(6)}_{2134}=B^{(6)}_{1243}=B^{(6)}_{2143}$. Since the spin-wave energy is modified by the first term of Eq. (2.14) in the first order of $1/2S$, this shift should be included in Eq. (3.16) to calculate the second-order correction. Inserting Eqs. (3.16)–(3.18) into Eqs. (3.14) and (3.15), we get the spectral function. The spectrum is composed of the continuum of the two-magnon excitations as a function of energy. (The explicit shape has not been evaluated in this paper.) Note that the spectral function of the TSCF is composed of the δ-function-like spike of the one-magnon excitation and the sideband of the three-magnon excitations.[17]

The equal-time correlation function is obtained from integrating the spectral function with respect to ω. For the staggered spins, it becomes

$$P_Q^{zz}(\mathbf{k})\equiv\int_{-\infty}^{\infty}d\omega\,P_Q^{zz}(\mathbf{k},\omega)$$
$$=\frac{2}{N}\sum_{\mathbf{p}}(l_{\mathbf{p}}m_{\mathbf{p}+\mathbf{k}}+m_{\mathbf{p}}l_{\mathbf{p}+\mathbf{k}})^2$$
$$-\frac{4}{N}\sum_{\mathbf{p},\mathbf{p}'}(l_{\mathbf{p}}m_{\mathbf{p}+\mathbf{k}}+m_{\mathbf{p}}l_{\mathbf{p}+\mathbf{k}})(l_{\mathbf{p}'}m_{\mathbf{p}'+\mathbf{k}}+m_{\mathbf{p}'}l_{\mathbf{p}'+\mathbf{k}})V_{1\mathbf{p},2\mathbf{p}'}(\mathbf{k})(\varepsilon_{\mathbf{p}+\mathbf{k}}+\varepsilon_{\mathbf{p}}+\varepsilon_{\mathbf{p}'+\mathbf{k}}+\varepsilon_{\mathbf{p}'})^{-1}\ . \qquad (3.21)$$

The first and second terms in Eq. (3.21) represent the first- and second-order corrections in $1/2S$, respectively. The terms coming from Eq. (3.17) vanish after summing over $\mathbf{p}$ and $\mathbf{p}'$. (For the total spins, the discussion is quite similar.) We evaluate numerically Eq. (3.21) by summing up 6400 points of $\mathbf{p}$ and 6400 points of $\mathbf{p}'$ in the first Brillouin zone. Figure 3 shows the calculated $P_Q^{zz}(\mathbf{k})$ as a function of $\mathbf{k}$ along a line of $k_x=k_y$. Note that the second-order correction is negative.

It may be interesting to consider the spherically averaged correlation function for the staggered spins, $\langle\mathbf{Q}(\mathbf{k})\cdot\mathbf{Q}(-\mathbf{k})\rangle$, since finite-size calculations can give only this correlation function due to the lack of the broken symmetry. Using the TSCF calculated in Ref. 17, together with $P_Q^{zz}(\mathbf{k})$ calculated above, we obtain $\langle\mathbf{Q}(\mathbf{k})\cdot\mathbf{Q}(-\mathbf{k})\rangle$. Figure 4 shows the function thus evaluated for $S=\frac{1}{2}$ as a function of $\mathbf{k}$. [The TSCF's up to $1/(2S)^2$ are also shown.] The reduction caused by the second-order correction in the TSCF is mostly compensated by the LSCF, thereby making the spherically aver-

