Phonon dynamics in a compressible classical Heisenberg chain

Jan Fivez*
Institut für Theoretische Physik, Universität des Saarlandes, D-6600 Saarbrücken, Germany

Hans De Raedt
Departement of Natuurkunde, Universitaire Instelling Antwerpen, B-2610 Wilrijk, Belgium

Bart De Raedt†
Institut für Theoretische Physik, Universität des Saarlandes, D-6600 Saarbrücken, Germany
(Received 3 October 1979)

The dynamic properties of the compressible classical Heisenberg chain with bilinear coupling are investigated. The sound velocity is calculated exactly. The Fourier-transformed displacement-displacement correlation function is studied as a function of temperature, wave vector, and the model parameters. For this calculation a continued-fraction approximation is used.

I. INTRODUCTION

In the last years, a lot of work has been devoted to the study of magnetic systems with translational degrees of freedom. The effect of the coupling of phonons to spins on the static properties has been examined in one- and three-dimensional compressible spin systems with Heisenberg or Ising interaction. As far as we know, dynamic properties have only been investigated for three-dimensional systems,[1-4] mostly for temperatures below T_c.

Recently, some studies have been made of a model Hamiltonian for a compressible classical Heisenberg chain. Starting from a Hamiltonian with nearest-neighbor interaction and a bilinear coupling term,[5] one is able to decouple the system into a pure phonon and a pure spin part,[5-8] such that all static quantities can be calculated exactly.[9-11] It is attractive to study the dynamics of this model system because no approximations for the statics have to be made. The aim of the present work is to investigate the influence of the spin degrees of freedom on the phonon dynamics.

We present a detailed study of the longitudinal displacement fluctuations. The dynamic correlation functions are calculated by means of a continued-fraction representation. The frequency moments, which determine the continued fraction completely, can be expressed rigorously in terms of the eigenvalues of a transfer operator.

The plan of the paper is as follows. In Sec. II we define our model. The principles of the calculation of the static quantities are exposed and they are used to determine the sound velocity. In Sec. III we briefly discuss the continued-fraction method. We show which static correlation functions we need and evaluate them in terms of eigenvalues of the transfer operator defined in Sec. II. We then investigate all possible limits as a function of the parameters of the model. In Sec. IV we present plots and a discussion of the results for the correlation functions. The conclusions of this work are summarized in Sec. V.

II. THE MODEL

A. Hamiltonian and static correlation functions

The model we will study is described by the Hamiltonian[5]

$$H = H_P + H_S + H_{SP} \ , \tag{2.1a}$$

$$H_P = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2}\alpha \sum_{i=1}^{N-1} (x_{i+1} - x_i)^2 \ , \tag{2.1b}$$

$$H_S = -J \sum_{i=1}^{N-1} \vec{S}_i \cdot \vec{S}_{i+1} \ , \tag{2.1c}$$

$$H_{SP} = -\epsilon \sum_{i=1}^{N-1} (x_{i+1} - x_i) \vec{S}_i \cdot \vec{S}_{i+1} \ , \tag{2.1d}$$

where α is an elastic constant and ϵ characterizes the strength of the spin-lattice interaction. The Hamiltonian clearly describes a chain of spins not fixed on a rigid, but on an elastic lattice. H_P, H_S, and H_{SP} stand for the pure harmonic phonon Hamiltonian, the Heisenberg Hamiltonian, and the spin-phonon coupling. The spins are assumed to be classical unit vectors. If we define

$$E_i = \vec{S}_i \cdot \vec{S}_{i+1} \ , \tag{2.2}$$

which is related to the local spin energy, it is clear that in Hamiltonian (2.1) the displacements are bilinearly coupled with the energy fluctuations. In Refs. 5

and 6 it is shown how the Hamiltonian (2.1) results if one assumes the exchange parameter J to depend linearly on the atom-atom separation.

A basic property of our model Hamiltonian is the possibility of its decoupling by means of a coordinate transformation.[5–7] We briefly recall the basic elements and give some comments.

Defining new coordinates u_i by

$$x_i = u_i + \frac{\epsilon}{\alpha} \sum_{j<i} \vec{S}_j \cdot \vec{S}_{j+1} \;, \tag{2.3}$$

the Hamiltonian becomes

$$H = \sum \frac{p_i^2}{2m} + \tfrac{1}{2}\alpha \sum (u_{i+1} - u_i)^2 - J \sum \vec{S}_i \cdot \vec{S}_{i+1} - \frac{\epsilon^2}{2\alpha} \sum (\vec{S}_i \cdot \vec{S}_{i+1})^2 \;. \tag{2.4}$$

The Jacobian of this transformation is 1. An advantage of the transformation (2.3) is that every pure spin correlation function can be calculated using the effective spin Hamiltonian

$$H^{\text{eff}} = -J \sum \vec{S}_i \cdot \vec{S}_{i+1} - \frac{\epsilon^2}{2\alpha} \sum (\vec{S}_i \cdot \vec{S}_{i+1})^2 \;, \tag{2.5}$$

A further consequence of the decoupling is

$$\langle (x_{i+1} - x_i) f(S) \rangle = (\epsilon/\alpha) \langle \vec{S}_i \cdot \vec{S}_{i+1} f(S) \rangle \;, \tag{2.6}$$

where $f(S)$ is a function of spins only. More generally, every correlation function of displacements and spins can be written as a sum of correlation functions of spins and the new variables u_i. After the decoupling, the pure spin correlation functions are calculated using Hamiltonian (2.5) and the u-correlation functions are that of a pure harmonic oscillator.

