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Soliton–magnon interaction in the sine–Gordon-like magnetic chain

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Abstract. We present theoretical results for the interference effects between solitons and two-magnon processes in the classical sine–Gordon model. We calculate the dynamical longitudinal structure factor where the two-magnon processes give an important contribution to the central peak. We compare our results with existing numerical simulation data.

1. Introduction

The classical properties of ferromagnetic linear chains, including the soliton features, the dynamics and the thermodynamics are important subjects of theoretical and experimental studies. The ferromagnet CsNiF₃ is one of the best-studied quasi-one-dimensional (1D) magnetic systems (Steiner and Bishop 1986). Its magnetic properties have been studied by different experimental techniques, as well as by means of different theoretical approaches. Central peak behaviour in the inelastic neutron scattering results for this compound in a magnetic field (Kjems and Steiner 1978, Steiner *et al* 1983) first suggested that solitons were present in this system. A theoretical examination of a single classical easy-plane ferromagnet described by the Hamiltonian

$$H = -2J \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1} + A \sum_n (S_n^z)^2 - g\mu_B H \sum_n S_n^x \quad (1.1)$$

was made by mapping it, in the low temperature limit, onto the sine–Gordon model (Mikeska 1978) whose dynamical properties are well known. The comparison between theory and experiment was ambiguous because of the differences in the physical and theoretical Hamiltonians, and because of the uncertainty in the validity range of the theory.

In order to interpret theoretically the available neutron scattering data we have to calculate the dynamical correlation functions $S^{\alpha\alpha}(q, \omega)$ ($\alpha = x, y, z$). The transverse component $S^{yy}(q, \omega)$ shows spin-wave peaks and, with increasing temperature, a Gaussian central peak develops, signalling the presence of solitons. The theory for this component consistently describes the experimental findings. The longitudinal component $S^{xx}(q, \omega)$ is expected to be more complicated since both solitons and two-spin-wave processes can be expected to play a role in the same region of the

spectrum. The simultaneous creation and annihilation of two-spin-waves results in a contribution to the cross section around zero energy transfer producing a central peak (CP) in the longitudinal component. However sine-Gordon theory also predicts a CP due to scattering from a gas of thermally activated solitons, and particular emphasis must then be placed on the experimental separation of the contributions. There are experimental results that agree quantitatively with soliton prediction while others agree better with the two-spin-wave theory (Steiner *et al* 1983, Reiter 1981). For instance, it has been observed that at small wavenumber q the CP shape is dominated by a narrow Gaussian central peak, while at large q the broad two-spin-wave cross section becomes dominant. Therefore, we have in the energy width of the CP at small q a behaviour consistent with the expectation of soliton theory, whereas at large q the widths are more consistent with two-spin-wave theory, suggesting that these processes dominate here. So, neither of the theories can give a consistent description of all results. The observations for $S^{xx}(q, \omega)$ cannot be explained by one of the theories alone and therefore seem to indicate that we observe a mixture of the contributions, whose weights vary, particularly with q and also with temperature T .

The discrepancies between theory and experiment could have several causes; for instance, differences between physical systems and theoretical models, quantum corrections and finite size effects. To overcome some of these complications Gerling and Landau (1990) performed computer simulation in the *classical* planar model and found, in general, excellent qualitative agreement with the theoretical predictions. However, they also observed some quantitative differences in $S^{xx}(q, \omega)$ between the results of the simulation and of the theoretical predictions, showing clearly that quantum corrections alone cannot account for the differences between theory and experiment.

Thus we see that, in order to understand the dynamics of the system described by Hamiltonian (1.1), more theoretical work should be done. To help attain this goal we will study in this paper the interference effects between solitons and two-magnon processes in the sine-Gordon model. This interaction has been neglected so far in theoretical calculations presented in the literature. Our work is an extension of that of Allroth and Mikeska (1981) who investigated the lowest order corrections to the non-interacting soliton-magnon picture. We will concentrate on the dynamical longitudinal structure factor $S^{xx}(q, \omega)$, because it is in this term that the two-magnon processes are important and where some controversy still remains. We will consider a sine-Gordon chain and include, in our treatment, terms up to second order in temperature.

