RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 45, NUMBER 17 1 MAY 1992-I

Spin-wave velocity renormalization in the two-dimensional Heisenberg antiferromagnet at zero temperature

C. M. Canali,* S. M. Girvin, and Mats Wallin
Department of Physics, Indiana University, Bloomington, Indiana 47405
(Received 9 September 1991)

We compute the spin-wave dispersion of the square-lattice Heisenberg antiferromagnet at $T=0$ within the Dyson-Maleev formalism, to order $1/S$. This allows us to calculate the spin-wave velocity renormalization factor, Z_c, to order $O(1/S^2)$. For the $S=\frac{1}{2}$ case, it is found that $Z_c=1.1765\pm0.0002$, in very good agreement with series-expansion estimates.

A renewed interest in two-dimensional antiferromagnets has been recently brought about by the discovery of high-T_c superconductivity, partly because the undoped parent La_2CuO_4 is a magnetic system which is believed to be well represented by a square-lattice spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model. The antiferromagnetic Heisenberg model (HAFM) has been a challenging problem for many years and very few exact results are known up to date. In particular, in contrast with the $S>\frac{1}{2}$ case,[1] the very nature of the ground state of the two-dimensional spin $S=\frac{1}{2}$ system is not known rigorously, and only through recent numerical work,[2] considerable evidence has been gained that the ground state indeed has long-range antiferromagnetic order.

Among the approximation techniques used to tackle the HAFM, spin-wave theory (SWT), in its different versions, has turned out to be an extremely useful tool providing very accurate results, even for the $S=\frac{1}{2}$ systems, despite the fact that SWT is believed to be only an asymptotic expansion in the parameter $1/S$.[3-5] Many authors have recently addressed the question of how good SWT is for $S=\frac{1}{2}$, by calculating higher order terms on this asymptotic expansion for several physical quantities and comparing the spin-wave theory results with the results obtained with other methods, e.g., series-expansion calculations. Recently Castilla and Chakravarty[5] have calculated the staggered magnetization of the square-lattice HAFM $T=0$ to order $O(1/S^2)$. They found that, up to this order, the spin-wave expansion generates asymptotically small terms, so that the inclusion of the $O(1/S^2)$-order term does not ruin the excellent agreement between spin-wave theory and recent Monte Carlo and series expansion estimates of the staggered magnetization.

In this paper we want to carry out a similar analysis for the $T=0$ spin-wave excitation energy of the square-lattice HAFM, given by the Hamiltonian

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

where the sum extends over distinct pairs of nearest neighbors. In particular, we shall study the long-wave limit of the spin-wave dispersion, which, on the basis of general principles, is supposed to vanish linearly for small wave vectors, according to the relation $\omega_\mathbf{k}\sim ck$ as $\mathbf{k}\rightarrow 0$, where c is the spin-wave velocity. Within spin-wave theory, c can be written in the form

$$c=\frac{2\sqrt{2}SJa}{\hbar}Z_c(S)\,, \tag{2}$$

where a is the nearest-neighbor distance. $Z_c(S)$ is a renormalization factor which is expanded in powers of $1/S$. The first two terms of the expansion have been known for a long time[6] and give

$$Z_c(S)=1+0.15795/2S+O(1/2S)^2\,. \tag{3}$$

The most precise estimate of $Z_c(S)$ comes from series expansion[7] which gives 1.18 ± 0.02 for $S=\frac{1}{2}$. The purpose of this paper is to determine the $O(1/S^2)$ term in the spin-wave expansion of Z_c and show that this correction is small but not negligible and, in fact, it makes the agreement between the SWT result and the series-expansion estimate almost perfect. We use the Dyson-Maleev (DM) transformation[8,9] to map the spin Hamiltonian of Eq. (1) into a boson Hamiltonian. The DM transformation must be preferred to the more familiar Holstein-Primakoff (HP) transformation, because the infrared singularities of the spin-wave interaction vertices are handled much better by the DM formalism. A correct treatment of the spin-wave interaction vertices is crucial for any calculations that want to go beyond the noninteracting SWT, such as the one that we are about to describe. The DM boson Hamiltonian, obtained from the spin Hamiltonian equation (1), is the sum of a quadratic term and a quartic term.[10] The quadratic term is then diagonalized by a Bogoliubov transformation; the quartic term is expressed in terms of the quasiparticle operators and normal ordered. The total Hamiltonian finally reads

