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A non-linear spin-wave theory of quasi-2D quantum Heisenberg antiferromagnets

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Abstract. Based on the Hartree–Fock approximation we propose a non-linear spin-wave theory of anisotropic 3D (or quasi-2D) quantum Heisenberg antiferromagnets, which reduces to the known spin-wave theories of isotropy when our anisotropy parameter δ takes special values. In the Hartree–Fock approximation the Dyson-transformed Hamiltonian is equivalent to the Holstein–Primakoff-transformed Hamiltonian truncated up to quartic operator terms. The spin-wave lifetime is obtained in the first-order approximation. For very small δ, the Néel temperature T_N is much smaller than the coupling constant J, in contrast with $T_N \sim J$ in the 3D isotropic case, so that our non-linear anisotropic spin-wave theory is suitable for a description of the ordering phase as well as the paramagnetic phase (up to J) of layer-like antiferromagnets. Applied to the antiferromagnetism of the cuprate La_2CuO_4, our quasi-2D non-linear spin-wave theory describes quite satisfactorily the existing experimental data of the Néel transition temperature, the correlation length above the Néel temperature, and staggered magnetization of the material if $J = 1034$ K and the anisotropy parameter is set to be 4×10^{-5}.

1. Introduction

Quantum Heisenberg antiferromagnets (QHAFM) have recently attracted much attention due to their relevance to high-temperature oxide superconductivity. Undoped materials La_2CuO_4 and $RBa_2Cu_3O_6$ (where R is a rare-earth element) are insulating antiferromagnets (AFM) that can be described by QHAFM models [1,2]. Lightly doped cuprates are antiferromagnetic insulators. Even in heavily doped superconducting materials there are antiferromagnetic fluctuations that are believed to play some important roles in the superconductivity of the cuprates [3].

Conventional non-linear spin-wave theory [4,5], an improved version of linear spin-wave theory [6–8] established on Dyson's transformations of sublattice spin operators and the Hartree–Fock approximation, is a good approximation to the ordering states of isotropic QHAFM. However, it works only when the temperature T is smaller than the Néel temperature T_N [5]. Chakravarty, Halperin and Nelson (CHN) [9] have made a renormalization-group analysis of a (2+1)-dimensional non-linear sigma model to approach 2D QHAFM, concluding that the correlation length has a renormalization classical behaviour $\exp(A/T)$ where A is not equivalent to zero when T tends to zero. Auerbach and Arovas (AA) [10] have developed a large-N theory of the quantum Heisenberg model based on a Schwinger boson representation

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for a rotation-symmetrical disordered state. Hirsch and Tang (HT) [11] have shown by means of the Bose–Einstein condensation viewpoint that the AA theory holds as well for the ordering state. Hirsch *et al* [12] have developed a linear sublattice-symmetrical spin-wave theory by requiring that the sublattice magnetization be set to be zero, and then have compared it with exactly-diagonalized results on finite-size lattices. Takahashi [13] has presented a variational-modified spin-wave theory for the 2D square lattice, in which the spin-correlation length is same as the CHN one-loop result. It has been established [11, 12] that at low temperature, the AA, Takahashi and Hirsch theories are equivalent to each other except for a factor 3/2 in the AA theory. All of the three spin-wave theories mentioned above are based on the following isotropic quantum Heisenberg Hamiltonian:

$$H = J \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{1}$$

where $\langle ij \rangle$ is the nearest-neighbouring site pair, as in the following. The isotropic Hamiltonian is not appropriate for a complete description of anisotropic antiferromagnets such as the quasi-2D insulating cuprate antiferromagnets, because it yields $T_N \approx J$ for the 3D case and $T_N = 0$ for the 2D case. In [14] the random phase approximation (RPA) was used to investigate an anisotropic 3D quantum Heisenberg antiferromagnetic Hamiltonian such as

$$H = \sum_{\langle ij \rangle} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{2}$$

where $J_{ij} = J$ if $\langle ij \rangle$ is in the xy plane and $J_{ij} = \delta J$ if $\langle ij \rangle$ is parallel to the z axis. The Hamiltonian (2), with an appropriate δ in the RPA, describes quite well the antiferromagnetic ordering of the insulating cuprate La_2CuO_4 and $RBa_2Cu_3O_6$ materials [14]. As well as its advantage for quasi-2D antiferromagnets, the anisotropic Hamiltonian can also be used to describe quasi-1D antiferromagnets by letting $\delta J = J'$ and J to be smaller than J'.

In this paper we shall formulate a non-linear spin-wave theory for quasi-2D quantum Heisenberg antiferromagnets defined by the Hamiltonian (2), which in isotropic cases reduces to the conventional non-linear spin-wave theory when $T < T_N$ [4, 5], and leads to the same result as the variation-modified spin-wave theory [13]. Different from the Takahashi variational method and the Hirsch *et al* linearization method, our method is a Hartree–Fock approximation for the higher operator power terms. We prove that in the Hartree–Fock approximation the Dyson-transformed Hamiltonian [15] is equivalent to the Holstein–Primakoff-transformed Hamiltonian [16] truncated up to quartic operator terms. The spin-wave lifetime is obtained in the first-order approximation. For the 2D isotropic case we obtain Takahashi's results, including the CHN one-loop renormalization-group behaviour of correlation length and the AA correlation functions except the factor of 3/2. The ground-state energy in our theory is $-0.335NJZ$ for the 2D square lattice, being equivalent to the digital result on 32×32 sites [17]. With the anisotropy parameter δ decreasing, our anisotropic theory yields a decreasing Néel temperature T_N; $T_N = 0$ if $\delta = 0$. The Néel temperature T_N is much smaller than J if δ is very small. When $T_N \ll J$, our theory is expected to work well not only for $T < T_N$ but also for $T \geqslant T_N$. Our theory is very suitable for a description of quasi-2D (or layer-like)

quantum Heisenberg antiferromagnets such as the interesting insulating cuprates. Applied to the antiferromagnetism of the cuprate La_2CuO_4, our quasi-2D non-linear spin-wave theory describes quite satisfactorily the existing experimental data of the Néel transition temperature, the correlation length above the Néel temperature, and staggered magnetization of the material if $J = 1034$ K and the anisotropy parameter is set to be 4×10^{-5}.

In section 2 we propose the general theoretical framework of our quasi-2D non-linear (Hartree–Fock) spin-wave theory. In section 3 we calculate the interaction correction beyond the Hartree–Fock theory. In section 4 we derive 2D and 3D isotropic theories as two special cases of the anisotropic theory, and compare the 2D theory with other results. In section 5 we discuss the quasi-2D case and its application to the insulating cuprate antiferromagnets. Section 6 includes some further discussions and our conclusion.

2. General Hartree–Fock theoretical framework

We first divide our lattice into two sublattices, A and B, such that any site of sublattice A has all its nearest-neighbouring sites in sublattice B, and *vice versa*. We shall make Dyson's transformations for spin operators in sublattices A and B, respectively. Afterwards we transform to momentum space, or k space. After making a Hartree–Fock approximation for the quartic terms of the Dyson boson operators, our Hamiltonian will be bilinear in the operators so that we can diagonalize it by means of a Bogoliubov transformation. As a result, we shall obtain a set of self-consistent equations. These equations will determine all physical properties at the Hartree–Fock level. In addition, we shall prove that at the Hartree–Fock approximate level the Dyson-transformed Hamiltonian is equivalent to Holstein–Primakoff-transformed Hamiltonian.