One has to realize that the transformation exploits the classical nature of the spins and has no quantum-mechanical analogue. Consequently, the transformed Hamiltonian (2.4) will be used only to calculate static expectation values. For all calculations of dynamic quantities such as commutators or Poisson brackets we will use the Hamiltonian (2.1).

As a result of the transformation, all spin correlation functions are those of a system with Hamiltonian (2.5). Such systems are known to have an ordered or disordered ground state depending on the value of J and ϵ^2/α.[9] Our system always has $\epsilon^2/\alpha > 0$ and is therefore ordered at $T=0$, because there is no competition between ferromagnetic and antiferromagnetic interactions.

In Ref. 9 it was shown how to obtain exact analytical results for the static spin correlation functions of a system with Hamiltonian (2.5) by means of the transfer operator method. We briefly recall the general idea of this method. For any one-dimensional system described by a Hamiltonian of the form

$$H = \sum_i h(x_i, x_{i+1}) \;,$$

the transfer operator K is defined by

$$(K\phi)(x) = \int K(x,y)\phi(y)\, dy \;, \tag{2.7}$$

with

$$K(x,y) = e^{-\beta h(x,y)} \tag{2.8}$$

and $\beta = 1/k_B T$. K is positive definite and symmetric and so it has real eigenvalues. Any static quantity can be expressed in terms of the eigenvalues and eigenfunctions of K. In our case the transfer operator (2.8) is given by

$$K(\vec{S}_i, \vec{S}_{i+1}) = (1/2\pi) \exp\{\beta[J\vec{S}_i \cdot \vec{S}_{i+1} + (\epsilon^2/2\alpha)(\vec{S}_i \cdot \vec{S}_{i+1})^2]\} \;. \tag{2.9}$$

Because the transfer operator has spherical symmetry, it is obvious that the eigenfunctions are the spherical harmonics. This makes it possible to find analytic expressions for the spin correlation functions in terms of the eigenvalues. In Ref. 9 it is shown that

$$\int K(\vec{S}_1, \vec{S}_2)\, Y_{lm}(\vec{S}_2)\, d\vec{S}_2 = \lambda_l Y_{lm}(\vec{S}_1) \;, \tag{2.10}$$

with

$$\lambda_l = \int_{-1}^{1} \exp\left[\beta\left(Jx + \frac{\epsilon^2}{2\alpha}x^2\right)\right] P_l(x)\, dx \;. \tag{2.11}$$

P_l are the Legendre polynomials. The largest eigenvalue is λ_0 because K is positive and P_0 has no nodes.

From here on, we will work with a new set of parameters. We define

$$u = \beta J \;, \tag{2.12a}$$

$$\gamma = \epsilon^2/\alpha J \;, \tag{2.12b}$$

$$\delta = J/(2\sqrt{2}\,\Omega) \;, \tag{2.12c}$$

$$\Omega = (\alpha/m)^{1/2} \;. \tag{2.12d}$$

These new parameters are of direct relevance to the dynamics of the system. As can be seen from Eq. (2.5), γ measures the importance of the coupling. Ω is the frequency of a single harmonic oscillator, and δ is a measure for the ratio of spin fluctuation energy to the phonon energy. Finally, u compares thermal energy with spin interaction energy.

It is possible to express all the eigenvalues in terms of λ_0. If one defines[7]

$$I_n = \int_{-1}^{1} x^n e^{u[x+(\gamma/2)x^2]}\, dx \;, \tag{2.13}$$

one has the recursion formula

$$\gamma u I_{n+1} = e^{\gamma u/2}[e^{u} + (-1)^{n+1} e^{-u}] - u I_n - n I_{n-1} \ . \tag{2.14}$$

Combining Eqs. (2.11)–(2.14) we find for the first three reduced eigenvalues $y_n = \lambda_n/\lambda_0$

$$y_1 = \frac{2}{u\gamma} e^{\gamma u/2} \frac{shu}{\lambda_0} - \frac{1}{\gamma} \ , \tag{2.15a}$$

$$y_2 = \frac{3chu}{\gamma u} \frac{e^{\gamma u/2}}{\lambda_0} - \frac{3y_1}{2\gamma} - \frac{3}{2\gamma u} - \frac{1}{2} \ , \tag{2.15b}$$

$$y_3 = \left(1 - \frac{5}{\gamma u}\right) y_1 + \frac{5}{3\gamma}(1 - y_2) \ . \tag{2.15c}$$

