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Dynamical central peak and spinon deconfinement in frustrated spin chains

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Studying the dynamical spin structure factor in frustrated spin chains with spontaneously dimerized ground state we show that besides the gapped spin-wave excitations there appears at finite temperatures also a sharp central peak. The latter can be attributed to deconfined spinons, accounted well within the variational approach. The central peak remains well pronounced within the local spin dynamics and may be relevant for experiments on materials with one-dimensional frustrated spin chains.

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Frustrated spin systems have been intensively investigated both theoretically and experimentally in the last decades,[1] offering novel phenomena and challenges as well as a broader view on strongly correlated electron systems. Among one-dimensional (1D) models the spin-1/2 antiferromagnetic (AFM) Heisenberg chain (nearest-neighbor interaction $J>0$) frustrated with the second-neighbor AFM interaction $J'>0$ (Ref. 2) has attracted wide attention also due to its relevance to the quasi-1D material $CuGeO_3$ exhibiting the spin-Peierls transition at $T_{SP}=14$ K. For particular parameters $J'/J=\alpha=0.5$ the exact ground state (g.s.) found by Majumdar and Ghosh (MG) (Ref. 3) is doubly degenerate and dimerized with a spin gap to excited states. Such a spin-liquid state without a long-range magnetic order has been shown to extend in a wider range around this point, i.e., in the regime $\alpha>\alpha_c\sim 0.241$.[4–6] Excited states at the MG point have been determined analytically[7,8] and can be represented to a good approximation as a pairs of $S=1/2$ solitons or spinons with a gapped dispersion, the concept confirmed by detailed numerical studies using the density-matrix renormalization-group (DMRG) method.[9]

The dynamical properties of the frustrated J-J' spin chain have been so far mostly studied via the dynamical spin structure factor $S(q,\omega)$ motivated again by the inelastic neutron-scattering (INS) results on $CuGeO_3$.[10] At $T=0$ the continuum of $S=1$ excitation in $S(q,\omega)$ in a wide range of α can be well represented with a pair of spinons,[9,11] in particular, if the phenomenologically introduced matrix elements are taken into account[12] in analogy to the basic $\alpha=0$ AFM Heisenberg model.[13] So far, there are very few theoretical results on finite-T properties of frustrated system. It has been shown that the upper boundary of spinon continuum in $S(q,\omega)$ persists even at $T>0$ (Ref. 14) while the maximum in the static structure factor $S(q)$ exhibit a shift to incommensurate $q<\pi$ at larger α and T.[15,16]

In the following we present evidence that $T>0$ dynamics of frustrated spin-chain model with the spontaneously dimerized g.s. exhibits several striking and rather unexpected features. Most evident, numerically calculated $S(q,\omega)$ reveals at low but finite $T>0$ a sharp central $\omega\sim 0$ peak well pronounced in the region $q\sim\pi$, coexisting with the gapped two-spinon continuum known already from $T=0$ studies.[9,11] The central peak has its manifestation in a unusual T dependence of static susceptibility $\chi_{q\sim\pi}(T)$ with a maximum at $T>0$. It shows up also in the local (q integrated) $S_L(\omega)$ as relevant, e.g., for the NMR spin-lattice relaxation. Using a variational presentation of excited two-spinon states and relevant matrix elements we show that the phenomenon can be directly traced back to spinons and their deconfined nature.