On this bipartite lattice our quasi-2D QHAFM Hamiltonian (2) is

$$H = \sum_{(mn)} J_{mn} \boldsymbol{S}_m \cdot \boldsymbol{S}_n = \sum_{(mn)} J_{mn}[S_m^3 S_n^3 + \tfrac{1}{2}(S_m^+ S_n^- + S_m^- S_n^+)] \tag{3}$$

where m labels the site of lattice A and n the site of lattice B. Here, for generality, J_{mn} is direction dependent, $J_{xy} = J$ and $J_z = \delta J$. We shall use the following Dyson transformation [15]:

$$S_m^3 = s - a_m^\dagger a_m \qquad S_m^+ = \sqrt{2s}\, a_m \qquad S_m^- = \sqrt{2s}\, a_m^\dagger (1 - a_m^\dagger a_m / 2s) \tag{4}$$

$$S_n^3 = b_n^\dagger b_n - s \qquad S_n^+ = \sqrt{2s}\, b_n^\dagger \qquad S_n^- = \sqrt{2s}(1 - b_n^\dagger b_n / 2s) b_n \tag{5}$$

where the Dyson boson operators $a_m^\dagger$ and $b_n^\dagger$ are Hermitian conjugate operators of a_m and b_n, respectively, and there are only the following non-zero commutation relations between these operators:

$$[a_m, a_{m'}^\dagger] = \delta_{mm'} \qquad [b_n, b_{n'}^\dagger] = \delta_{nn'}. \tag{6}$$

Substituting the transformations (4) and (5) into Hamiltonian (3) and making the following Fourier transformation

$$a_m = \frac{1}{\sqrt{N}} \sum_k e^{imk} a_k \qquad b_n^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{ink} b_k^\dagger \tag{7}$$

we obtain our transformed Hamiltonian

$$H = JZs\sum_k[(1+\mu')(a_k^\dagger a_k + b_k^\dagger b_k) + r_k(a_k b_k + a_k^\dagger b_k^\dagger)]$$
$$-JZ\frac{1}{N}\sum_{1,2,3,4}\delta_{1+4,2+3}[r_{3-4}a_1^\dagger a_2 b_3^\dagger b_4 + \tfrac{1}{2}(r_1 a_{-1} b_2^\dagger b_{-3} b_4 + r_2 a_1^\dagger b_2^\dagger a_{-3}^\dagger a_{-4})] \tag{8}$$

where $r_k = (2/Z)(\cos k_x + \cos k_y + \delta\cos k_z)$ and $Z = 4 + 2\delta$ is the effective coordination number. We have introduced a chemical potential $\mu = JZs\mu'$ in the above Hamiltonian. It should be noted that Hamiltonian (8) is not Hermitian.

Following [4] and [5], we make the Hartree–Fock approximation (HFA) in Hamiltonian (8). Letting

$$\langle a_k^\dagger a_k\rangle = \langle b_k^\dagger b_k\rangle = \eta_k \qquad \langle a_k b_k\rangle = \langle a_k^\dagger b_k^\dagger\rangle = \xi_k \tag{9}$$

we obtain the following effective Hamiltonian in HFA:

$$H_{\mathrm{HF}} = \sum_k[e_k(a_k^\dagger a_k + b_k^\dagger b_k) + f_k(a_k b_k + a_k^\dagger b_k^\dagger)] \tag{10}$$

where e_k and f_k are given by

$$e_k = JZs\left((1+\mu') - \frac{1}{Ns}\sum_{k_1}(\eta_{k_1} + r_{k_1}\xi_{k_1})\right) \tag{11}$$

$$f_k = JZs\left(r_k - \frac{1}{Ns}\sum_{k_1}(r_k\eta_{k_1} + r_{k-k_1}\xi_{k_1})\right). \tag{12}$$

The Hamiltonian (10) can be diagonalized by a Bogoliubov transformation [8]. The diagonal Hamiltonian is given by

$$H_{\mathrm{HF}} = \sum_k \omega_k(A_k^\dagger A_k + B_k^\dagger B_k) + E_0 \tag{13}$$

where

$$\omega_k = \sqrt{e_k^2 - f_k^2} \qquad E_0 = \sum_k(\omega_k - e_k). \tag{14}$$

The Bogoliubov transformation is defined by

$$a_k = \mu_k A_k + \nu_k B_k^\dagger \qquad b_k^\dagger = \mu_k B_k^\dagger + \nu_k A_k \tag{15}$$

where μ_k and ν_k are given by

$$\mu_k^2 - \nu_k^2 = 1 \qquad \mu_k^2 + \nu_k^2 = e_k/\omega_k \qquad 2\mu_k\nu_k = -f_k/\omega_k. \tag{16}$$

From the effective Hamiltonian (13) and the Bogoliubov transformation (15) we can formally obtain η_k and ξ_k as functions of e_k, f_k, and ω_k:

$$\eta_k = -\frac{1}{2} + \left(\frac{1}{2} + \frac{1}{e^{\beta\omega_k} - 1}\right)\frac{e_k}{\omega_k} \tag{17}$$

$$\xi_k = -\left(\frac{1}{2} + \frac{1}{e^{\beta\omega_k} - 1}\right)\frac{f_k}{\omega_k}. \tag{18}$$

The average sublattice spin is given by

$$\langle S^3 \rangle = s - \langle a_k^\dagger a_k \rangle = s - \frac{1}{N}\sum_k \eta_k. \tag{19}$$

Because ω_k, e_k and f_k all are functions of η_k and ξ_k, η_k and ξ_k must be determined consistently by (17) and (18) together with (11), (12) and (14).

Define

$$a = \frac{1}{Ns}\sum_k \eta_k \qquad b = \frac{1}{Ns}\sum_k \frac{2}{Z}\cos k_x \xi_k \qquad c = \frac{1}{Ns}\sum_k \frac{2}{Z}\cos k_z \xi_k \tag{20}$$

where e_k, f_k, and ω_k can be expressed in terms of a, b and c:

$$e_k = JZs(1 - a - 2b - \delta c)(1 + \mu'') \tag{21}$$

$$f_k = JZs(1 - a - 2b - \delta c)r_{\delta'}(k) \tag{22}$$

$$\omega_k = JZs(1 - a - 2b - \delta c)\sqrt{(1 + \mu'')^2 - r_{\delta'}^2(k)} \tag{23}$$

where

$$\mu'' = \mu'/(1 - a - 2b - \delta c) \tag{24}$$

$$\delta' = \delta\frac{1 - a - c(2 + \delta)}{1 - a - b(2 + \delta)}. \tag{25}$$

Our problem now reduces to solving consistently (20)–(23). As in [12,13], we shall set $\mu = 0$ in the ordering states. In fact, the chemical potential μ can be considered as a variational parameter in the above derivations. Varying the zero-temperature energy E_0 with respect to μ, we conclude that $\mu = 0$ makes the zero-temperature energy reach its minimum. Therefore it is reasonable to set $\mu = 0$ for the ordering states. Keeping $\mu = 0$, $\langle S_m^3 \rangle$ will decrease with increasing temperature. There is a temperature at which $\langle S_m^3 \rangle = 0$ and above which $\langle S_m^3 \rangle$ becomes negative. This temperature is called the Néel transition temperature T_N. This Néel transition temperature T_N is determined by (20) together with $\mu = 0$ and $\langle S^3 \rangle = s(1 - a) = 0$. However, from our original postulation, $\langle S_m^3 \rangle$ must be non-negative. To keep $\langle S_m^3 \rangle$ non-negative, we must allow μ to be non-zero above the Néel temperature T_N. Following Hirsch *et al* [12] and Takahashi [13], we require $\langle S^3 \rangle = 0$ when $T > T_N$. This leads μ to be non-zero above T_N. In summary, T_N with (b, c), as functions of the two parameters J and δ, will be determined by the conditions $\mu = 0$ and $a = 1$ ($\langle S_m^3 \rangle = 0$). Below T_N $\langle S_m^3 \rangle = s(1 - a)$ with (b, c), as functions of

temperature T and parameters (b, c), will be determined by the condition $\mu = 0$. Above T_N, μ with (b, c), as functions of T and (b, c), will be determined by $a = 1$ or $\langle S_m^3 \rangle = s(1 - a) = 0$.