2. Soliton-magnon interference effects in the dynamical longitudinal structure factor

The classical sine-Gordon chain is defined by the Hamiltonian density

$$\mathcal{H} = E_0 \left\{ \frac{1}{2} \left(\frac{\partial \phi}{\partial z} \right)^2 + \frac{1}{2c^2} \left(\frac{\partial \phi}{\partial t} \right)^2 + m^2 (1 - \cos \phi) \right\}. \quad (2.1)$$

We are interested in the following dynamical structure factor

$$S^{xx}(q, \omega) = \frac{S^2}{4\pi^2} \int dt dz e^{i(qz - \omega t)} g^{xx}(z, t) \quad (2.2)$$

where

$$g^{xx}(z, t) = \langle \cos \phi(z, t) \cos \phi(0, 0) \rangle. \quad (2.3)$$

For an investigation of the influence of the soliton-magnon interference on the zeroth order magnon and soliton peaks, we describe the field ϕ as a linear superposition of N solitons and antisolitons and the real part of a general magnon solution (Allroth and Mikeska 1981):

$$\phi(z, t) = \sum_{n=1}^N \phi_{\text{sol}}^n(z - v_n t - z_{0n}) + \Re \left\{ \sum_q \lambda_q \psi_q(z, t) \right\} \quad (2.4)$$

where

$$\psi_q(z, t) = e^{i(qz - \omega_q t)} \prod_{n=1}^N A_{q_n}(z, t) e^{i\phi_{q_n}(z, t)} \quad (2.5)$$

and $\omega_q = c\sqrt{m^2 + q^2}$. Here \Re means that we are taking the real part of the function. Using the procedure adopted by Allroth and Mikeska (1981) up to fourth order in magnon amplitude, we have

$$\begin{aligned} g^{xx}(z, t) = & g_0^{xx}(z, t) - \frac{1}{2} \left\langle (R^2(z, t) + R^2(0, 0) - \frac{1}{12}[R^4(z, t)] - \frac{1}{12}[R^4(0, 0)] \right. \\ & - \frac{1}{2}[R^2(z, t)R^2(0, 0)]) \left[1 - N \left(1 - \frac{1}{N} \sum_n \cos \phi_{\text{sol}}^n(z, t) \right. \right. \\ & \left. \left. \times \cos \phi_{\text{sol}}^n(0, 0) \right) \right] \right\rangle + \left\langle (R(z, t)R(0, 0) - \frac{1}{6}[R(z, t)R^3(0, 0)] \right. \\ & \left. - \frac{1}{6}[R^3(z, t)R(0, 0)]) \sum_n \sin \phi_{\text{sol}}^n(z, t) \sin \phi_{\text{sol}}^n(0, 0) \right\rangle \quad (2.6) \end{aligned}$$

where we have defined

$$R(z, t) = \Re \left\{ \sum_q \lambda_q \psi_q(z, t) \right\}. \quad (2.7)$$

Here we are only interested in those terms that have not been considered by Allroth and Mikeska (1981). These terms are

$$\begin{aligned} G_1(z, t) = & \frac{1}{4} \left\langle \frac{1}{6}[R^4(z, t) + R^4(0, 0) + 6R^2(z, t)R^2(0, 0)] \right. \\ & \left. \times \left[1 - N \left(1 - \frac{1}{N} \sum_n \cos \phi_{\text{sol}}^n(z, t) \cos \phi_{\text{sol}}^n(0, 0) \right) \right] \right\rangle \quad (2.8) \end{aligned}$$

and

$$\begin{aligned} G_2(z, t) = & -\frac{1}{6} \left\langle [R^3(z, t)R(0, 0) + R(z, t)R^3(0, 0)] \sum_n \sin \phi_{\text{sol}}^n(z, t) \right. \\ & \left. \times \sin \phi_{\text{sol}}^n(0, 0) \right\rangle. \quad (2.9) \end{aligned}$$

