SPIN WAVES IN A CLASSICAL COMPRESSIBLE HEISENBERG CHAIN

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The effect of the spin–lattice interaction on the spin dynamics of a classical Heisenberg chain is studied by means of a truncated continued fraction. At low temperature, the spin correlation length and the spin wave frequency show the same simple dependence on the coupling.

In ref. [1] we presented a detailed study of the phonon dynamics in a compressible classical Heisenberg chain (CHC). Here we will deal with the influence of the phonons on the spin dynamics.

The hamiltonian is given by [1]:

$$H = H_P + H_S + H_{SP},\qquad(1a)$$

$$H_P = \sum p_i^2/2m + \tfrac{1}{2}\alpha \sum(x_{i+1} - x_i)^2 ,\qquad(1b)$$

$$H_S = -J\sum S_i \cdot S_{i+1} \quad (S = 1) ,\qquad(1c)$$

$$H_{SP} = -\epsilon \sum(x_{i+1} - x_i)S_i \cdot S_{i+1} .\qquad(1d)$$

The spins are located on a harmonic lattice and the exchange interaction is supposed to depend linearly on the atom–atom separation. If we define the transformation

$$x_j = u_j + (\epsilon/\alpha)\sum_{i<j} S_i \cdot S_{i+1} ,\qquad(2)$$

the hamiltonian decouples as follows:

$$H = H'_P + H'_S ,\qquad(3a)$$

$$H'_P = \sum p_i^2/2m + \tfrac{1}{2}\alpha \sum(u_{i+1} - u_i)^2 ,\qquad(3b)$$

$$H'_S = -J\sum S_i \cdot S_{i+1} - (\epsilon^2/2\alpha)\sum(S_i \cdot S_{i+1})^2 .\qquad(3c)$$

Then every static correlation function can be calculated exactly by means of the transfer operator method. If we define new parameters

$$u = \beta J \quad (\beta = 1/k_B T) ,\qquad(4)$$

$$\gamma = \epsilon^2/\alpha J ,\qquad(5)$$

the transfer operator [2] has eigenfunctions Y_{lm} and the eigenvalues are given by

$$\lambda_l = \int_{-1}^{1} \exp[u(x + \tfrac{1}{2}\gamma x^2)] P_l(x)\, dx ,\qquad(6)$$

where P_l are the Legendre polynomials. In order to study the time-dependent spin–spin correlation function we write its Fourier transform in the exact continued fraction expansion [3] and truncate it following the method given in ref. [4]. Then we need the frequency moments

$$\langle \omega^{2n}\rangle_q = \frac{\langle[[...[S^z_{-q}, H]...,H],S^z_q]\rangle}{\beta\langle S^z_{-q}S^z_q\rangle},\qquad(7)$$

where the number of Poisson brackets is $2n$. These moments can be expressed in terms of the model parameters and the reduced eigenvalues $y_n = \lambda_n/\lambda_0$. For the rigid Heisenberg chain (RHC), this requires already a considerable amount of work and for the CHC the computational problem is enormous. For example, the fourth moment of the CHC is much more complex than the sixth moment of the RHC. Recently, we have developed

a powerful computer program [5] which, among other things, is able to calculate analytic expressions for the frequency moments.

Our aim here is to present results for the dynamic correlation functions as obtained from a three pole approximation. Truncating the continued fraction at the corresponding level, the imaginary part of the spin relaxation function reads [4]

$$\frac{-\Phi_{ss}''(q,\omega)}{S(q)} = (\langle\omega^4\rangle_q - \langle\omega^2\rangle_q^2)\left(\frac{\langle\omega^4\rangle_q}{\langle\omega^2\rangle_q}\right)^{1/2}$$

$$\times \left[\omega^2\left(\omega^2 - \frac{\langle\omega^4\rangle_q}{\langle\omega^2\rangle_q}\right)^2 + (\omega^2 - \langle\omega^2\rangle_q)^2\frac{\langle\omega^4\rangle_q}{\langle\omega^2\rangle_q}\right]^{-1},$$

(8)

where

$$S(q) = \langle S_{-q}S_q\rangle = \tfrac{1}{3}(1 - y_1^2)/(1 - 2y_1\cos q + y_1^2) \quad (9)$$

is the static structure factor. The zeroth moment or static structure factor (9) is formally the same as for the RHC, but y_1 is different. The inverse correlation length is defined by

$$\kappa = -\ln|y_1|. \quad (10)$$

For low temperatures ($|u| \gg 1$) one finds

$$\kappa \approx [|u|(1 + |\gamma|)]^{-1}. \quad (11)$$

Thus, the correlation length is enhanced with a factor $(1 + |\gamma|)$ by the coupling. Remark that both κ and q are measured in units of the lattice parameter. For example, κ^{-1} measures the number of strongly correlated spins. In order to compare the real correlation lengths of RHC and CHC, one has to take the lattice parameter and thus the thermal expansion into account. The second moment reads

$$\langle\omega^2\rangle_q = 4J^2(1 - \cos q)\,[y_1 + \tfrac{1}{3}\gamma(1 + 2y_2)]$$