$$H_{\rm DM}={\rm const}+H_0+V_{\rm DM}\,. \tag{4}$$

The quadratic part H_0 is given by

$$H_0=\sum_\mathbf{k}\hbar\,\Omega_\mathbf{k}(\alpha_\mathbf{k}^\dagger\alpha_\mathbf{k}+\beta_\mathbf{k}^\dagger\beta_\mathbf{k})\,, \tag{5}$$

where $\Omega_\mathbf{k}=[JzS\alpha(S)/\hbar]\epsilon_\mathbf{k}$, $\epsilon_\mathbf{k}=(1-\gamma_\mathbf{k})^{1/2}$, and $\alpha(S)=1+r/2S$. The function $\gamma_\mathbf{k}$ is defined as

$$\gamma_\mathbf{k}=\frac{1}{z}\sum_{\boldsymbol\delta}e^{ia\mathbf{k}\cdot\boldsymbol\delta}\,, \tag{6}$$

and the sum over $\boldsymbol\delta$ is over the $z=4$ (for the square lattice) unit vectors connecting site i with its nearest neighbors. The constant r is the $\mathbf{k}$-independent correction to the linear spin-wave dispersion coming from the normal ordering of the α and β boson operators in the quartic term. It is known in the literature as the Oguchi correction[6] and it is approximately 0.15795 in two dimensions. The quartic part of the Hamiltonian is expressed as

$$V_{\rm DM}=-\frac{zJ}{4N}\sum_{(1,2,3,4)}\delta_{\bf G}(1+2-3-4)[V^{(1)}\alpha_1^\dagger\alpha_2^\dagger\alpha_3\alpha_4+V^{(2)}\alpha_1^\dagger\beta_2\alpha_3\alpha_4+V^{(3)}\alpha_1^\dagger\alpha_2^\dagger\beta_3^\dagger\alpha_4+V^{(4)}\alpha_1^\dagger\alpha_3\beta_4^\dagger\beta_2+V^{(5)}\beta_4^\dagger\alpha_3\beta_2\beta_1$$
$$+V^{(6)}\beta_4^\dagger\beta_3^\dagger\alpha_2^\dagger\beta_1+V^{(7)}\alpha_1^\dagger\alpha_2^\dagger\beta_3^\dagger\beta_4^\dagger+V^{(8)}\beta_1\beta_2\alpha_3\alpha_4+V^{(9)}\beta_4^\dagger\beta_3^\dagger\beta_2\beta_1]\,. \quad (7)$$

We shall use the abbreviations 1 for $\mathbf{k}_1$, 2 for $\mathbf{k}_2$, and so on. In Eq. (7) the Kronecker delta function $\delta_{\bf G}(1+2-3-4)$ expresses the conservation of momentum to within a reciprocal-lattice vector $\mathbf{G}$. The vertex functions $V^{(i)}\equiv V^{(i)}_{(1234)}$, $i=1,\ldots,9$ are the DM vertices. Their explicit expressions have been derived by several authors.[11,12] We have recently rederived them using a slightly different parametrization[13] in order to implement the umklapp processes that are possible when $\mathbf{G}\neq 0$. Following Ref. 13, the vertex functions can be written in the form