We will split (2.8) into three contributions:

$$G_1(z, t) = \Delta_1(z, t) + \Delta_2(z, t) + \Delta_3(z, t). \quad (2.10)$$

For Δ_1 we have

$$\begin{aligned} \Delta_1(z, t) = & \frac{1}{8} \sum_k \sum_{k'} (|\lambda_k|^2) (|\lambda_{k'}|^2) (\langle A_{kn}^2(z, t) \rangle^N \langle A_{k'n}^2(z, t) \rangle^N \\ & + \Re \{ e^{i(kz - \omega_k t)} \} \langle A_{kn}(0, 0) A_{kn}(z, t) e^{i\phi_{kn}(z, t)} \rangle \\ & \times \Re \{ e^{i(k'z - \omega_{k'} t)} \} \langle A_{k'n}(0, 0) A_{k'n}(z, t) e^{i\phi_{k'n}(z, t)} \rangle). \end{aligned} \quad (2.11)$$

In the non-relativistic limit, we have

$$A_{kn}(z, t) = \sqrt{1 - m^2 \frac{\sinh^2(m(z - v_n t - z_{0n}))}{m^2 + k^2}} \quad (2.12)$$

$$\phi_{kn}(z, t) = \arctan \left\{ \frac{m \tanh(m(z - v_n t - z_{0n}))}{k} \right\} + \arctan \left(\frac{m \tanh(m z_{0n})}{k} \right). \quad (2.13)$$

The averages in (2.11) have been calculated by Allroth and Mikeska (1981) and are

$$\langle |\lambda_k|^2 \rangle = 2/\beta L (k^2 + m^2) \quad (2.14)$$

where β^{-1} is the temperature measured in units of E_0/κ_B , and L is the chain length,

$$\langle A_k^2(z, t) \rangle^N = 1 - 4nm/(m^2 + k^2) \quad (2.15)$$

and

$$\langle A_{kn}(z, t) A_{kn}(0, 0) \exp(i\phi_{kn}(z, t)) \rangle^N = \exp(-r(k)|z| - s(k)|t| + iD(k)kz) \quad (2.16)$$

where n is the soliton density given by $n = 4m\sqrt{\beta m/\pi} \exp(-8\beta m)$ and

$$r(k) = 4m^2 n / (m^2 + k^2) \quad (2.17)$$

$$s(k) = (1/\sqrt{\beta m \pi}) 2m^2 n c / (m^2 + k^2) \quad (2.18)$$

$$D(k) = 4mn / (m^2 + k^2). \quad (2.19)$$

Fourier transforming we obtain

$$\begin{aligned} \Delta_1(q, \omega) = & \frac{1}{8(\beta\pi)^2} \int_{-\infty}^{+\infty} \frac{dk dk'}{(m^2 + k^2)(m^2 + k'^2)} \\ & \times \left\{ \left(1 - \frac{4nm}{m^2 + k^2} \right) \left(1 - \frac{4nm}{m^2 + k'^2} \right) \delta(q) \delta(\omega) + \frac{1}{4\pi^2} \right. \\ & \times \left(\frac{a(k, k')}{a^2(k, k') + (\omega + \omega_k + \omega_{k'})^2} \frac{b(k, k')}{b^2(k, k') + (q + kB_k + k'B_{k'})^2} \right. \\ & + (\omega_k \rightarrow -\omega_k, k \rightarrow -k) + (\omega_{k'} \rightarrow -\omega_{k'}, k' \rightarrow -k') \\ & \left. \left. + (\omega_k \rightarrow -\omega_k, \omega_{k'} \rightarrow -\omega_{k'}, k \rightarrow -k, k' \rightarrow -k') \right) \right\} \end{aligned} \quad (2.20)$$

where

$$a(k, k') = r(k) + r(k') \quad (2.21)$$

$$b(k, k') = s(k) + s(k') \quad (2.22)$$

$$B_k = 1 + D(k) \quad (2.23)$$

and the density $\rho(k)$ of magnon states in k -space is (Allroth and Mikeska 1981)

$$\rho(k) = \frac{L}{2\pi} \left(1 - \frac{4nm}{m^2 + k^2} \right). \quad (2.24)$$

