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Dynamical properties of quantum spin systems in magnetically ordered product ground states

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The one-dimensional spin-s XYZ model in a magnetic field of particular strength has a ferro- or antiferromagnetically ordered product ground state. The recursion method is employed to determine $T=0$ dynamic structure factors for systems with $s=\frac{1}{2}, 1, \frac{3}{2}$. The line shapes and peak positions differ significantly from the corresponding spin-wave results, but their development for increasing values of s suggests a smooth extrapolation to the spin-wave picture.

It is not necessarily the presence of strong quantum fluctuations in the ground state that is primarily responsible for turning the $T=0$ dynamics of a quantum many-body system into a challenging topic of condensed-matter theory. Even for systems with no correlated quantum fluctuations in their ground state, the dynamically relevant excitation spectrum may be exceedingly complex, and the spectral weight in dynamical quantities may be distributed over frequency bands of infinite width. This will be demonstrated for a system of localized spins with an exact ferro- or antiferromagnetic product ground state. The shortcomings of the *harmonic* alias *linear spin-wave* alias *single-mode* approximation are found to be considerable.

We consider the spin-s XYZ ferromagnet in a magnetic field,

$$H=-\sum_{l=1}^{N}\{J_xS_l^xS_{l+1}^x+J_yS_l^yS_{l+1}^y+J_zS_l^zS_{l+1}^z+hS_l^z\}, \quad (1)$$

for $J_x\geq J_y\geq J_z\geq 0$, even N, and periodic boundary conditions. If the magnetic field has a particular strength, $h=h_N=2s[(J_x-J_z)(J_y-J_z)]^{1/2}$, that system is known to have a product ground state wave function,

$$|G\rangle=\bigotimes_{l=1}^{N}U_l(\vartheta)|s\rangle_l, \quad (2)$$

where the unitary transformation represented by $U_l(\vartheta)$ describes a rotation of the spin direction at site l by an angle $\vartheta=\arccos\sqrt{(J_y-J_z)/(J_x-J_z)}$ away from the z axis into the xz plane.[1] $|G\rangle$ is a state of maximum ferromagnetic order, $\langle\mathbf{M}\rangle=\langle G|\mathbf{S}_l|G\rangle=(s\sin\vartheta,\ 0,\ s\cos\vartheta)$. The ground state energy is $E_G=-Ns^2(J_x+J_y-J_z)$.

Previous studies of this system, motivated by the search for new rigorous results in quantum many-body dynamics, led to two general conclusions:[2–4] (i) The conditions under which ferromagnetic spin waves are exact eigenstates of H are much more restrictive than those for the existence of the product ground state, namely $J_x=J_y$ or $q=\pi$ or $s\rightarrow\infty$, in addition to $h=h_N$. (ii) The realization of the product ground state $|G\rangle$ implies the following rigorous relations between the $T=0$ dynamic structure factors $S_{\mu\mu}(q,\omega)$:

$$S_{xx}(q,\omega)=S_{yy}(q,\omega)\cos^2\vartheta+4\pi^2s^2\sin^2\vartheta\,\delta(\omega)\,\delta(q),$$

$$S_{zz}(q,\omega)=S_{yy}(q,\omega)\sin^2\vartheta+4\pi^2s^2\cos^2\vartheta\,\delta(\omega)\,\delta(q). \quad (3)$$

The only known rigorous and explicit results pertain to the $s=\frac{1}{2}$ XY model ($J_x=1+\gamma$, $J_y=1-\gamma$, $J_z=0$), and can be evaluated in the form of a two-particle Green's function for free lattice fermions,[5] in combination with relations (3):[2–4]

$$S_{yy}(q,\omega)=\frac{\gamma}{2(1-\gamma)}\frac{\sqrt{4(1-\gamma^2)\cos^2(q/2)-(\omega-2)^2}}{[\omega-2\sin^2(q/2)]^2+\gamma^2\sin^2 q}\times\Theta[4(1-\gamma^2)\cos^2(q/2)-(\omega-2)^2]. \quad (4)$$

Whereas spin-wave theory predicts a single spectral line in $S_{\mu\mu}(q,\omega)$ at the frequency $\omega_{SW}=2s(J_x-J_y\cos q)$, expression (4) is represented by a spectral-weight distribution that consists of a peak shifted relative to ω_{SW} and with nonzero intrinsic width.[2] However, the result (4) does not yet fully reflect the generic structure of $S_{\mu\mu}(q,\omega)$ for this situation.

