Spin dynamics and antiferromagnetic short-range order in the two-dimensional Heisenberg model

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We investigate the spin dynamics in the presence of short-range order in the square lattice $S=\frac{1}{2}$ Heisenberg antiferromagnet by a spin-rotation-invariant Green's-function theory for the dynamic spin susceptibility. The self-energy is calculated in the lowest-order Born approximation using the results of a sum-rule–conserving mean-field approximation. In the spin-wave region, where the damping of magnons is found to be small compared with their energy, the dynamic structure factor is obtained in reasonable agreement with Monte Carlo data. Moreover, the structure factor yields an indication of the crossover to the relaxation region. [S0163-1829(99)00809-7]

To explain the unconventional magnetic properties of high-T_c superconductors,[1] the understanding of the spin dynamics in the undoped compounds (e.g., La_2CuO_4), described by the two-dimensional spin-$\frac{1}{2}$ antiferromagnetic (AFM) Heisenberg model $H=(J/2)\Sigma_{\langle i,j\rangle}\mathbf{S}_i\mathbf{S}_j$ (hereafter, we set $J=1$ and the lattice spacing $a=1$), is of primary importance. At finite temperatures, the dynamics in two dimensions is determined by the AFM short-range order (SRO). Of particular interest is the crossover from propagating spin wave to diffusion and relaxational behavior near characteristic wave numbers q_c and k_c [$\mathbf{k}=\mathbf{q}-\mathbf{Q}$, $\mathbf{Q}=(\pi,\pi)$], respectively. These wave numbers are the lowest boundaries for weakly damped magnons.

From general sum-rule arguments, Capellmann *et al.*[2] estimated $k_c\simeq T/c$ (c is the spin-wave velocity). Recently, the crossover has been studied at low temperatures using renormalization-group techniques[3] as well as at intermediate and high temperatures by a mode-mode coupling theory.[4] In the approaches describing the spin-wave region by perturbation expansions within the Dyson-Maleev formalism,[5,6] the crossover to the diffusion region is indicated by the breakdown of perturbation theory (divergent vertex corrections, cf. Ref. 5) near $q_c\propto\xi^{-1}\ll T$ (ξ is the correlation length). As argued in Refs. 2 and 7, the boundaries q_c, $k_c\propto\xi^{-1}$ are too small, which may be due to shortcomings of the bosonic representations. Barabanov and Maksimov[7] examined the spin-wave damping $\Gamma_{\mathbf{k}}$ at $\omega=\omega_{\mathbf{k}}$ (magnon energy) and $\mathbf{k}$ close to zero within a spin-rotation-invariant theory based on the Green's-function projection method[8,9] using the initial spin operators. In the range $T^{3/2}\ll\omega_{\mathbf{k}}\ll T$, the soft magnons are found to be well-defined quasiparticles ($\Gamma_{\mathbf{k}}\ll\omega_{\mathbf{k}}$) with the lowest boundary $k_c\simeq T^{3/2}/c\gg\xi^{-1}$. In a previous paper,[10] hereafter referred to as I, we presented a spin-rotation invariant theory of SRO based on the projection method[8,9] and elaborated in detail the mean-field approximation with site-dependent vertex parameters as introduced by Shimahara and Takada.[11] Note that in Ref. 7 the same projection method was used, but vertex parameters were not considered.

In this paper we extend the previous work of I and Ref. 7 and calculate the self-energy of the dynamic spin susceptibility $\chi^{+-}(\mathbf{q},\omega)=-\langle\langle S^+_{\mathbf{q}};S^-_{-\mathbf{q}}\rangle\rangle_\omega$ over the whole frequency and wave-vector region, whereby our perturbational approach is analogous to that of Ref. 7. To examine the validity of the spin-wave description, we compare our results for the dynamic structure factor with available Monte Carlo (MC) data[12] and calculate the magnon damping $\Gamma_{\mathbf{q}}$ at $\omega=\omega_{\mathbf{q}}$.