$$V^{(i)}_{(1234)}=u_1u_2u_3u_4\tilde{V}^{(i)}_{(1234)}\,, \quad (8)$$

where $u_{\bf k}=[(1+\epsilon_{\bf k})/2\epsilon_{\bf k}]^{1/2}$. The singularity of the vertices is entirely contained in the prefactor $u_1u_2u_3u_4$, which diverges like $k^{-1/2}$, when any one of the momenta vanishes. On the other hand, $\tilde{V}^{(i)}_{(1234)}$ are regular functions of the momenta, which furthermore *vanish linearly* when $\mathbf{k}_3$ or $\mathbf{k}_4$ vanishes. As we show below, this property turns out to be essential to take care of the divergences of the vertices in the calculation of the second-order self-energy. The noninteracting spin-wave dispersion $\Omega_{\bf k}$, which is the lowest-order spin-wave dispersion renormalized by the Oguchi correction, immediately yields the first two terms of the $1/S$ expansion of Z_c given in Eq. (3). In order to compute the $1/S^2$ correction, we need to take the magnon interaction into account. We do this by using a Green's function formalism. We define the following time-ordered magnon Green's functions

$$\begin{aligned} iG_{\alpha\alpha}(\mathbf{k};t-t')&=\langle\psi_0|T\alpha_{\bf k}(t)\alpha^\dagger_{\bf k}(t')|\psi_0\rangle\,,\\ iG_{\beta\beta}(\mathbf{k};t-t')&=\langle\psi_0|T\beta^\dagger_{\bf k}(t)\beta_{\bf k}(t')|\psi_0\rangle\,,\\ iG_{\alpha\beta}(\mathbf{k};t-t')&=\langle\psi_0|T\alpha_{\bf k}(t)\beta_{\bf k}(t')|\psi_0\rangle\,,\\ iG_{\beta\alpha}(\mathbf{k};t-t')&=\langle\psi_0|T\beta^\dagger_{\bf k}(t)\alpha^\dagger_{\bf k}(t')|\psi_0\rangle\,. \end{aligned} \quad (9)$$

For the unperturbed propagators we obtain[13]

$$\begin{aligned} G^{(0)}_{\alpha\alpha}(\mathbf{k},\omega)&=\frac{1}{\omega-\Omega_{\bf k}+i\eta}\,,\\ G^{(0)}_{\beta\beta}(\mathbf{k},\omega)&=-\frac{1}{\omega+\Omega_{\bf k}-i\eta}\,,\\ G^{(0)}_{\alpha\beta}(\mathbf{k};\omega)&=G^{(0)}_{\beta\alpha}(\mathbf{k};\omega)=0\,. \end{aligned} \quad (10)$$

$G^{(0)}_{\alpha\alpha}$ and $G^{(0)}_{\beta\beta}$ are represented by the diagrams shown in Fig. 1.

The Green's functions $G_{\mu\nu}$ satisfy a matrix Dyson's equation[11]

$$G_{\mu\nu}(\mathbf{k},\omega)=G^{(0)}_{\mu\nu}(\mathbf{k},\omega)+\sum_{\gamma,\delta}G^{(0)}_{\mu\gamma}(\mathbf{k},\omega)\Sigma_{\gamma\delta}(\mathbf{k},\omega)G_{\delta\nu}(\mathbf{k},\omega)\,, \quad (11)$$

where the self-energy $\Sigma_{\gamma\delta}(\mathbf{k},\omega)$ can be expressed in the usual kind of diagrammatic expressions. It turns out[11–13] that $\Sigma_{\gamma\delta}(\mathbf{k},\omega)$ is small compared to the unperturbed energy $\Omega_{\bf k}$, so that, to leading order in $||\Sigma(\mathbf{k},\omega)||/\Omega_{\bf k}$ Eq. (11) can be decoupled and we obtain

$$G_{\alpha\alpha}(\mathbf{k},\omega)=\frac{1}{\omega-\Omega_{\bf k}-\Sigma_{\alpha\alpha}(\mathbf{k},\omega)+i\eta}\,. \quad (12)$$

The dispersion for an α spin wave with wave vector $\mathbf{k}$ is given by the pole of the propagator $G_{\alpha\alpha}(\mathbf{k},\omega)$, that is by the real part of the solution of the equation

$$\omega-\Omega_{\bf k}-\Sigma_{\alpha\alpha}(\mathbf{k},\omega)=0\,. \quad (13)$$