The term in $\delta(q)\delta(\omega)$ modifies the intensity of the Bragg peak, while the other terms modify the two-magnon peaks. In the non-interacting case we have a step-like two-spin-wave difference process central peak and a second peak, due to two-spin-wave processes, that begins with a square root singularity at the threshold frequency $2\omega_{q/2}$. In addition, the width of the central peak depends on the wavevector but not on temperature. The interference effects between solitons and magnons remove the singularity occurring in the non-interacting case and lead to a temperature dependence for the width of the central peak.

For the Δ_2 term we have

$$\begin{aligned} \Delta_2(z, t) = & -\frac{N}{16} \sum_k \sum_{k'} \langle |\lambda_k|^2 \rangle \langle |\lambda_{k'}|^2 \rangle \langle (1 - \cos \phi_{\text{sol}}^n(z, t) \cos \phi_{\text{sol}}^n(0, 0)) \\ & \times (A_{kn}^2(z, t) A_{k'n}^2(z, t) + A_{kn}^2(z, t) A_{k'n}(0, 0)^2) \rangle. \end{aligned} \quad (2.25)$$

The average in the soliton term is calculated over the possible soliton positions and velocities. Using $\cos \phi(\xi) = 1 - 2\text{sech}^2(m\xi)$, where $\xi = z - vt - z_0$, and (2.12) we obtain, after Fourier transformation,

$$\begin{aligned} \Delta_2(q, \omega) = & -\frac{N}{16} \sum_k \sum_{k'} \langle |\lambda_k|^2 \rangle \langle |\lambda_{k'}|^2 \rangle S_{\text{sol},0}^{xx}(q, \omega) \left\{ 2 - B \left(\frac{1}{m^2 + k^2} + \frac{1}{m^2 + k'^2} \right) \right. \\ & \left. + C \frac{1}{m^2 + k^2} \frac{1}{m^2 + k'^2} \right\} \end{aligned} \quad (2.26)$$

where we have defined

$$B = (m^2 + q^2)/3 \quad \text{and} \quad C = (q^2 + 4m^2)(13q^2 - 2m^2)/360. \quad (2.27)$$

In (2.26) $S_{\text{sol},0}^{xx}(q, \omega)$ is the non-interacting soliton contribution to $S^{xx}(q, \omega)$ which is given by

$$S_{\text{sol},0}^{xx}(q, \omega) = \frac{4nq\sqrt{a\pi}}{m^4} e^{-a(\omega/q)^2} \sinh^{-2} \left(\frac{\pi q}{2m} \right) \quad (2.28)$$

where $a = 4\beta m/c^2$. Performing the k, k' -summation in (2.26) we arrive at the following inelastic soliton contribution of order T^2 to the longitudinal structure factor

$$\Delta_2(q, \omega) = \frac{S_{\text{sol},0}^{\text{xx}}(q, \omega)}{(4\beta m)^2} \left\{ 2 \left(1 - \frac{4n}{m} + \frac{4n^2}{m^2} \right) - \frac{B}{m^2} \left(1 - \frac{5n}{m} + \frac{6n^2}{m^2} \right) + \frac{C}{4m^4} \left(1 - \frac{6n}{m} - \frac{9n^2}{m^2} \right) \right\}. \quad (2.29)$$