On the other hand, we can consider our Hamiltonian (8) to represent a system of the boson operators a_k and b_k. At high temperature there is no spin order so that $\langle a_m^\dagger a_m \rangle = \langle b_n^\dagger b_n \rangle = s$ for all m and n, or $\frac{1}{N}\sum_k \langle a_k^\dagger a_k \rangle = \frac{1}{N}\sum_k \langle b_k^\dagger b_k \rangle = s$. It demands a chemical potential to keep the total a boson number and the total b boson number unchanged, respectively, at different temperatures. It is expected that at a temperature, T_N, our boson system will experience a Bose condensation so that the chemical potential will be zero. The U(1) symmetry of Hamiltonian (8) makes $\frac{1}{N}\sum_k \langle a_k^\dagger a_k \rangle = \frac{1}{N}\sum_k \langle b_k^\dagger b_k \rangle$. The total condensed a boson number $s - \frac{1}{N}\sum_k \langle a_k^\dagger a_k \rangle$ and the total condensed b boson number $s - \frac{1}{N}\sum_k \langle b_k^\dagger b_k \rangle$ are identical with $\langle S_m^3 \rangle$ and $-\langle S_n^3 \rangle$, so that we have an antiferromagnetic order below T_N. In this interpretation, T_N is the Bose condensation temperature of our boson system, at which the chemical potential becomes zero and $\langle S_m^3 \rangle = \langle S_n^3 \rangle = 0$.

As we have emphasized, the Dyson-transformed Hamiltonian (8) is not Hermitian. But the effective Hamiltonian in HFA, (10), is Hermitian. If we make use of the Holstein–Primakoff transformation [16] instead of the Dyson transformations (4) and (5), we shall obtain a Hermitian Hamiltonian. Truncated up to quartic terms, it is equivalent to the Hermitian part of the Dyson-transformed Hamiltonian (8), or $(H + H^\dagger)/2$:

$$H^{HP} = JZs\sum_k [(1+\mu')(a_k^\dagger a_k + b_k^\dagger b_k) + r_k(a_k b_k + a_k^\dagger b_k^\dagger)]$$
$$- JZ\frac{1}{N}\sum_{1,2,3,4} \delta_{1+4;2+3}[r_{3-4}a_1^\dagger a_2 b_3^\dagger b_4 + \tfrac{1}{4}r_1(a_{-1}b_2^\dagger b_{-3}b_4 + b_4^\dagger b_{-3}^\dagger b_2 a_{-1}^\dagger)$$
$$+ \tfrac{1}{4}r_2(a_1^\dagger b_2^\dagger a_{-3}^\dagger a_{-4} + a_{-4}^\dagger a_{-3} b_2 a_1)]. \qquad (26)$$

It is obvious that at the Hartree–Fock level H^{HP} leads to the same results as does the Dyson-transformed non-Hermitian Hamiltonian (8). It is our Hartree–Fock approximation that cuts off the non-Hermitian part of the Dyson-transformed Hamiltonian (8).

3. Interaction correction beyond the Hartree–Fock approximation

To go beyond the Hartree–Fock approximation, we shall take into account the contribution of the Hartree–Fock (non-linear) spin-wave interaction. It is expected that the interaction will modify the Hartree–Fock spin-wave spectra and lead to a finite lifetime for the Hartree–Fock spin waves. Because the original Dyson Hamiltonian (8) is non-Hermitian, we shall make use of its Hermitian part, $(H + H^\dagger)/2$ or H^{HP} in (26), for our further work. We split the complete Hermitian Hamiltonian H in (26) into two parts

$$H = H_0 + H_1$$

where H_0 is defined as the Hartree–Fock approximated version of H given by formula (13), and $H_1 \simeq H - H_0$ describes the interactions of the spin waves. The term H_1 can

be expressed in terms of the operators A_k and B_k. Since H_0 is diagonal with respect to the non-linear spin-wave operators A_k and B_k, H_1 will be the interaction between the non-linear spin-waves A_k and B_k. We can obtain the interaction correction by means of the Green function method in the cutoff approximation. Detailed calculation of the Green function will be presented in appendix 1. In the Fourier-transformed form our result is

$$\langle\langle A_k, A_k^\dagger\rangle\rangle(\omega) = 1/[\omega - \omega_k - X_k(\omega)] \tag{27}$$

where $X_k(\omega)$ is defined by

$$X_k(\omega) = \frac{JZ}{N^2}\sum_{1,2}\left(\frac{L^{\mathrm{A}}_{k,1,2}\bar{D}_{k,1+2-k,1,2}}{\omega - \omega_1 - \omega_2 + \omega_{1+2-k}} + \frac{L^{\mathrm{AB}}_{k,1,2}\bar{D}_{k,1,1+2-k,2}}{\omega + \omega_1 - \omega_2 - \omega_{1+2-k}}\right) \tag{28}$$

where ω has been defined in (14), and the L and D will be defined in appendix 1. Here we give only the A_k Green function. The B_k Green function has the same form. It should be noticed that $X_k(\omega) = 0$ when $T = 0$. This implies that there is no interaction contribution to the spin-wave spectra and lifetime at zero temperature. At zero temperature the spin waves have infinite lifetime. At finite temperature, however, we have $X_k(\omega \pm \mathrm{i}0^+) = X_{1k}(\omega) \mp \mathrm{i}X_{2k}(\omega)$. The spin-wave interaction has a contribution to the spin-wave spectra $X^1_k(\omega)$, and gives the spin wave a finite lifetime $1/X_{2k}(\omega)$ at finite temperature. It is very difficult to work out analytical expressions for low-frequency and long-wave limits.

