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Excitation spectrum and $T = 0$ dynamics of the one-dimensional planar spin-1/2 ferromagnet

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The $T = 0$ dynamics of the one-dimensional $S = 1/2$ ferromagnet with planar exchange anisotropy is studied by finite-chain calculations and a Green function approach. We demonstrate that the excitation spectrum relevant for appropriate low- T inelastic neutron scattering experiments is much more complex than predicted by linear spin-wave theory. It includes two continua and a set of discrete branches. Some of the low-lying excitations predicted by rigorous calculations, on the other hand, are shown to contribute no spectral weight to the $T = 0$ dynamic structure factor $S_{zz}(q, \omega)$. We provide quantitative results for the spectral-weight distribution in $S_{zz}(q, \omega)$ at $T = 0$ from bound states and continuum states, including a detailed analysis of the singularity in $S_{zz}(q, \omega)$ at the lower band edge. Further evidence is found for the prediction that some $T = 0$ critical properties of the planar $S = 1/2$ ferro- and antiferromagnet are governed by exponents which depend continuously on the planar anisotropy.

1. Introduction

The static and dynamic properties of one-dimensional (1D) ferromagnets (FM) have been studied extensively for some time, both theoretically and experimentally [1]. By far the most prominent physical realization of such systems has been the quasi-1D $S = 1$ easy-plane FM CsNiF_3 . Its excitation spectrum and low-temperature dynamical properties have been interpreted – not without controversy – mostly in terms of classical spin waves and solitons [2]. More recently, the discovery of a number of compounds characterized as quasi-1D spin-1/2 FM's has attracted much attention from both experimentalists [3] and theorists [4,5], in the belief that quantum effects will be important. A neutron scattering study completed very recently [6] has indeed confirmed that the dynamical properties of the quasi-1D FM $\text{CuCl}_2 \cdot \text{DMSO}$ cannot be understood in terms of the excitations predicted by classical theories.

The object of the present work is the 1D $S = 1/2$ FM

$$\mathcal{H} = -J \sum_{l=1}^N [S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z] \quad (1)$$

with planar exchange anisotropy $0 \leq \Delta \leq 1$. It is well-known that this system has a singlet ground state without true long-range order [7,8]. Therefore, linear spin-wave theory is not applicable. The energies of two classes of low-lying excitations of (1) were found by Johnson et al. [9] by exploiting the mapping between the eight-vertex model and the quantum spin chain. According to their rigorous calculations, the excitation spectrum of (1) consists for $0 \leq \Delta \leq 1$ of two partly overlapping continua of "free" states and a set of discrete branches of "bound" states. The states of the continua \mathcal{C} and $\bar{\mathcal{C}}$, respectively, have energies

$$\mathcal{C} : \epsilon_L(q) < \omega < \epsilon_U(q); \quad \bar{\mathcal{C}} : \bar{\epsilon}_L(q) < \omega < \bar{\epsilon}_U(q) \quad (2a)$$

$$\epsilon_L(q) = J(\pi \sin \mu/2\mu) |\sin q|, \quad \bar{\epsilon}_L(q) = \epsilon_L(q) \quad (2b)$$

$$\epsilon_U(q) = J(\pi \sin \mu/\mu) |\sin(q/2)|, \quad \bar{\epsilon}_U(q) = \epsilon_U(\pi - q) \quad (2c)$$

where $\Delta = -\cos \mu$, $\pi/2 \leq \mu \leq \pi$, $-\pi \leq q \leq \pi$ (see Fig. 1). The energies of the bound states are given by

$$\epsilon_r(q) = J(\pi \sin \mu / \mu \sin y) \sin(q/2) \sqrt{\sin^2(q/2) + \sin^2 y \cos^2(q/2)} \quad (3)$$

where $y = (\pi r / 2\mu)(\pi - \mu)$, and the r -th branch exists only for $\mu > \pi/(1 + 1/r)$. In the XY limit ($\Delta = 0$) only the two continua are present. The bound-state branches $r = 1, 2, 3, \dots$ progressively emerge from the top of continuum \mathcal{C} at $\Delta = 0, 0.5, 0.707 \dots$, etc. In the Heisenberg limit ($\Delta = 1$) the continua vanish altogether leaving behind an infinite set of discrete branches. Fig. 1 shows the bound-state branches $\epsilon_r(q)$, $r = 1, 2, 3$ existing at $\Delta = 0.8$ together with the continua \mathcal{C} and $\bar{\mathcal{C}}$.