In the following we study the frustrated spin model on a 1D chain

$$H=J\sum_i [\mathbf{S}_i\cdot\mathbf{S}_{i+1}+\alpha\mathbf{S}_i\cdot\mathbf{S}_{i+2}], \tag{1}$$

where $\mathbf{S}_i$ are local $S=1/2$ operators and the only relevant parameter is $\alpha=J'/J$ (we choose further on $J=1$). The model has been invoked as the microscopic model for $CuGeO_3$ with $\alpha\sim 0.36$ (realized above $T<T_{SP}$ where lattice-deformation-induced dimerization is zero). But it as well represents the 1D zigzag spin system, examples are double-chain compound $SrCuO_2$ within the opposite limit of large $|\alpha|\sim 5-10$ (Ref. 17) and Li_2CuO_2 with ferromagnetic coupling $J<0$.[18]

As the central quantity we calculate dynamical $S(q,\omega)$ at $T>0$. We employ two numerical approaches. Finite-T Lanczos method (FTLM) (Ref. 19) based on the Lanczos diagonalization of small systems covers the whole T range but is restricted to system sizes $N\leq 28$ whereby we use periodic boundary conditions (b.c.). Finite-T dynamical extensions of the DMRG (FTD-DMRG) method recently developed by the present authors[20] combines the DMRG optimization of basis states with the FTLM method for dynamical correlations at $T>0$ and offers more powerful method for low T. The model, Eq. (1), is here studied with open b.c. The reachable system sizes depend on T and the method shows good convergence, at least for low ω, for systems $N<60$ for $T\leq 0.5$ presented here, with the typical subblock dimension $m\leq 256$. Concentrating on the low-ω dynamical window the method is used as presented in Ref. 20 while high-ω results are improved by the application of correction vectors increasing at the same time computation demand. The advantage of both methods is very good spectral resolution so that typically only a minor additional ω dependent broadening of $\delta\sim 0.02$ at $\omega\sim 0$ and $\delta\sim 0.06$ at higher ω is employed in presentations.

Let us first present results for the MG model with $\alpha=0.5$. While $S(q,\omega)$ at $T=0$ is rather well understood and investigated numerically,[11] we concentrate in Figs. 1 and 2 on $T>0$ FTD-DMRG results for different $T/J\leq 0.5$. The high-ω continuum appearing at $T=0$ above the two-spinon

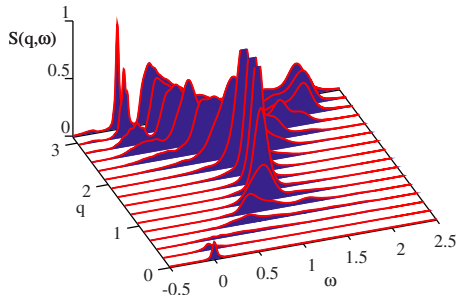

FIG. 1. (Color online) Dynamical spin structure factor $S(q,\omega)$ for the MG model at $T/J=0.1$ within the whole range of $q\leq\pi$, calculated by the FTD-DMRG method on a system of $N=60$ sites. Correction vector improvement of high ω part was preformed only for $q\geq 13\pi/15$.

gap $\Delta_0\sim 0.25J$ (Ref. 6) is qualitatively not changed from $T=0$ spectra. The evident new feature is the central peak at $\omega\sim 0$ most pronounced at $q\sim\pi$. Its width w is very narrow but still of intrinsic nature (being larger than the additional broadening $\delta=0.02$). It is evident that at fixed T the width w increases away from $q=\pi$ whereby the peak also looses the intensity. Still it remains well pronounced in wide region $q>0.7\pi$. The comparison of Figs. 1 and 2 also reveals that w increases as well with T and finally merges in a broader continuum for high T.

In the following we present the analysis showing that the emergence of the central peak in $S(q,\omega)$ at low $T<J$ can be described well in terms of spinons as relevant excitations of the system and their deconfinement. At the MG point $\alpha=0.5$ the g.s. (for even N and periodic b.c.) has the energy $E_0=-3NJ/8$ and the wave function which can be written as the product of local singlets $\Psi_0=[1,2][3,4]\cdots[N-1,N]$. It is doubly degenerate with the corresponding eigenstate $\tilde{\Psi}_0$ having for one site shifted singlets. It has been already realized[2,7,8] that lowest excitations can be well represented in terms of spinon states. In particular, the lowest branch of approximate triplet $(S=1,S^z=1)$ eigenstates can be constructed from the local triplet two-spinon states