4. Two- and three-dimensional isotropic cases

For general δ our Hartree–Fock spin-wave theory is a 3D anisotropic theory. However, if we let $\delta = 1$, we shall obtain a 3D isotropic theory. Similarly, if we let $\delta = 0$, we shall obtain a 2D isotropic theory. As its first application we shall discuss its 2D and 3D isotropic cases and compare it with other spin-wave theories. For isotropic cases, it is easy to prove that $\sum_{k_1} r_{k-k_1}\xi_{k_1} = r_k\sum_{k_1} r_{k_1}\xi_{k_1}$. The terms ω_k and $\langle S^3\rangle$ can be simplified to

$$\omega_k = JZs(1-C)\sqrt{(1+\mu'')^2 - r_k^2} \tag{29}$$

$$\langle S^3\rangle = s - \frac{1}{2N}\sum_k \frac{1+\mu''}{\sqrt{(1+\mu'')^2 - r_k^2}}\coth\tfrac{1}{2}\beta\omega_k \tag{30}$$

$$C = \frac{1}{Ns}\sum_k(\eta_k + r_k\xi_k) = \frac{1}{2Ns}\sum_k\left(-1 + \frac{(1+\mu'') - r_k^2}{\sqrt{(1+\mu'')^2 - r_k^2}}\coth\tfrac{1}{2}\beta\omega_k\right). \tag{31}$$

For the SC lattice, $\eta = 0.45824$ [18]. The function $\zeta(n)$ is the Riemann ζ function of order n. The term $C_0 = [(1/N)\sum_k\sqrt{1-r_k^2} - 1]/2s = -0.097/2s$; E_0 and S_0^3 are the average energy and sublattice spin of the HAFM ground state:

$$E_0 = -NJZs^2(1-C_0)^2 \qquad S_0^3 = s - 0.078. \tag{32}$$

The average sublattice spin of the ground state is the same as that of linear spin theory [6]; it is 0.422 for $s = \frac{1}{2}$. The ground-state energy is lower than the linear spin-wave result; it is $-0.301NJZ$ for $s = \frac{1}{2}$, in contrast with $-0.2985NJZ$ in linear spin-wave theory [6]. As T increases, $\langle S^3 \rangle$ decreases. This can be seen in (30). When T approaches the Néel temperature T_N, $\langle S^3 \rangle$ tends to zero. The Néel temperature T_N has to be determined consistently with $\langle S^3 \rangle = 0$. The result is $T_N = 1.079J$, being larger than the $0.989J$ of RPA theory [7, 14] and the $0.951J$ of the series expansion method [19].

In two dimensions the summation in (30) with $\mu'' = 0$ diverges when the temperature T is non-zero. So there is a Néel ordering state only at $T = 0$ in two dimensions, in agreement with the Mermin–Wagner theorem [20]. In the case $C_0 = -0.158/2s$, the average energy and sublattice spin of the ground state are $E_0 = -NJZs^2(1-C_0)^2$ and $S_0^3 = s-0.197$. For $s = \frac{1}{2}$, we have $E_0 = -0.335NJZ$ and $S_0^3 = 0.303$. This ground-state energy is equivalent to Carlson's digital result $-0.335NJZ$ on 32×32 sites [17]. The sublattice spin value is equivalent to the linear theory result, but the energy is lower than the $-0.329NJZ$ of linear theory [6]. In one dimension, the summation in (30) with $\mu'' = 0$ diverges even at $T = 0$. So there is no Néel ordering state in one dimension.

When $T > T_N$, μ'' should be non-zero in order to keep $\langle S^3 \rangle = 0$. This is different from the situation discussed above. In three dimensions T_N is so large that for $T > T_N$ large thermal effects make any spin-wave theory give way to a high-temperature series expansion theory. We will discuss no further the $T > T_N$ case in three dimensions. In contrast with the 3D isotropic case, we have $T_N = 0$ in two dimensions. Spin-wave theories should be good up to some, quite high, temperature. The terms η_k and ξ_k are given in this case by

$$\eta_k = -\frac{1}{2} + \frac{1+\mu''}{\sqrt{(1+\mu'')^2 - r_k^2}}\left(\frac{1}{2} + \frac{1}{e^{\beta\omega_k} - 1}\right) \tag{33}$$

$$\xi_k = -\frac{r_k}{\sqrt{(1+\mu'')^2 - r_k^2}}\left(\frac{1}{2} + \frac{1}{e^{\beta\omega_k} - 1}\right). \tag{34}$$

Correlation functions $\langle a_m^\dagger a_{m'} \rangle$, $\langle b_n^\dagger b_{n'} \rangle$, and $\langle a_m b_n \rangle$ can be expressed in terms of η_k and ξ_k:

$$\langle a_m^\dagger a_{m'} \rangle = \frac{1}{N}\sum_k \eta_k e^{ik(m'-m)} \qquad \langle b_n^\dagger b_{n'} \rangle = \frac{1}{N}\sum_k \eta_k e^{ik(n-n')}$$
$$\langle a_m b_n \rangle = \frac{1}{N}\sum_k \xi_k e^{ik(m-n)}. \tag{35}$$

Using a technique similar to the Takahashi method, we shall make use of Dyson's transformation and Wick's theorem in the derivation of spin-correlation functions. Detailed calculations are presented in appendix 2. As a result, the spin-correlation function $\langle S_0 \cdot S_r \rangle$ has the following large-r asymptotic behaviour:

$$\langle S_0 \cdot S_r \rangle = \exp(i\pi r)\frac{4T^2}{\pi J^2 Z^2 s^2 (1-C_0)^2}\frac{\xi}{r}\exp(-r/\xi) \tag{36}$$

where the spin-correlation length is given by

$$\xi(T) = \frac{1}{4\sqrt{\mu''}} = \frac{\sqrt{2}JZs(1-C_0)}{4T}\exp(\rho/T) \tag{37}$$

where ρ is defined by $\rho = \pi JZss_0(1-C_0)/2$. It is interesting that this correlation length is in agreement with the CHN one-loop renormalization group result [9]. In the same way, we can derive our magnetic susceptibility $\chi(T)$:

$$\chi(T) = \frac{1}{3T}\sum_r \langle S_0 \cdot S_r\rangle = \frac{1}{3T}\left(\sum_{r_A}\langle S_0 \cdot S_{r_A}\rangle + \sum_{r_B}\langle S_0 \cdot S_{r_B}\rangle\right)$$
$$= \frac{s_0}{3JZ(1-C_0)} + \frac{2T}{3\pi J^2Z^2s^2(1-C_0)^2} + o(T^3). \tag{38}$$

Since we have $T_N = 0$ in the 2D case, the above correlation function, correlation length and magnetic susceptibility work within a wide temperature range, from zero to a temperature comparable with the coupling constant J. It should be pointed out that our main results in the 2D square lattice case have been obtained by Takahashi in his variational modified spin-wave theory. But our Hartree–Fock theory is very different from the Takahashi variational theory [13]. Furthermore, our theory can work not only in the 2D case but also in 3D cases including isotropic and anisotropic cases.

5. Quasi-2D case and its application to the insulating cuprates

It is established experimentally that the cuprates, such as $La_{2-x}(Sr,Ba)_xCuO_4$ and $RBa_2Cu_3O_{7-y}$, are quasi-2D materials. The undoped cuprates, such as La_2CuO_4, are quasi-2D antiferromagnets. Essentially they are three-dimensional, but their coupling in the z direction is very weak with respect to their in-plane coupling. As a result they exhibit 2D behaviour at very high temperatures, but the interplane coupling is indispensable for them to maintain a finite Néel temperature. Our theory, with a small δ, is very suitable for a theoretical description of these materials. We shall calculate the Néel temperature, spin-correlation function, correlation length and sublattice spin for the quasi-2D case, and fit the theoretical results with corresponding experimental data. Because there are only two parameters, J and δ, in our theory, we shall consider the agreement to be successful. In addition we shall present the sublattice spin of linear spin-wave theory for contrast with our theory.