Our analysis of generic cases ($s>\frac{1}{2}$ XY or XYZ with arbitrary s) employs the recursion method. For this application, it is based on an orthogonal expansion of the wave function $|\Psi_q^\mu(t)\rangle=S_q^\mu(-t)|G\rangle$, where $S_q^\mu=N^{-1/2}\sum_l e^{iql}S_l^\mu$.[6–8] The recursion algorithm produces (after some intermediate steps) a sequence of continued-fraction coefficients $\Delta_1^{\mu\mu}(q)$, $\Delta_2^{\mu\mu}(q)$,..., for the relaxation function,

$$c_0^{\mu\mu}(q,z)=\cfrac{1}{z+\cfrac{\Delta_1^{\mu\mu}(q)}{z+\cfrac{\Delta_2^{\mu\mu}(q)}{z+\cdots}}}, \quad (5)$$

which is the Laplace transform of the symmetrized correlation function $\Re\langle S_q^\mu(t)S_{-q}^\mu\rangle/\langle S_q^\mu S_{-q}^\mu\rangle$. The dynamic structure factor $S_{\mu\mu}(q,\omega)$, which is the Fourier transform of $\langle S_q^\mu(t)S_{-q}^\mu\rangle$, can be obtained directly from (5) as follows (for $T=0$):

$$S_{\mu\mu}(q,\omega)=4\langle S_q^\mu S_{-q}^\mu\rangle\Theta(\omega)\lim_{\epsilon\rightarrow 0}\Re[c_0^{\mu\mu}(q,\epsilon-i\omega)]. \quad (6)$$

The simple dependence of the product wave function $|G\rangle$ on the size of the system offers the advantage that we can compute a significant number of size-independent coefficients $\Delta_k^{\mu\mu}(q)$.[9] In Fig. 1 we have plotted the sequences $\Delta_k^{\mu\mu}(q=0)$ for four different applications of the recursion method. Each one of the four qualitatively different patterns

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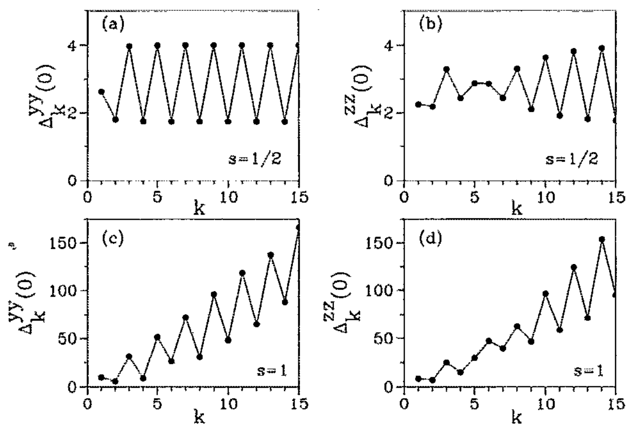

FIG. 1. Continued-fraction coefficients $\Delta_k^{yy}(0)$ and (rescaled) $\Delta_k^{zz}(0)$, as obtained from the recursion method for the determination of the $T=0$ dynamic structure factors $S_{\mu\mu}(q=0,\omega),\mu=y,z,$ of the 1D spin-s XY model ($J_x=1+\gamma,\ J_y=1-\gamma,\ J_z=0,\ h=h_N$) with $\gamma=\frac{3}{4}$, and the spin quantum number s, as specified in each of the four panels.

