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Dynamics of the quantum integer spin *S* one-dimensional Heisenberg antiferromagnet coupled to phonons

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Abstract
We present the low-temperature dynamic properties of the quantum one-dimensional Heisenberg antiferromagnet with integer spin S coupled to phonons. The calculation of the relaxation function is performed using the combination of the memory function formalism with the modified spin-wave theory. The procedure includes up to two-magnon and magnon–phonon processes. We show that the phonon–magnon coupling smooths the double-peak structure obtained for the model in the absence of phonons, when the wavevector q moves from $q = \pi$.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Since Haldane's conjecture [1] in 1983, quantum antiferromagnetism has become a very exciting field. Now, the existence of an excitation gap and a finite correlation length in an integer spin one-dimensional Heisenberg antiferromagnet is very well established theoretically, numerically and experimentally. A great number of theoretical studies have been devoted to the understanding of the properties of low-dimensional antiferromagnets when features such as interchain coupling, anisotropies and external fields are included in the model. However, the dynamics of the magnetic system when the spin–phonon coupling is taken into account have not been studied so far.

As is well known, in low-dimension quantum magnetic systems, spin–phonon coupling plays an important role. The lattice vibrations modulate the exchange interaction by varying the interatomic distances. Therefore, the exchange interaction can be expanded in powers of the atomic displacements, keeping only the linear terms. This gives an interaction Hamiltonian which is linear in the phonon operators and quadratic in the spin operators.

The dynamic properties of the classical Heisenberg chain coupled to phonons was studied by Fivez *et al* [2] using the memory function formalism. The influence of spin–phonon coupling on the two-dimensional spin-$1/2$ antiferromagnet was treated in [3] using a unitary transformation approach within the framework of the modified spin-wave theory. In both papers the authors calculated the phonon structure factor, but not the spin structure factor. Some works treating the spin–phonon coupling can be found in [4–7].

However, as far as we know, there are no calculations for the spin–spin dynamic correlation function for the antiferromagnet in one dimension when the phonon coupling is taken into account for $S = 1/2$ or $S \to \infty$. So we cannot compare our results with the ones in those cases. For $S = 1/2$, the elementary excitations are spinons and the coupling to phonons leads to a dimerization of the chain. The behavior is completely different to that of integer spins. In the classical limit ($S \to \infty$) the Haldane gap vanishes and we do not have a double-peak structure for the spin correlation function. The effect of the coupling would be, therefore, less dramatic.

In the present work, we calculate the relaxation function for the quantum one-dimensional integer spin S Heisenberg antiferromagnet taking into account the magnon–phonon coupling using the memory function method, following a procedure proposed originally by Reiter [8] and further developed by other authors [9]. This method has proven successful in the study of the classical and quantum Heisenberg models in one [10] and two dimensions [11, 12], showing good agreement with experimental data, molecular dynamic simulations, and, also, with other theories [13]. For the purpose of numerical calculations we will take $S = 1$. The dynamics of the one-dimensional $S = 1$ antiferromagnet was studied by Pires and Gouvea in [14]. As a consequence of the Haldane gap a double-peak structure was found for the dynamical correlation function. In that reference it was suggested that the effect of higher-order processes could smooth the sharp peaks obtained. One of such processes is the magnon–phonon coupling that we consider in the present paper.

The calculation of the memory function, which plays a central role in the formalism, does not require long-range order to be valid, for it depends only on correlations between nearest neighbors. The frequency of the local spin-wave modes and static correlations, required as input to the method, are obtained via the modified spin-wave (MSW) treatment. It is well known that the standard spin-wave theory is not applicable to low-dimensional quantum magnets without modifications [15]. In the MSW theory [16], the consequence of the Mermin–Wagner theorem is enforced by hand in a variational density-matrix approach. The procedure has been applied to one- (1D) and two-dimensional (2D) ferromagnets [16] and antiferromagnets [17, 18], giving results in excellent agreement with results obtained via exact diagonalization [19] and renormalization-group theory [20]. We have used the MSW theory to obtain the static quantities required by the memory function formalism.

The combination of these two techniques, the memory function method and the MSW theory, has already been applied by some co-workers of our group to study the low-temperature properties of the quantum 1D [14] spin-1 and 2D [12] spin-$1/2$ Heisenberg models.

The structure of this paper is as follows. In section 2 we describe the steps in the calculation of the spin–spin relaxation function and present the expression obtained for the memory function. In section 3 we discuss the numerical result obtained for the spin–spin relaxation function for different values of temperatures, wavevectors q, and spin–phonon coupling constant. In section 4 we present our conclusions.