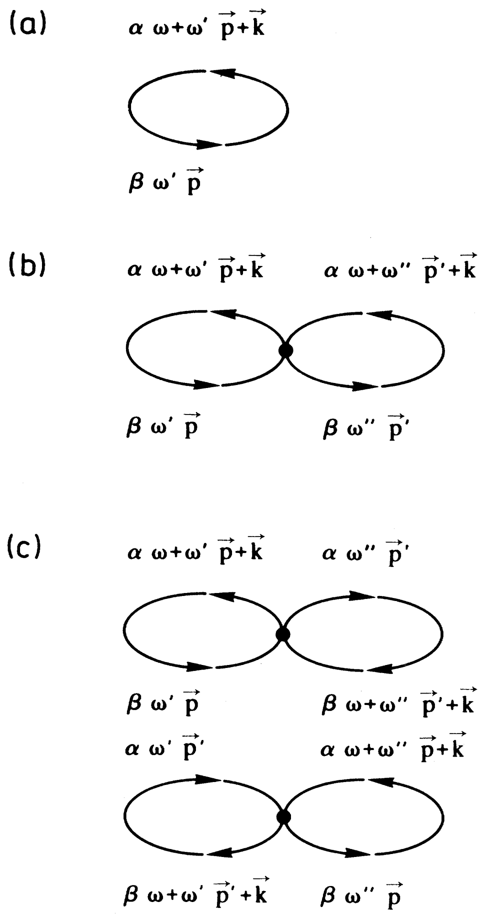

FIG. 2. Diagrams for the two-particle Green function $W(\mathbf{k},\omega)$: (a) the first-order contribution to $[W(\mathbf{k},\omega)]_{1\mathbf{p},1\mathbf{p}}$, (b) the second-order contribution to $[W(\mathbf{k},\omega)]_{1\mathbf{p},1\mathbf{p}'}$, and (c) the second-order contribution to $[W(\mathbf{k},\omega)]_{1\mathbf{p},2\mathbf{p}'}$ and $[W(\mathbf{k},\omega)]_{2\mathbf{p}',1\mathbf{p}}$. The solid lines represent the unperturbed single-particle Green functions, $(\omega-\varepsilon_{\mathbf{k}}+i\delta)^{-1}$ for $\alpha,\omega,\mathbf{k}$, and $(-\omega-\varepsilon_{\mathbf{k}}+i\delta)^{-1}$ for $\beta,\omega,\mathbf{k}$, with $\delta\rightarrow 0^+$. The Green functions are integrated over the frequencies ω' and ω''. The solid circle in (b) represents the interaction $V_{1\mathbf{p},1\mathbf{p}'}(\mathbf{k})$, and the solid circles in (c) are $V_{1\mathbf{p},2\mathbf{p}'}(\mathbf{k})$ and $V_{2\mathbf{p}',1\mathbf{p}}(\mathbf{k})$.

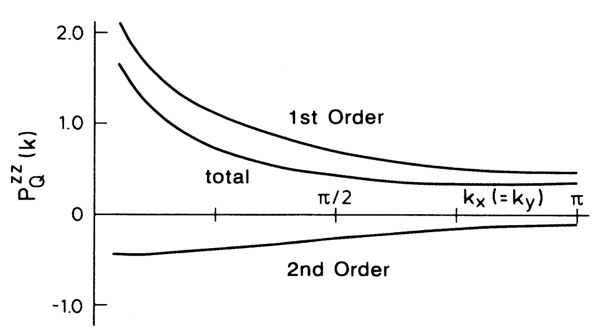

FIG. 3. Equal-time longitudinal spin-correlation function for the staggered spins, as a function of $\mathbf{k}$ along a line $k_x=k_y$. The curve with "1st order" is the contribution of the first term in Eq. (3.21), and the curve with "2nd order" is the contribution of the last term in Eq. (3.21). $S=\frac{1}{2}$.

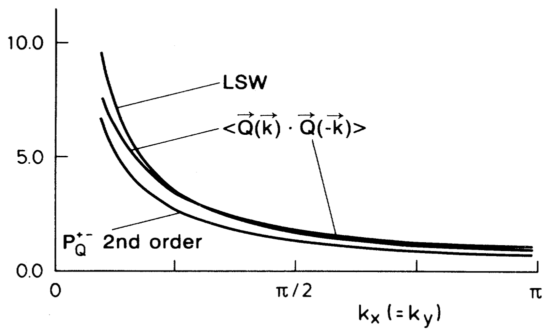

FIG. 4. Spherically averaged spin-correlation function for the staggered spins, $\langle \mathbf{Q}(\mathbf{k})\cdot\mathbf{Q}(-\mathbf{k})\rangle$, as a function of $\mathbf{k}$ along a line $k_x=k_y$. The curve with "LSW" represents the lowest-order result (given by LSW theory). The curve with "2nd order" represents the transverse spin-correlation function calculated up to $1/(2S)^2$ (Ref. 17). $S=\frac{1}{2}$.

aged correlation function very close to the value given by LSW theory. Our finding is consistent with Horsch and von der Linden,[8] who obtained a good agreement with the lowest-order value in the spherically averaged function for $S=\frac{1}{2}$ by using a variational method and an exact diagonalization in finite systems. Note that the good compensation is only possible for $S=\frac{1}{2}$, since the compensation takes place between the first-order correction in the LSCF and the second-order correction in the TSCF.