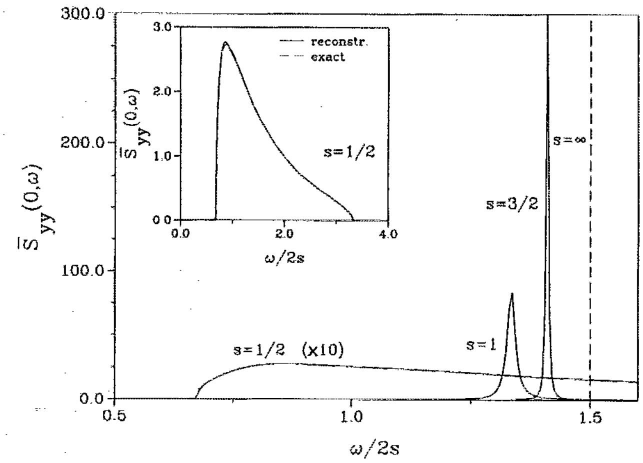

FIG. 2. Normalized dynamic structure factor $\bar{S}_{yy}\equiv S_{yy}(q,\omega)/\langle S_q^y S_{-q}^y\rangle$ (for $q=0$) at $T=0$ of the 1D XY model ($J_x=1+\gamma, J_y=1-\gamma, J_z=0, h=h_N$) with $\gamma=\frac{3}{4}$. The three curves in the main plot represent the results for $s=\frac{1}{2},1,\frac{3}{2}$, as obtained from the recursion method combined with the continued-fraction analysis outlined in the text. For better visibility, we have expanded the vertical scale by a factor of 10 for the spin-$\frac{1}{2}$ curve. The number of continued-fraction coefficients used is $K=16$. The vertical dashed line represents the classical spin-wave result for the same function. The inset shows again the spin-$\frac{1}{2}$ result (solid line) on different scales, now in comparison with the exact expression (4) (dashed line).

displayed by these sequences bears the signature of a characteristic property of the associated $S_{\mu\mu}(q=0,\omega)$.

In panels (a) and (b), the Δ_{2k-1} and the Δ_{2k} tend to converge to different (finite) values $\Delta_\infty^{(o)}$ and $\Delta_\infty^{(e)}$, respectively. If $\Delta_\infty^{(o)}>\Delta_\infty^{(e)}$ as in (a), the implication for the dynamic structure factor is that all its spectral weight is confined to the interval $\omega_{\min}\leqslant\omega\leqslant\omega_{\max}$, with $\omega_{\min}=|\sqrt{\Delta_\infty^{(e)}}-\sqrt{\Delta_\infty^{(o)}}|$, $\omega_{\max}=\sqrt{\Delta_\infty^{(e)}}+\sqrt{\Delta_\infty^{(o)}}$. If $\Delta_\infty^{(o)}<\Delta_\infty^{(e)}$ as indicated in (b) for $k>5$, the dynamic structure factor has a $\delta(\omega)$ contribution, in addition to the continuous part.[8] These are precisely the properties of the known functions $S_{yy}(0,\omega)$ and $S_{zz}(0,\omega)$ for the $s=\frac{1}{2}$ XY model, as inferred from (4) and (3).

In panels (c) and (d), the two subsequences Δ_{2k} and Δ_{2k-1} grow roughly linearly with k to infinity, but with different average slopes. The linear average growth of a Δ_k sequence implies that the associated dynamic structure factor has unbounded support and that the spectral weight tapers off by a Gaussian decay law, $\sim e^{-\omega^2}$, at high frequencies. If the Δ_{2k-1} grow more steeply than the Δ_{2k} as in (c), it can be concluded that the dynamic structure factor has a gap at $0<\omega<\Omega$. If that pattern is reversed asymptotically, as in (d) for $k>5$, it signals the presence of an additional $\delta(\omega)$ contribution in the dynamic structure factor. Our observations indicate that patterns (c) and (d) are generic for $S_{yy}(0,\omega)$ and $S_{zz}(0,\omega)$, $S_{xx}(0,\omega)$, respectively, of the spin-s XYZ model. The exception is the $s=\frac{1}{2}$ XY case, where patterns (a) and (b) obtain.

For fixed $q\neq 0$, the Δ_k sequences of all three functions $S_{\mu\mu}(q,\omega),\mu=x,y,z$ are the same in consequence of (3). For $q=0$, by contrast, the additional $\delta(\omega)$ contributions in $S_{xx}(0,\omega)$ and $S_{zz}(0,\omega)$ lead to a pattern reversal from (a) to (b) or from (c) to (d), with two characteristic properties: (i) it leaves the sum of successive pairs of coefficients, $\Delta_{2k-1}^{\mu\mu}(0)+\Delta_{2k}^{\mu\mu}(0)$, invariant; (ii) the factor by which the first coefficient changes determines the weight of the $\delta(\omega)$ contribution: $\Delta_1^{xx}(0)/\Delta_1^{yy}(0)=\cos^2\vartheta$, $\Delta_1^{zz}(0)/\Delta_1^{yy}(0)=\sin^2\vartheta$.