2. Dynamics

We start from the following Hamiltonian:

$$H = H_S + H_{SP} + H_P, \tag{1}$$

where

$$H_S = J\sum_{l=1}^{N}[\mathbf{S}_l \cdot \mathbf{T}_{l+1} + \mathbf{T}_{l-1} \cdot \mathbf{S}_l] \tag{2}$$

$$H_{SP} = \alpha\sum_{l=1}^{N}[(\mathbf{x}_l - \mathbf{y}_{l+1})\mathbf{S}_l \cdot \mathbf{T}_{l+1} + (\mathbf{y}_{l-1} - \mathbf{x}_l)\mathbf{T}_{l-1} \cdot \mathbf{S}_l] \tag{3}$$

$$H_P = \sum_{l=1}^{N}\left\{\frac{m}{2}(\dot{\mathbf{x}}_l^2 + \dot{\mathbf{y}}_l^2) + \frac{K}{2}[(\mathbf{x}_l - \mathbf{y}_{l+1})^2 + (\mathbf{y}_{l-1} - \mathbf{x}_l)^2]\right\}, \tag{4}$$

where $\mathbf{x}_l$, $\mathbf{y}_l$, $\mathbf{S}_l$ and $\mathbf{T}_l$ are the displacement operators and spin operators of the sublattices A and B respectively, J is the exchange constant and α is the spin–phonon coupling. Taking the Fourier transform gives

$$H_S = 2\sum_{k=1}^{N} J(k)[\mathbf{S}_k \cdot \mathbf{T}_{-k} + \mathbf{T}_k \cdot \mathbf{S}_{-k}] \tag{5}$$

$$H_{SP} = 2\mathrm{i}\alpha\sum_{q,k}[-\mathbf{x}_q \sin(q+k) + \mathbf{y}_q \sin(k)]\mathbf{S}_k \cdot \mathbf{T}_{-q-k} \tag{6}$$

$$H_P = K\sum_{q}[\mathbf{x}_q\mathbf{x}_{-q} + \mathbf{y}_q\mathbf{y}_{-q} - \cos(q)(\mathbf{x}_q\mathbf{y}_{-q} + \mathbf{x}_{-q}\mathbf{y}_q)], \tag{7}$$

where $J(q) = 2J\cos(q)$.

Using the Dyson–Maleev representation,

$$\begin{array}{lll} \mathbf{S}_l^+ = \sqrt{2S}a_l & \mathbf{S}_l^- = \sqrt{2S}a_l^+ & \mathbf{S}_l^z = S - a_l^+a_l \\ \mathbf{T}_l^+ = \sqrt{2S}b_l^+ & \mathbf{T}_l^- = \sqrt{2S}b_l & \mathbf{T}_l^z = -S + b_l^+b_l \end{array}, \tag{8}$$

and a transformation defined by

$$\begin{aligned} \mathbf{x}_q &= \varepsilon_q + \eta_{-q} \\ \mathbf{y}_q &= \varepsilon_q - \eta_{-q}, \end{aligned} \tag{9}$$

where

$$\begin{aligned} \varepsilon_q &= \frac{1}{\sqrt{2m\omega_c(q)}}(\alpha_q + \alpha_{-q}^+), \\ \eta_q &= \frac{1}{\sqrt{2m\omega_d(q)}}(\beta_q + \beta_{-q}^+) \end{aligned} \tag{10}$$

and

$$\begin{aligned} \omega_c(q) &= \sqrt{\frac{2K}{m}}(1-\cos(q))^{1/2}, \\ \omega_d(q) &= \sqrt{\frac{2K}{m}}(1+\cos(q))^{1/2} \end{aligned} \tag{11}$$

are the phonon frequencies of the A and B sublattice respectively, we obtain

$$H_S = 2JS\sum_k\{a_k^+a_k + b_k^+b_k + \cos(k)(a_kb_k + a_k^+b_k^+)\} \tag{12}$$

$$H_{SP} = -4\mathrm{i}\alpha S\sum_{q,k}\{\varepsilon_q\Gamma_{q,k}\sin(q/2) - \eta_{-q}\Delta_{q,k}\cos(q/2)\}, \tag{13}$$

where

$$\Gamma_{q,k} = \cos(q/2)(a_{q+k}^+a_k + b_k^+b_{q+k}) + \cos(k+q/2)(a_kb_{q+k} + a_{q+k}^+b_k^+) \tag{14}$$

$$\Delta_{q,k} = \sin(q/2)(a_{q+k}^+a_k - b_k^+b_{q+k}) + \sin(k+q/2)(a_{q+k}^+b_k^+ - a_kb_{q+k}) \tag{15}$$

and

$$H_P = \sum_q \{\omega_c(q)\alpha_q^+\alpha_q + \omega_d(q)\beta_q^+\beta_q\}. \tag{16}$$