In order to determine our model completely, we still have to choose the boundary conditions. Salinas[12] pointed out that the Hamiltonian (2.1) exhibits different properties under different constraints. It turns out that periodic boundary conditions on x_i and $\vec{S}_i$ result in an effective spin Hamiltonian with long-range interactions. Then we cannot use the transfer operator method to calculate the static correlation functions exactly. Furthermore, periodic boundary conditions on x_i would suppress thermal expansion. We impose periodic boundary conditions on u_i and the spins after the transformation (2.3). In this way we avoid these problems.

B. Sound velocity

We are now able to calculate the longitudinal sound velocity exactly. The starting point is the well-known formula for the phonon frequency[14]

$$\omega_q^2 = 1/m\,(x;x)_q \ , \tag{2.16}$$

where $(x;x)_q$ denotes the Fourier-transformed static displacement-displacement susceptibility. In the classical limit, the static susceptibility is given by

$$(A;B) = \beta(\langle A^* B\rangle - \langle A^*\rangle\langle B\rangle) \ . \tag{2.17}$$

Using Eq. (2.3) and

$$(\vec{S}_0\cdot\vec{S}_1;\vec{S}_n\cdot\vec{S}_{n+1}) = \tfrac{1}{3}\beta\delta_{n,0}(1 - 3y_1^2 + 2y_2) \ , \tag{2.18}$$

we obtain

$$\omega_q^2 = 6\Omega^2(1-\cos q)/[3 + \gamma u(1 - 3y_1^2 + 2y_2)] \ . \tag{2.19}$$

The sound velocity is then found to be

$$C \equiv \lim_{q\to 0} \frac{\omega_q}{q} = \frac{C_0}{[1 + \frac{1}{3}\gamma u(1 - 3y_1^2 + 2y_2^2)]^{1/2}} \ , \tag{2.20}$$

where $C_0 = \Omega$ denotes the sound velocity of the harmonic phonon system.

III. DYNAMIC CORRELATION FUNCTIONS

The Laplace-transformed displacement relaxation function is defined by

$$\phi(z,q) = -i\int_0^\infty e^{izt}(x(t);x)_q\,dt \ ,$$

$$z = \omega + i\epsilon, \quad \epsilon > 0 \ . \tag{3.1}$$

The dynamic structure factor $S(\omega,q)$ is related to $\phi(z,q)$ by

$$S(\omega,q) = (-1/\beta)\phi''(\omega,q) \ , \tag{3.2}$$

with

$$\phi''(\omega,q) = \lim_{\epsilon\to 0} \mathrm{Im}\phi(z,q) \ . \tag{3.3}$$

We want to study the influence of the spin-lattice coupling on the phonon dynamics in detail. An appropriate way to do this is to use Mori's formalism.[13–16] The Laplace-transformed relaxation function is then written as a continued fraction. The coefficients of this expansion are combinations of frequency moments of the relaxation function. The frequency moments are static quantities and consequently they can be computed by means of the theory given in Sec. II. The normalized continued-fraction representation is given by

$$\phi(z,q) = \cfrac{1}{z - \cfrac{\Delta_1^2(q)}{z - \cfrac{\Delta_2^2(q)}{z - \ddots \cfrac{\Delta_{n-1}^2(q)}{z - \Delta_n^2(q)\phi^{(n)}(z,q)}}}} \ . \tag{3.4}$$

The first three coefficients $\Delta_n^2(q)$ are

$$\Delta_1^2(q) = \langle\omega^2\rangle_q \ , \tag{3.5a}$$

$$\Delta_2^2(q) = \langle\omega^4\rangle_q/\langle\omega^2\rangle_q - \langle\omega^2\rangle_q \ , \tag{3.5b}$$

$$\Delta_3^2(q) = (\langle\omega^6\rangle_q/\langle\omega^2\rangle_q - \langle\omega^4\rangle_q^2/\langle\omega^2\rangle_q^2)/\Delta_2^2(q) \ , \tag{3.5c}$$

where

$$\langle\omega^{2n}\rangle_q = (L^n x;L^n x)_q/(x;x)_q \tag{3.6}$$

denote the frequency moments of the relaxation function. The Liouville operator L is related to the Hamiltonian by

$$LA = [H,A] \ . \tag{3.7}$$

If we terminate the continued fraction at some stage, the problem of calculating $\phi(z,q)$ is reduced to the problem of finding an approximation for $\phi^{(n)}(z,q)$.