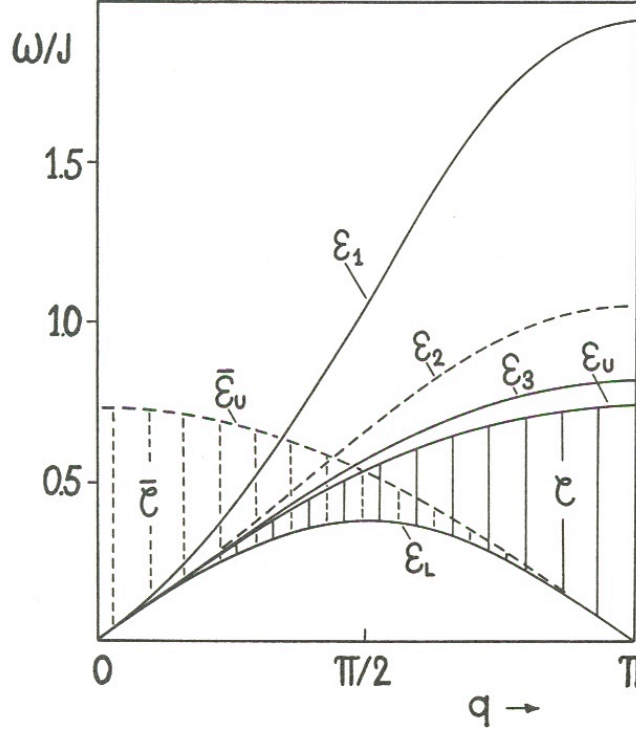


Figure 1. Excitation spectrum of the 1D $S = 1/2$ planar FM (i) with $\Delta = 0.8$, consisting of two continua and three discrete branches of bound states. Only the states of continuum \mathcal{C} and of branches $\epsilon_r(q)$ with odd r (solid lines) contribute to $S_{zz}(q, \omega)$ at $T = 0$.

Apart from the knowledge of their energies it has remained unclear whether these excitations are relevant for the dynamics because the corresponding matrix elements have, generally, not been known. A set of excitations of (1) can be called relevant for the dynamics at a given temperature if it contributes significantly to the dynamic structure factor $S_{\mu\mu}(q, \omega)$, the Fourier transform of the time-dependent two-spin correlation function $\langle S_l^\mu(t) S_{l+R}^\mu \rangle$. Such a relevant set of excitations should then be observable in an appropriate inelastic neutron scattering experiment. At $T = 0$ $S_{\mu\mu}(q, \omega)$ can be written in the simple form

$$S_{\mu\mu}(q, \omega) = \sum_{\lambda} M_{\lambda}^{\mu} \delta(\omega - E_{\lambda} + E_G), \quad M_{\lambda} = 2\pi |\langle G | S^{\mu}(q) | \lambda \rangle|^2 \quad (4)$$

where $S^{\mu}(q) = N^{-1/2} \sum_l \exp(iql) S_l^{\mu}$, $|G\rangle$ is the ground state with energy E_G , and λ runs over all eigenstates $|\lambda\rangle$ of (1) with energies E_{λ} .

This communication reports the results of a purely quantum mechanical approach to the $T = 0$ dynamics of the planar $S = 1/2$ FM (1). We investigate the observability of the excitations (2),

(3) predicted by Johnson et al. [9] and find observable excitations not present in any classical calculation. Preliminary, rather qualitative results, are already published [5]. The approach of the present work, which was proposed in Ref. 5, is paralleled to some extent by work of Schneider and Stoll [10].