Our aim is the calculation of the dynamic structure factor, which is the Fourier transform of the relaxation function, defined by

$$S^\alpha(q,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t\mathrm{e}^{-\mathrm{i}\omega t}\frac{(\mathbf{S}^\alpha(t),\mathbf{S}^\alpha(0))}{(\mathbf{S}^\alpha,\mathbf{S}^\alpha)}, \tag{17}$$

where $\alpha = x, y, z$. $\mathbf{S}_q$ is the Fourier transform of spins belonging to both sublattices A and B. The inner product (A, B) of two operators A and B is defined by [21]

$$(A,B) = \frac{1}{\beta}\int_0^\beta \langle \mathrm{e}^{\lambda H}A^+\mathrm{e}^{-\lambda H}B\rangle\,\mathrm{d}\lambda, \tag{18}$$

where $\langle\cdots\rangle$ denotes the thermal average and $\beta = 1/k_\mathrm{B}T$, k_B being the Boltzmann constant. In our work we will take $k_\mathrm{B} = 1$ and do the numerical calculations for $S = 1$.

It can be shown that the Laplace transform of the relaxation function

$$R^\alpha(z) = -\mathrm{i}\int_0^\infty \mathrm{e}^{\mathrm{i}zt}(\mathbf{S}_q^\alpha(t),\mathbf{S}_q^\alpha(0))\,\mathrm{d}t \tag{19}$$

can be written as [22]

$$R^\alpha(z) = (\mathbf{S}_q^\alpha,\mathbf{S}_q^\alpha)\left\{z - \frac{\langle\omega_q^2\rangle}{[z+\Sigma_q(z)]}\right\}^{-1}, \tag{20}$$

where

$$\langle\omega^2\rangle = \frac{(\dot{\mathbf{S}}_q^\alpha,\dot{\mathbf{S}}_q^\alpha)}{(\mathbf{S}_q^\alpha,\mathbf{S}_q^\alpha)} \tag{21}$$

is the second moment and $\Sigma_q(t)$ is the memory function given by

$$\Sigma_q(t) = -\frac{M(t)}{(\dot{\mathbf{S}}_q,\dot{\mathbf{S}}_q)} \tag{22}$$

$$M(t) = (QL^2\mathbf{S}_q, \exp(-\mathrm{i}QLQt)QL^2\mathbf{S}_q) \tag{23}$$

and

$$QL^2\mathbf{S}_q = L^2\mathbf{S}_q - \langle\omega^2\rangle\mathbf{S}_q. \tag{24}$$

L is the Liouville operator defined by $LA = \mathrm{i}\dot{A} = -\mathrm{i}[A, H]$ and Q is the projection operator, which applied on an operator B_q gives

$$QB_q = B_q - \frac{(\mathbf{S}_q,B_q)}{(\mathbf{S}_q,\mathbf{S}_q)}\mathbf{S}_q - \frac{(L\mathbf{S}_q,B_q)}{(L\mathbf{S}_q,L\mathbf{S}_q)}L\mathbf{S}_q. \tag{25}$$

The dynamic structure factor $S(q, w)$, which is the imaginary part of $R_q(z)$, can be written as

$$S(q,\omega) = (\mathbf{S}_q^\alpha,\mathbf{S}_q^\alpha)\langle\omega_q^2\rangle\left\{\frac{\Sigma_q''(\omega)}{[\omega^2-\langle\omega_q^2\rangle+\omega\Sigma_q'(\omega)]^2+[\omega\Sigma_q''(\omega)]^2}\right\}. \tag{26}$$

$\Sigma_q'(\omega)$ and $\Sigma_q''(\omega)$ are the real and imaginary parts of $\Sigma_q(\omega)$.

It was shown by Pires and Gouvea [13] that the memory function technique is equivalent to the Green's function approach (at least up to the second order) for the calculation of the phonon structure factor (and the amount of work involved in the calculation is the same). However, in the calculation of the symmetrized spin–spin correlation function we have a term with two boson operators in the component S^z. In this case we would have to use a two-particle Green's function, and the memory function approach is more convenient. That is the reason why this formalism has been largely used in the literature.