To determine the dynamic spin susceptibility in the presence of AFM SRO, we employ the projection method outlined in I and choose the two-operator basis $\mathbf{A}=(S^+_{\mathbf{q}},i\dot{S}^+_{\mathbf{q}})^T$. The two-time retarded matrix Green's function $\mathbf{G}(\omega)=\langle\langle\mathbf{A};\mathbf{A}^+\rangle\rangle_\omega$ is exactly represented as

$$\langle\langle\mathbf{A};\mathbf{A}^+\rangle\rangle_\omega=[\omega-\mathbf{M}'\mathbf{M}^{-1}-\Sigma(\omega)]^{-1}\mathbf{M}, \tag{1}$$

with the moments $\mathbf{M}=\langle[\mathbf{A},\mathbf{A}^+]\rangle$ and $\mathbf{M}'=\langle[i\dot{\mathbf{A}},\mathbf{A}^+]\rangle$, and the self-energy matrix $\mathbf{\Sigma}(\omega)=\langle\langle i\dot{\mathbf{A}}^{(\mathrm{ir})};\mathbf{A}^+\rangle\rangle_\omega\langle\langle\mathbf{A};\mathbf{A}^+\rangle\rangle_\omega^{-1}$ expressed by

$$\Sigma(\omega)=(\langle\langle i\dot{\mathbf{A}};-i\dot{\mathbf{A}}^+\rangle\rangle_\omega-\langle\langle i\dot{\mathbf{A}};\mathbf{A}^+\rangle\rangle_\omega\langle\langle\mathbf{A};\mathbf{A}^+\rangle\rangle_\omega^{-1}\times\langle\langle i\dot{\mathbf{A}};\mathbf{A}^+\rangle\rangle_\omega)\mathbf{M}^{-1}. \tag{2}$$

The irreducible part $-\ddot{S}^{+(\mathrm{ir})}_{\mathbf{q}}$ is given by

$$-\ddot{S}^{+(\mathrm{ir})}_{\mathbf{q}}=-\ddot{S}^+_{\mathbf{q}}-\omega^2_{\mathbf{q}}S^+_{\mathbf{q}};\omega^2_{\mathbf{q}}=M^{(3)}_{\mathbf{q}}/M^{(1)}_{\mathbf{q}}, \tag{3}$$

where $M^{(1)}_{\mathbf{q}}=\langle[i\dot{S}^+_{\mathbf{q}},S^-_{-\mathbf{q}}]\rangle=-8C_{1,0}(1-\gamma_{\mathbf{q}})$ and $M^{(3)}_{\mathbf{q}}=\langle[-\ddot{S}^+_{\mathbf{q}},-i\dot{S}^-_{-\mathbf{q}}]\rangle$, with $C_{n,m}=\langle S^+_0S^-_{\mathbf{R}}\rangle$, $\mathbf{R}=n\mathbf{e}_x+m\mathbf{e}_y$, and $\gamma_{\mathbf{q}}=1/2(\cos q_x+\cos q_y)$.

In the mean-field approximation ($-\ddot{S}^{+(\mathrm{ir})}_{\mathbf{q}}=0$, cf. I) we have $\chi_0^{+-}(\mathbf{q},\omega)=-M^{(1)}_{\mathbf{q}}(\omega^2-\omega^2_{\mathbf{q}})^{-1}$, where the spectrum $\omega_{\mathbf{q}}$ is calculated by the decoupling of $-\ddot{S}^+_i$ with vertex parameters α_i as proposed by Shimahara and Takada.[11] We get

$$\omega^2_{\mathbf{q}}=2(1-\gamma_{\mathbf{q}})[1-2\alpha_1C_{1,0}+2\alpha_2(C_{2,0}+2C_{1,1})-8\alpha_1C_{1,0}\gamma_{\mathbf{q}}]. \tag{4}$$

The parameter α_1 is determined by the sum rule $C_{0,0}=\frac{1}{2}$ yielding $\alpha_1=\alpha_1(T)$. To obtain $\alpha_2(T)$, we take, as in our previous paper,[13] the Monte Carlo value of the ground-state energy [$3C_{1,0}=-0.6693$ (Ref. 14)] and assume the ratio $[\alpha_2(T)-1]/[\alpha_1(T)-1]=0.8530$ as temperature independent.

