Quantum-field-theory approach to the Heisenberg Hamiltonian, modified spin-wave theory, and application to an antiferromagnet with a square lattice

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(Received 3 August 1994; revised manuscript received 28 December 1994)

This paper proposes a quantum-field-theory approach to treat the anisotropic Heisenberg Hamiltonian, and gives a general temperature-dependent modified spin-wave theory. For a square-lattice antiferromagnet, the numerical calculations give several results in agreement with experiments or the Monte Carlo results, and several predictions which need future verification.

I. INTRODUCTION

There has been a lot of interest in two-dimensional spin-$\frac{1}{2}$ magnetic systems since the discovery of high-T_c superconductivity.[1-8] The ground-state staggered magnetization per spin, $m^*=\frac{1}{2}-\Delta$, in the spin-1/2 square lattice of a Heisenberg antiferromagnet has been calculated in linear spin-wave (LSW) theory ($\Delta=0.197$),[9] in perturbation theory ($\Delta=0.187$),[2] in exact diagonalization on a small finite-size lattice ($\Delta=0.257$),[10] in a Monte Carlo simulation on a small finite-size lattice ($\Delta=0.20$),[1] and in the equation-of-motion method ($\Delta=0.14$).[11] Experimental measurements have been made in K_2MnF_4 and Rb_2MnF_4 ($\Delta=0.17\pm0.03$),[12] and in K_2MnF_4 and K_2NiF_4 ($\Delta=0.20\pm0.03$).[13] House thinks that LSW theory is valid only in the limit of large S, and therefore LSW theory overestimates the spin reduction in this unfavorable ($S=\frac{1}{2}$) case.[2] Anderson also thinks that LSW theory is not a good approximation for the case of $S=\frac{1}{2}$ because it takes $1/S=2$ as a small expansion parameter.[9] Recently, many papers concerned only with the ground state of the Heisenberg antiferromagnet have appeared.[3-6] The temperature-dependent properties have not yet had the attention they deserve. Some modified spin-wave theories, such as the Dyson-Maleev transformation[7] and the Wigner-Jordan transformation[8] for spin operators, have been proposed. We will propose a modified spin-wave theory with temperature-dependent spin-wave spectrum and magnetization for anisotropic ferromagnets and antiferromagnets, and apply our theory to the square-lattice antiferromagnet.

In Sec. II and the Appendix, we show that the Abrikosov pseudofermion method can be extended to the Heisenberg Hamiltonian with spin $\frac{1}{2}$, and quantum field theory can be used very conveniently to treat the anisotropic Heisenberg Hamiltonian with spin $\frac{1}{2}$. In Sec. III, we derive the anisotropic and temperature-dependent spin-wave spectrum for the Heisenberg ferromagnet. In Sec. IV, we derive the anisotropic and temperature-dependent spin-wave spectrum and staggered magnetization for the antiferromagnet. In Sec. V are the numerical calculations for the two-dimensional (2D) square-lattice Heisenberg antiferromagnet and some discussion.

II. PSEUDOFERMION METHOD FOR THE ANISOTROPIC HEISENBERG HAMILTONIAN WITH SPIN $\frac{1}{2}$

The Heisenberg Hamiltonian is

$$H=-2\sum_{i>j}[J_z\hat{\mathbf{S}}_i^z\hat{\mathbf{S}}_j^z+J_x\hat{\mathbf{S}}_i^x\hat{\mathbf{S}}_j^x+J_y\hat{\mathbf{S}}_i^y\hat{\mathbf{S}}_j^y]\ , \tag{1}$$

where $\hat{\mathbf{S}}_i$ is the spin operator with spin $\frac{1}{2}$ on site i and $J\gtrless0$. We consider only the nearest-neighbor interaction. To treat the Kondo s-d Hamiltonian, Abrikosov introduced the pseudofermion representation for the local spin operator[14-16] $\hat{\mathbf{S}}_i$ as follows:

$$\hat{\mathbf{S}}_i=\sum_{ss'}\mathbf{S}_{ss'}a_{is}^{\dagger}a_{is'}\ , \tag{2}$$

where $a_{is}^{\dagger}$ and $a_{is'}$ are the so-called pseudofermion operators obeying the usual fermion anticommutation rules, $\mathbf{S}=\boldsymbol{\sigma}/2$, $\boldsymbol{\sigma}$ is the Pauli matrix, s and s' are the z components of $\hat{S}_i^z$, and $s=-\frac{1}{2},\frac{1}{2}$. We will show that one can also very conveniently use the pseudofermion representa-

tion to treat the Heisenberg Hamiltonian with spin $\frac{1}{2}$.

Using Eq. (2), Eq. (1) can be rewritten as

$$H=-2\sum_{i>j\alpha\alpha'\beta\beta'}[J_zS^z_{\alpha\alpha'}S^z_{\beta\beta'}+J_xS^x_{\alpha\alpha'}S^x_{\beta\beta'}+J_yS^y_{\alpha\alpha'}S^y_{\beta\beta'}]\times a^\dagger_{i\alpha}a_{i\alpha'}a^\dagger_{j\beta}a_{j\beta'}\ . \tag{3}$$