We find from the equation of motion defining the Liouville operator and from the Hamiltonian the following expression:

$$\begin{aligned} L^2\mathbf{S}_q^x &= 4S^2J^2(1-\cos^2 q)\mathbf{S}_q^x \\ &\quad - 2\mathrm{i}\alpha JS^2\sqrt{N}\sum_k\{[\cos(q)\sin(q) - \cos(q-k)\sin(q-k)]\mathbf{x}_k\mathbf{S}_{k-q}^x \\ &\quad - \sin(k)\mathbf{y}_k\mathbf{S}_{k-q}^x + \cos(q)\sin(k)\mathbf{x}_k\mathbf{T}_{k-q}^x + \cos(k-q)\sin(k)\mathbf{y}_k\mathbf{T}_{k-q}^x\}. \end{aligned} \tag{27}$$

For the y-component we find an identical expression by replacing $x \leftrightarrow y$, while for the z-component we find the same result obtained in [14]. The expression for $\mathbf{T}_q$ is obtained by the replacement $\mathbf{S} \leftrightarrow \mathbf{T}$.

We introduce the Bogoliubov transformation given by

$$a_k = u_k c_k + v_k d_{-k}^+ \qquad b_{-k}^+ = v_k c_k + u_k d_{-k}^+, \tag{28}$$

where a_k and b_k^+ are the Fourier transforms of a_l and b_l^+, with k going up half of the first Brillouin zone.

Using the modified spin-wave theory we have the magnon frequency

$$\omega_k = \lambda(1-\eta^2\cos^2 k)^{1/2}, \tag{29}$$

and

$$\begin{aligned} u_k^2 &= \frac{1}{2(1-\eta^2\cos^2 k)^{1/2}} + \frac{1}{2} \\ v_k^2 &= \frac{1}{2(1-\eta^2\cos^2 k)^{1/2}} - \frac{1}{2} \\ v_k^2 &= u_k^2 - 1. \end{aligned} \tag{30}$$

The dependences of the η and λ parameters on the temperature are obtained by solving the self-consistent equations presented in [18].

Equation (29) has a gap at $k = 0$ given by $\omega_0 = \lambda(1-\eta^2)^{1/2}$. The correlation length is given by $\varepsilon\alpha e^{\pi S}$ and, therefore, for large S the spin chain has long-range order. The gap decreases with the increase of S. The MSW formalism, as was discussed by Arovas and Auerbach [23], is equivalent to a treatment using the Schwinger boson technique and gives a gap. This gap can be associated with the Haldane gap, and it was studied in [14].

Following the procedure described in detail in [8], we evaluated $\Sigma_q(t)$, obtaining

$$\Sigma_q(t) = \frac{1}{N}\sum_k\{A_-^c\cos(\Omega_-^c t) + A_-^d\cos(\Omega_-^d t) + A_+^c\cos(\Omega_+^c t) + A_+^d\cos(\Omega_+^d t)\}, \tag{31}$$

where

$$A_-^c(q,k) = \frac{1}{(L\mathbf{S}_q^x, L\mathbf{S}_q^x)} n_k^c n_{q-k} \frac{(\mathrm{e}^{\beta\omega_c(k)} - \mathrm{e}^{\beta\omega_{q-k}})}{\beta\Omega_-^c}\Gamma_1(q,k) \tag{32}$$

$$A_-^d(q,k) = \frac{1}{(L\mathbf{S}_q^x, L\mathbf{S}_q^x)} n_k^d n_{q-k} \frac{(\mathrm{e}^{\beta\omega_d(k)} - \mathrm{e}^{\beta\omega_{q-k}})}{\beta\Omega_-^d}\Gamma_2(q,k) \tag{33}$$

$$A_+^c(q,k) = \frac{1}{(L\mathbf{S}_q^x, L\mathbf{S}_q^x)} n_k^c n_{q-k} \frac{(\mathrm{e}^{\beta\Omega_+^c} - 1)}{\beta\Omega_+^c}\Gamma_1(q,k) \tag{34}$$

$$A_+^d(q,k) = \frac{1}{(L\mathbf{S}_q^x, L\mathbf{S}_q^x)} n_k^d n_{q-k} \frac{(\mathrm{e}^{\beta\Omega_+^d} - 1)}{\beta\Omega_+^d}\Gamma_2(q,k) \tag{35}$$