Calculating the self-energy matrix, we express the renormalization of all Green's functions in Eq. (2) in terms of

$$T(\mathbf{q},\omega)=-(M_{\mathbf{q}}^{(1)})^{-2}\langle\langle-\ddot{S}_{\mathbf{q}}^{+(\mathrm{ir})};-\ddot{S}_{-\mathbf{q}}^{-(\mathrm{ir})}\rangle\rangle_{\omega}. \quad (5)$$

Note that in Ref. 7 the renormalization of $\langle\langle\ddot{S}_{\mathbf{q}}^{+};\ddot{S}_{-\mathbf{q}}^{-}\rangle\rangle_{\omega}$ only was considered. The elements of $\mathbf{\Sigma}(\omega)$ are found to vanish except for $\Sigma_{21}\equiv\Sigma(\mathbf{q},\omega)$ given by

$$\Sigma(\mathbf{q},\omega)=-M_{\mathbf{q}}^{(1)}T(\mathbf{q},\omega)\left(1-\frac{M_{\mathbf{q}}^{(1)}T(\mathbf{q},\omega)}{\omega^{2}-\omega_{\mathbf{q}}^{2}}\right)^{-1}. \quad (6)$$

From Eq. (1) we get the dynamic spin susceptibility

$$\chi^{+-}(\mathbf{q},\omega)=-\frac{M_{\mathbf{q}}^{(1)}}{\omega^{2}-\omega_{\mathbf{q}}^{2}-\Sigma(\mathbf{q},\omega)}. \quad (7)$$

Rewriting Eq. (6) as $-M_{\mathbf{q}}^{(1)}T(\mathbf{q},\omega)=\Sigma(\mathbf{q},\omega)+\Sigma(\mathbf{q},\omega)\chi_{0}^{+-}(\mathbf{q},\omega)T(\mathbf{q},\omega)$, and following the diagrammatic arguments by Plakida,[9] the self-energy $\Sigma(\mathbf{q},\omega)$ is just the irreducible part of $-M_{\mathbf{q}}^{(1)}T(\mathbf{q},\omega)$ which has no parts connected by a single Green's function $\chi_{0}^{+-}(\mathbf{q},\omega)$. Thus, $\Sigma(\mathbf{q},\omega)$ is exactly expressed as

$$\Sigma(\mathbf{q},\omega)=\frac{1}{M_{\mathbf{q}}^{(1)}}\langle\langle-\ddot{S}_{\mathbf{q}}^{+(\mathrm{ir})};-\ddot{S}_{-\mathbf{q}}^{-(\mathrm{ir})}\rangle\rangle_{\omega}^{(\mathrm{ir})}, \quad (8)$$

with the imaginary part

$$\Sigma''(\mathbf{q},\omega)=-[2M_{\mathbf{q}}^{(1)}n(\omega)]^{-1}\int_{-\infty}^{\infty}dt\, e^{i\omega t}\langle\ddot{S}_{-\mathbf{q}}^{-(\mathrm{ir})}\ddot{S}_{\mathbf{q}}^{+(\mathrm{ir})}(t)\rangle^{(\mathrm{ir})}, \quad (9)$$

where $n(\omega)=(e^{\beta\omega}-1)^{-1}$. Note that $\Sigma''(\mathbf{q},-\omega)=-\Sigma''(\mathbf{q},\omega)$. Because the site representation of $\ddot{S}_{\mathbf{q}}^{+}$ in Eq. (9) contains spin operators on different sites only, we obtain