The eigenstates of $\hat{n}_i=\sum_s a^\dagger_{is}a_{is}$ are $|n\rangle_i=|n_{i\uparrow}n_{i\downarrow}\rangle$ $=|01\rangle$, $|10\rangle$, $|00\rangle$, and $|11\rangle$, in which only two eigenstates, $|01\rangle$ and $|10\rangle$, correspond to correct magnitudes of the spin at site i. These are called true states. The other two states do not correspond to correct magnitudes of the spin at site i and are called spurious states. The eigenstates of $\hat{n}_i\hat{n}_j=\sum_\alpha a^\dagger_{i\alpha}a_{i\alpha}\sum_\beta a^\dagger_{j\beta}a_{j\beta}$ are $|n\rangle_{ij}$ $=|n_{i\uparrow}n_{i\downarrow}\rangle|n_{j\uparrow}n_{j\downarrow}\rangle$. There are altogether 16 states, where only four eigenstates, $|01\rangle|01\rangle$, $|10\rangle|10\rangle$, $|01\rangle|10\rangle$, and $|10\rangle|01\rangle$, correspond to true states, and the other 12 eigenstates do not correspond to correct magnitudes of spins at sites i or j, and are thus called spurious states. If we consider the 16 eigenstates in statistical average, i.e., the total state average, then we are able to use the standard diagram method of quantum statistical theory to treat the Heisenberg Hamiltonian, Eq. (3). For example, we consider the pseudofermion Green's function. The definition of the Green's function is

$$\begin{aligned}G_{(ij)}&=-\langle T_\tau\{\bar{a}_{i\uparrow}(\tau)\bar{a}^\dagger_{j\uparrow}\}\rangle\\&=-\langle T_\tau\{e^{\tau H}a_{i\uparrow}e^{-\tau H}a^\dagger_{j\uparrow}\}\rangle\\&=-\langle D\rangle_{(N)}\ ,\end{aligned} \tag{4}$$

where the subscripts (ij) and (N) mean the total state average on the lattice, T_τ is the imaginary-time-ordering operator,

$$\langle\cdots\rangle=\frac{\mathrm{Tr}(\rho\cdots)}{\mathrm{Tr}\rho}\ , \tag{5}$$

$$\rho=e^{-H/T}\ , \tag{6}$$

$$\mathrm{Tr}(\cdots)=\sum_{\{n_1,\ldots,n_N\}_{(N)}1,2,\ldots,N}\langle n|\cdots|n\rangle_{1,2,\ldots,N}\ , \tag{7}$$

where the subscript (N) means the total states of the lattice and $|n\rangle_{1,2,\ldots,N}$ is the state of N sites. We should freeze out the spurious states from the thermal statistical average, and thus obtain the true Green's function G corresponding to the true state average. We show in the Appendix that

$$G=G_{(ij)}\ . \tag{8}$$

That the spurious states do not contribute to the average is similar to Abrikosov's idea that the infinite-energy limit of the pseudofermion can freeze out the spurious states.[14] Equation (8) is a very useful formula which tells us that, to calculate the Green's function corresponding to the true state average, one can directly calculate the Green's function corresponding to the total state average. For the latter, one can use the standard quantum-field-theory method including the Wick theorem.

III. TEMPERATURE-DEPENDENT SPIN-WAVE SPECTRUM OF THE ANISOTROPIC HEISENBERG FERROMAGNET

First let us calculate the spin-wave spectrum of the Heisenberg ferromagnet with spin $\frac{1}{2}$ ($J>0$) by using Eq. (8). To obtain the spin-wave spectrum, we should treat the following spin-flip Green's function:[17]

$$G(i,j;\tau)=-\langle T_\tau(\tilde{S}^+_i(\tau)\tilde{S}^-_j(0))\rangle\ , \tag{9}$$

where

$$\tilde{S}^+_i(\tau)=e^{\tau H}a^\dagger_{i\uparrow}e^{-\tau H}e^{\tau H}a_{i\downarrow}e^{-\tau H}\ , \tag{10}$$

$$\tilde{S}^-_j(0)=a^\dagger_{j\downarrow}a_{j\uparrow}\ , \tag{11}$$

$$G(i,j;\tau)=\frac{1}{N}\sum_{\mathbf{k}'}e^{i\mathbf{k}'\cdot(\mathbf{R}_i-\mathbf{R}_j)}G(\mathbf{k}',\tau)\ , \tag{12}$$

where N is the number of local spins. Substituting Eqs. (9)–(11) into Eq. (12) and making the Fourier transformation for $a_{i\uparrow}$ and so on gives

$$\begin{aligned}G(\mathbf{k},\tau)&=-\frac{1}{N}\sum_{\mathbf{k}_2\mathbf{k}_4}\langle T_\tau(\bar{a}^\dagger_{-k+k_2\uparrow}(\tau)\bar{a}_{k_2\downarrow}(\tau)\bar{a}^\dagger_{k+k_4\downarrow}(0)\bar{a}_{k_4\uparrow}(0))\rangle\\&=\frac{1}{N}\sum_{\mathbf{k}_2\mathbf{k}_4}G_{k_2k_4}(\mathbf{k},\tau)=\frac{1}{N}\sum_{\mathbf{k}_2\mathbf{k}_4}T\sum_{\omega_n}e^{-i\omega_n\tau}G_{k_2k_4}(\mathbf{k},\omega_n)=T\sum_{\omega_n}e^{-i\omega_n\tau}G(\mathbf{k},\omega_n)\ ,\end{aligned} \tag{13}$$

where $\omega_n=2n\pi T$ and n are positive and negative integers. To write the expression of the Feynman diagrams, we should do the Fourier transformation for the Hamiltonian given in Eq. (3):