2. Finite-Chain Calculations

By using exact finite-chain results for $S_{zz}(q, \omega)$, i.e. by diagonalizing the Hamiltonian (1) for $N = 4$ to 10 and evaluating the (squared) matrix elements M_λ^z of (4), we have analyzed the spectral weight of the various excitations contributing to $S_{zz}(q, \omega)$ at $T = 0$.

At $\Delta = 0$ we observe that only the excitations of continuum \mathcal{C} carry spectral weight (i.e. have $M_\lambda^z \neq 0$), in agreement with exact analytic results for the XY model [11]. With increasing Δ “branches” of states out of continuum \mathcal{C} are progressively transformed into branches of bound state $\epsilon_r(q)$ with odd r . In the Heisenberg limit $\Delta = 1$, finally, all states of continuum \mathcal{C} have “evaporated” into odd- r bound states. These states keep nonzero spectral weight in the finite system for $0 \leq \Delta \leq 1$ either as continuum states or as bound states. The bound states in branches with even r , on the other hand, are of different origin and have zero spectral weight in $S_{zz}(q, \omega)$ at any value of Δ [12]. A simple but not rigorous argument explaining this empirical selection rule is presented in Sect. 3.

The states of continuum $\bar{\mathcal{C}}$ and any excitations not considered so far are observed not to contribute significantly to $S_{zz}(q, \omega)$ for any Δ . Their matrix elements M_λ^z for $N = 10$ are at least two orders of magnitude smaller than the matrix element of any \mathcal{C} state.

At $\Delta = 1$ the eigenstates can be characterized according to their quantum number S^T of the total spin $\sum_l \vec{S}_l^2 = S^T(S^T + 1)$. For the bound states $S^T = N/2 - r$ holds. The ground state has $r = 0$. The $r = 1$ states are the familiar FM magnons and the $r > 1$ excitations are bound r -spin complexes. At $\Delta = 1$ a selection rule based on the Wigner-Eckart theorem allows only the magnons ($r = 1$) to contribute to $S_{zz}(q, \omega)$ at $T = 0$.

Finally, we should remark that the well-known two-magnon continuum states found for the Heisenberg-Ising FM ($\Delta > 1$) [13] are not related to the continuum states (2) of the Heisenberg-XY FM ($0 < \Delta < 1$).

3. Green Function Approach to $S_{zz}(q, \omega)$

The finite-chain calculations have proved to be very useful in identifying which classes of excitations play an important role in the $T = 0$ dynamics. They provide a very reliable though qualitative picture of the excitation spectrum relevant in $S_{zz}(q, \omega)$ at $T = 0$. For an analytic approach we use the well-known mapping of (1) onto a Fermion system [14],

$$\mathcal{H} = \sum_k \epsilon_0(k) a_k^\dagger a_k + (2N)^{-1} \sum_q V(q) \rho(q) \rho(-q) \quad (5)$$

with $\epsilon_0(k) = -J \cos k$, $V(q) = -2\Delta J \cos q$, $\rho(q) = \sum_k a_k^\dagger a_{k+q}$. The dynamic structure factor $S_{zz}(q, \omega)$ of the spin chain (1) is related to the two-particle Green function G_2 of (5) which is the solution of a Bethe-Salpeter equation. In the Hartree-Fock approximation the latter reads

$$G_2(q, p, z) = H(q, p, z) \left[1 + N^{-1} \sum_{p'} \{V(q) - V(p - p')\} G_2(q, p', z) \right], \quad (6)$$

where

$$H(q, p, z) = \frac{N_F(p - q/2) - N_F(p + q/2)}{z + \epsilon(p - q/2) - \epsilon(p + q/2)} \quad (7)$$

with $N_F(p) = [\exp(\beta\epsilon(p)) + 1]^{-1}$ comes from the product of the two one-particle propagators. Incorporation of Hartree-Fock corrections to the one-particle spectrum leads (at $T = 0$) to the