$$\ddot{S}_{\mathbf{q}}^{+}=-\sum_{\mathbf{q}_1,\mathbf{q}_2}B_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}(\tfrac{1}{2}S_{\mathbf{q}_1}^{-}S_{\mathbf{q}_2}^{+}+S_{\mathbf{q}_1}^{z}S_{\mathbf{q}_2}^{z})S_{\mathbf{q}_3}^{+}, \quad (10)$$

with

$$B_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}=4[4(\gamma_{\mathbf{q}_1+\mathbf{q}_3}-\gamma_{\mathbf{q}_2})(\gamma_{\mathbf{q}_3}-\gamma_{\mathbf{q}_1})-\gamma_{\mathbf{q}_1}+\gamma_{\mathbf{q}_2+\mathbf{q}_3}-\gamma_{\mathbf{q}_1+\mathbf{q}_2}+\gamma_{\mathbf{q}_3}], \quad (11)$$

where $\mathbf{q}_3=\mathbf{q}-\mathbf{q}_1-\mathbf{q}_2$.

Considering the spin-wave region, we make the Born approximation, i.e., we decouple the irreducible correlation function in Eq. (9) with Eqs. (10) and (11) in terms of two-spin correlation functions $C_{\mathbf{q}}(t)=\langle S_{\mathbf{q}}^{+}S_{-\mathbf{q}}^{-}(t)\rangle$. This yields

$$\Sigma''(\mathbf{q},\omega)=-[8\pi^{2}M_{\mathbf{q}}^{(1)}n(\omega)]^{-1}\sum_{\mathbf{q}_1,\mathbf{q}_2}B_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}^{2}\int_{-\infty}^{\infty}d\omega_1\times\int_{-\infty}^{\infty}d\omega_2 C_{\mathbf{q}_1}(\omega_1)C_{\mathbf{q}_2}(\omega_2)C_{\mathbf{q}_3}(\omega-\omega_1-\omega_2), \quad (12)$$

where $C_{\mathbf{q}}(\omega)=FT\{C_{\mathbf{q}}(t)\}=2n(\omega)\mathrm{Im}\,\chi^{+-}(\mathbf{q},\omega)$. In the lowest order, we insert the mean-field results for $C_{\mathbf{q}}(\omega)$ (cf. I) and get

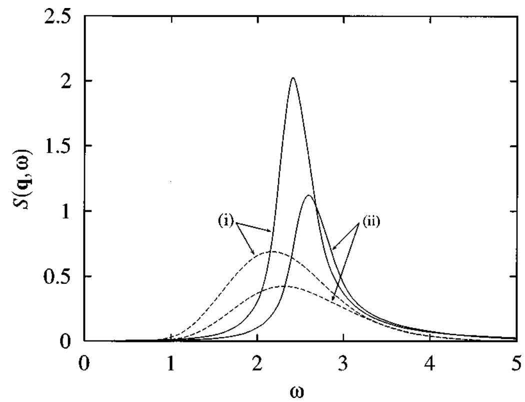

FIG. 1. Dynamic structure factor at $T=0.38$ and (i) $\mathbf{q}=[(5/8)\pi,(5/8)\pi]$, (ii) $\mathbf{q}=[(\pi/2),(\pi/2)]$ compared with the Monte Carlo data (dashed line) of Ref. 12.

$$\Sigma''(\mathbf{q},\omega)=-\pi[8M_{\mathbf{q}}^{(1)}n(\omega)]^{-1}\times\sum_{\mathbf{q}_1,\mathbf{q}_2}B_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}^{2}\left(\prod_{i=1}^{3}\frac{M_{\mathbf{q}_i}^{(1)}}{\omega_{\mathbf{q}_i}}\right)I_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}(\omega), \quad (13)$$

with $\mathbf{q}_3=\mathbf{q}-\mathbf{q}_1-\mathbf{q}_2$ and

$$I_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}(\omega)=\sum_{\sigma_1,\sigma_2,\sigma_3=\pm}\left[\prod_{i=1}^{3}\sigma_i n(\sigma_i\omega_{\mathbf{q}_i})\right]\times\delta\left(\omega-\sum_{i=1}^{3}\sigma_i\omega_{\mathbf{q}_i}\right). \quad (14)$$