$$\begin{aligned}H=&-\frac{J_z}{4N}\sum_{\mathbf{k}'_2\mathbf{k}'_3\mathbf{k}'_4\mathbf{R}_i-\mathbf{R}_j}(a^\dagger_{k'_2-k'_3+k'_4\uparrow}a_{k'_2\uparrow}-a^\dagger_{k'_2-k'_3+k'_4\downarrow}a_{k'_2\downarrow})(a^\dagger_{k'_3\uparrow}a_{k'_4\uparrow}-a^\dagger_{k'_3\downarrow}a_{k'_4\downarrow})e^{i(\mathbf{k}'_3-\mathbf{k}'_4)\cdot(\mathbf{R}_i-\mathbf{R}_j)}\\&-\frac{J_x+J_y}{4N}\sum_{\mathbf{k}'_2\mathbf{k}'_3\mathbf{k}'_4\mathbf{R}_i-\mathbf{R}_j}(a^\dagger_{k'_2-k'_3+k'_4\uparrow}a_{k'_2\downarrow}a^\dagger_{k'_3\downarrow}a_{k'_4\uparrow}+a^\dagger_{k'_2-k'_3+k'_4\downarrow}a_{k'_2\uparrow}a^\dagger_{k'_3\uparrow}a_{k'_4\downarrow})e^{i(\mathbf{k}'_3-\mathbf{k}'_4)\cdot(\mathbf{R}_i-\mathbf{R}_j)}\\=&H_{zz}+H_{\uparrow\downarrow}\ .\end{aligned} \tag{14}$$

Now our task is to find the Green's function under the two-body interaction given by Eq. (14) by using the ordinary quantum field theory including the linked-cluster theorem, i.e., Wick's theorem. In the random-phase approximation (RPA), $G(\mathbf{k},\omega_n)$ can be expressed as in Fig. 1,

$$J_{\parallel}(\mathbf{k})=\frac{J_x+J_y}{2}\sum_{\mathbf{a}_i} e^{i\mathbf{k}\cdot\mathbf{a}_i} , \tag{15}$$

where the summation is over the nearest-neighbor sites of the original site. The reason that the dot in Fig. 1 is $-J_{\parallel}(\mathbf{k})$ is as follows. The sign of the diagram with two bubbles is $(-1)(-1)2$, where the first -1 comes from first-order perturbation of $H_{\uparrow\downarrow}$ in Eq. (14), the second -1 comes from one fermion bubble, and 2 comes from two possibilities of connection of the two bubbles in using $H_{\uparrow\downarrow}$. The pseudofermion Green's function $g_{\uparrow(\downarrow)}$ in Fig. 1 can be expressed as in Fig. 2. We define

$$\langle \hat{S}_i^z\rangle_I=\langle \tfrac{1}{2}(a_{i\uparrow}^{\dagger}a_{i\uparrow}-a_{i\downarrow}^{\dagger}a_{i\downarrow})\rangle$$
$$=\frac{1}{2N}\sum_{\mathbf{k}_1} T\sum_{\omega_{n'}} e^{-i\omega_{n'}(-0^+)}[g_{\uparrow}(\mathbf{k}_1,\omega_{n'}-g_{\downarrow}(\mathbf{k}_1,\omega_{n'})] , \tag{16}$$

$$g_{0\uparrow}(\mathbf{k},\omega_{n'})=\frac{1}{i\omega_{n'}} , \tag{17}$$

where $\omega_{n'}=(2n'+1)\pi T$. Substituting Eqs. (16) and (17) into Fig. 2 gives

$$g_{\downarrow}(\mathbf{k},\omega_{n'})=\frac{1}{i\omega_{n'}+J_z(0)\langle \hat{S}_i^z\rangle_I} , \tag{18}$$

$$J_z(0)=J_z\sum_{\mathbf{a}_i} 1 . \tag{19}$$

Similarly,

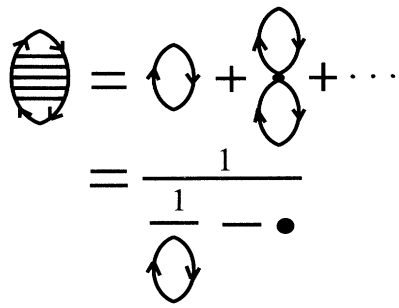

FIG. 1. Feynman diagram representation in the RPA for $G(\mathbf{k},\omega_n)$. The thick line is a pseudofermion Green's function $g_{\uparrow(\downarrow)}(\mathbf{k},\omega_n)$, and is determined by Fig. 2. The dot is $-J_{\parallel}(\mathbf{k})$ [see Eq. (15)].

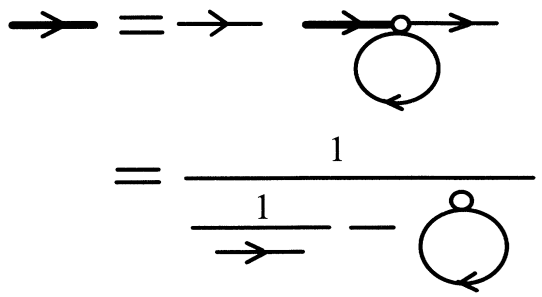

FIG. 2. Feynman diagram representation for the pseudofermion Green's function $g_{\uparrow}(\mathbf{k},\omega_n)$. The fine line is the free pseudofermion Green's function $g_{0\uparrow}(\mathbf{k},\omega_n)$. The small circle is $-J_z(0)$ [see Eq. (19)]. The thick-line circle is the average value of the z component of the local spin at site i in the Ising model, $\langle \hat{S}_i^z\rangle_I$ [see Eqs. (16) and (21)].

$$g_{\downarrow}(\mathbf{k},\omega_{n'})=\frac{1}{i\omega_{n'}-J_z(0)\langle \hat{S}_i^z\rangle_I} . \tag{20}$$