In terms of the theoretical framework proposed in section 2, the Néel temperature T_N is determined by solving the following equations:

$$\frac{1}{N}\sum_k \eta_k = s \qquad \frac{1}{N}\sum_k \frac{2}{Z}\cos k_x\xi_k = bs \qquad \frac{1}{N}\sum_k \frac{2}{Z}\cos k_z\xi_k = cs \tag{39}$$

where

$$\eta_k = -\tfrac{1}{2} + \kappa_k \qquad \xi_k = -r_{\delta'}(k)\kappa_k \tag{40}$$

$$\kappa_k = \left(\frac{1}{2} + \frac{1}{e^{\omega_k/T_N}-1}\right)\frac{1}{\sqrt{1-r_{\delta'}^2(k)}} \tag{41}$$

$$\omega_k = JZs(-2b-\delta c)\sqrt{1-r_{\delta'}^2(k)} \tag{42}$$

where $\delta' = \delta c/b$. If $\delta = 1$, $b = c$ so that the b equation in (39) is identified with the c equation in (39). We need to solve only two of the three equations in (39) for T_N and b. If $\delta = 0$, the anisotropic 3D theory reduces to a 2D theory so that the summations in the first two equations in (39) diverge for $T > 0$. It implies that the equations in (39) have no solution for $T > 0$ in two dimensions. Detailed discussions on the 2D case has been included in section 4. For very small δ, we can solve the equation set (39) analytically. The k summations for very small δ in (39) are dominated by those in the region of small k_x and k_y. It is easy to solve the three equations in (39). The solutions are given by

$$b = -\tfrac{1}{2} \qquad c = -\frac{s}{2\ln(1/\delta)} \qquad T_N = \frac{4\pi J s^2}{\ln(1/\delta)}. \tag{43}$$

It should be pointed that the above asymptotic T_N solution is not an accurate expression for T_N because T_N depends very weakly on δ when δ approaches to zero, and it is very difficult to calculate the coefficients more precisely. It can be used only for quality usage. T_N decreases with decreasing δ; $T_N = 0$ if $\delta = 0$. This is the above result that there is an ordering state only for $T = 0$ in the 2D isotropic model. When $s = 1/2$, we have $T_N = \pi J/\ln(1/\delta)$, half the RPA result [14]. For other δ, a digital calculation is required to obtain accurate T_N. Figure 1 is our digital T_N result for $0 \leqslant \delta \leqslant 1$. The (A) curve is normally scaled; the (B) curve is logarithmically scaled to emphasize the T_N for very small δ. For $\delta = 1$ we obtain $T_N = 1.079J$, a little larger than the series expansion result $0.951J$ [19] and the RPA result $0.989J$ [14].

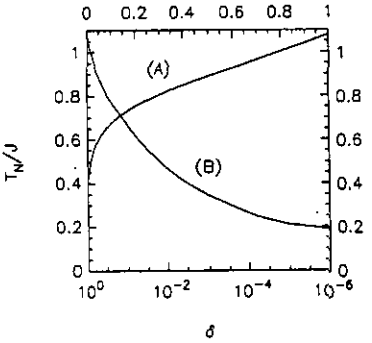

Figure 1. T_N/J as a function of δ for $s = 1/2$. Curve A is normally scaled. Curve B is scaled logarithmically to emphasize the region of very small δ. For $\delta = 1$, $T_N/J = 1.079$.

In general for all temperatures, our consistent equation set is (20), with η_k and ξ_k defined in the following way:

$$\eta_k = -\tfrac{1}{2} + (1 + \mu'')F_k \qquad \xi_k = -r_{\delta'}(k)F_k \tag{44}$$

and

$$F_k = \left(\frac{1}{2} + \frac{1}{e^{\omega_k/T} - 1}\right)\frac{1}{\sqrt{(1+\mu'')^2 - r_{\delta'}^2(k)}} \tag{45}$$

where ω_k is defined by

$$\omega_k = JZs(1-a-2b-\delta c)\sqrt{(1+\mu'')^2 - r_{\delta'}^2(k)}. \tag{46}$$

The μ'' and δ' terms in the above three equations are defined by (24) and (25). Following the discussion on the 2D isotropic case, we derive the following correlation functions:

$$\langle S_m \cdot S_{m'}\rangle = s\delta_{mm'} + [(s - \langle a_m^\dagger a_m\rangle) + \langle a_m^\dagger a_{m'}\rangle]^2 \tag{47}$$

$$\langle S_m \cdot S_n\rangle = -[(s - \langle a_m^\dagger a_m\rangle) - \langle a_m b_n\rangle]^2 \tag{48}$$

where

$$\langle a_m^\dagger a_{m'}\rangle = \frac{1}{N}\sum_k \eta_k e^{ik\cdot(m'-m)} \qquad \langle a_m a_n\rangle = \frac{1}{N}\sum_k \xi_k e^{ik\cdot(m-n)}. \tag{49}$$

From expression (47) we obtain $\langle S_m \cdot S_m\rangle = s(s+1)$ for all temperatures, the result we expect.

For $T < T_N$, we have $\langle a_m^\dagger a_m\rangle = \frac{1}{N}\sum_k \eta_k = as$. In section 2 it was shown that $\langle S^3\rangle = s(1-a)$, and $a = 1$ for $T \geqslant T_N$. Therefore, the correlation functions (47) and (48) for $T \geqslant T_N$ reduce to

$$\langle S_m \cdot S_{m'}\rangle = (\langle a_m^\dagger a_{m'}\rangle)^2 \qquad \langle S_m \cdot S_n\rangle = -(\langle a_m b_n\rangle)^2. \tag{50}$$

Since μ'' is small for $T_N \leqslant T \leqslant J$, we obtain $\xi_k = -\eta_k$ in the region of small (k_x, k_y, k_z) so that the correlation functions of large r can be expressed in a unified way:

$$\langle S_0 \cdot S_r\rangle = e^{i\pi\cdot r}(\alpha_r)^2 \tag{51}$$

where

$$\alpha_r = \frac{1}{N}\sum_k \alpha_k e^{ik\cdot r} \tag{52}$$

and α_r for large r is dominated by α_k for small momentum k. For small k, we derive in momentum space

$$\alpha_k \approx \frac{2T}{JZs(-2b-\delta c)}\frac{1}{k_x^2 + k_y^2 + \delta k_z^2 + 4\mu''} \tag{53}$$

so that for large r in real space

$$\alpha_r \propto \exp\{-[2\sqrt{\mu''}(r_x + r_y) + 2\sqrt{\mu''/\delta}]\}. \tag{54}$$

As a result, we obtain the spin-correlation function

$$\langle S_0 \cdot S_r\rangle \propto e^{i\pi\cdot r}\exp\{-[(r_x + r_y)/\xi_{xy} + r_z/\xi_z]\} \tag{55}$$

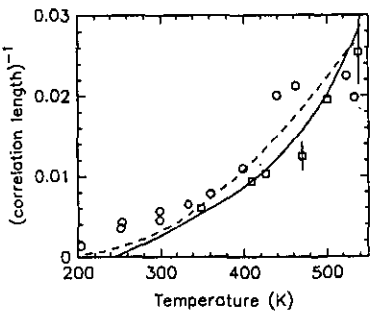

Figure 2. Correlation length as a function of temperature. The circles and squares are experimental data for NTT#2 (T_N = 195 K) and NTT#7 (T_N = 245 K). The broken curve is the CHN result fitting to the both data. Their theoretical T_N is zero because of the two-dimensionality of their model. The full curve is our best-fitted result for NTT#7 with J = 1034 K and $\delta = 0.00004$.

where the correlation lengths ξ_{xy} in the xy plane and ξ_z in the z direction are defined by

$$\xi_{xy} = 1/4\sqrt{\mu''} \qquad \xi_z = \sqrt{\delta/\mu''}/4. \tag{56}$$

The correlation lengths in (56), as all the above quantities, are in units such that the lattice constant d is equal to 1. In normal units, the correlation lengths are given by

$$\xi_{xy} = d/4\sqrt{\mu''} \qquad \xi_z = \sqrt{\delta/\mu''}d/4. \tag{57}$$

The correlation lengths are functions of T, δ and J.