For the reconstruction of the dynamic structure factor $S_{yy}(0,\omega)$ from the known coefficients $\Delta_1^{yy}(0),\ldots,\Delta_K^{yy}(0)$, such as is shown for two distinct cases in panels (a) and (c) of Fig. 1, we proceed according to the well-tested method outlined previously.[7,8,10] At first, we select a model spectral density $\bar{\Phi}_0(\omega)$, which is compatible with the general structure of $S_{yy}(0,\omega)$ identified above. For case (a) we choose the function

$$\bar{\Phi}_0(\omega)=\frac{\pi}{\omega_{\max}-\omega_{\min}}\,\Theta(|\omega|-\omega_{\min})\Theta(\omega_{\max}-|\omega|), \quad (7)$$

which has bounded support and a gap, and for the case (c) the function

$$\bar{\Phi}_0(\omega)=\frac{2\sqrt{\pi}}{\omega_0}\,\Theta(|\omega|-\Omega)e^{-(|\omega|-\Omega)^2/\omega_0^2}, \quad (8)$$

which has unbounded support and a gap. Each function has two parameters, whose values are determined by matching the coefficients $\Delta_k^{yy}(0)$ of panels (a) and (c) with the continued-fraction coefficients of the corresponding model relaxation function,

$$\bar{c}_0(z)=\frac{1}{2\pi i}\int_{-\infty}^{+\infty}d\omega\frac{\bar{\Phi}_0(\omega)}{\omega-iz}. \quad (9)$$

Next, we expand the model relaxation function into a continued fraction down to level K and replace its continued-fraction coefficients by those from panels (a) and (c) for the two situations, respectively. That yields an approximation of (5), which is of high precision, as we shall see. The dynamic structure factor $S_{yy}(0,\omega)$ is then obtained via (6). The practical aspects of this procedure have been described in previous applications to different physical situations.[7,10]

In order to demonstrate the degree of accuracy of our method, we first reconstruct the function $S_{yy}(0,\omega)$ for the $s=\frac{1}{2}$ XY model with $\gamma=\frac{3}{4}$, from the $\Delta_k^{yy}(0)$ of panel (a) and compare it with the exact expression (4). The two results are plotted in the inset to Fig. 2. The coefficients $\Delta_k^{yy}(0)$ of panel (c) pertain to spin quantum number $s=1$. The reconstructed dynamic structure factor $S_{yy}(0,\omega)$ is shown in the main plot of Fig. 2. Note the different vertical and horizontal scales. Also shown are the results for $s=\frac{1}{2}$ (the same as in the inset) and for $s=\frac{3}{2}$. The latter has been reconstructed from 16 coefficients $\Delta_k^{yy}(0)$, which also exhibit pattern (c). The spectral line shown dashed represents the spin-wave result $S_{yy}(0,\omega)=2\pi\delta(\omega-4s\gamma)$, which is exact in the classical limit $s=\infty$. We conclude that quantum effects are very significant. They produce nontrivial line shapes and move the peak positions by as much as a factor of 2.1 relative to the spin-wave prediction. Nevertheless, convergence of the quantum results for increasing s toward the classical result is indicated.

Our results thus expose the limitations of spin-wave theory in quantum spin dynamics very clearly. No matter how favorable the circumstances for the application of a harmonic analysis or single-mode approximation are, the generic structure of the functions $S_{\mu\mu}(q,\omega)$ for quantum spin systems at $T=0$ deviates considerably from the results produced on that basis, especially for small spin quantum numbers: The spectral weight is distributed over bands of infinite width (unbounded support),[11] and is dominated by lines with nonzero intrinsic width at frequencies that differ significantly from the spin-wave dispersion. Since these quantum effects cannot be attributed to the strongly fluctuating nature of typical 1D phenomena, there is no reason to assume that they are less pronounced in 2D and 3D magnetic systems.

All the conclusions reached in this study for the spin-s XYZ ferromagnet ($J_\mu \geqslant 0$) can be translated into similar conclusions for the same model with antiferromagnetic coupling ($J_\mu \leqslant 0$). That model has a spin-flop ground state at a particular strength of the magnetic field. Therefore, the order parameter causes a pattern reversal at $q=\pi$ in $S_{xx}(q,\omega)$ and at $q=0$ in $S_{zz}(q,\omega)$.

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