Substituting Eqs. (20) and (18) into Eq. (16) gives

$$\langle \hat{S}_i^z\rangle_I=\frac{1}{2}\frac{e^{J_z(0)\langle \hat{S}_i^z\rangle_I/2T}-e^{-J_z(0)\langle \hat{S}_i^z\rangle_I/2T}}{e^{J_z(0)\langle \hat{S}_i^z\rangle_I/2T}+e^{-J_z(0)\langle \hat{S}_i^z\rangle_I/2T}} . \tag{21}$$

At $T=0$ K,

$$\langle \hat{S}_i^z\rangle_I=\tfrac{1}{2} . \tag{22}$$

Using Eqs. (18) and (20)–(22), the bubble consisting of two pseudofermion Green's functions in Fig. 1, $g_{2\uparrow\downarrow}$, is

$$g_{2\uparrow\downarrow}=\frac{2\langle \hat{S}_i^z\rangle_I}{i\omega_n-2J_z(0)\langle \hat{S}_i^z\rangle_I} . \tag{23}$$

Substituting Eq. (23) into Fig. 1 and considering Eq. (13) gives

$$G(\mathbf{k},\omega_n)=\frac{2\langle \hat{S}_i^z\rangle_I}{i\omega_n-2\langle \hat{S}_i^z\rangle_I[J_z(0)-J_{\parallel}(\mathbf{k})]} , \tag{24}$$

$$G(\mathbf{k},\omega+i0^+)=\frac{2\langle \hat{S}_i^z\rangle_I}{\omega+i0^+-2\langle \hat{S}_i^z\rangle_I[J_z(0)-J_{\parallel}(\mathbf{k})]} . \tag{25}$$

From Eq. (25), we have the spin-wave spectrum $\epsilon(\mathbf{k})$:

$$\epsilon(\mathbf{k})=2\langle \hat{S}_i^z\rangle_I[J_z(0)-J_{\parallel}(\mathbf{k})] . \tag{26}$$

IV. THE ANISOTROPIC HEISENBERG ANTIFERROMAGNET

Now let us derive the spin-wave spectrum for the Heisenberg antiferromagnet ($J<0$) with spin $\frac{1}{2}$. For simplicity, we consider only a simple lattice. We denote the up spins as the A sublattice and the down spins as the B sublattice. In the case of two sublattices, the Hamiltonian in Eq. (14) becomes

$$H=-\frac{J_z}{4}\frac{2}{N}\sum_{\mathbf{k}_2'\mathbf{k}_3'\mathbf{k}_4'\mathbf{R}_{iA}-\mathbf{R}_{jB}}(a^{\dagger}_{Ak_2'-k_3'+k_4'\uparrow}a_{Ak_2'\uparrow}-a^{\dagger}_{Ak_2'-k_3'+k_4'\downarrow}a_{Ak_2'\downarrow})(a^{\dagger}_{Bk_3'\uparrow}a_{Bk_4'\uparrow}-a^{\dagger}_{Bk_3'\downarrow}a_{Bk_4'\downarrow})e^{i(\mathbf{k}_3'-\mathbf{k}_4')\cdot(\mathbf{R}_{iA}-\mathbf{R}_{jB})}$$
$$-\frac{J_x+J_y}{4}\frac{2}{N}\sum_{\mathbf{k}_2'\mathbf{k}_3'\mathbf{k}_4'\mathbf{R}_{iA}-\mathbf{R}_{jB}}(a^{\dagger}_{Ak_2'-k_3'+k_4'\uparrow}a_{Ak_2'\downarrow}a^{\dagger}_{Bk_3'\downarrow}a_{Bk_4'\uparrow}+a^{\dagger}_{Ak_2'-k_3'+k_4'\downarrow}a_{Ak_2'\uparrow}a^{\dagger}_{Bk_3'\uparrow}a_{Bk_4'\downarrow})e^{i(\mathbf{k}_3'-\mathbf{k}_4')\cdot(\mathbf{R}_{iA}-\mathbf{R}_{jB})}$$
$$=H_{zz}+H_{\uparrow\downarrow}\ . \tag{27}$$

To find the spectrum, we introduce the following spin-flip Green's functions,

$$G(iA,jA;\tau)=-\langle T_\tau[\tilde{S}^+_{iA}(\tau)\tilde{S}^-_{jA}(0)]\rangle$$
$$=\frac{2}{N}\sum_{\mathbf{k}'}e^{i\mathbf{k}'\cdot(\mathbf{R}_{iA}-\mathbf{R}_{jA})}G_{AA}(\mathbf{k}',\tau)\ , \tag{28}$$

$$G_{AA}(\mathbf{k},\tau)=\frac{2}{N}\sum_{\mathbf{k}_2\mathbf{k}_4}-\langle T_\tau[\tilde{a}^{\dagger}_{A-k+k_2\uparrow}(\tau)\tilde{a}_{Ak_2\downarrow}(\tau)\times\tilde{a}^{\dagger}_{Ak+k_4\downarrow}a_{Ak_4\uparrow}]\rangle$$
$$=T\sum_{\omega_n}e^{-i\omega_n\tau}G_{AA}(\mathbf{k},\omega_n)\ , \tag{29}$$

$$G_{AB}(iA,jB;\tau)=-\langle T_\tau[\tilde{S}^+_{iA}(\tau)\tilde{S}^-_{jB}(0)]\rangle$$
$$=\frac{2}{N}\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot(\mathbf{R}_{iA}-\mathbf{R}_{jB})}G_{AB}(\mathbf{k},\tau)\ , \tag{30}$$

$$G_{AB}(\mathbf{k},\tau)=T\sum_{\omega_n}e^{-i\omega_n\tau}G_{AB}(\mathbf{k},\omega_n)\ . \tag{31}$$