Here, we will use the approximation proposed in Ref. 15. It has the advantage that it is simple and systematic and $\phi(z,q)$ satisfies as many sum rules as possible. The result reads

$$\phi^{(n)}(z,q)=[z+i\tau_n^{-1}(q)]^{-1} \ . \tag{3.8}$$

Here the relaxation time $\tau_n(q)$ can again be written as a function of the frequency moments and we have

$$\tau_n^{-2}(q)=\Delta_n^2(q)+\Delta_{n-1}^2(q) \ . \tag{3.9}$$

In Eq. (3.5) we wrote down the Δ_n^2 up to $n=3$. For the computation of Δ_4^2 we need $\langle\omega_q^8\rangle$, but at the moment we are not able to calculate this quantity for practical reasons. This means that we will not go further than a four-pole expansion.

We now calculate the frequency moments as a function of the reduced eigenvalues y_n. Using the formula[15]

$$(A;LB)=\langle[A^*,B]\rangle \ , \tag{3.10}$$

we find for the first three moments

$$\langle\omega^2\rangle_q=6\Omega^2(1-\cos q)/[3+\gamma u(1-3y_1^2+2y_2)] \ , \tag{3.11a}$$

$$\langle\omega^4\rangle_q=12\Omega^4(1-\cos q)^2/[3+\gamma u(1-3y_1^2+2y_2)] \ , \tag{3.11b}$$

$$\begin{aligned}\langle\omega^6\rangle_q=&24\Omega^6(1-\cos q)^3/[3+\gamma u(1-3y_1^2+2y_2)]\\&+128\Omega^6\gamma\delta^2(1-\cos q)^2\{\gamma[\tfrac{2}{3}(1-y_2)(\tfrac{1}{2}+y_2)-\tfrac{3}{5}y_1(y_1-y_3)\cos q]\\&+y_1(1-y_2)(1-\cos q)\}/[3+\gamma u(1-3y_1^2+2y_2)] \ .\end{aligned} \tag{3.11c}$$

As $\langle\omega^2\rangle_q$, $\langle\omega^4\rangle_q$ involves spin expectation values only through the static structure factor $(x;x)_q$. This is due to the linear appearance of x in the spin-phonon coupling (2.1d). The second term of Eq. (3.11c) has been obtained with the help of a computer program.[17]

Combination of Eqs. (3.6) and (3.11) gives

$$\Delta_1^2=6\Omega^2(1-\cos q)/[3+\gamma u(1-3y_1^2+2y_2)] \ , \tag{3.12a}$$

$$\Delta_2^2=2\Omega^2(1-\cos q)\frac{\gamma u(1-3y_1^2+2y_2)}{3+\gamma u(1-3y_1^2+2y_2)} \ , \tag{3.12b}$$

$$\Delta_3^2=32\Omega^2\delta^2\{\tfrac{1}{3}(1-\cos q)y_1(1-y_2)+\gamma[\tfrac{2}{9}(1-y_2)(\tfrac{1}{2}+y_2)-\tfrac{1}{5}y_1(y_1-y_3)\cos q]\}\frac{3+\gamma u(1-3y_1^2+2y_2)}{u(1-3y_1^2+2y_2)} \ . \tag{3.12c}$$

Because the y_m only depend on u and γ, the parameters u, γ, and δ are sufficient to describe the dynamics if we measure all frequencies in units of Ω. Using

$$y_n(-u,-\gamma)=(-1)^n y_n(u,\gamma) \ , \tag{3.13}$$

it is clear from Eqs. (3.4) and (3.12) that the dynamic displacement correlation functions are exactly the same for a ferromagnetic as for an antiferromagnetic interaction. From Eq. (3.12) we conclude that a three-pole approximation for the relaxation function is too simple because it does not depend on δ.

We first investigate some limits that will be helpful for the interpretation of the parameter dependence of the dynamic structure factor.

For the low-temperature limit ($u\rightarrow\infty$), one can use the asymptotic expansion of λ_0 given in Ref. 7 and the recursion relations (2.15) to find

$$\Delta_1^2\rightarrow 2\Omega^2(1-\cos q) \ , \tag{3.14a}$$

$$\Delta_2^2\rightarrow 0 \ , \tag{3.14b}$$

$$\Delta_3^2\rightarrow 32\Omega^2\delta^2(1+|\gamma|)^2(1-\cos q) \ . \tag{3.14c}$$

Consequently, for $u=\infty$, the continued fraction is terminated at the second stage and the dynamic form factor consists of two δ functions at $\pm$ the harmonic frequency.

In the high-temperature limit, we have

$$y_n\rightarrow\delta_{n,0} \ ,$$

and we obtain

$$\Delta_1^2\rightarrow 2\Omega^2(1-\cos q) \ , \tag{3.15a}$$

$$\Delta_2^2\rightarrow 0 \ , \tag{3.15b}$$

$$\Delta_3^2\rightarrow\infty \ . \tag{3.15c}$$

Consequently, for $u=0$, the Fourier-transformed x-x correlation function again consists of two δ functions at $\pm$ the harmonic frequency.