$$\psi^t(p,m)=[1,2]\cdots[2p-3,2p-2]\uparrow_{2p-1}[2p,2p+1]\cdots [2m-2,2m-1]\uparrow_{2m}[2m+1,2m+2]\cdots, \qquad (2)$$

where the first spinon is on site $2p-1$ and the second on site $2m$. Since the total momentum Q is conserved due to periodic b.c., the relevant two-spinon functions are

$$\psi^t_Q(k)=\frac{1}{M}\sum_{p,m}^{M} e^{i(Q+k)p+i(Q-k)m}\psi^t(p,m), \qquad (3)$$

where sums run over $M=N/2$ double cells. In the further analysis difficulties arise since $\psi^t(p,m)$ are not orthogonal even for distant $|p-m|\gg 1$ and furthermore for $p\sim m$. To find proper eigenfunctions we follow the procedure and notation of Ref. 7 which for each momentum subspace Q yields nontrivial matrix elements

$$\langle\psi^t_Q(k')|\psi^t_Q(k)\rangle=\frac{9J^2}{64\omega_-\omega_+}\delta_{k,k'}+\frac{1}{M}\chi_Q(k,k'),$$

$$\langle\psi^t_Q(k')|\tilde{H}|\psi^t_Q(k)\rangle=\frac{9\epsilon_Q(k)J^2}{64\omega_-\omega_+}\delta_{k,k'}+\frac{1}{M}h_Q(k,k'), \qquad (4)$$

where $\tilde{H}=H-E_0$, $\omega_\pm=\omega((Q\pm k)/2)$, and $\omega(p)=(5/4+\cos 2p)J/2$ are (approximate) single-spinon energies and

$$\epsilon_Q(k)=\omega_+ +\omega_-=\left(\frac{5}{4}+\cos Q\cos k\right)J. \qquad (5)$$

The off-diagonal terms $\chi_Q(k,k'),h_Q(k,k')$ (not presented here) emerging from nonorthogonality of $\psi^t_Q(k)$ are the same as given in Ref. 7. Within the triplet two-spinon basis, Eqs. (2) and (3), proper eigenstates [nevertheless not yet exact eigenstates of Eq. (1)] are obtained via the diagonalization of Eq. (4) and can be denoted $\Psi^t_Q(k)$ (whereby k remains only a label and not a well-defined wave vector). In contrast to $\psi^t_Q(k)$, $\Psi^t_Q(k)$ are orthonormalized. The corresponding two-spinon excitation energies $e^t_Q(k)$ are well approximated as the sum of two (deconfined) free spinons, i.e., $e^t_Q(k)\sim\epsilon_Q(k)$, Eq. (5).

Our goal is, however, to understand low-T properties of $S(q,\omega)$. Before discussing $T>0$ results, we first have to reconsider the $T=0$ spectrum $S_0(q,\omega)$ which has been already interpreted in terms of two-spinon excitations.[9,11,21] Still the corresponding matrix element has been postulated so far only phenomenologically[12,22] in analogy with previous works on the unfrustrated Heisenberg model.[13] We note that at $T=0$ within the chosen subspace, Eq. (2), we can express

$$S_0(q,\omega)=\frac{1}{2}\sum_k |\langle\Psi^t_q(k)|S^+_q|\Psi_0\rangle|^2\delta[\omega-e_q(k)] \qquad (6)$$

and

$$S^+_q|\Psi_0\rangle=\frac{1-e^{-iq}}{2M}\sum_k \psi^t_q(k). \qquad (7)$$

Since Eq. (7) is an exact representation of the S^+_q operator, we can evaluate matrix elements $\zeta_q(k)=\langle\Psi^t_q(k)|S^+_q|\Psi_0\rangle$ by diagonalizing numerically equations, Eq. (4). Taking into account that $e^t_q(k)\sim\epsilon_q(k)$ we can then evaluate $S_0(q,\omega)$ in the two-spinon approximation. Results within such a framework are presented for $q=\pi$ in Fig. 3 along with the full numerical results obtained via the $T=0$ FTD-DMRG (for $T=0$ identical