$G_{AA}(\mathbf{k},\omega_n)$ and $G_{AB}(\mathbf{k},\omega_n)$ are shown in Figs. 3 and 4. The dot in Figs. 3 and 4 is $-J_\parallel(\mathbf{k})/2$ because there is only one possibility to connect the two bubbles. We obtain Fig. 5 from Figs. 3 and 4. The bubbles consisting of two pseudofermion Green's functions in Fig. 5, $g_{2AA\uparrow\downarrow}$ and $g_{2BB\uparrow\downarrow}$, can be calculated as we did for $g_{2\uparrow\downarrow}$ in Eq. (23),

$$g_{2AA\uparrow\downarrow}=\frac{2\langle\hat{S}^z_{iA}\rangle_I}{i\omega_n-J_z(0)\langle\hat{S}^z_{iB}\rangle_I}\ , \tag{32}$$

$$g_{2BB\uparrow\downarrow}=\frac{-2\langle\hat{S}^z_{iA}\rangle_i}{i\omega_n-J_z(0)\langle\hat{S}^z_{iA}\rangle_I}\ , \tag{33}$$

$$\langle\hat{S}^z_{iA}\rangle_I=\frac{1}{2}\frac{e^{|J_z(0)|\langle\hat{S}^z_{iA}\rangle_I/4T}-e^{-|J_z(0)|\langle\hat{S}^z_{iA}\rangle_I/4T}}{e^{|J_z(0)|\langle\hat{S}^z_{iA}\rangle_I/4T}+e^{-|J_z(0)|\langle\hat{S}^z_{iA}\rangle_I/4T}}\ . \tag{34}$$

Substituting Eqs. (32)–(34) into Fig. 5 and noting that $\langle\hat{S}^z_{iB}\rangle_I=-\langle\hat{S}^z_{iA}\rangle_I<0$ gives

$$G_{AA}(\mathbf{k},\omega_n)=\frac{2\langle\hat{S}^z_{iA}\rangle_I[i\omega_n-J_z(0)\langle\hat{S}^z_{iA}\rangle_I]}{\{i\omega_n+\langle\hat{S}^z_{iA}\rangle_I\sqrt{J_z(0)^2-J_\parallel(\mathbf{k})^2}\}\{i\omega_n-\langle\hat{S}^z_{iA}\rangle_I\sqrt{J_z(0)^2-J_\parallel(\mathbf{k})^2}\}}\ . \tag{35}$$

From the expression of $G_{AA}(\mathbf{k},\omega+i0^+)$, we know the spin-wave spectrum is

$$\epsilon(\mathbf{k})=\langle\hat{S}^z_{iA}\rangle_I\sqrt{[J_z(0)]^2-[J_\parallel(\mathbf{k})]^2}$$
$$=\langle\hat{S}^z_{iA}\rangle_I 4|J_z|\times\left[1-\left[\frac{1}{z}\sum_{\mathbf{a}_i}\cos\mathbf{k}\cdot\mathbf{a}_i\right]^2\left[\frac{J_x+J_y}{2J_z}\right]^2\right]^{1/2}\ . \tag{36}$$

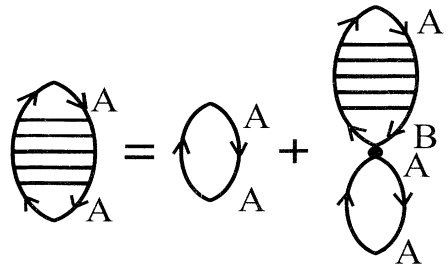

FIG. 3. Feynman diagram of $G_{AA}(\mathbf{k},\omega_n)$. The dot is $-J_\parallel(\mathbf{k})/2$.

Considering Eqs. (34), (36), (15), and (19), we know the spin-wave spectrum at $T=0$ K is

$$\epsilon(\mathbf{k})=|J_z|zS\times\left[1-\left[\frac{1}{z}\sum_{\mathbf{a}_i}\cos(\mathbf{k}\cdot\mathbf{a}_i)\right]^2\left[\frac{J_x+J_y}{2J_z}\right]^2\right]^{1/2}\ , \tag{37}$$

where $\mathbf{a}_i$ is a vector connecting any local spin with any of its z nearest neighbors. Equation (37) with

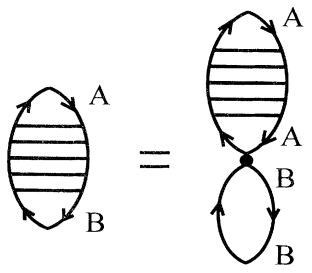

FIG. 4. Feynman diagram of $G_{AB}(\mathbf{k},\omega_n)$.

$J_z=(J_x+J_y)/2$ is the same as given by LSW theory.[9] In LSW theory, there is doubt as to the validity of Eq. (37) because $1/S=2$ is not a small parameter. In our pseudofermion method, Eq. (37) comes from the RPA, $T=0$ K, and anisotropy, and does not use the condition of $S=\frac{1}{2}$. The staggered magnetization for a simple lattice can be calculated as follows. We know

$$\hat{S}_{iA}^{-}\hat{S}_{iA}^{+}=\tfrac{1}{2}-\hat{S}_{iA}^{z} . \tag{38}$$

So

$$\langle \hat{S}_{iA}^{z} \rangle=\tfrac{1}{2}+G(iA,iA;-0^{+})$$
$$=\frac{1}{2}+\frac{2}{N}\sum_{\mathbf{k}} T\sum_{\omega_n} e^{-i\omega_n(-0^{+})} G_{AA}(\mathbf{k},\omega_n) . \tag{39}$$