In the strong-coupling limit ($\gamma\rightarrow\infty$), we obtain

$$y_1\simeq\tanh u-\frac{1}{\gamma}\left(\operatorname{sech}^2u+\frac{\tanh u}{u}\right)+\cdots \ , \tag{3.16a}$$

$$y_2\simeq 1-3/\gamma u+\cdots \ , \tag{3.16b}$$

$$y_3\simeq\tanh u-\frac{1}{\gamma}\left(\operatorname{sech}^2u+6\frac{\tanh u}{u}\right)+\cdots \ , \tag{3.16c}$$

and consequently,

$$\Delta_1^2 \to 0 \ , \tag{3.17a}$$

$$\Delta_2^2 \to 2\Omega^2(1-\cos q) \ , \tag{3.17b}$$

$$\Delta_3^2 \to \infty \ . \tag{3.17c}$$

The dynamic structure factor becomes a δ function at $\omega = 0$.

Because $\delta \to 0$ results in $\Delta_3^2 \to 0$, the correlation function consists of a very narrow central peak and two very narrow peaks centered at $\pm$ the harmonic frequency. If $\delta \to \infty$, $\Delta_3^2 \to \infty$, and the dynamic form factor is given by a pair of δ functions at $\pm \langle \omega_q^2 \rangle^{1/2}$.

The limits $u \to 0$ and $\gamma \to \infty$ are unphysical. For $u \to 0$ the displacements become infinitely large. It is obvious that the model (2.1) breaks down. The limit $\gamma \to \infty$ means that the coupling term is dominant.

We close this section with two remarks.

Of interest is the limiting case where both u and γ become very large. From Eqs. (3.14) and (3.17) it is clear ordering is important if one takes the limits $u \to \infty$ and $\gamma \to \infty$. From Eqs. (3.16) we obtain

$$E = \gamma u (1 - 3y_1^2 + 2y_2) \simeq 3\gamma u \,\mathrm{sech}^2 u, \quad \gamma >> 1 \tag{3.18}$$

and consequently

$$\lim_{\gamma\to\infty}\left[\lim_{u\to\infty} E\right] = 0 \neq \lim_{u\to\infty}\left[\lim_{\gamma\to\infty} E\right] = \infty \ .$$

If we compare Eq. (3.18) to Eqs. (3.12), this illustrates the origin of the difficulties. But the problem is artificial in some sense. Indeed, our model allows γ to be very, but not infinitely large. Then we can simply use Eq. (3.18). It is important to note that E vanishes much more quickly for large u than it increases with increasing γ.

The four-pole approximation given by Eqs. (3.4), (3.8), and (3.9) satisfies the sum rules

$$\langle \omega^{2n} \rangle_q = \int_{-\infty}^{\infty} S(q,\omega)\omega^{2n}\,d\omega \Big/ \int_{-\infty}^{\infty} S(q,\omega)\,d\omega \ ; \quad n = 0,1,2,3 \tag{3.19}$$

if $\Delta_n \neq 0$ for all $n \leq 3$. If, however, $\Delta_m = 0$ for some $0 < m < 3$, the sum rules for $n > m$ can be violated because the continued fraction does not contain information about higher moments [see Eq. (3.4)]. In fact, the continued fraction and the moment expansion are not necessarily related anymore[18] if one of the Δ's is zero. Mathematically, this is connected with the fact that the integrals in Eq. (3.19) are not well defined in such a case. The limits given in Eqs. (3.15) and (3.17) are examples of such cases, but, as mentioned above, these limits are unphysical for our model.

IV. RESULTS

In Fig. 1 the dependence of the sound velocity on u and γ is plotted. Note the minimum of c as a function of temperature and the fact that $c \to c_0$ if $u \to 0$ or $u \to \infty$. A minimum was also found in three-dimensional compressible magnetic systems below T_c.[4] There, however, one has a discontinuity in the derivative with respect to T. Because of Eq. (2.12), Fig. 1 shows at the same time the dependence of the static susceptibility on u and γ. The wave-vector dependence is that of the pure phonon system, as can be seen from Eq. (2.19).

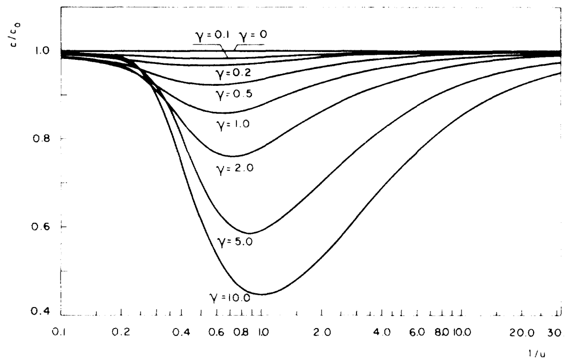

FIG. 1. Semilogarithmic plots of the sound velocity as a function of temperature and the coupling strength γ. c_0 is the harmonic sound velocity ($\gamma = 0$).