The Δ_3 term is given by

$$\Delta_3(z, t) = -\frac{N}{8} \sum_k \sum_{k'} \langle |\lambda_k|^2 \rangle \langle |\lambda_{k'}|^2 \rangle \langle (1 - \cos \phi_{\text{sol}}^n(z, t) \cos \phi_{\text{sol}}^n(0, 0)) \times \Re[e^{i(kz - \omega_k t)} A_{k_n}(z, t) A_{k_n}(0, 0) e^{i\phi_{k_n}(z, t)}] \times \Re[e^{i(k'z - \omega_{k'} t)} A_{k'_n}(z, t) A_{k'_n}(0, 0) e^{i\phi_{k'_n}(z, t)}] \rangle. \quad (2.30)$$

Calculating the average and Fourier transforming, we obtain

$$\Delta_3(q, \omega) = \frac{1}{64} \sum_k \sum_{k'} \frac{\langle |\lambda_k|^2 \rangle \langle |\lambda_{k'}|^2 \rangle}{(m^2 + k^2)(m^2 + k'^2)} \left\{ S_{\text{sol},0}^{\text{xx}}(Q^*, \Omega) \left\{ 2(m^2 - kk') \times (2m^2 - kk') + (k + k')|Q^*| \left[(3m^2 - 2kk') - \frac{1}{3}(Q^{*2} + 4m^2) \right] - \frac{1}{3}(3m^2 - 2kk') (Q^{*2} + 4m^2) + \frac{1}{18}(Q^{*2} + 4m^2)^2 + \frac{1}{2}(k + k')^2 Q^{*2} - [m^2(k + k')^2 + 2(m^2 - kk')(k + k')m^2/|Q^*| - m^2(k + k')(Q^{*2} + 4m^2)/3|Q^*|] \tanh(\pi|Q^*|/m) \right\} + (\omega_k \rightarrow -\omega_k, k \rightarrow -k) + (\omega_{k'} \rightarrow -\omega_{k'}, k' \rightarrow -k') + (\omega_k \rightarrow -\omega_k, \omega_{k'} \rightarrow -\omega_{k'}, k \rightarrow -k, k' \rightarrow -k') \right\} \quad (2.31)$$

where $Q^* = q + k + k'$ and $\Omega = \omega + \omega_k + \omega_{k'}$. This term gives the $O(T^2)$ soliton contribution to the two-magnon process peak.

Let us now consider $G_2(z, t)$. We have

$$G_2(z, t) = -\frac{N}{4} \sum_k \sum_{k'} \langle |\lambda_k|^2 \rangle \langle |\lambda_{k'}|^2 \rangle \Re \left\{ e^{i(kz - \omega_k t)} \right\} \langle A_{K'_n}^2(0, 0) \times A_{k_n}(z, t) A_{k_n}(0, 0) e^{i\phi_{k_n}(z, t)} \sin \phi_{\text{sol}}^n(z, t) \sin \phi_{\text{sol}}^n(0, 0) \rangle. \quad (2.32)$$

Performing the average, Fourier transforming, and summing over k' we obtain

$$G_2(q, \omega) = \frac{1}{8\beta\pi m^6} \sum_k \langle |\lambda_k|^2 \rangle S_{\text{sol},0}^{\text{yy}}(Q', \Omega') \left\{ K_1 \left(k + \frac{m^2 - Q'^2}{2|Q'|} \right)^2 - \frac{K_2}{48m^2} \frac{m^2 + Q'^2}{Q'^2} \times (m^2 - Q'^2 + 2k|Q'|)(4k|Q'| + 3m^2 - Q'^2) \right\} \times (\omega_k \rightarrow -\omega_k, k \rightarrow -k) \quad (2.33)$$

where $Q' = q + k$, $\Omega' = \omega + \omega_k$ and

$$K_1 = 2(m - 2n) \tan^{-1}(\pi/m) - 4\pi n m / (m^2 + \pi^2) \quad (2.34)$$

$$K_2 = (m - 3n) \tan^{-1}(\pi/m) + \pi m(m - 4n) / (m^2 + \pi^2) - \pi n m(m^2 - \pi^2) / (m^2 + \pi^2)^2. \quad (2.35)$$