Substituting Eq. (35) into Eq. (39) gives

$$\langle \hat{S}_{iA}^{z} \rangle=\frac{1}{2}-\langle \hat{S}_{iA}^{z} \rangle_I \frac{2}{N}\sum_{\mathbf{k}} \left\{ \coth\frac{\epsilon(\mathbf{k})}{2T} \Big/ \left[1-\left[\frac{1}{z}\sum_{\mathbf{a}_i} \cos\mathbf{k}\cdot\mathbf{a}_i \right]^2 \left[\frac{J_x-J_y}{2J_z} \right]^2 \right]^{1/2} -1 \right\} . \tag{40}$$

V. NUMERICAL CALCULATIONS FOR THE SQUARE-LATTICE HEISENBERG ANTIFERROMAGNET

The quantum antiferromagnetic Heisenberg model on a square lattice has aroused much interest recently due to its connection to high-T_c superconductivity, but many important issues remain unresolved. Based on the general formulas given in Sec. IV, this section makes some numerical calculations.

First we calculate the temperature dependence of the staggered magnetization to find the Néel temperature. Assume $J_x=J_y=J_z=J<0$. Substituting Eqs. (36) and (34) into Eq. (40) and performing numerical integration, we obtain the curve of the staggered magnetization $\langle \hat{S}_{iA}^{z} \rangle$ versus temperature $T/|J|$, which is shown in Fig. 6. From the numerical calculation, we obtain the staggered magnetization at $T=0$ K as 0.3017. The corresponding Monte Carlo value is 0.30.[1] The antiferromagnetic transition temperature, i.e., the Néel temperature T_N, can be determined by $\langle \hat{S}_{iA}^{z} \rangle=0$ from Fig. 6, and it is $T_N=0.323|J|$. The experimental value of $|J|$ is 0.1 eV.[18] So our theoretical value is $T_N=374$ K. The experimental value for La_2CuO_4 is $T_N=326$ K.[19]

The coefficient of the spin-wave spectrum in Eq. (36) is $\langle \hat{S}_{iA}^{z} \rangle_I 4|J|$. The temperature dependence of $\langle \hat{S}_{iA}^{z} \rangle_I$ is shown in Fig. 6 as well. The coefficients at $T=0$ K and $T=0.5|J|$ are $2|J|$ and 0, respectively. However, the corresponding coefficients in Ref. 8 are $1.479|J|$ and $1.46|J|$, respectively. In Ref. 8, even if $T=4.0|J|$, the coefficient is still not equal to zero. The discrepancy between Ref. 8 and our theory on the coefficient awaits further experimental discrimination. At this time, we would like to say that the conclusion of Ref. 8 is not physically reasonable. For example, $|J|=0.1$ eV for high-T_c superconductors, and thus $T=4|J|=4600$ K $\gg T_N$. As we know, there should be no spin wave and long-range order when $T>T_N$.

The anisotropy has an important effect on the staggered magnetization. Assuming $|(J_x+J_y)/(2J_z)|=0.99$ and $T=0$ K, we obtain $\langle \hat{S}_{iA}^{z} \rangle=0.34$ for a square lattice from Eq. (40). Thus the anisotropy might be the origin of the dispersion of the experimental data in Refs. 12 and 13.

Note that the equation-of-motion method is different from our Eq. (40). In the former, the $\langle \hat{S}_{iA}^{z} \rangle_I$ in our Eq. (40) is substituted by $\langle \hat{S}_{iA}^{z} \rangle$, and thus $\langle S_{iA}^{z} \rangle=0.36$ at $T=0$ K, which is different from the experimental data.[12,13] The most serious defect of the equation-of-motion method is that it contradicts charge neutrality,[16] but our quantum-field-theory approach can solve the problem without contradicting charge neutrality.[16]

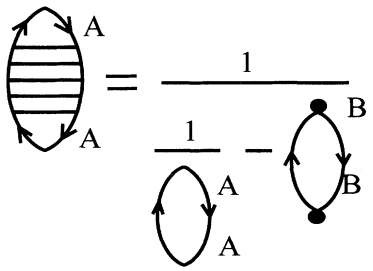

FIG. 5. Feynman diagram of $G_{AA}(\mathbf{k},\omega_n)$ in the RPA.

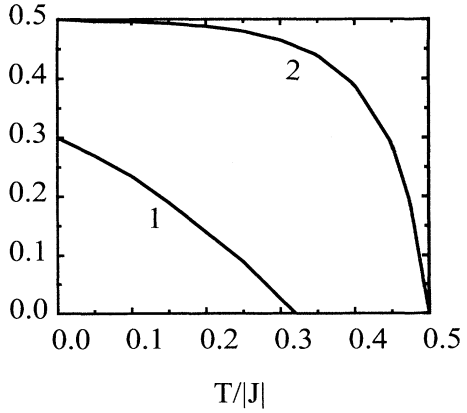

FIG. 6. Line 1 is the curve of the staggered magnetization $\langle \hat{S}_{iA}^{z} \rangle$ vs $T/|J|$, and line 2 is the curve of the coefficient $\langle \hat{S}_{iA}^{z} \rangle_I$ in Eq. (36) vs $T/|J|$.

There is a major difference between our Eqs. (26) and (36) and Ref. 20. For the Ising model ($J_x=J_y=0$, $J_z\neq 0$), there is no spin wave in our theory, but there is a spin wave in the case of the 2D Ising model in Ref. 20.

