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The time- and frequency dependent energy fluctuations in the Heisenberg chain are studied by means of a continued fraction representation. In a broad wave vector and temperature range, the energy fluctuations are found to display dominant oscillatory behavior.

It is well known that the time evolution of the energy density of the Heisenberg chain in the hydrodynamic region is governed by the diffusion equation. In particular, the diffusion constant at infinite temperature has been calculated by computer simulation [1, 2].

The aim of this paper is to investigate the dynamic properties of the energy fluctuations at low temperature and to shed light on the question whether the diffusive nature of the energy fluctuations in the hydrodynamic region persists in the wave vector range where hydrodynamic theory is not valid.

Here, we will confine ourselves to the analytic results obtained by means of a continued fraction representation for the energy-energy correlation functions for the classical Heisenberg chain. The Hamiltonian is given by

$$H = -J \sum_{i=1}^N \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \quad (1)$$

and the energy density  $E_q$  is given by the Fourier transformed local energy

$$E_n = -\frac{J}{2} \mathbf{S}_n \cdot (\mathbf{S}_{n+1} + \mathbf{S}_{n-1}). \quad (2)$$

In order to study the time-dependent energy-energy correlation functions we write its Fourier transform in the exact continued fraction representation [3] and we truncate this expansion following the method given in ref. [4]. Application of this method requires the knowledge of the frequency moments

$$\langle \omega^{2n} \rangle_q = \frac{\langle [ [\dots [E_{-q}, H] \dots, H], E_q ] \rangle}{\beta (\langle E_{-q} E_q \rangle - \langle E \rangle^2 \delta_{q,0})}, \quad (3)$$

where the number of commutators equals  $2n$ , and because of the nature of the spin commutation relations evaluation results in complicated expressions.

In order to evaluate the commutators analytically, we have developed an interactive computer program. This program takes the various symmetry properties of the Hamiltonian into account and writes the final results in terms of eigenvalues of the transfer operator of the Hamiltonian (1). The final results for the second and fourth moment are

$$\langle \omega^2 \rangle_q = (12/\beta^2) y_1^2 u / (1 - 3y_1^2 + 2y_2), \quad (4)$$

$$\langle \omega^4 \rangle_q = \frac{8u y_1^2 - 4y_1^2 y_2 + 3y_2^2 + y_1^2 (4 + 5y_2) u}{\beta^2 (1 - 3y_1^2 + 2y_2)}, \quad (5)$$

where  $y_1 = \coth \beta - 1/\beta$ ,  $y_2 = 1 - 3y_1/\beta$  [5],  $u = 1 - \cos q$  and  $\beta$  denotes the inverse temperature in units of  $JS(S + 1)$ . Note that these expressions do not depend on the sign of  $J$ . To our knowledge, the general result eq. (5) is new. For infinite temperature, our expressions reduce to those given in ref. [1]. We were unable to calculate higher moments because of lack of sufficient computer time.

Truncating the continued fraction at the corresponding level, we have [4]

$$\begin{aligned} S_{EE}(q, \omega) / S_{EE}(q, 0) &= (\langle \omega^4 \rangle_q - \langle \omega^2 \rangle_q^2) \\ &\quad \times (\langle \omega^4 \rangle_q / \langle \omega^2 \rangle_q)^{1/2} \\ &\quad / \left[ \omega^2 (\omega^2 - \langle \omega^4 \rangle_q / \langle \omega^2 \rangle_q)^2 \right. \\ &\quad \left. + \langle \omega^4 \rangle_q (\omega^2 - \langle \omega^2 \rangle_q)^2 \right. \\ &\quad \left. / \langle \omega^2 \rangle_q \right], \quad (6) \end{aligned}$$