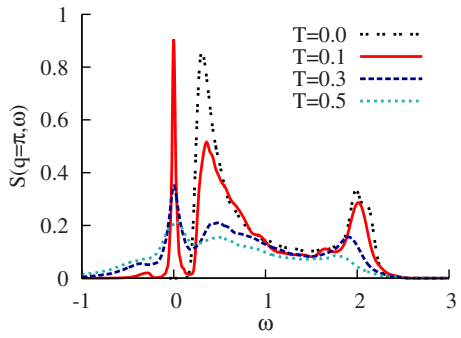

FIG. 2. (Color online) $S(q=\pi,\omega)$ for different $T/J=0.0$, 0.1, 0.3, and 0.5 where the broadening of central peak with increasing T is well pronounced.

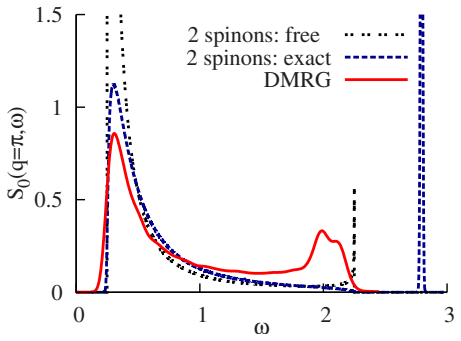

FIG. 3. (Color online) $T=0$ dynamical spin structure factor $S_0(q=\pi,\omega)$ as calculated via the DMRG for $N=100$ sites (full line), numerically within the two-spinon approximation (dashed line) and using simplified $\tilde{\zeta}_q(k)$ (dotted line).

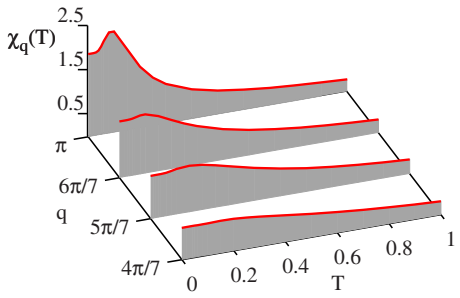

FIG. 4. (Color online) Static susceptibility $\chi_q(T)$ vs T for different $q \leq \pi$ for $\alpha=0.5$ as obtained with the FTLM.

to the more standard dynamical DMRG) evaluated within a system of $N=100$ sites. The agreement is very satisfactory except at the higher ω end where the obtained intensity is too low as well as Eq. (4) seem to generate a high two-spinon antibound state [peak in $S_0(\pi,\omega)$] besides the free two-spinon dispersion, Eq. (5). It should be noted that obtained $\zeta_q(k)$ is quite far from the oversimplified spinon picture with $\zeta_q(k)\sim 1$.[22] Still it is hard to find for it an appropriate analytical expression.[7,22] One possibility is to neglect nonorthogonalities in Eq. (4) which yields $\tilde{\zeta}_q(k) \propto 1/(\omega_+\omega_-)^{1/2}$. Corresponding "free" spinons results for $S_0(q=\pi,\omega)$ also presented in Fig. 3 show qualitatively reasonable trend (falloff for higher ω). Still they give an incorrect behavior at lower and higher cutoff due to divergent two-spinon density of states.

The above agreement of numerical $T=0$ results with the description in terms of the two-spinon basis, Eq. (2), gives firm support also to the interpretation of $T>0$ dynamics. In the low-T regime we are in $S(q,\omega)$ predominantly dealing with excitations increasing the number of spinons, $n_s \to n_s+2$, analogous to those in $S_0(q,\omega)$, Eqs. (6) and (7). Their contribution analogous to $T=0$ in Fig. 3 is evident also at $T>0$ in Figs. 1 and 2.