Again, to leading order in $||\Sigma(\mathbf{k},\omega)||/\Omega_{\bf k}$ the solution of Eq. (13) can be approximated as

$$\omega_{\bf k}\simeq\Omega_{\bf k}+{\rm Re}\Sigma_{\alpha\alpha}(\mathbf{k},\Omega_{\bf k})\,, \quad (14)$$

where we have used the fact that the imaginary part of the *on shell* (i.e., $\omega=\Omega_{\bf k}$) magnon self-energy is identically zero at $T=0$.[13]

It is possible to show that the first-order correction to the self-energy, which is of order $O(1/S^0)$, is identically zero at $T=0$, both for ω on shell and off shell. This is due to the fact that all the quartic vertices have been normal ordered.[13] The second-order self-energy,[14] which is of order $O(1/S)$, is given by the two diagrams shown in Fig. 2. The analytical expression is

$$\Sigma^{(2)}_{\alpha\alpha}(\mathbf{k},\omega)=\Omega_{\max}\frac{1}{[4Sa(S)]^2}\frac{1}{N^2}\sum_{(2,3,4)}\delta_{\bf G}(\mathbf{k}+2-3-4)\left[2V^{(2)}_{(\mathbf{k}234)}V^{(3)}_{(432\mathbf{k})}\frac{1}{\tilde\omega-\epsilon_2-\epsilon_3-\epsilon_4+i\eta}-8V^{(7)}_{(\mathbf{k}234)}V^{(8)}_{(432\mathbf{k})}\frac{1}{\tilde\omega+\epsilon_2+\epsilon_3+\epsilon_4-i\eta}\right]\,, \quad (15)$$

where $\Omega_{\max}=JzSa(S)$ and $\tilde\omega=\omega/\Omega_{\max}$. Using the property of the vertex functions given in Eq. (8), it is possible to see that the products $V^{(2)}_{(\mathbf{k}234)}V^{(3)}_{(432\mathbf{k})}$ and $V^{(7)}_{(\mathbf{k}234)}V^{(8)}_{(432\mathbf{k})}$ are regular functions of the momenta.[12,13]

FIG. 1. The single-arrow line corresponds to the bare α propagator. The double-arrow line corresponds to the bare β propagator.

The on-shell self-energy $\Sigma_{\alpha\alpha}^{(2)}(\mathbf{k},\Omega_{\mathbf{k}})$ gives a $1/S$ correction to the magnon dispersion. We have evaluated this correction by computing numerically the phase-space integrals in Eq. (15) in different ways, including lattice summations and the Monte Carlo method. In Fig. 3 we show the result for

$$R_{\mathbf{k}}=[2Sa(S)]^2\frac{\Sigma_{\alpha\alpha}^{(2)}(\mathbf{k},\Omega_{\mathbf{k}})}{\Omega_{\mathbf{k}}}\,, \tag{16}$$

as a function of $\mathbf{k}$ inside the antiferromagnetic Brillouin zone. We find that the correction is small and positive —i.e., the magnon dispersion becomes slightly stiffer. We can see that the second-order term increases the dispersion by approximately 2% for a wave vector close to the zone center and by approximately 4% for some of the wave vectors on the zone boundary. In order to compute the correction to Z_c, a precise evaluation of $R_{\mathbf{k}}$ for $\mathbf{k}\to 0$ is needed. First we attempted to calculate $R_{\mathbf{k}}$ for small but finite $\mathbf{k}$ and extrapolated to $\mathbf{k}=0$. This procedure is not very stable numerically, though, since close to the zone center $R_{\mathbf{k}}$ contains the difference between almost equal terms, whose magnitude diverges as $\mathbf{k}\to 0$. However, it is possible to show analytically[13] that $\Sigma_{\alpha\alpha}^{(2)}(\mathbf{k},\Omega_{\mathbf{k}})$ vanishes linearly as $\mathbf{k}\to 0$. This is expected, since, because of the rotational invariance of the Hamiltonian, the elementary excitations must be gapless.[15] Therefore, in order to obtain a more precise result we expanded $\Sigma_{\alpha\alpha}^{(2)}(\mathbf{k},\Omega_{\mathbf{k}})$ in a power series around $\mathbf{k}=0$, removed the canceling terms at $\mathbf{k}=0$ and computed the coefficient δ of the linear term by the Monte Carlo method. It is important to note that a correct treatment of the umklapp is essential here. The result is

$$\delta=\lim_{\mathbf{k}\to 0}\frac{[2Sa(S)]^2\Sigma_{\alpha\alpha}^{(2)}(\mathbf{k},\Omega_{\mathbf{k}})}{\Omega_{\mathbf{k}}}=0.0215\pm 0.0002\,. \tag{17}$$