APPENDIX

To use Larsen's method[15] to freeze out the spurious states, we rewrite Eq. (3) as

$$H=-2\sum_{i>j}^{(N-1)}[J_z\hat{S}_i^z\hat{S}_i^z+J_x\hat{S}_i^x\hat{S}_j^x+J_y\hat{S}_i^y\hat{S}_j^y]-2\sum_{j(>1)ss'}[J_z\hat{S}_j^z\hat{S}_{1ss'}^z+J_x\hat{S}_j^x\hat{S}_{1ss'}^x+J_y\hat{S}_j^y\hat{S}_{1ss'}^y]a_{1s}^{\dagger}a_{1s'}$$

$$=H^{(N-1)}-2\sum_{j(>1)ss'}[J_z\hat{S}_j^zS_{1ss'}^z+J_x\hat{S}_j^xS_{1ss'}^x+J_y\hat{S}_j^yS_{1ss'}^y]a_{1s}^{\dagger}a_{1s'}\ , \tag{A1}$$

where the superscript $(N-1)$ means that there is no site 1 in the summation over i and j. Only the site 1 is shown by the pseudofermion representation in Eq. (A1), so the spurious states are only contained at site 1. From the definition, we have the following equation:

$$\langle D\rangle^{(N-1)1}=\frac{\mathrm{Tr}^{(N-1)1}(\rho D)}{\mathrm{Tr}^{(N-1)1}\rho}$$

$$=\frac{\mathrm{Tr}_1^{(N-1)}(\rho D)}{\mathrm{Tr}_1^{(N-1)}\rho}\frac{\mathrm{Tr}^{(N-1)1}(\rho D)}{\mathrm{Tr}_1^{(N-1)}(\rho D)}\frac{\mathrm{Tr}_1^{(N-1)}\rho}{\mathrm{Tr}^{(N-1)1}\rho}$$

$$=\langle D\rangle_1^{(N-1)}\frac{\mathrm{Tr}^{(N-1)1}(\rho D)}{\mathrm{Tr}_1^{(N-1)}(\rho D)}\frac{\mathrm{Tr}_1^{(N-1)}\rho}{\mathrm{Tr}^{(N-1)1}\rho}\ , \tag{A2}$$

where the superscript $(N-1)1$ means the true state average on the lattice as well as (N), the single subscript 1 means the total state on site 1, and the superscript $(N-1)$ the true states on $N-1$ sites. From the definition, we have

$$\mathrm{Tr}_1^{(N-1)}(\rho D)=\sum_{\{n_2,\ldots,n_N\}^{(N-1)}}{}_{2,\ldots,N}\langle n|\{{}_1\langle 00|\rho D|00\rangle_1+{}_1\langle 11|\rho D|11\rangle_1+{}_1\langle 10|\rho D|10\rangle_1$$

$$+{}_1\langle 01|\rho D|01\rangle_1\}|n\rangle_{2,\ldots,N}\ . \tag{A3}$$

We define

$$\rho^{(N-1)}=e^{-H^{(N-1)}/T}\ , \tag{A4}$$

$$D^{(N-1)}=T_\tau e^{\tau H^{(N-1)}}a_{i\uparrow}e^{-\tau H^{(N-1)}}a_{j\uparrow}^{\dagger}\ . \tag{A5}$$

Considering[15]

$$\sum_{ss'}\mathbf{S}_{ss'}a_{1s}^{\dagger}a_{1s'}|00\rangle_1=\sum_{ss'}\mathbf{S}_{ss'}a_{1s}^{\dagger}a_{1s'}|11\rangle_1=0\ , \tag{A6}$$

Eq. (A3) can be rewritten as

$$\mathrm{Tr}_1^{(N-1)}(\rho D)=\tfrac{1}{2}\mathrm{Tr}_1^{(N-1)}(\rho^{(N-1)}D^{(N-1)})+\mathrm{Tr}^{(N-1)1}(\rho D)\ . \tag{A7}$$

The second factor in Eq. (A2) can be rewritten as

$$\frac{\mathrm{Tr}^{(N-1)1}(\rho D)}{\mathrm{Tr}_1^{(N-1)}(\rho D)}=1-\frac{1}{2}\frac{\langle D^{(N-1)}\rangle_1^{(N-1)}}{\langle D\rangle_1^{(N-1)}\mathrm{Tr}_1^{(N-1)}\rho/\mathrm{Tr}_1^{(N-1)}\rho^{(N-1)}}\ . \tag{A8}$$

Substituting Eq. (A8) into Eq. (A2) gives

$$\langle D\rangle^{(N-1)1}=\langle D\rangle_1^{(N-1)}\frac{\mathrm{Tr}_1^{(N-1)}\rho}{\mathrm{Tr}^{(N-1)1}\rho}-\frac{1}{2}\frac{\langle D^{(N-1)}\rangle_1^{(N-1)}\mathrm{Tr}_1^{(N-1)}\rho^{(N-1)}}{\mathrm{Tr}^{(N-1)1}\rho}\ . \tag{A9}$$

Because there is no site 1 in $D^{(N-1)}$ and $\rho^{(N-1)}$, we know from the definitions of $\langle\cdots\rangle$ and Tr that

$$\langle D^{(N-1)}\rangle_1^{(N-1)}=\langle D^{(N-1)}\rangle^{(N-1)}\ , \tag{A10}$$

$$\mathrm{Tr}_1^{(N-1)(N-1)}=4\,\mathrm{Tr}^{(N-1)}\rho^{(N-1)}\ . \tag{A11}$$

Equation (A9) can be rewritten as

$$\langle D\rangle^{(N-1)1}=\langle D\rangle_1^{(N-1)}\frac{\mathrm{Tr}_1^{(N-1)}\rho}{\mathrm{Tr}^{(N)}\rho}-\langle D^{(N-1)}\rangle^{(N-1)}\frac{2\,\mathrm{Tr}^{(N-1)}\rho^{(N-1)}}{\mathrm{Tr}^{(N)}\rho}\ . \tag{A12}$$