effective exchange J' :

$$\epsilon(k) = -J' \cos k, \quad J' = J(1 - 2\Delta/\pi). \quad (8)$$

Eq. (6) has been applied earlier to the Heisenberg antiferromagnet (AFM) [15]. $S_{zz}(q, \omega)$ is obtained from the imaginary part (at $z = \omega + i\epsilon$) of

$$\chi_{zz}(q, z) + N^{-1} \sum_p G_2(q, p, z), \quad (\chi \equiv \chi' - i\chi'') \quad (9)$$

as

$$S_{zz}(q, \omega) = \frac{2\chi''_{zz}(q, \omega)}{1 - \exp(-\beta\omega)}. \quad (10)$$

Solving eq. (6) yields [15]

$$\chi_{zz}(q, \omega) = \frac{\chi_0(q, z)}{1 - W(q, z)\chi_0(q, z)}. \quad (11)$$

Here $W(q, z) = 2[\Delta z^2/4J' \sin^2(q/2) - \Delta J \cos q]$, and $\chi_0(q, z) = N^{-1} \sum_p H(q, p, z)$ is the response function for the noninteracting system. For $T = 0$ the real and imaginary parts read, respectively

$$\begin{aligned} \chi'_0(q, \omega) &= \frac{2\theta(\omega^2 - \omega_U^2(q))}{\pi\sqrt{\omega^2 - \omega_U^2(q)}} \arctan \frac{\omega_U^2(q)/2J'}{\sqrt{\omega^2 - \omega_U^2(q)}} \\ &\quad - \frac{\theta(\omega_U^2(q) - \omega^2)}{\pi\sqrt{\omega_U^2(q) - \omega^2}} \ln \left| \frac{\sqrt{\omega_U^2(q) - \omega^2} + \omega_U^2(q)/2J'}{\sqrt{\omega_U^2(q) - \omega^2} - \omega_U^2(q)/2J'} \right| \end{aligned} \quad (12a)$$

$$\chi''_0(q, \omega) = \text{sgn}(\omega) \frac{\theta(\omega^2 - \omega_L^2(q))\theta(\omega_U^2(q) - \omega^2)}{\sqrt{\omega_U^2(q) - \omega^2}} \quad (12b)$$

with the spectral boundaries $\omega_L(q) = J' \sin q$, $\omega_U(q) = 2J' \sin(q/2)$. The result (11) yields the following information on $S_{zz}(q, \omega)$ at $T = 0$:

(i) The Hartree-Fock correction (8) leads to a renormalization of the boundaries $\omega_L(q)$, $\omega_U(q)$ of continuum \mathcal{C} , which agrees with (2) to first order in Δ .

(i i) For $\Delta > 0$ χ_{zz} has a pole at the energy

$$\omega_1(q) = [4J'^2 \sin^2(q/2) + 16\Delta^2 J'^2 \sin^4(q/2)]^{1/2} \quad (13)$$

above the continuum \mathcal{C} . $\omega_1(q)$ agrees with $\epsilon_1(q)$ of (3) to first order in Δ . Thus our approximation reproduces the first branch of bound states in a satisfactory way. The residuum is readily evaluated, yielding the contribution

$$S_{zz}^B(q, \omega) = 4\pi\Delta \sin(q/2)\delta(\omega - \omega_1(q)) \quad (14)$$

to the dynamic structure factor. The occurrence of discrete energies in the spectrum of S_{zz} above the continuum is easily understood by realizing that, according to (6), G_2 is the Green function of a two-particle scattering problem. In an appropriate continuum approximation we can concentrate on the p -range $p \simeq \pi/2$ close to the upper bound $\omega_U(q)$ of the particle-hole continuum. Then

$$\hat{G}_2(q, R, z) \equiv \sum_p e^{ipR} G_2(q, p, z) = \sum_\lambda \frac{\psi_\lambda^*(q, R)\psi_\lambda(q, 0)}{z - E_\lambda} \quad (15)$$