However, in addition there are possible transitions between excited states conserving n_s. In particular, the matrix element $\gamma_{qQ}(k,k')=\langle \Psi^t_{q+Q}(k)|S^+_q|\Psi^s_Q(k')\rangle$ as introduced already in Ref. 22 is finite and nontrivial. Here $\Psi^s_Q(k')$ are singlet two-spinon eigenstates. We evaluate $\gamma_{qQ}(k,k')$ numerically assuming two-spinon approximation, Eq. (4). Results show that elements are nearly diagonal, i.e., $\gamma_{qQ}(k,k')\sim \delta_{k',k+Q}$ leading in $S(q,\omega)$ to the contribution at $\omega \sim e^t_{q+Q}(k+q)-e^s_Q(k)$. Since at low T favored are lowest excited states, i.e., from Eq. (5) $Q\sim 0$, $k\sim\pi$ and $Q\sim\pi$, $k\sim 0$ with a Boltzmann weight $p\propto \exp(-\Delta_0/T)$ [where $\Delta_0 \sim \epsilon_\pi(0)=J/4$]. Numerical solution of two-spinon problem shows that $e^s_Q(k)\sim e^t_Q(k)\sim \epsilon_Q(k)$ consistent with the picture of unbound (deconfined) spinons. Hence, the strongest transitions are at $\omega \sim \epsilon_{q+Q}(k+q)-\epsilon_Q(k)$. This evidently leads at $q\sim\pi$ to a sharp central peak at $\omega\sim 0$ with the strength increasing as $\propto \exp(-\Delta_0/T)$.

From above perspective we therefore conclude that the pronounced central peak in Figs. 1 and 2 at $q\sim\pi$ confirm the presented analysis of nearly free or deconfined spinons as excited states at the MG point. On the other hand, even without the extensive calculations it is evident that the central peak can only appear if triplet and singlet spinon states are nearly degenerate again only possible for deconfined spinons.

The emergence of the central peak is, however, not restricted to the MG point $\alpha=0.5$ but appears to be related closely to the existence of the spontaneous dimerization at $\alpha>\alpha_c$ and the spin gap $\Delta_0>0$. We tested numerically also the case $\alpha=0.7$ (only partly presented here) where the spin gap is larger $\Delta_0\sim 0.4J$.[6] Consequently also the central peak feature is even more pronounced and extended in the q space as well as persists to higher T.

It is evident that the central peak has a substantial effect on the static susceptibility $\chi_q(T)$,

$$\chi_q(T) = \int_{-\infty}^{\infty} \frac{d\omega}{\omega}[1-e^{-\omega/T}]S(q,\omega), \tag{8}$$

being sensitive to low-ω dynamics. In Fig. 4 we show the FTLM results obtained on systems with $N=28$ sites for $\chi_q(T)$ with various q and again $\alpha=0.5$. Most pronounced is the variation at $q=\pi$ where the g.s. value $\chi_\pi(0)$ is determined with the dimerization gap, i.e., $\chi_\pi(0)\propto 1/\Delta_0$. Instead of naively expected monotonously decreasing $\chi_q(T)$, we observe in Fig. 4 simultaneously with the emergence of the central peak an increasing $\chi_\pi(T)$ in the regime $0<T<T^*$ whereby $T^*\sim\Delta_0/2$. On the other hand, for $T>T^*$ the falloff is uniform with $\chi_\pi(T)\propto 1/T$ which is close to the characteristic critical $q=\pi$ behavior for the simple AFM Heisenberg model.[20] Results for $q<\pi$ are quite analogous taking into account that the relevant spin gap is $\Delta_q>\Delta_0$.