$$\Gamma_1(q,k) = \tfrac{1}{2}(v_{q-k}v_{q-k} + u_{q-k}u_{q-k})B_1(q,k) + v_{q-k}u_{q-k}C_1(q,k),$$
$$\Gamma_2(q,k) = \tfrac{1}{2}(v_{q-k}v_{q-k} + u_{q-k}u_{q-k})B_2(q,k) + v_{q-k}u_{q-k}C_2(q,k),$$
$$\begin{aligned}B_1(q,k) = 16\alpha^2 J^2 S^4\sqrt{N}\bigg\{&\frac{S}{2m\omega_c(k)}\{4\sin^2(k/2)\cos^2(q-k/2)\\ &\times[\cos^2(q)+\cos(q-k)\cos(q)+\cos^2(q-k)]\\ &-4\sin(k)\sin(k/2)\cos(q-k/2)[\cos(q)+\cos(k-q)]\\ &+\sin^2(k)[\cos^2(q)+\cos(q-k)\cos(q)+\cos^2(q-k)+4]\}\bigg\},\end{aligned}$$
$$\begin{aligned}B_2(q,k) = 16\alpha^2 J^2 S^4\sqrt{N}\bigg\{&\frac{S}{2m\omega_d(k)}\{4\cos^2(k/2)\sin^2(q-k/2)\\ &\times[\cos^2(q)-\cos(q-k)\cos(q)+\cos^2(q-k)]\\ &-4\sin(k)\cos(k/2)\sin(q-k/2)[\cos(q)-\cos(k-q)]\\ &+\sin^2(k)[\cos^2(q)-\cos(q-k)\cos(q)+\cos^2(q-k)+4]\}\bigg\},\end{aligned}$$
$$\begin{aligned}C_1(q,k) = 16\alpha^2 J^2 S^4\sqrt{N}\bigg\{&\frac{S}{2m\omega_c(k)}\{2\sin(k)\sin(k/2)\cos(q-k/2)\\ &\times[\cos^2(q)+\cos(q-k)\cos(q)+\cos^2(q-k)+\cos(q-k)]\\ &-2\sin^2(k)[1+\cos(k-q)]\}\bigg\},\end{aligned}$$
$$\begin{aligned}C_2(q,k) = 16\alpha^2 J^2 S^4\sqrt{N}\bigg\{&\frac{S}{2m\omega_d(k)}\{2\sin(k)\cos(k/2)\sin(q-k/2)\\ &\times[\cos^2(q)+\cos(q-k)\cos(q)-\cos^2(q-k)-\cos(q-k)]\\ &+2\sin^2(k)[1-\cos(k-q)]\}\bigg\}\end{aligned}$$

and $n_k = (\exp(\beta\omega_k)-1)^{-1}$ is the boson occupation number.

The quantities $\Omega_\pm$ are defined for the x- and y-components by

$$\Omega^c_\pm = \omega_c(k) \pm \omega_{q-k} \tag{36}$$
$$\Omega^d_\pm = \omega_d(k) \pm \omega_{q-k}; \tag{37}$$

for the z-component, the result for $\Omega_\pm$ is the same as the one obtained in [14]. $\omega_c(k)$ and $\omega_d(k)$ are the phonon frequencies defined by equation (11). We have also obtained the expression for $(\dot{\mathbf{S}}_q, \dot{\mathbf{S}}_q)$ using the identity

$$(\dot{A}, \dot{B}) = -\mathrm{i}\beta^{-1}\langle[\dot{A}, B]\rangle \tag{38}$$

leading to the x-component, for instance,

$$(\dot{\mathbf{S}}^x_q, \dot{\mathbf{S}}^x_q) = -2\mathrm{i}JT\sum_k \cos(q-k)\{u_{q-k}v_{q-k}(1+\mathrm{e}^{\beta\omega_{q-k}})n_{q-k}\}. \tag{39}$$

The second moment $\langle\omega_q^2\rangle$, which is necessary for the calculation of $S(q,\omega)$, is given by $\langle\omega^2\rangle = \omega_q^2$. The spin structure factor can be expressed in terms of two operators: $\boldsymbol{M}^\alpha_q = \mathbf{S}^\alpha_q + \mathbf{T}^\alpha_q$, which describes the contribution of the usual magnetization, and $\boldsymbol{R}^\alpha_q = \mathbf{S}^\alpha_q - \mathbf{T}^\alpha_q$, which correspond to the staggered magnetization. At low temperature the $\boldsymbol{R}^\alpha_q$ correlation function is the leading contribution to the structure factor near the antiferromagnetic wavevector.

We emphasize that only rotationally invariant quantities such as $\boldsymbol{R}_q = \frac{1}{3}(\boldsymbol{R}^x_q + \boldsymbol{R}^y_q + \boldsymbol{R}^z_q)$ are calculated here. Due to the isotropic character of Hamiltonian (1), each of the three spin components gives the same contribution to the dynamical behavior of the model. However, the Dyson–Maleev transformation breaks the symmetry of the spin-space, giving a privileged role to the z-component. Therefore, we restore the model's symmetry by computing rotationally invariant quantities.