In Figs. 2–6, we present plots for the normalized Fourier-transformed dynamic correlation functions. The normalization is such that

$$\frac{-1}{\pi}\int_{-\infty}^{+\infty} \phi''(\omega)\,d\omega = 1 \ . \tag{4.1}$$

In each plot only one parameter is changed in order to demonstrate the dependence on the various model parameters.

Figure 2 shows the dependence on temperature. To a good approximation, the peak position is given by $\langle \omega^2 \rangle_q^{1/2}$ and therefore the temperature dependence of the peak position is given by Eq. (2.19) and is plotted in Fig. 1. The frequency is renormalized by a factor independent of q. Hence, the relative frequency shift due to the coupling with the spins is frequency independent. Such a result was also found in theoretical calculations for Ising systems and in corresponding experiments. (See Ref. 1 and references quoted therein.)

If a well-defined phonon excitation exists, the linewidth can be associated with the spin-lattice relaxation time. The evolution of the linewidth as a function of temperature is understood considering the limits investigated in Sec. III. The plot with $|u| = 10$ is very close to the harmonic oscillator, although $|\gamma| = 10$ is rather large, and this is understood using Eq. (3.18). Large u dominates equally large γ. Physically spoken, both the phonon and the spin system are frozen in and this reduces the coupling seriously.

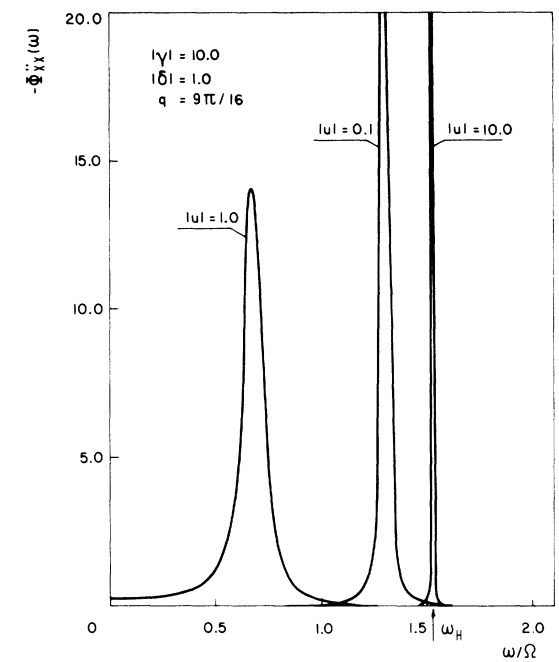

FIG. 2. Fourier-transformed normalized displacement-displacement correlation function for some values of $|u|$ and the other parameters fixed. ω_H is the harmonic oscillator frequency. The temperature dependence of the peak position is the same as that of c (see Fig. 1). For low temperature ($u=10$), the harmonic oscillator is approached, although γ is large. Because the results are the same for a ferromagnet and an antiferromagnet, only the absolute value of the parameters is important.

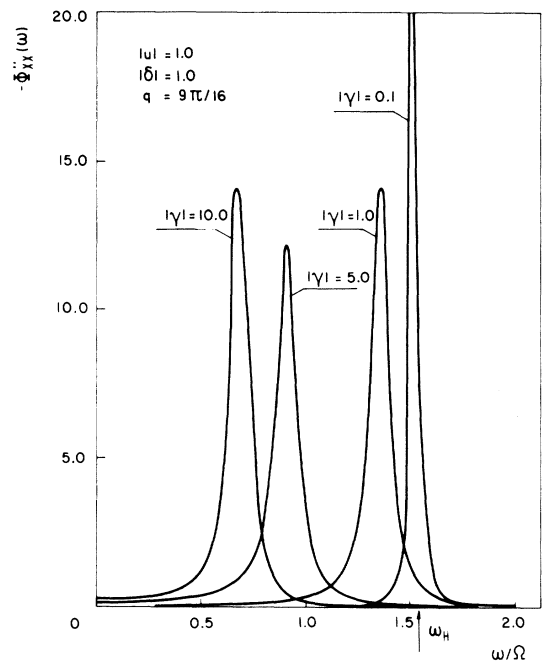

FIG. 3. Fourier-transformed (FT) correlation function as a function of the coupling strength γ. Note that the height of the peak has a minimum for $1 < |\gamma| < 10$.

Figure 3 shows the dependence of the line shape on the coupling strength γ. In this case, the excitation frequency decreases with increasing γ, but this is not generally true (see, e.g., Fig. 1 for large u). The phonon system becomes a harmonic system for $\gamma \to 0$. For $\gamma \to \infty$, one gets a δ function at zero frequency. Therefore, the height of the peak shows a minimum or, equivalently, the linewidth has a maximum.