The effect of the central peak is visible also in local spin correlations $S_L(\omega)=(1/N)\Sigma_q S(q,\omega)$ as presented in Fig. 5. They are accessible directly via FTD-DMFT by calculating local spin correlations $\langle S^z_i, S^z_i\rangle_\omega$ locating the site $i\sim N/2$ to avoid effects of open b.c. As well we can evaluate them within the FTLM and periodic b.c. summing all $S(q\neq 0,\omega)$ ($q=0$ contribution is delta function due to the conserved S^z_{tot}). Clearly, in both approaches the diffusion contribution $q\sim 0$ is not represented correctly but it is expected to be subdominant.[23] FTD-DMRG results in Fig. 5 presented for $\alpha=0.5,0.7$ reveal a central peak at $\omega\sim 0$ well separated from the higher ω two-spinon continuum as far as $T\lesssim\Delta_0$. The

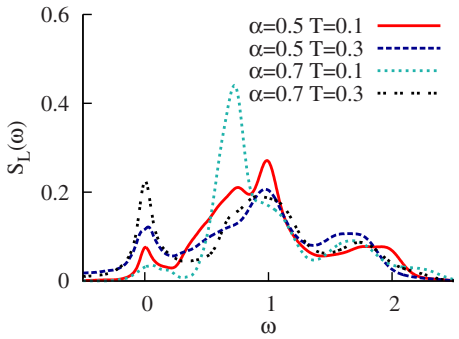

FIG. 5. (Color online) Local spin correlations $S_L(\omega)$ for $\alpha=0.5$ and 0.7 at $T=0.1$ and 0.3 as obtained with the FTD-DMRG method.

peak gains the weight at $T\sim T^*$ and for $T>T^*$ steadily becomes broader, finally merging with the continuum for $T>\Delta_0$. Moreover we observe for both α that $S_L(\omega=0)$ is nearly constant in a broad range $T^*<T<2J$.

It should be noted that within the simplest approximation (with q-independent form factor) the NMR or nuclear quadrupole resonance spin-lattice relaxation should be a closely related to $S_L(\omega)$, i.e., the relaxation rate is given by $1/T_1\propto S_L(\omega=0)$. Following above results we would obtain for considered systems $1/T_1\sim$const in a broad range $T>T^*$ similar to theoretical predictions for the 1D (unfrustrated) AFM Heisenberg model and $CuGeO_3$.[23] While the agreement for higher $T>\Delta_0$ with the Heisenberg model is not surprising the novel contribution of the central peak is that the validity of this universality is extended to lower $T>T^*$. It should be also reminded that such relaxation is far from the usual Korringa relaxation with $1/(TT_1)\sim$const.

In conclusion, we have shown that the frustrated spin chain as manifested within the 1D J-J' model with $\alpha>\alpha_c$ reveals besides the gap in spin excitations at $T=0$ also very unusual spin dynamics at finite but low $T<\Delta_0$. The central peak which appears in $S(q,\omega)$ at $q\sim\pi$ as well in the q-integrated local $S_L(\omega)$ is very sharp and dominates the low-ω response at low T. It is a direct consequence and the signature of spinons as the elementary excitations in such systems. It remains to be investigated whether such a behavior is restricted to the particular case of investigated model or there are other gapped spin systems with similar phenomena. As far as experimental relevance is concerned extensively investigated $CuGeO_3$ above the spin-Peierls transition $T>T_{SP}$ is interpreted with a frustrated spin-chain model with $\alpha\sim0.36$. Although theoretically estimated scale frustration-induced gap for this case is quite small, i.e., $\Delta_0\sim0.01J$ (Ref. 9) the actual scale and its relevance could be verified by more detailed INS experiments. On the other hand, many recently found and emerging materials[18] with, e.g., zigzag spin geometry modeled with frustrated spin-chain models with a variety of $\alpha=J_2/J_1$ offer also possibility to approach the regime $\alpha\sim0.5$ where above phenomena should be more pronounced.

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