The discrete sum in equation (31) can be transformed into an integral after performing the Laplace transform, leading to integrals of the form

$$G(z) = \frac{1}{\pi}\int_0^{\pi} \frac{A(q,k)\,\mathrm{d}k}{z - \Omega(q,k)} \tag{40}$$

where $z = \omega + \mathrm{i}\varepsilon$. For instance:

$$\Sigma'_q(\omega) = \frac{1}{2\pi^2} P\int_0^{\pi} \mathrm{d}k \left\{ \frac{A_-(q,k)}{\omega^2 - \Omega_-^2(q,k)} + \frac{A_+(q,k)}{\omega^2 - \Omega_+^2(q,k)} \right\} \tag{41}$$

$$\Sigma''_q(\omega) = \frac{1}{2\pi} \left\{ \frac{A_-(q,k)}{|\mathrm{d}\Omega_-/\mathrm{d}k|_{ki}} + \frac{A_+(q,k)}{|\mathrm{d}\Omega_+/\mathrm{d}k|_{ki}} \right\}, \tag{42}$$

where k_i with $i = 1, 2$ are the roots of $\omega = \Omega_+(q,k)$ and $\omega = \Omega_-(q,k)$ respectively, and P is the principal value.

The first term in equations (38) and (39) corresponds to the creation of two magnons when ω is above the magnon frequency, and the second term corresponds to the absorption and re-emission of a magnon when ω is below the magnon frequency.

3. Numerical results

The understanding of the k_i roots of $\omega = \Omega_\pm(q,k)$ and the behavior of $\Omega_\pm$ are crucial for the interpretation of $S(q,\omega)$. The real part of the memory function gives the peak position of $S(q,\omega)$. The points where $\Sigma''_q(\omega)$ diverges correspond to $\mathrm{d}\Omega_\pm(q,k_i)/\mathrm{d}k = 0$ or, as discussed by De Raedt *et al* [9], the place where the two-magnon density of states, $n_\pm = |\mathrm{d}k/\mathrm{d}\Omega_\pm(q,k)|$, diverges. For the model without taking into account the coupling with phonons there is a frequency range where $\Sigma''_q(\omega)$ vanishes that corresponds to the range between the maximum of $\Omega_-(q,k)$ and the minimum of $\Omega_+(q,k)$; in this case, Ω_- and Ω_+ never overlap. This behavior is a consequence of the gap in w_k at $k = 0$ given by equation (29). For a gapless model the two curves would touch one another. It is important to remark that in this case the single spin-wave energy, ω_q, is inside this frequency region. For frequencies larger than the maximum of Ω_+ there will be no contribution. The two-magnon processes are forbidden in the frequency range where $\Sigma''_q(\omega)$ vanishes and, therefore, their contribution to the damping is zero. However, the magnon–phonon scattering is allowed for all values of the energy, and the contribution of this process to the damping smoothes out the sharp peaks.

In figure 1 we show the magnon energy spectrum. We see that the softening of the magnon energy becomes significant for q in the middle of the Brillouin zone and for large values of α, which corresponds to strong magnon–phonon coupling. This softening occurs because the phonon absorbs the magnon's energy in the magnon–phonon coupling process.

Figure 2 shows the spin structure factor for $\alpha = 0$ and three values of the wavevector. We can observe the double-peak structure discussed in the text. Figure 3 is similar to figure 2, but using $\alpha = 0.1$. As we can see, for $q = 5\pi/6$ we can still detect a slight influence of the two-peak structure. For the other values of q we have a smooth peak. Thus the wavevector q plays a fundamental role in the dynamics.

Figures 4 and 5 show the variation of the magnon damping as a function of the wavevector q for $\alpha = 0.1$ and 0.005, and $K/m = 0.2$. The primary result is that the ratio of the damping Γ rate to the magnon frequency ω_q satisfies $\Gamma/\omega_q \ll 1$, leading to well-defined magnon

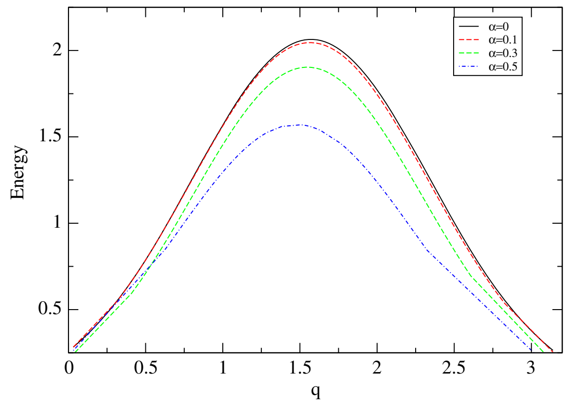

Figure 1. The magnon energy spectrum for different values of α.