In (2.33), $S_{\text{sol},0}^{yy}(q, \omega)$ is the non-interacting soliton contribution to $S^{yy}(q, \omega)$; its expression can be obtained from (2.28) if $\sinh^{-2}(x)$ is replaced by $\cosh^{-2}(x)$. $G_2(q, \omega)$ contributes to the magnon peak to order (T^2) . It is an easy task to integrate (2.33) over frequency because only $S_{\text{sol},0}^{yy}(Q', \Omega')$ depends on the frequency ω . For $q\pi \gg 2m$, the integrand will be sharply peaked around $k = -q$ and we can get an estimate of the magnon intensity as

$$G_2(q) = \frac{n}{4\beta^2 m^6} \frac{1}{q^2 + m^2} \left(K_1 - \frac{K_2}{4} \right). \quad (2.36)$$

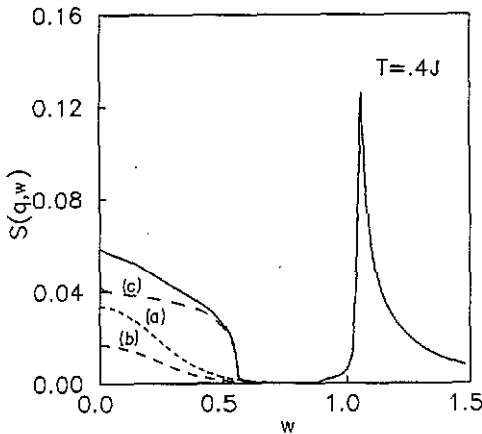


Figure 1. $S^{xx}(q, \omega)$ (full line) as a function of ω for temperature $T = 0.4J$, magnetic field $h = 0.1J$, and wavevector $qa = \pi/8$. (a) represents the non-interacting soliton contribution $S_{\text{sol},0}^{xx}$; (b) is the sum of the soliton non-interacting contribution and the soliton-magnon interaction up to the order calculated by Allroth and Mikeska; (c) is the two-magnon contribution that has been obtained in this work.

3. Conclusion

In the last section we calculated, using the approach of Allroth and Mikeska (1981) all corrections to order T^2 due to interference effects between solitons and magnons, to the longitudinal dynamical structure factor in the classical sine-Gordon-like magnetic chain. Figures 1 and 2 give the $S^{xx}(q, \omega)$ spectra (full line) obtained for $q = \pi/8$ at $T/J = 0.4$ and $T/J = 0.8$, respectively. Keeping in mind (as discussed in section 1) that the most important corrections are the ones for the central peak

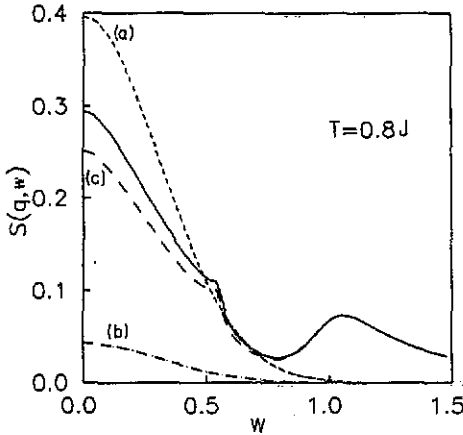


Figure 2. $S^{xx}(q, \omega)$ (full line) as a function of ω for temperature $T = 0.8J$, magnetic field $h = 0.1J$, and wavevector $qa = \pi/8$. (a), (b) and (c) represent partial contributions, as explained in figure 1.