First we calculate the dynamic structure factor $S(\mathbf{q},\omega)=2(1-e^{-\beta\omega})^{-1}\,\mathrm{Im}\,\chi^{zz}(\mathbf{q},\omega)[2\chi^{zz}=\chi^{+-}]$ from Eqs. (7), (13), and (14), where we drop the real part $\Sigma'(\mathbf{q},\omega)$ of the self-energy. This may be justified as follows. Approximating $\Sigma'(\mathbf{q},\omega)$ by $\Sigma'(\mathbf{q},\omega_{\mathbf{q}})$, the magnon spectrum becomes renormalized. On the other hand, an effective renormalization has already been achieved by the introduction of vertex parameters in $\omega_{\mathbf{q}}$ [Eq. (4)]. Hence, we neglect $\Sigma'(\mathbf{q},\omega)$.

In Fig. 1 our numerical results at $T=0.38$ are depicted and compared with the MC data of Ref. 12. For the $\mathbf{q}$ values used we have $q\gg\xi^{-1}\simeq0.1$ (cf. I) and $\omega_{\mathbf{q}}\gg T$. The spin-wave peaks in $S(\mathbf{q},\omega)$ occur nearly at $\omega_{\mathbf{q}}$ (cf. Fig. 3) and, as compared with the MC values, are slightly shifted (by about 10%) to higher frequencies. The more pronounced peak structures may be due to an underestimation of the magnon damping in the lowest-order Born approximation. Note the essential role played by SRO in describing the spin-wave dynamics. In the mode-mode coupling theory of Ref. 4, the structure factor for $T=0.4$ and $\mathbf{q}=(\pi/2,\pi/2)$ exhibits a very broad maximum around relatively high frequencies indicating, as argued in Ref. 4, that the SRO is not sufficiently taken into account.

Considering $\mathbf{q}$ close to $\mathbf{Q}$, where MC data are available,[12] we have calculated $S(\mathbf{q},\omega)$ at $T=0.38$ and $\mathbf{q}=[(15/16)\pi,(15/16)\pi]$. Here, we have $k\xi\simeq2.8$ and $\omega_{\mathbf{q}}=0.54>T$, i.e., we are in the boundary region of spin-wave behavior. Our result (narrow peak at $\omega_{\mathbf{q}}$,) qualitatively disagrees with the broad MC curve. The breakdown of the spin-wave description, seen by the comparison of $S(\mathbf{q},\omega)$

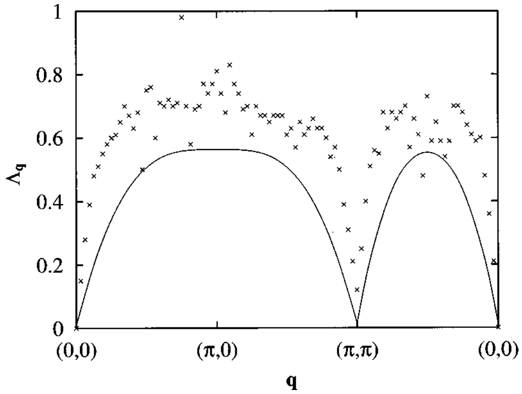

FIG. 2. Linewidth $\Lambda_{\mathbf{q}}$ at $T=0.35$ in comparison with the MC data ($\times$) of Ref. 12.