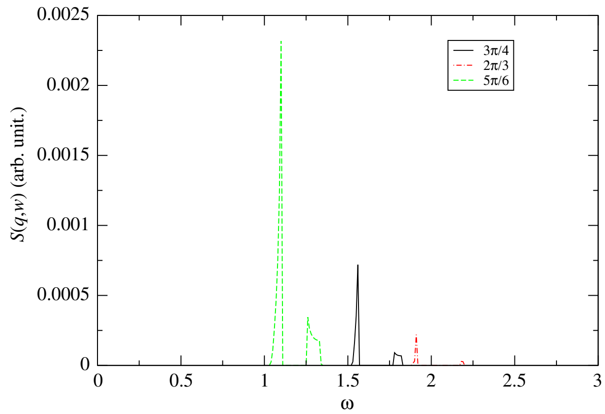

Figure 2. Dynamic structure factor for $\alpha = 0$ and $q = 3\pi/4$, $2\pi/3$ and $5\pi/6$.

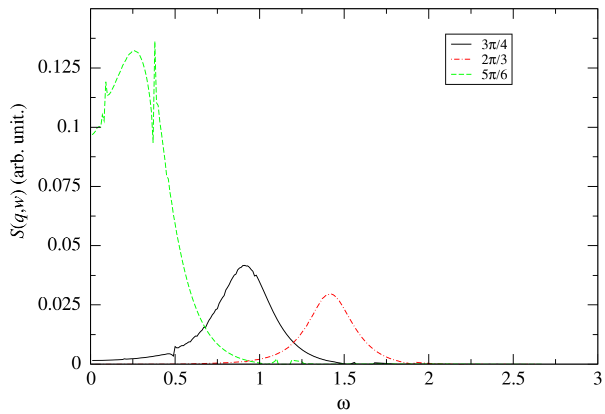

Figure 3. Dynamic structure factor for values of the wavevector $q = 2\pi/3, 3\pi/4, 5\pi/6$ with $\alpha = 0.1$ and $K/m = 0.2$ fixed.

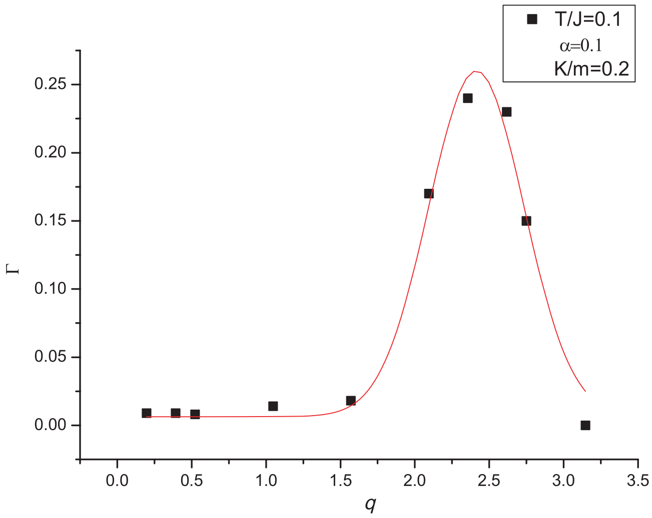

Figure 4. The dependence of Γ (half-width) with the wavevector q with the parameters $\alpha = 0.1$, $T = 0.1J$ and $K/m = 0.2$ fixed.

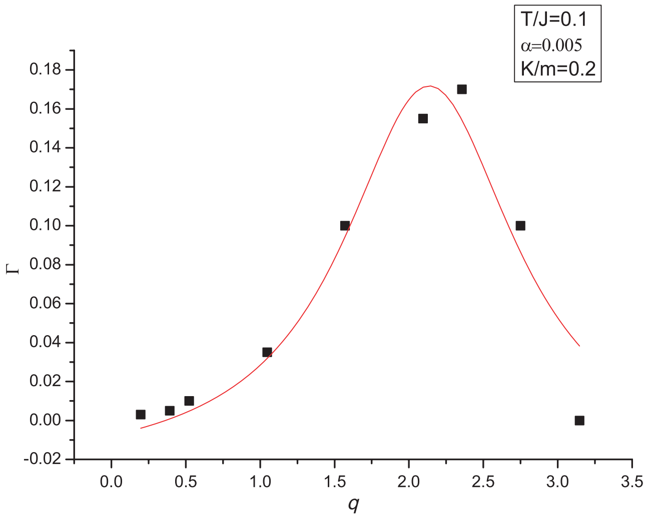

Figure 5. The dependence of Γ (half-width) with the wavevector q with the parameters $\alpha = 0.005$, $T = 0.1J$ and $K/m = 0.2$ fixed.

excitations in all the situations. We see that, for $\alpha = 0.1$, Γ is nearly constant for small values of q up to $q = 1.5$ and then increases, reaching a maximum at $q = 2.5$, and after that it drops rapidly. For $\alpha = 0.005$, Γ is nearly constant for small values of q up to $q = 0.39$, and then increases, reaching a maximum at $q = 2.0$, and after that it drops rapidly too. The spin–phonon coupling depends strongly on q.