The error estimate corresponds to 1 standard deviation, and 10^7 terms were used in the evaluation. This result is in complete agreement with the results from evaluations at small $\mathbf{k}$, described above. Now Z_c can finally be rewritten as

$$Z_c(S)=1+0.15795/2S+\delta(1/2S)^2+O(1/2S)^3\,, \tag{18}$$

which for $S=\frac{1}{2}$ yields $Z_c=1.1795\pm 0.0002$. As we mentioned above,[14] Eq. (18) is obtained by expanding the

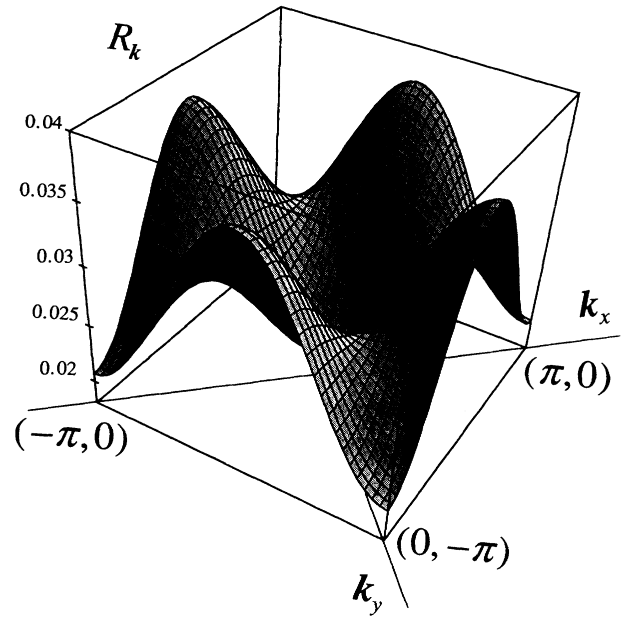

FIG. 3. Normalized self-energy $R_{\mathbf{k}}$, defined in Eq. (16), as a function of the wave vector inside the HAFM Brillouin zone.

second-order self-energy in powers of $1/S$ and keeping only the term of order $O(1/S)$. If instead we want the correction to Z_c given by the "total" second-order self-energy we obtain

$$Z_c(S)=1+0.15795/2S+[\delta/a(S)](1/2S)^2\,, \tag{19}$$

which may be interpreted as a perturbation expansion in the quartic term, V_{DM}. For $S=\frac{1}{2}$, Eq. (19) gives $Z_c=1.1765\pm 0.0002$. Both Eqs. (18) and (19) are in excellent agreement with the series-expansion result 1.18 ± 0.02. Recently, Igarashi and Watabe[16] have calculated the second-order correction to the self-energy by using the HP formalism. They found that the correction is negative for all the wave vectors and quite large near the zone boundary. Their Z_c is decreased by approximately 2% by the $1/S^2$ correction. We believe that our result is more reliable because of the aforementioned property of the DM vertices, that all the infrared singularities cancel out order-by-order. This property is not shared by the HP formalism. In addition, our calculation retained the umklapp processes which were neglected in Ref. 16. Our result strengthens the belief that the SWT expansion is a useful and reliable tool, whose low-order terms indeed give very precise results. A lengthy calculation, within the same formalism, of the Raman spectrum will be presented elsewhere.[13]

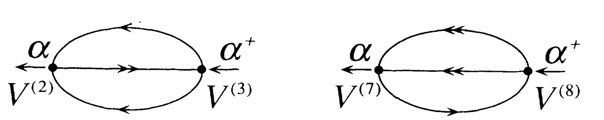

FIG. 2. Second-order self-energy diagrams for the α magnon.