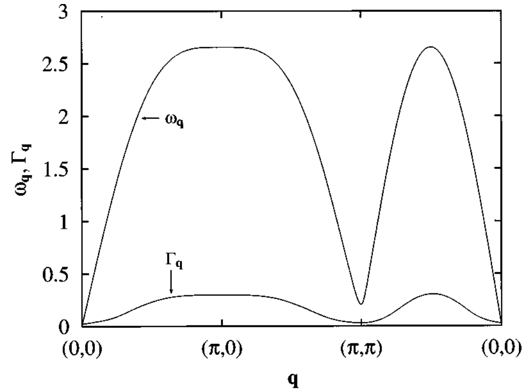

FIG. 3. Magnon energy $\omega_{\boldsymbol{q}}$ and damping $\Gamma_{\boldsymbol{q}}$ at $T=0.35$.

with the MC data, indicates the crossover to the relaxation region which cannot be described by our theory.

To further test our spin-wave approach within the validity region in **q** space (**q** not too close to zero or **Q**), in Fig. 2 we compare the linewidth $\Lambda_{\mathbf{q}}$ of the relaxation function $F(\mathbf{q},\omega)=2(1-e^{-\beta\omega})[\beta\omega\chi(\mathbf{q})]^{-1}S(\mathbf{q},\omega)$ with the MC data at $T=0.35$,[12] and we find a good agreement. The linewidth is defined by $\Lambda_{\mathbf{q}}^2=\langle\omega^2\rangle_{\mathbf{q}}-\langle\omega\rangle_{\mathbf{q}}^2$, where $\langle\omega^n\rangle_{\mathbf{q}}=\int_0^\infty d\omega\,\omega^n F(\mathbf{q},\omega)/\int_0^\infty d\omega\,F(\mathbf{q},\omega)$, and yields a measure for the spin-wave damping.

Finally, we consider the magnon damping at $\omega=\omega_{\mathbf{q}}$ in more detail. Rewriting Eq. (7) as $\chi^{+-}(\mathbf{q},\omega)=-M_{\mathbf{q}}^{(1)}(2\omega_{\mathbf{q}})^{-1}\Sigma_{\sigma=\pm}\sigma[\omega-\sigma\omega_{\mathbf{q}}-\Sigma_\sigma(\mathbf{q},\omega)]^{-1}$ with $\Sigma_\sigma(\mathbf{q},\omega)=\Sigma(\mathbf{q},\omega)(\omega+\sigma\omega_{\mathbf{q}})^{-1}$, we define the magnon damping as

$$\Gamma_{\mathbf{q}}=-\Sigma_\sigma''(\mathbf{q},\sigma\omega_{\mathbf{q}})=-\frac{\Sigma''(\mathbf{q},\omega_{\mathbf{q}})}{2\omega_{\mathbf{q}}}. \qquad (15)$$

Here, only two-magnon scattering processes [cf. Eq. (14) with $\omega=\omega_{\mathbf{q}}$] contribute.[15]

Figure 3 shows our result for $\Gamma_{\mathbf{q}}$ compared with $\omega_{\mathbf{q}}$ at $T=0.35$. As can be seen, the **q** dependence of $\Gamma_{\mathbf{q}}$ resembles that of $\Lambda_{\mathbf{q}}$, where we get $\Gamma_{\mathbf{q}}\simeq\Lambda_{\mathbf{q}}/2$. In the spin-wave region, we have a well-defined quasiparticle picture ($\Gamma_{\mathbf{q}}/\omega_{\mathbf{q}}\simeq0.1$). On the other hand, as revealed by the frequency dependence of $S(\mathbf{q},\omega)$ discussed above, the spin-wave description is no longer valid at $T=0.38$ and $\mathbf{q}=[(15/16)\pi,(15/16)\pi]$, although we have $\Gamma_{\mathbf{q}}/\omega_{\mathbf{q}}\simeq0.07$. We conclude that the consideration of magnon damping (at $\omega=\omega_{\mathbf{q}}$) alone does not provide a sufficient criterion for the validity of the spin-wave description, but, in addition, the dynamic structure factor has to be considered.

To summarize, we presented a spin-rotation-invariant theory of spin-wave dynamics in the presence of SRO in the two-dimensional Heisenberg antiferromagnet. The dynamic structure factor is calculated in reasonable agreement with MC data and is found to be indicative of the crossover to the relaxation region.

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