$\langle D\rangle_1^{(N-1)}$ means that the average is taken on the total state at site 1 and on the true states at all other sites. Let us continue the transformation to obtain $\langle D\rangle_{(N)}$ $(=\langle D\rangle_{1,2,\ldots,N})$ on the right side of Eq. (A12). From the same method as Eq. (A2), we obtain

$$\langle D\rangle_1^{(N-1)}=\langle D\rangle_{1,2}^{(N-1-2)}\frac{\mathrm{Tr}_1^{(N-1)}(\rho D)}{\mathrm{Tr}_{1,2}^{(N-1-2)}(\rho D)}\frac{\mathrm{Tr}_{1,2}^{(N-1-2)}\rho}{\mathrm{Tr}_1^{(N-1)}\rho}\ . \tag{A13}$$

Note that the 1 and 2 represent site 1 and site 2, respectively. Considering

$$\mathrm{Tr}_{1,2}^{(N-1-2)}(\rho D)=\mathrm{Tr}_1^{(N-1)}(\rho D)+2\,\mathrm{Tr}_{1,2}^{(N-1-2)}(\rho^{(N-2)}D^{(N-2)}) \tag{A14}$$

and Eq. (20), Eq. (19) an be rewritten as

$$\langle D\rangle^{(N)}=\langle D\rangle_{1,2}^{(N-1-2)}\frac{\mathrm{Tr}_{1,2}^{(N-1-2)}\rho}{\mathrm{Tr}^{(N)}\rho}$$
$$-\langle D^{(N-2)}\rangle_{1}^{(N-1-2)}\frac{2\,\mathrm{Tr}_{1}^{(N-1-2)}\rho^{(N-2)}}{\mathrm{Tr}^{(N)}\rho}-\langle D^{(N-1)}\rangle^{(N-1)}2\,\mathrm{Tr}^{(N-1)}\rho^{(N-1)}\,. \tag{A15}$$

We continue the transformations until $\langle D\rangle_{1,2,\ldots,N}$ appears on the right side of Eq. (A15). Finally, we obtain

$$\langle D\rangle^{(N)}=\frac{1}{\mathrm{Tr}^{(N)}\rho}[\langle D\rangle_{1,2,\ldots,N}\mathrm{Tr}_{1,2,\ldots,N}\rho-\langle D^{(N-N)}\rangle_{1,2,\ldots,N-1}2\,\mathrm{Tr}_{1,2,\ldots,N-1}\rho^{(N-N)}-\cdots$$
$$-\langle D^{(N-1)}\rangle^{(N-1)}2\,\mathrm{Tr}^{(N-1)}\rho^{(N-1)}]\,. \tag{A16}$$

From the basic definitions, $\mathrm{Tr}_{1,2,\ldots,N}\rho$ in Eq. (A16) can be rewritten as

$$\mathrm{Tr}_{1,2,\ldots,N}\rho=\mathrm{Tr}^{(N)}\rho+2\sum_{i=1}^{4}\mathrm{Tr}_{1,2,\ldots,i-1}^{(N-1-2\cdots-i)}\rho^{(N-i)}\,, \tag{A17}$$

where the factor 2 in Eq. (A17) comes from the fact that there are two spurious states at site i. For large systems, the averages on both the N local spin system and $(N-1)$ local spin system should be equal. Considering Eq. (A17), the consistent solution of Eq. (A6) is

$$\langle D\rangle^{(N)}=\langle D^{(N-1)}\rangle^{(N-1)}$$
$$=\cdots=\langle D^{(N-i)}\rangle_{1,2,\ldots,i-1}^{(N-1-2-\cdots-i)}$$
$$=\cdots=\langle D\rangle_{1,2,\ldots,N}\,, \tag{A18}$$

which means that the averages on both the true states and the total states are the same, i.e., the averages on spurious states do not contribute to the statistical averages. Because Eq. (A18) is very important, let us prove it in detail. If we assume that

$$\langle D\rangle^{(N)}=(1-Na)\langle D\rangle_{1,2,\ldots,N}\,, \tag{A19}$$

then

$$\langle D^{(N-i)}\rangle_{1,2,\ldots,i-1}^{(N-1-2-\cdots-i)}=[1-(N-i)a]\langle D\rangle_{1,2,\ldots,N}\,. \tag{A20}$$

Substituting Eqs. (A17), (A19), and (A20) into Eq. (A16) gives

$$(1-Na)=1+\frac{a}{\mathrm{Tr}^{(N)}\rho}[2\,\mathrm{Tr}_{1,2,\ldots,N-2}^{[N-1-2-\cdots-(N-1)]}\times\rho^{[N-(N-1)]}+\cdots$$
$$+(N-1)2\,\mathrm{Tr}^{(N-1)}\rho^{(N-1)}]\,. \tag{A21}$$

Because

$$\frac{1}{\mathrm{Tr}^{(N)}\rho}[2\,\mathrm{Tr}_{1,2,\ldots,N-2}^{[N-1-2-\cdots-(N-1)]}\rho^{[N-(N-1)]}+\cdots+(N-1)2\,\mathrm{Tr}^{(N-1)}\rho^{(N-1)}>0\,, \tag{A22}$$

we obtain $a=0$. From Eqs. (A18) and (4), we know that the true Green's function G is equal to $G_{(ij)}$.

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