IV. SPIN-STIFFNESS CONSTANT

Let the order parameter be twisted by an angle θ per lattice constant along the y direction. Then we can define the stiffness constant ρ_s through the increase of the ground-state energy:

$$\Delta E=\tfrac{1}{2}N\rho_s\theta^2+O(\theta)\ . \tag{4.1}$$

In this section we use a coordinate frame whose x and y axes are along the crystal axes (see Fig. 1).

In order to calculate the increase of the ground-state energy, following Singh and Huse,[18] we express the Hamiltonian *in terms of the spin variables in the local coordinate frame,* which is rotated by an angle θ per lattice constant along the y axis in spin space. The expression is

$$H=J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j+J\theta\sum_i(S_i^xS_{i+\mathbf{b}}^z-S_i^zS_{i+\mathbf{b}}^x)-J\tfrac{1}{2}\theta^2\sum_i(S_i^xS_{i+\mathbf{b}}^x+S_i^zS_{i+\mathbf{b}}^z)+O(\theta)\ , \tag{4.2}$$

where i runs over all lattice sites, and $i+\mathbf{b}$ indicates the nearest neighbor to the ith site in the positive y direction. The Holstein-Primakoff transformation is applied to spins in this local coordinate frame in which the spins are aligned in the $\pm z$ directions. To the change of the ground-state energy within the order θ^2, there are two kinds of contribution: One term is the contribution of the second-order perturbation energy coming from the second term in Eq. (4.2), which we call "paramagnetic," and another term is the contribution of the third term in Eq. (4.2) averaged over the ground state, which we call "diamagnetic," i.e., $\rho_s = \rho_s^{\rm para} + \rho_s^{\rm dia}$.[19]

Let us first consider the diamagnetic term. From Eqs. (4.1) and (4.2), it is expressed as

$$\rho_s^{\rm dia} = -\frac{J}{N}\sum_i \langle S_i^x S_{i+\mathbf{b}}^x + S_i^z S_{i+\mathbf{b}}^z \rangle \ . \tag{4.3}$$

Rewriting the spin operators in terms of the magnon operators, we obtain

$$\begin{aligned}\rho_s^{\rm dia} &= JS^2 \left[1 - \frac{4}{2S}\frac{2}{N}\sum_{\mathbf{p}} \left[\frac{1}{4} l_{\mathbf{p}} m_{\mathbf{p}} \tilde{\gamma}_{\mathbf{p}} + m_{\mathbf{p}}^2 \right] + \frac{2}{(2S)^2}\left[\frac{2}{N}\right]^2 \sum_{\mathbf{p},\mathbf{q}} (l_{\mathbf{p}} m_{\mathbf{p}} m_{\mathbf{q}}^2 \tilde{\gamma}_{\mathbf{p}} + 2 m_{\mathbf{p}}^2 m_{\mathbf{q}}^2 + l_{\mathbf{p}} m_{\mathbf{p}} l_{\mathbf{q}} m_{\mathbf{q}} \tilde{\gamma}_{\mathbf{p}-\mathbf{q}}) \right] \\ &= JS^2 \left[1 - \frac{1}{2S}(2\Delta S - A) + \frac{1}{(2S)^2}[4(\Delta S)^2 + 2(\Delta S)A + A^2] \right] \ ,\end{aligned} \tag{4.4}$$

where

$$\tilde{\gamma}_{\mathbf{k}} = 2\cos\left[\frac{k_x + k_y}{2}\right] \ . \tag{4.5}$$