Figure 4 shows how the relaxation function changes if only δ is varied. If δ is large, the energy of the magnetic fluctuations is much larger than the energy of the phonons. Consequently, the phonons cannot transfer energy to the magnetic excitations.

In all but one case, the frequency is nearly exactly given by $\langle \omega^2 \rangle_q^{1/2}$. For $\delta = 0.1$, we find a completely different structure. Both a central peak and a very narrow one at the harmonic frequency are observed. This can be explained by a physical argument. For small δ, the frequency of the fluctuations of the magnetic energy density is much smaller than the phonon frequency. Because in the Hamiltonian (2.1) E_i and x_i are coupled bilinearly, we could use use the results

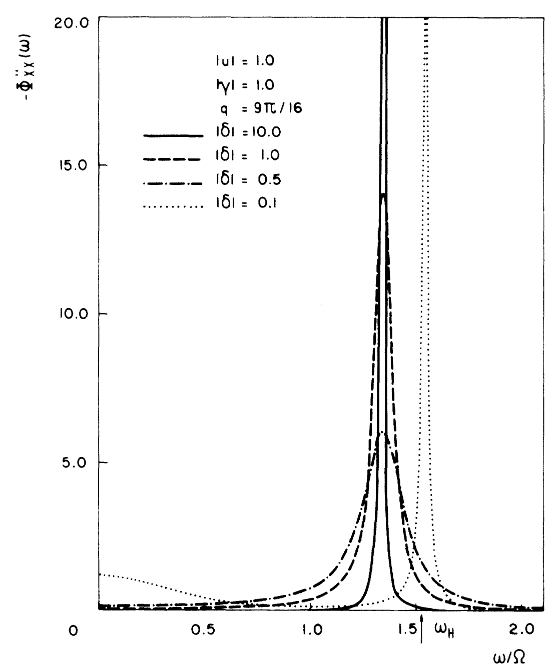

FIG. 4. FT correlation function for some values of δ. Except for $|\delta| = 0.1$, the peak positions are nearly exactly at $\langle \omega^2 \rangle_q^{1/2}$. Note the central peak for $|\delta| = 0.1$.

of a system of two bilinearly coupled harmonic oscillators as a first approximation. That system has as eigenfrequencies a very small frequency and the frequency of the strongest oscillator, just as we find here.

A typical illustration of the dependence on q is given in Fig. 5. For $q \rightarrow 0$, a δ function at $\omega = 0$ is obtained because of translational invariance.

Because $\phi''(\omega) = \phi''(-\omega)$, all graphs shown in Figs. 2–5 show a two-peak structure. The only exception is the three-peak structure of Fig. 4. We also found four-peak structures. In most cases the peak with the largest frequency is dominant, but we also found parameter values for which both peaks are comparable. In Fig. 6 we demonstrate that a small change in q can have a drastic effect on the line shape. A two-peak structure evolves to a well-defined four-peak and then to a three-peak structure. We also found pure central peaks for some values of the parameters. We can get an idea of how good the four-pole approximation is by comparing the absolute value of the poles with the transport coefficient τ_n^{-1}.[13,19] The poles should lie in a circle with radius τ_n^{-1}, the closer to the origin the better. For our two peak structures this criterion is well satisfied. In those cases where we find three or four peaks or a pure central peak, this criterion is not or only badly satisfied. Hence, it is not sure that the four-pole approximation is quantitatively correct there.

Our results also apply directly to a system with

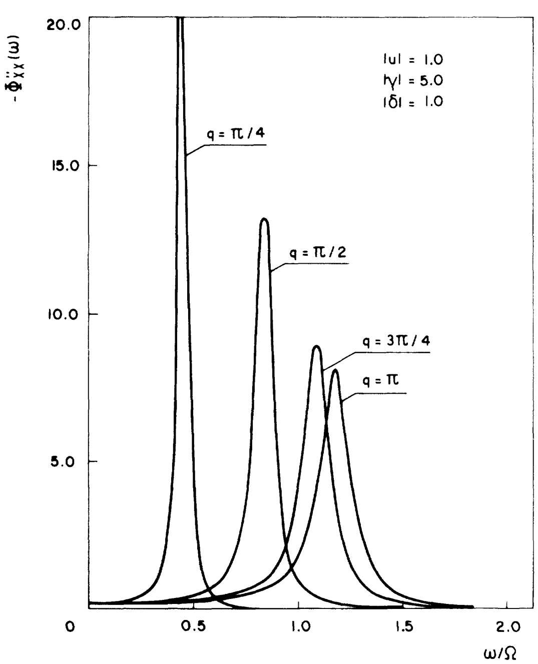

FIG. 5. In this plot, the wave-vector dependence of the peak position is the same as for the pure phonon system.