Figure 6 shows the variation of the damping as a function of the spin–phonon coupling constant α for different values of q. The behavior of Γ with α can be understood by looking at figures 4 and 5.

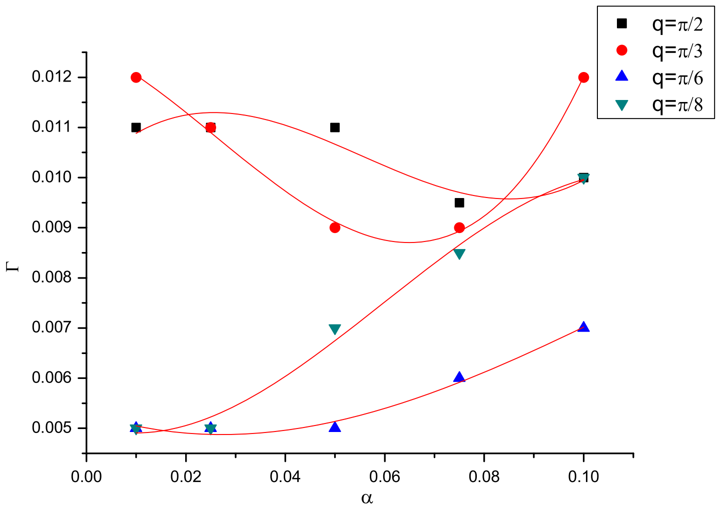

Figure 6. The dependence of Γ (half-width) with the spin–phonon coupling α to different values of the wavevector q and with $T = 0.1J$, $K/m = 0.2$ fixed.

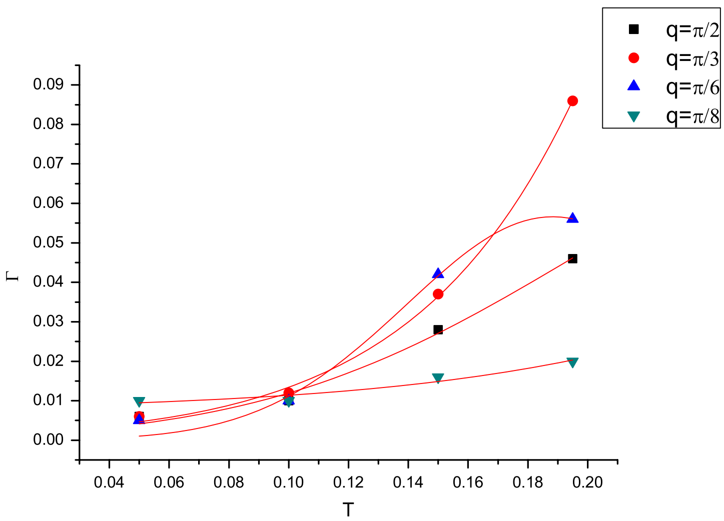

Figure 7. Variation of Γ (half-width) with T for different values of q with $\alpha = 0.1$ and $K/m = 0.2$ fixed.

Finally, in figure 7 we present the variation of the damping with temperature. The damping is larger for larger values of the wavevector q. One can see also that the magnon widths increase with the increase of temperature, indicating a more significant influence of the phonon excitations at elevated temperatures.

4. Conclusion

In summary, we have studied the quantum one-dimensional $S = 1$ Heisenberg antiferromagnet coupled to phonons. In the limit $\alpha = 0$ our theory reduces to the one studied by Pires and

Gouvea [14]. The coupling of the lattice and the spins produces interesting modifications in the excitation spectra. Our calculation indicates that the spin–phonon coupling is strongly q dependent, and the coupling can have more significant influence at elevated temperatures: the phonon absorbs the energy of the magnon, in the coupling process, leading to a magnon softening, which is more pronounced in the middle of the Brillouin zone. Another important effect of the magnon–phonon interaction, which is also q dependent, is the destruction of the two-peak structure present in the absence of this coupling. The damping also strongly varies with the wavevector and has its maximum value at intermediate q values. The spin–spin correlation function can be an effective probe of the spin–phonon coupling, and neutron scattering experiments will show the effect of the coupling.

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