Let us next consider the paramagnetic term. In the magnon language, the second term of Eq. (4.2) is expressed as

$$\begin{aligned} J\theta \sum_i (S_i^x S_{i+\mathbf{b}}^z - S_i^z S_{i+\mathbf{b}}^x) &= -J\theta \frac{1}{2}\sqrt{2S}\left[\frac{2}{N}\right]^{1/2} \sum_{123} \delta(1-2-3)\eta_3 (a_1^\dagger a_2 b_3 + a_1^\dagger a_2 b_{-3}^\dagger - a_3 b_1^\dagger b_2 - a_{-3}^\dagger b_1^\dagger b_2) \\ &= -J\theta\frac{1}{2}\sqrt{2S}\left[\frac{2}{N}\right]^{1/2} \sum_{123} [\delta(1-2+3)(l_1 m_2 m_3 - m_1 l_2 l_3)\eta_{-3}\alpha_1^\dagger \beta_{-2}^\dagger \alpha_3^\dagger \\ &\qquad + \delta(1-2-3)(l_1 m_2 l_3 - m_1 l_2 m_3)\eta_3 \alpha_1^\dagger \beta_{-2}^\dagger \beta_{-3}^\dagger + \text{H.c.}] + \cdots \ ,\end{aligned} \tag{4.6}$$

where

$$\eta_{\mathbf{k}} = -2i\sin\left[\frac{k_x + k_y}{2}\right] \ . \tag{4.7}$$

The conventional second-order perturbation theory concerning the perturbation given by Eq. (4.6) gives

$$\rho_s^{\rm para} = -\frac{J}{2z}\left[\frac{2}{N}\right]^2 \sum_{\mathbf{p},\mathbf{q}} l_{\mathbf{p}+\mathbf{q}}^2 l_{\mathbf{p}}^2 l_{\mathbf{q}}^2 \frac{|M(\mathbf{p},\mathbf{q})|^2}{\varepsilon_{\mathbf{p}+\mathbf{q}} + \varepsilon_{\mathbf{p}} + \varepsilon_{\mathbf{q}}} \ , \tag{4.8}$$

where

$$M(\mathbf{p},\mathbf{q}) = \eta_{-\mathbf{q}}(x_{\mathbf{p}+\mathbf{q}} x_{\mathbf{q}} + x_{\mathbf{p}}) + \eta_{-\mathbf{p}}(x_{\mathbf{p}+\mathbf{q}} x_{\mathbf{p}} + x_{\mathbf{q}}) \ . \tag{4.9}$$

We evaluate numerically Eq. (4.8) by dividing the first Brillouin zone into a finite number of meshes, $N_m = 80\times 80$, 100×100, and 120×120, and extrapolate the sum to $N_m \to \infty$ (see Fig. 5). The result is

$$\rho_s^{\rm para} = JS^2\left[-\frac{s_2^{\rm para}}{(2S)^2}\right] \ , \quad s_2^{\rm para} \simeq 0.29 \ . \tag{4.10}$$

Thus the sum of the diamagnetic and paramagnetic terms becomes

$$\rho_s = JS^2\left[1 - \frac{0.236}{2S} - \frac{s_2}{(2S)^2}\right] \ , \quad s_2 \simeq 0.05 \ . \tag{4.11}$$

The second-order correction is small due to a partial cancellation between the diamagnetic and paramagnetic terms. Our previous estimate[17] of s_2 based on the hydrodynamic relation is a little larger than the present value (of course, the first-order correction is the same), probably due to a rough estimate of the spin-wave velocity in Ref. 17. Our value for $\rho_s/(JS^2)$ at $S=\frac{1}{2}$ is 0.714, which is compared with other theoretical estimates, 0.738,[6] 0.73,[18] 0.88,[20] 0.636,[21] and 0.796.[22] (The last three values are the estimates by Monte Carlo calculations.)

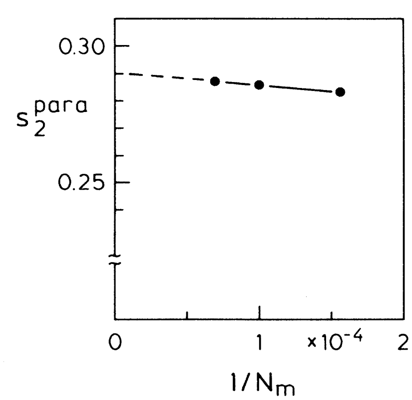

FIG. 5. Numerical estimates of $s_2^{\rm para}$ as a function of the inverse of the mesh number N_m^{-1}.