This work was supported by NSF Grant No. DMR-9113911 and a grant of computer time from the National Center for Supercomputer Applications. M.W. was supported by the Swedish Natural Science Research Council through Contract No. F-PD 9901-302.

*Present address: Department of Physics, King's College London, Strand, London WC2R 2LS, United Kingdom.

[1]For $S > \frac{1}{2}$ in two dimensions, it is rigorously known that the HAFM has long-range order at $T=0$. See the appendix in I. Affleck *et al.*, Comm. Math. Phys. **115**, 477 (1988), and references therein.

[2]J. D. Reger and A. P. Young, Phys. Rev. B **37**, 5978 (1988); Mark Gross, Eduardo Velasco-Sanchez, and Eric D. Siggia, *ibid.* **39**, 2484 (1989); J. D. Reger, J. A. Riera, and A. P. Young, J. Phys. Condens. Matter **1**, 1855 (1989).

[3]R. Kubo, Rev. Mod. Phys. **24**, 344 (1953).

[4]S. J. Miyake, Prog. Theor. Phys. **74**, 468 (1985).

[5]Guillermo E. Castilla and Sudip Chakravarty, Phys. Rev. B **43**, 13687 (1991).

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

[7]R. R. P. Singh, Phys. Rev. B **39**, 9760 (1989); R. R. P. Singh and D. A. Huse, *ibid.* **40**, 7247 (1989).

[8]F. J. Dyson, Phys. Rev. **102**, 1217 (1956); **102**, 1230 (1956).

[9]S. V. Maleev, Zh. Eksp. Teor. Fiz. **30**, 1010 (1957) [Sov. Phys. JETP **64**, 654 (1958)].

[10]Details of the derivation of these results can be found in Refs. 11-13.

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

[12]P. Kopietz, Phys. Rev. B **41**, 9228 (1990).

[13]C. M. Canali and S. M. Girvin, Phys. Rev. B **45**, 7127 (1992).

[14]As one can see from Eq. (15), since the Oguchi correction renormalizes the noninteracting spin-wave dispersion, $\Omega_{\mathbf{k}}$, the second-order self-energy contains a factor $1/\alpha(S)$. When we say that the second-order self-energy is of order $O(1/S)$, we mean that the *leading term,* obtained by expanding $1/\alpha(S)$ in powers of $1/S$, is of order $O(1/S)$.

[15]In fact, the elementary excitations of the nearest-neighbor HAFM vanish *linearly.*

[16]Jun-ichi Igarashi and Akihiro Watabe, Phys. Rev. B **43**, 13456 (1991).

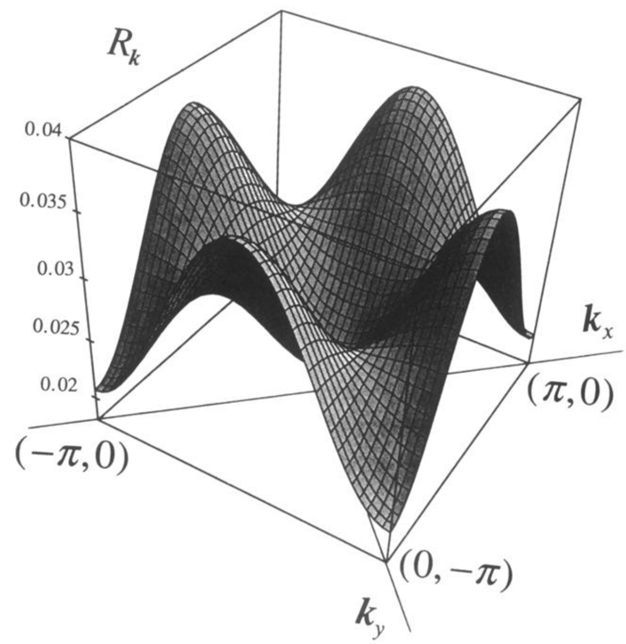

FIG. 3. Normalized self-energy $R_{\mathbf{k}}$, defined in Eq. (16), as a function of the wave vector inside the HAFM Brillouin zone.