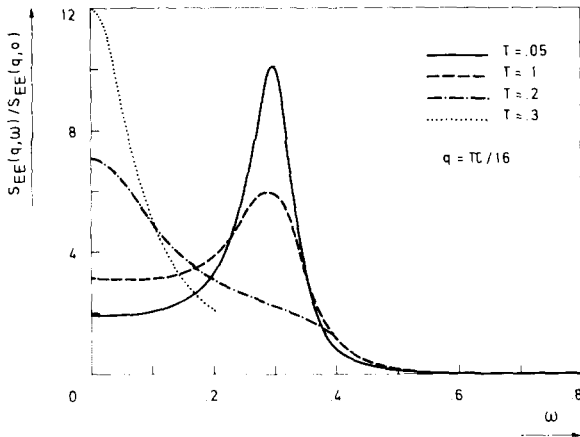


Fig. 1. The normalized energy-energy structure factor for  $q = \pi/16$  and some temperatures. The propagating mode has the largest spectral weight if the wave vector is larger than the inverse correlation length.

with

$$S_{EE}(q, 0) = (1 - 3y_1^2 + 2y_2)(1 + \cos q)/6. \quad (7)$$

In the limit  $T \rightarrow 0$ , we obtain

$$S_{EE}(q, 0) = T^2(1 + \cos q)/2, \quad (8)$$

$$\langle \omega^2 \rangle_q = 8 \sin^2 q/2, \quad (9)$$

$$\langle \omega^4 \rangle_q = 96 \sin^4 q/2, \quad (10)$$

From eq. (8), it follows that the probability for energy excitations to occur vanishes for  $T \rightarrow 0$ . From eqs. (9) and (10) we conclude that, in contrast with the spin excitation spectrum, the normalized excitation spectrum for  $T = 0$  cannot be written as a sum of two delta functions because this requires  $\langle \omega^4 \rangle_q = \langle \omega^2 \rangle_q^2$ .

In the limit  $T \rightarrow \infty$  and  $q \rightarrow 0$ , eq. (6) reduces to a Lorentzian centered around  $\omega = 0$ . The width is determined by  $D_E q^2$ . The energy diffusion constant  $D_E = 0.82|J|S$  is larger than the one obtained by a Gaussian approximation [1] but is in serious disagreement with the result  $D_E = (3 \pm 1)|J|S$  obtained by computer simulation [1, 2]. This can be due to the fact that the approximations that lead to

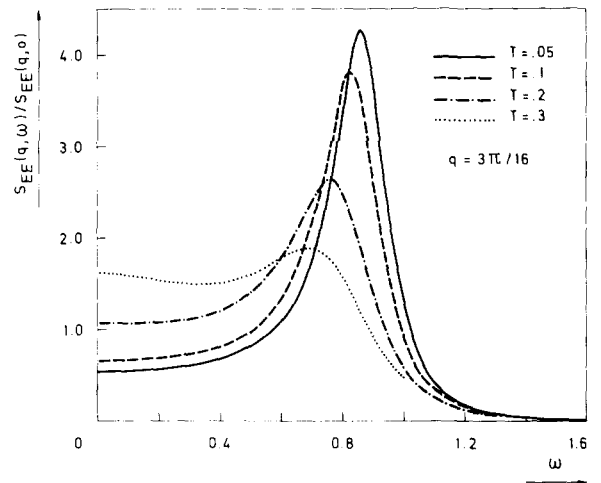


Fig. 2. The normalized energy-energy structure factor for  $q = 3\pi/16$  and a set of temperatures.

eq. (6) are invalid at infinite temperature. In figs. 1, 2 some typical lineshapes for the energy density fluctuations are depicted. It is clear that for small wave vectors and low temperatures, energy fluctuations are characterized by a dominant propagating mode and a relaxation mode. The spectral weight of the propagating part decreases with increasing temperature. In general, we find that the propagating mode disappears if the inverse correlation length  $\kappa = -\ln y_1$  is larger than the wave vector. It is remarkable that the three pole expansion for the energy-energy correlation function does not lead to the criterion  $q \gg \kappa^{1/2}$  which seems to be the typical criterion for the three pole approximation of the spin-spin correlation function [4, 5].

## References

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