V. CONCLUDING REMARKS

We have calculated the dynamical LSCF up to terms of order $1/(2S)^2$ by using the Holstein-Primakoff transformation. The spectral function is composed of the continuum of two-magnon excitations as a function of energy. The equal-time LSCF is evaluated through the spectral function. Comparing the equal-time LSCF with the equal-time TSCF, which has been calculated up to terms of order $1/(2S)^2$ in Ref. 17, we have found an interesting cancellation between the LSCF and the second-order correction to the TSCF for $S=\frac{1}{2}$, which makes the spherically averaged correlation function very close to the value of LSW theory.

We have also calculated the spin-stiffness constant up to $1/(2S)^2$ by formulating it in terms of the response to the twist of the order parameter. We have found a partial cancellation between the "diamagnetic" and "paramagnetic" terms, which makes the remaining second-order correction small.

The second-order corrections to the above quantities are small due to cancellation . The second-order corrections to other quantities are not large.[17] This happens in spite of the absence of the obvious cancellation, indicating that the $1/2S$ expansion works well and has quantitative meaning.

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[1]Y. Endoh, K. Yamada, R. J. Birgenau, D. R. Gabbe, H. P. Jenssen, M. A. Kastner, C. J. Peters, P. J. Picone, T. R. Thurston, J. M. Tranquada, G. Shirane, Y. Hidaka, M. Oda, Y. Enomoto, M. Suzuki, and T. Murakami, Phys. Rev. B **37**, 7443 (1988); C. J. Peters, R. J. Birgeneau, M. A. Kastner, H. Yoshizawa, Y. Endoh, J. Tranquada, G. Shirane, Y. Hidaka, M. Oda, M. Suzuki, and T. Murakami, *ibid.* **37**, 9761 (1988).

[2]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. Sánchez-Velasco, and E. D. Siggia, *ibid.* **40**, 11 328 (1989).

[3]J. D. Reger and A. P. Young, Phys. Rev. B **37**, 5978 (1988).

[4]S. Miyashita, J. Phys. Soc. Jpn. **57**, 1934 (1988); Y. Okabe and M. Kikuchi, *ibid.* **57**, 4351 (1988); Y. Okabe, M. Kikuchi, and A. D. S. Nagi, Phys. Rev. Lett. **61**, 2971 (1988).

[5]S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. Lett. **60**, 1057 (1988); Phys. Rev. B **39**, 2344 (1989).

[6]A. Auerbach and D. P. Arovas, Phys. Rev. Lett. **61**, 617 (1988); D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988).

[7]D. A. Huse and V. Elser, Phys. Rev. Lett. **60**, 2531 (1988).

[8]P. Horsch and W. von der Linden, Z. Phys. B **72**, 181 (1988).

[9]W. von der Linden, M. Ziegler, and P. Horsch, Phys. Rev. B **40**, 7435 (1989).

[10]K. W. Becker, H. Won, and P. Fulde, Z. Phys. B **75**, 335 (1989).

[11]T. Holstein and H. Primakoff, Phys. Rev. **58**, 1098 (1940).

[12]P. W. Anderson, Phys. Rev. **86**, 694 (1952); R. Kubo, *ibid.* **87**, 568 (1952).

[13]T. Oguchi, Phys. Rev. **117**, 117 (1960).

[14]Y. Itoh and J. Kanamori, J. Phys. Soc. Jpn. **33**, 315 (1972).

[15]A. B. Harris, D.Kumar, B. I. Halperin, and P. C. Hohenberg, Phys. Rev. B **3**, 961 (1971).

[16]R. M. White and R. Freedman, Phys. Rev. B **10**, 1039 (1974).

[17]J. Igarashi and A. Watabe, Phys. Rev. B **43**, 13 456 (1991).

[18]R. R. P. Singh and D. A. Huse, Phys. Rev. B **40**, 7247 (1989).

[19]The momentum-dependent stiffness constant is evaluated at finite temperature in the Heisenberg ferromagnet by P. Kopietz and G. Castilla, Phys. Rev. B **43**, 11 100 (1991).

[20]E. Manousakis and E. Salvador, Phys. Rev. Lett. **60**, 840 (1988); Phys. Rev. B **39**, 575 (1989).

[21]G. Gomez-Santos, J. D. Joannopoulos, and J. W. Negele, Phys. Rev. B **39**, 4435 (1989).

[22]M. S. Makivic and H.-Q. Ding, Phys. Rev. B **43**, 3562 (1991).