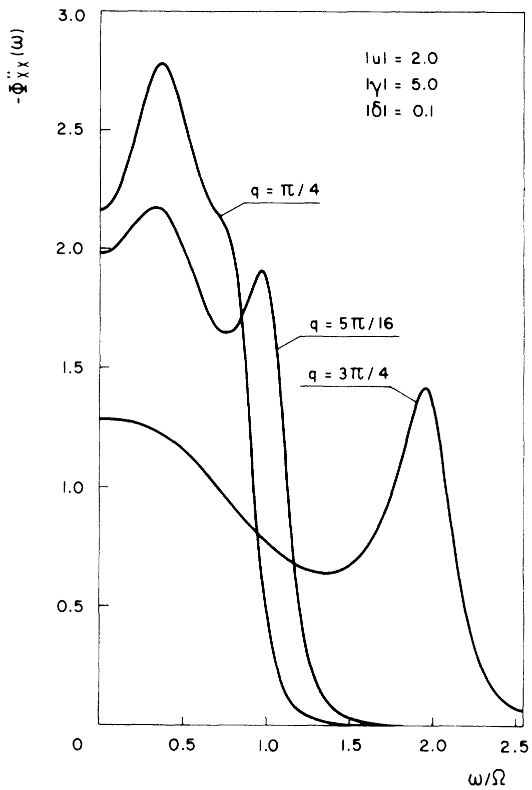

FIG. 6. Transition between different kinds of line shapes for small $|\delta|$ as a function of q. Note that a small change in q has a drastic effect on the line shape. In each plot, the rightmost peak is located near the harmonic frequency.

Hamiltonian (2.1) plus a biquadratic term $-J_1 \sum_n (\vec{S}_n \cdot \vec{S}_{n+1})^2$. After the transformation, this term has to be added to the effective biquadratic interaction. The only difference is that now $\epsilon^2/2\alpha$ is replaced by $A = \epsilon^2/2\alpha + J_1$. If $A > 0$, nothing is really changed. If, however, $A < 0$, some modifications can be expected.

V. CONCLUSIONS

The dynamic properties of a classical compressible Heisenberg chain with bilinear interaction have been investigated. We found the same dynamic behavior for ferromagnetic or antiferromagnetic interaction.

The sound velocity has been calculated exactly and it displays a minimum as a function of the temperature.

The Fourier-transformed displacement-displacement correlation function has been studied by means of a four-pole approximation. In most cases, the dependence of the peak position on the various model parameters can be understood in terms of the static displacement correlation function.

ACKNOWLEDGMENT

Financial support by the Sonderforschungsbereich Ferroelektrika der Deutschen Forschungsgemeinschaft and the Interuniversitair Instituut voor Kernwetenschappen (Belgium) project "Neutron Scattering" is gratefully acknowledged.

---

*Aspirant van het N.F.W.O. Present address: Dept. Natuurkunde, Universitaire Instelling Antwerpen, B-2610 Wilrijk, Belgium.

†Present address: Institut für Festkörperforschung der Kernforschungsanlage Jülich, Postfach 1913, D-5170 Jülich, Germany.

[1]G. K. Roy and B. K. Chakrabarti, Phys. Rev. Lett. A 58, 197 (1976).

[2]V. A. Timofeev, Sov. Phys. Solid State 19, 758 (1977).

[3]C. M. Care and J. W. Tucker, Physica (Utrecht) 86-88B, 975 (1977).

[4]R. H. Lemmer and J. de P. Viljoen, J. Magn. Magn. Mater. 5, 161 (1977).

[5]B. S. Lee, Prog. Theor. Phys. 50, 2093 (1973).

[6]M. Barma, Phys. Rev. B 16, 593 (1977).

[7]M. Barma, Phys. Rev. B 12, 2710 (1975).

[8]I. K. Kudryavtsev and A. S. Shumovsky, Phys. Lett. A 62, 253 (1977).

[9]M. F. Thorpe and M. Blume, Phys. Rev. B 5, 1961 (1972).

[10]L. L. Liu and R. I. Joseph, Phys. Rev. Lett. 26, 1378 (1971).

[11]K. Nagata and I. Yamamoto, Phys. Lett. A 60, 237 (1977).

[12]S. R. Salinas, J. Phys. A 6, 1527 (1973).

[13]H. Mori, Prog. Theor. Phys. 34, 399 (1965).

[14]W. Götze and K. H. Michel, in *Dynamical Properties of Solids*, edited by G. K. Horton and A. A. Maradudin (North-Holland, Amsterdam, 1974).

[15]H. De Raedt and B. De Raedt, Phys. Rev. B 15, 5379 (1977).

[16]M. Dupuis, Prog. Theor. Phys. 37, 502 (1967).

[17]H. De Raedt and B. De Raedt, Phys. Rev. B 21, 304 (1980).

[18]G. A. Baker, Jr., *Essentials of Padé approximants* (Academic, New York, 1975).

[19]H. De Raedt, Phys. Rev. B 19, 2585 (1979).