is the Green function of a continuum scattering problem with potential $W_q(R) = N^{-1} \sum_p \exp(ipR) \times [V(p) - V(q)]$, wave functions ψ_λ and eigenvalues E_λ . In a similar way, the wave function $(q, R)\psi(q, R)$ of an exciton in a semiconductor is built up by electron and hole states such that the pair has total momentum $\hbar q$ and a relative coordinate R [16]. The signs in the Schrödinger equation for ψ_λ in (15) are such that discrete “bound state” of the potential occur at energies $E_\lambda > \omega_L(q)$, i.e. above the continuum. Although the full physical content of (6) is more complicated than a

simple potential scattering problem (due to the presence of the filled Fermi sea) we can use this simple picture to illustrate the role of bound states in the spectrum of $S_{zz}(q, \omega)$: (a) In 1D potential well problems there is no threshold for the formation of a first bound state. Accordingly the first branch of bound states (3) shows up at arbitrarily small $\Delta > 0$. (b) If the potential has inversion symmetry (like our $W_q(R)$) the bound-state wave functions have alternating parity, the lowest being even. Obviously, the states with odd wave functions do not contribute to $\chi_{zz}(q, \omega)$ in (9). If the same holds true for the full Bethe-Salpeter equation (where higher-order terms will lead to nonlocal, energy-dependent potentials), it is clear why every other bound state branch has zero spectral weight in S_{zz} , as we have observed in finite-chain results.

(iii) The continuum part of $S_{zz}(q, \omega)$ as given by

$$S_{zz}^c(q, \omega) = \frac{\chi_0''(q, \omega)}{[1 - W(q, \omega)\chi_0'(q, \omega)]^2 + [W(q, \omega)\chi_0''(q, \omega)]^2} \quad (16)$$

is illustrated in Fig. 2(a) for the noninteracting case $\Delta = 0$ and (b) for the weakly coupled case $\Delta = 0.1$ (solid curve). Here the Hartree-Fock approximation is expected to give a qualitatively correct picture. Clearly, such details as the rounded-off singularities at the band edges should not be taken too literally. A more useful way to analyse (16), on which more elaborate renormalization group techniques [17] in the continuum limit are based, consists in simply calculating the first order correction to the singularities of χ_{zz} . At the lower edge $\omega_L(q)$ the discontinuity of $\chi_0''(q, \omega)$ changes to a logarithmic singularity for $\Delta \neq 0$. If we postulate a power-law behavior of $S_{zz}(q, \omega)$ – which, in fact, was predicted by calculations in the (Luttinger model) continuum limit for $q \simeq \pi$ [7,8] – with an exponent $\alpha(\Delta)$, we can formally expand

$$S_{zz}(q, \omega) \propto [\omega^2 - \omega_L^2(q)]^{-\alpha} = 1 - \alpha \ln(\omega^2 - \omega_L^2(q)) + O(\alpha^2). \quad (17)$$

Comparison with the same form found from (16) for $\omega \gtrsim \omega_L(q)$ yields

$$\alpha(\Delta) = -\frac{2\Delta}{\pi} + O(\Delta^2). \quad (18)$$

This agrees to $O(\Delta)$ with the corresponding exponent obtained in the continuum approximation