since this is where discrepancies between theory and experiment have been reported (Steiner and Bishop 1986), we have not included the contributions related to one-magnon peaks in our numerical calculations. The soliton non-interacting contribution is given by curves (a), note its dependence on temperature and the drastic reduction (curves (b): $S_{sol,0}^{xx}(q, \omega)$ + soliton-magnon interaction as calculated by Allroth and Mikeska (1981)) it suffers when the magnon interaction is taken into account. Curves (c) represent the contribution due to two-magnon processes as given by (2.20), (2.29) and (2.31); the singularity predicted to occur at $(\omega - 2\omega_{q/2})$ when the soliton effect on two-magnon processes is not considered is now completely removed. We also note that our results lead to a temperature dependent width for this contribution. The full lines shown in figures 1 and 2 correspond to the sum of curves (b) and (c); the contribution due to two-magnon processes is always dominant.

In figure 3 we present the half-width at half height of the central peak for $S^{xx}(q, \omega)$ as a function of temperature, comparing our theoretical calculations with simulation data from Gerling and Landau (1990). Also shown in figure 3 are the non-interacting soliton and the pure two-magnon contributions. As we can see, the longitudinal correlation function shows a crossover from a two-spin-wave process, dominating the low temperature region, to a soliton process, at higher temperature. Our results are in much better agreement with the simulation data than the non-interacting theory: two-spin-wave and soliton processes. The remaining discrepancy can be attributed to out-of-plane effects present in Gerling and Landau's simulations.

In conclusion we emphasize that this is the first time that soliton-magnon interactions up to second-order terms in temperature are taken into account. Of course, since our theory is an extension of the work of Allroth and Mikeska (1981) it suffers from the same limitations: for instance, lack of complete self-consistency. Also, the theory presented here was developed for the XY model. Its application to a realistic magnetic chain (such as that used to describe CsNiF_3) would require the inclusion of other effects such as quantum corrections, out-of-plane motion and discreteness effects. These effects have been discussed recently by Mikeska and Steiner (1991) in an excellent review paper. Our work complements their discussion showing that,

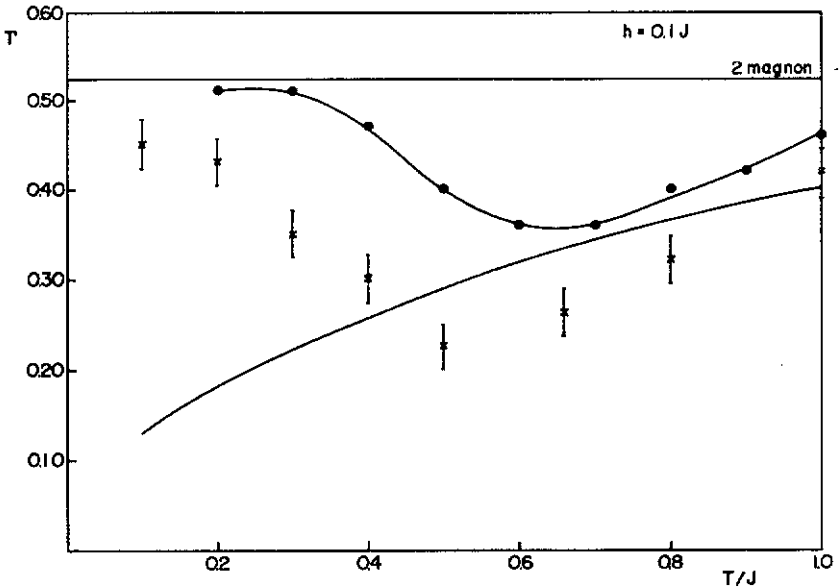


Figure 3. The half-width at half-height of the central peak for $S^{zz}(q, \omega)$ as a function of temperature for $h = 0.1J$ and $q = \pi/8$. The dots (connected by a guide line) are the results of our theory. The full lines are the results for the two-spin-wave difference process and for the central soliton peak. Also shown are the computer simulation data obtained from Gerling and Landau (1990).

besides the contributions pointed out in their work (Mikeska and Steiner 1991), the second-order soliton-magnon interaction must be taken into account.

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