When $T < T_N$, the averaged sublattice spin $\langle S^3\rangle = s(1-a)$. The a with b and c is determined by (20) and (44)–(46) with $\mu'' = 0$. It requires digital calculation. Through a, $\langle S^3\rangle$ is a function of T, δ and J.

There are two parameters, J and δ, in our theory. To apply our non-linear quasi-2D spin-wave theory to the insulating cuprate antiferromagnets, we fit our theoretical T_N and correlation length as a function of temperature with the real experimental T_N and correlation length, respectively. This determines the two parameters. With fixed J and δ, we compare our theoretical sublattice spin with the experimental one. The circles and squares in figure 2 are experimental correlation length data of La_2CuO_4 NTT#2 (T_N = 195 K) by Endoh *et al* [2] and NTT#7 (T_N = 245 K) by Yamada *et al* [2], respectively. The broken curve is the CHN result fitting to the data by Yamada *et al* [2]. The CHN T_N is zero because of the two-dimensionality of their model. The full curve is our best-fit theoretical correlation length result for NTT#7 with J = 1034 K and $\delta = 0.00004$. Our T_N is 245 K. Since we have used the SC lattice to describe the materials, we have taken a constant d = 3.79 Å, as did Yamada *et al* [2]. The Néel temperature T_N is very sensitive to holes doped into La_2CuO_4; NTT#7 has T_N = 245 K, but NTT#2 has only T_N = 195 K. There are many holes in NTT#2 so that the effect of the holes should be considered for fitting a theory to the experiment. Since our theory is formulated without considering the hole effect, we do not fit our theory to NTT#2. We present our sublattice spin $\langle S^3\rangle$ as a function of reduced temperature T/T_N in figure 3. The full curves in figure 3 are our theoretical $\langle S^3\rangle$ for $\delta = 0.00004$ and 1. The $\langle S^3\rangle$ for $\delta = 1$ is presented

for comparison. For contrast, we present sublattice spins of linear spin-wave theory (broken curves). Comparing with RPA and high-temperature series expansion results, linear spin-wave theory yields too large a Néel temperature. Although both theories agree at very low temperature, there is a large difference between them at relatively high temperature, as figure 3 shows. At low temperature the $\langle S^3 \rangle$ for $\delta = 1$ decreases with T very slowly. But the $\langle S^3 \rangle$ for $\delta = 0.00004$ decreases with T quite quickly. At $T = T_N/2$, the $\langle S^3 \rangle$ for $\delta = 0.00004$ become smaller than 0.2. This is consistent with the experimental result by Yamada *et al* [2].

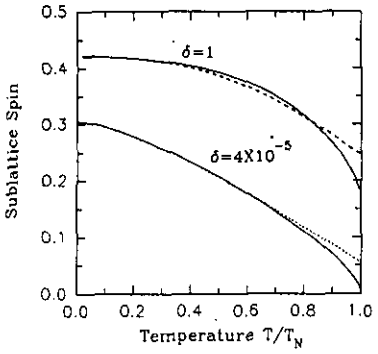

Figure 3. Sublattice spins as a function of reduced temperature T/T_N. The full curves are the sublattice spins of our Hartree–Fock (non-linear) spin-wave theory. The result of linear spin-wave theory is presented for comparison. Linear spin-wave theory overestimates the Néel temperature.

6. Discussions and conclusion

Based on the HT proof [11], the AA Schwinger boson theory is equivalent to Anderson's linear spin-wave theory [6]. The sublattice-symmetrical theory by Hirsch *et al* is also a linear spin-wave theory because they have used the linear spin-wave transformation [12]. The variation modified spin-wave theory [13] includes the quartic operator terms so that it is a non-linear spin-wave theory. At very low temperature, all three theories are equivalent to each other except for the factor 3/2 in the AA theory in the light of the Bose–Einstein condensation viewpoint. But at higher temperature some differences appear. The non-linear theory can work at higher temperatures because it takes into account the quartic operator terms. Our theory is also a non-linear spin-wave theory, taking into account the quartic operator terms. Besides, it is an anisotropic theory based on the anisotropic Hamiltonian (2), in contrast with the other theories based on the isotropic Hamiltonian (1). In isotropic cases, it is identical with the conventional non-linear spin-wave theory for $T \leqslant T_N$, and leads to the same result as the modified spin-wave theory for the 2D square lattice. The ground-state energy in our theory is $-0.335NJZ$, being equivalent to the digital result on the 32×32 site [17], for the 2D square lattice. For very small δ, $T_N \ll J$, so that our can work satisfactorily at $T \leqslant T_N$ as well as at $T > T_N$ (up to J). Therefore, our anisotropic theory is advantageous over other theories in the description of anisotropic antiferromagnets such as the insulating cuprate La_2CuO_4 and $RBa_2Cu_3O_6$.

As for the one-dimensional case, we should say that our theory does not work as well as other spin-wave theories. This results from the fact that we postulate a long-range antiferromagnetic order in spin-wave theories, but there is no long-range order in one dimension. In our theory, if we try to make it work, we shall have a non-zero chemical potential for all temperatures. As a result we shall obtain a gap in our spin-wave spectra even at zero temperature, and an exponential decay, not power decay, for our spin-correlation functions at zero temperature. It is a drawback not only in our theory, but also in all other spin-wave theories.

In summary, we have formulated a non-linear spin-wave theory that reduces to conventional non-linear spin-wave theory for $T \leqslant T_N$, and leads to the same result as the modified spin-wave theory for the 2D square lattice. We have proved that in the Hartree–Fock approximation the Dyson-transformed Hamiltonian is equivalent to the Holstein–Primakoff-transformed Hamiltonian truncated up to quartic terms. The spin-wave lifetime has been obtained in the first-order approximation. For the 2D square lattice we have obtained Takahashi's results, including the CHN one-loop renormalization-group behaviour of the correlation length and the AA spin-correlation functions except the factor of 3/2. Our theory is suitable for a description of quasi-two-dimensional quantum Heisenberg antiferromagnets such as the cuprate La_2CuO_4. Since for very small δ, $T_N \ll J$, so that our theory can work satisfactorily at $T \leqslant T_N$ as well as $T > T_N$ (up to J). Applied to the antiferromagnetism of the cuprate La_2CuO_4, our quasi-2D non-linear spin-wave theory describes quite satisfactorily the existing experimental data of the Néel transition temperature, correlation length above the Néel temperature, and staggered magnetization of the material if $J = 1034$ K and the anisotropy parameter is set to be 4×10^{-5}.