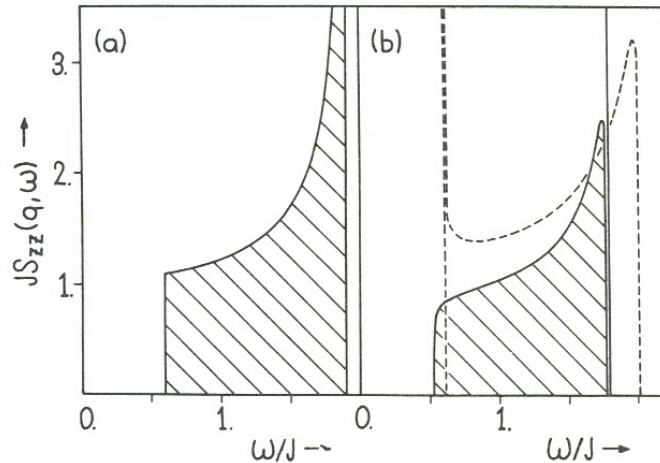


Figure 2. Dynamic structure factor $S_{zz}(q, \omega)$ for the system (I) at $T = 0$, as obtained by the Green function approach. The two plots represent $S_{zz}(q, \omega)$ at fixed $q = 4\pi/5$ as a function of ω for (a) $\Delta = 0$ (exact result), (b) $\Delta = 0.1$ (solid lines), $\Delta = -0.1$ (dashed line). In the case $\Delta > 0$ there is a δ -function type contribution from a bound state in addition to the continuum.

for $q \simeq \pi$ [7,8] and with the exponent

$$\alpha = \frac{\pi/2 - \mu}{\pi - \mu}, \quad \cos \mu = -\Delta \quad (19)$$

as derived from known critical exponents of the eight-vertex model [7]. We stress that our present calculation justifies the form (17) for the whole Brillouin zone, at least to $O(\Delta)$, whereas previous calculations [7,8] for continuum models, only cover the domains $q \simeq 0, \pi$. The same analysis applied to the singularity at $\omega_U(q)$ would require a higher order approximations to $S_{zz}(q, \omega)$ than (6).

(iv) The result (16) evaluated at small negative Δ yields the dynamic structure factor $S_{zz}(q, \omega)$ for the planar AFM [18]. Fig. 2(b) shows the case $\Delta = -0.1$ as the dashed curve. Here $S_{zz}(q, \omega)$ has a two-peak structure with peaks close to $\omega_L(q)$ and $\omega_U(q)$, respectively. In the Hartree-Fock approximation both peaks are rounded off, one of them being very tall and sharp for the example shown in Fig. 2(b). The analysis used above for the planar FM, however, suggests that $S_{zz}(q, \omega)$ for the planar AFM also has a power-law singularity of the form (17) at $\omega_L(q)$ with an exponent (18). In the AFM case, the positive α leads to a divergence of $S_{zz}(q, \omega)$ at $\omega_L(q)$ in agreement with calculations in the continuum approximation at $q \simeq \pi$ [7,8]. It is interesting to note that the general shape of $S_{zz}(q, \omega)$ for $\Delta = -0.1$ from (16) is in remarkably good agreement with $S_{zz}(q, \omega)$ as obtained in Ref. 19 by a completely different approach. The Hartree-Fock result (16) evaluated at $\Delta = -1$, on the other hand, has serious deficiencies [15]. Note also that the exponent α in (17) determines (for $\alpha > 0$) the $T_c = 0$ critical exponent η as it appears in $|\langle S_i^z S_{i+R}^z \rangle| \sim R^{1-\eta}$ to be $\eta(\Delta) = 3 - 2\alpha(\Delta)$.

4. Behavior of $S_{xx}(q, \omega)$

We have also investigated the transverse components $S_{xx}(q, \omega)$ of the dynamic structure factor. Finite-chain results show that the spectral weight is distributed over both continua \mathcal{C} and $\bar{\mathcal{C}}$ for $0 \leq \Delta \ll 1$. As the limit $\Delta = 1$ is approached the spectral weight is progressively transferred to the $r = 1$ branch of (3), i.e. to the FM magnon states. An analytic expression for $S_{xx}(q, \omega)$ in the limit $\Delta = 0$ obtained by a different approach has been given in Ref. 19 including figures of lineshapes [18]. An extension of that approach for $S_{xx}(q, \omega)$ and $S_{zz}(q, \omega)$ to $\Delta > 0$ together with a more detailed account of the present calculations including second-order terms in $V(q)$ will be published in due course.

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