$$\times (1 - 2y_1\cos q + y_1^2)\,[u(1 - y_1^2)]^{-1}. \quad (12)$$

For $T = 0$ we find

$$\langle\omega^2\rangle_q = 4J^2(1 - \cos q)(1 \mp \cos q)(1 + |\gamma|)^2, \quad (13)$$

where the upper sign refers to the ferromagnetic case ($J > 0$). The formula for the fourth moment would exceed the length of this letter. It is available on request. For $\gamma = 0$, we obtain the well-known results for the second and fourth moment of the RHC [6].
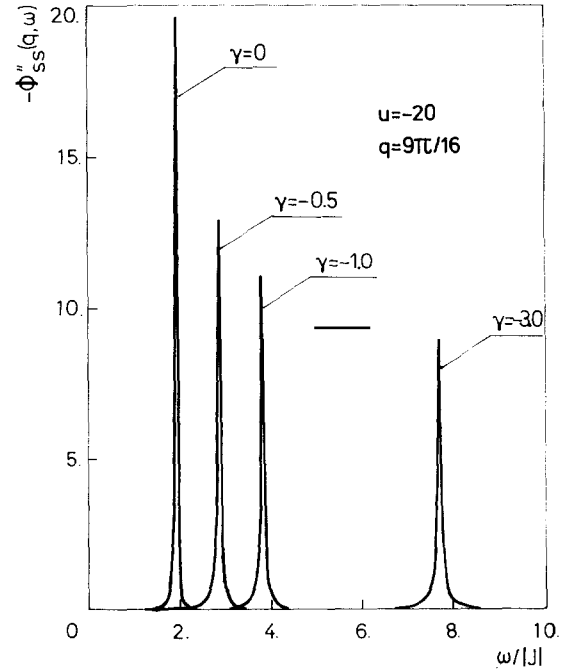

Fig. 1. The normalized spin wave excitation spectrum as a function of the coupling γ at low temperature. Because the area of each peak is the same, the line width increases as $|\gamma|$ increases.

For $T = 0$, we have

$$\langle\omega^4\rangle_q = \langle\omega^2\rangle_q^2. \quad (14)$$

Consequently, at $T = 0$ the spin system oscillates harmonically. Its dispersion is then given by

$$\Omega(q) = 2|J|(1 + |\gamma|)\,[(1 - \cos q)(1 \mp \cos q)]^{1/2}, (15)$$

with the same sign convention as in eq. (13).

In fig. 1 we see how at low temperatures the spin–phonon coupling results in a renormalised dispersion. As γ increases, the height of the peak decreases and consequently the lines become broader. This, however, is difficult to see in the figures. In principle there is also a dependence on a third parameter δ defined by [1]

$$\delta = J/2(2\alpha/m)^{1/2}. \quad (16)$$

This dependence is found to be minor for low temperatures and therefore it has been omitted in the figures.

For the RHC and low temperatures, the three pole approximation for the spin correlation function leads to the criterion $q > \kappa^{1/2}$ for the observability of the
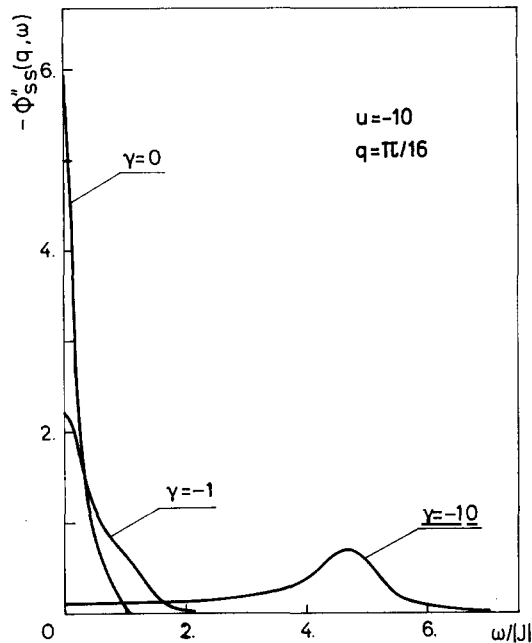
Fig. 2. For small wave vectors, the excitations in the RHC are overdamped because the correlation length is small. The correlation length increases with $|\gamma|$ and consequently propagating modes are present in the CHC for large coupling $|\gamma|$.

spin waves. Here, this criterion is still reasonably satisfied for the antiferromagnet. For the ferromagnet, however, it does not seem to apply anymore. By eq.

(11), it is then possible to find a propagating mode in the antiferromagnet where the RHC only displays relaxational behavior. In fig. 2 we show that this is indeed the case. Finally, we remark that the relaxation functions for ferro- and antiferromagnet do not coincide at $q = \pi/2$, while they do in the RHC.

To discuss the temperature dependence of line width or the criterion for the occurrence of spin waves, at least a four pole approximation is required [4]. Then we need the sixth moment. Because of the complexity of the calculation, it takes a considerable amount of computer time and therefore we are not yet in the possession of the complete result. However, we will present an extensive study of the four pole approximation in the near future.

References

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