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Appendix 1. Green function of the interacting HF spin-waves

H_0 is diagonal in the operators A_k and B_k. Expressed in terms of the operators A_k and B_k, the interaction part H_I is

$$H_I = \frac{1}{N}\sum_{1,2}(A^\dagger_{k_1}A_{k_1} + B^\dagger_{k_1}B_{k_1})R_{k_1,k_2} - \frac{JZ}{N}\sum_{1,2,3,4}[\delta_{1+2,3+4}\tilde{D}_{1,2,3,4} \times (A^\dagger_1A^\dagger_2A_3A_4 + B^\dagger_1B^\dagger_2B_3B_4) + \delta_{1+3,2+4}\tilde{D}^{AB}_{1,2,3,4}A^\dagger_1B^\dagger_2B_3A_4] \quad \text{(A1.1)}$$

where

$$R_{1,2} = n_2[(\mu_1^2+\nu_1^2)(\mu_2^2+\nu_2^2+2\mu_2\nu_2r_2) + 2\mu_1\nu_1r_1(\mu_2^2+\nu_2^2) + 2\mu_2\nu_2r_{1-2}] \quad \text{(A1.2)}$$

$$\tilde{D}_{1,2,3,4} = r_{1-4}\mu_1\mu_4\nu_2\nu_3 + \tfrac{1}{4}r_4(\nu_1\nu_2\nu_3\mu_4 + \mu_1\mu_2\mu_3\nu_4) + \tfrac{1}{4}r_1(\mu_1\nu_2\nu_3\nu - 4 + \nu_1\mu_2\mu_3\mu_4)$$

(A1.3)

$$\bar{D}^{AB}_{1,2,3,4} = r_{2-3}(\mu_1\mu_2\mu_3\mu_4 + \nu_1\nu_2\nu_3\nu_4) + \tfrac{1}{2}r_{1-2}(\mu_1\mu_3\nu_2\nu_4 + \nu_1\nu_3\mu_2\mu_4) + \tfrac{1}{2}r_{3-4}(\mu_2\mu_4\nu_1\nu_3 + \mu_1\mu_3\nu_2\nu_4) + \tfrac{1}{2}r_4(\mu_1\nu_2\nu_3\nu_4 + \nu_1\mu_2\mu_3\mu_4) + \tfrac{1}{2}r_1(\mu_1\mu_2\mu_3\nu_4 + \nu_1\nu_2\nu_3\mu_4) + \tfrac{1}{2}r_2(\nu_1\nu_2\mu_3\nu_4 + \mu_1\mu_2\nu_3\mu_4) + \tfrac{1}{2}r_3(\nu_1\mu_2\nu_3\nu_4 + \mu_1\nu_2\mu_3\mu_4). \tag{A1.4}$$

We shall use the equation-of-motion method of the Green function to calculate the lifetime of the spin waves. A detailed description of the method can be found in [7] and [14]. We define retarded and advanced Green functions of the operator A_k by $\langle\langle A_k(t), A_k^\dagger(t')\rangle\rangle_{R,A} = \langle[A_k(t), A_k^\dagger(t')]\rangle_{R,A}$. The retarded and advanced Green functions of the operator A_k satisfy the same equation of motion:

$$\left(i\frac{d}{dt} - \omega_k\right)\langle\langle A_k(t), A_k^\dagger(t')\rangle\rangle = \delta(t-t') + \langle\langle[A_k, H_1](t), A_k^\dagger(t')\rangle\rangle. \tag{A1.5}$$

The second term in the right-hand side represents the interaction of the spin waves; $[A_k(t), H_1] = -JZ\frac{1}{N}\sum_{1,2} W_{k,1,2}$ where $W_{k,1,2}$ is defined by

$$W_{k,1,2} = \bar{D}^{AB}_{k,1,1+2-k,2}(B_1^\dagger B_{1+2-k}A_2 - \delta_{k,2}\langle B_1^\dagger B_1\rangle A_k) + (\bar{D}_{k,1+2-k,1,2} + \bar{D}_{1+2-k,k,1,2})(A^\dagger_{1+1-k}A_1A_2 - \delta_{k,2}\langle A_1^\dagger A_1\rangle A_k - \delta_{k,1}\langle A_2^\dagger A_2\rangle A_k).$$

In order to take in account the interaction in the Green function method, we make equations of motion of $\langle\langle B_1^\dagger B_{1+2-k}A_2 - \delta_{k,2}\langle B_1^\dagger B_1\rangle A_k(t), A_k^\dagger(t')\rangle\rangle$ and $\langle\langle A^\dagger_{1+2-k}A_1A_2 - (\delta_{k,1}\langle A_2^\dagger A_2\rangle + \delta_{k,2}\langle A_1^\dagger A - 1\rangle)A_k(t), A_k^\dagger(t')\rangle\rangle$, and use a cutoff approximation in their equations of motion. In the first-order approximation they can be expressed in terms of the Green function $\langle\langle A_k(t), A_k^\dagger(t')\rangle\rangle$:

$$\langle\langle B_1^\dagger B_{1+2-k}A_2 - \delta_{k,2}\langle B_1^\dagger B_1\rangle A_k(t), A_k^\dagger(t')\rangle\rangle = -\frac{1}{N}\frac{L^{AB}_{k,1,2}}{i(d/dt) + \omega_1 - \omega_2 - \omega_{1+2-k}} \langle\langle A_k(t), A_k^\dagger(t')\rangle\rangle\langle\langle A^\dagger_{1+2-k}A_1A_2 - (\delta_{k,1}\langle A_2^\dagger A_2\rangle + \delta_{k,2}\langle A_1^\dagger A_1\rangle)A_k(t), A_k^\dagger(t')\rangle\rangle$$

$$= -\frac{1}{N}\frac{L^{A}_{k,1,2}}{i(d/dt) - \omega_1 - \omega_2 + \omega_{1+2-k}}\langle\langle A_k(t), A_k^\dagger(t')\rangle\rangle$$

where $L^{AB}_{k,1,2}$ and $L^{A}_{k,1,2}$ are defined by

$$L^{AB}_{k,1,2} = JZ\bar{D}^{AB}_{2,1+2-k,1,k}(n_1 + n_1n_{1+2-k} + n_1n_2 - n_2n_{1+2-k}) \tag{A1.6}$$

$$L^{A}_{k,1,2} = JZ[n_{1+2-k}(1+n_1) + n_2n_{1+2-k} - n_1n_2](\bar{D}_{1,2,1+2-k,k} + \bar{D}_{2,1,1+2-k,k} + \bar{D}_{1,2,k,1+2-k} + \bar{D}_{2,1,k,1+2-k}). \tag{A1.7}$$

As a result, we obtain $[A_k(t), H_1] = X_kA_k(t)$, where X_k is defined by

$$X_k\left(i\frac{d}{dt}\right) = \frac{JZ}{N^2}\sum_{1,2}\left(\frac{L^{A}_{k,1,2}\bar{D}_{k,1+2-k,1,2}}{i(d/dt) - \omega_1 - \omega_2 + \omega_{1+2-k}} + \frac{L^{AB}_{k,1,2}\bar{D}_{k,1,1+2-k,2}}{i(d/dt) + \omega_1 - \omega_2 - \omega_{1+2-k}}\right). \tag{A1.8}$$

Substitution of $[A_k(t), H_1] = X_k A_k(t)$ into (A1.6) leads to the Green function that includes the spin-wave interaction effect:

$$\langle\langle A_k(t), A_k^\dagger(t')\rangle\rangle = \frac{1}{\mathrm{i}(\mathrm{d}/\mathrm{d}t) - \omega_k - X_k(\omega)}\delta(t-t'). \tag{A1.9}$$

In Fourier-transformed form it is

$$\langle\langle A_k, A_k^\dagger\rangle\rangle(\omega) = 1/[\omega - \omega_k - X_k(\omega)]. \tag{A1.10}$$

Appendix 2. 2D spin-correlation functions

Similar to the Takahashi method, we shall make use of Dyson's transformation and Wick's theorem in the derivation of spin-correlation functions. Define $\eta = \frac{1}{N}\sum_k \eta_k$. After using Wick's theorem the spin-correlation function $\langle \boldsymbol{S}_m \cdot \boldsymbol{S}_{m'}\rangle$ is derived:

$$\begin{aligned}\langle \boldsymbol{S}_m \cdot \boldsymbol{S}_{m'}\rangle = s^2 &- s(\langle a_m^\dagger a_m\rangle + \langle a_{m'}^\dagger a_{m'}\rangle - \langle a_m^\dagger a_{m'}\rangle - \langle a_{m'}^\dagger a_m\rangle - \delta_{m,m'}) \\ &+ \langle a_m^\dagger a_m\rangle\langle a_{m'}^\dagger a_{m'}\rangle + \langle a_m^\dagger a_{m'}\rangle\langle a_{m'}^\dagger a_m\rangle \\ &- \langle a_m^\dagger a_m\rangle\langle a_m^\dagger a_{m'}\rangle - \langle a_{m'}^\dagger a_{m'}\rangle\langle a_{m'}^\dagger a_m\rangle.\end{aligned} \tag{A2.1}$$

Noticing that $\langle a_m^\dagger a_{m'}\rangle = \langle a_{m'}^\dagger a_m\rangle$ and $\langle a_m^\dagger a_m\rangle = \eta$, we derive

$$\langle \boldsymbol{S}_m \cdot \boldsymbol{S}_{m'}\rangle = s\delta_{m,m'} + [(s-\eta) + \langle a_m^\dagger a_{m'}\rangle]^2 \tag{A2.2}$$

where $s - \eta$ is the average sublattice spin at the zero temperature. In the same way, noticing $\langle a_m b_n\rangle = \langle a_m^\dagger a_n^\dagger\rangle$, we derive

$$\langle \boldsymbol{S}_m \cdot \boldsymbol{S}_n\rangle = -[(s-\eta) - \langle a_m b_n\rangle]^2. \tag{A2.3}$$

In (A2.2) we have $\langle \boldsymbol{S}_m \cdot \boldsymbol{S}_m\rangle = s(s+1)$, as it should be. When the temperature T is equivalent to zero, the correlation functions have the following asymptotic behaviour for very large r:

$$\langle a_0^\dagger a_r\rangle = 1/\sqrt{2}\pi r \qquad \langle a_0 b_r\rangle = -1/\sqrt{2}\pi r \tag{A2.4}$$

$$\langle \boldsymbol{S}_0 \cdot \boldsymbol{S}_r\rangle = \mathrm{e}^{\mathrm{i}\pi\cdot r}[s-\eta) + 1/\sqrt{2}\pi r]^2. \tag{A2.5}$$

μ'' should be small when the temperature T is low. Suppose that

$$\beta J Z s(1-C) \gg 1 \qquad \beta J Z s(1-C)\sqrt{(1+\mu'')^2 - 1} \ll 1. \tag{A2.6}$$

Keeping the relation $\langle S^3\rangle = 0$ in mind, we derive

$$s + \tfrac{1}{2} = \frac{1}{N}\sum_k \frac{1+\mu''}{\sqrt{(1+\mu'')^2 - r_k^2}}\left(\frac{1}{2} + \frac{1}{\mathrm{e}^{\beta\omega_k} - 1}\right) \tag{A2.7}$$

$$sC = \frac{1}{N}\sum_k \left[-\frac{1}{2} + \frac{1+\mu'' - r_k^2}{\sqrt{(1+\mu'')^2 - r_k^2}}\left(\frac{1}{2} + \frac{1}{\mathrm{e}^{\beta\omega_k} - 1}\right)\right]. \tag{A2.8}$$

On the conditions in (A2.6), the k summations in (A2.7) and (A2.8) are dominated by contributions of the domain $k \sim 0$. Noticing $r_k = \frac{1}{2}(\cos k_x + \cos k_y) \simeq 1 - k^2/2$ or $\sqrt{(1+\mu'')^2 - r_k^2} \simeq \sqrt{2\mu'' + k^2/2}$, we derive

$$s - \delta S_0 = \frac{2(1+\mu'')}{\pi D} \ln \frac{1}{1 - \exp(-t_0)} \tag{A2.9}$$

$$\begin{aligned} C - C_0 &= \frac{2}{\pi s D^3} \int_{-\infty}^{\infty} \frac{\mathrm{d}t}{\mathrm{e}^t - 1}(t^2 - \tfrac{1}{2}t_0^2) \\ &= \frac{1}{\pi s D^3}\left[4\zeta(3) - \exp\left(-\frac{\pi D s_0}{1+\mu''}\right)\left(1 + \frac{\pi s_0 D}{2(1+\mu'')}\right)\right] \end{aligned} \tag{A2.10}$$

where $D = \beta J Z s(1-C)$ and $t_0 = D\sqrt{2\mu''}$. In the present 2D case, $C_0 = -0.078/s$ and $\delta S_0 = 0.197$. Equations (A2.8) and (A2.9) constitute a set of non-linear equations. They are solved approximately by

$$C = C_0 + \alpha T^3 - \frac{3}{1 - C_0}\alpha^2 T^6 + \mathrm{o}(T^9) \tag{A2.11}$$

$$\sqrt{\mu''} = \exp(-\rho/T)\left(\frac{2\sqrt{3}\rho}{\pi s_0 T} + \mathrm{o}(T)\right)^{-1} \tag{A2.12}$$

where $\alpha = 4\zeta(3)/\pi J^3 Z^3 s^4(1 - C_0)$ and $\rho = \pi J Z s s_0(1 - C_0)/2$. When r tends to infinity, the correlation function $\langle a_0^\dagger a_r \rangle$ has the asymptotic behaviour

$$\langle a_0^\dagger a_r \rangle = \frac{2\sqrt{\xi/\pi r}}{J Z s \beta(1 - C_0)} \exp(-r/2\xi). \tag{A2.13}$$

Substituting this asymptotic correlation function into (A2.2) and (A2.3), we obtain our spin-correlation function for large r:

$$\langle S_0 \cdot S_r \rangle = \exp(\mathrm{i}\pi r) \frac{4T^2}{\pi J^2 Z^2 s^2 (1 - C_0)^2} \frac{\xi}{r} \exp(-r/\xi) \tag{A2.14}$$

where the spin-correlation length is given by

$$\xi(T) = \frac{1}{4\sqrt{\mu''}} = \frac{\sqrt{2} J Z s(1 - C_0)}{4T} \exp(\rho/T) \tag{A2.15}$$

where ρ is defined by $\rho = \pi J Z s s_0(1 - C_0)/2$.

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