Fractional and Integer Excitations in Quantum Antiferromagnetic Spin 1/2 Ladders

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Spectral densities are computed in unprecedented detail for quantum antiferromagnetic spin 1/2 two-leg ladders. These results were obtained due to a major methodical advance achieved by optimally chosen unitary transformations. The approach is based on dressed integer excitations. Considerable weight is found at high energies in the two-particle sector. Precursors of fractional spinon physics occur supporting the conclusion that there is no necessity to resort to fractional excitations in order to describe features at higher energies.

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Low-dimensional quantum antiferromagnets are of fundamental and enduring interest. One reason is that high-temperature superconductivity depends crucially on the interplay of charge carriers with the magnetic excitations of a two-dimensional (2D) quantum antiferromagnet. A vivid debate concerns the nature of the elementary excitations of such an antiferromagnet. In terms of integer spin waves ($S = 1$), no quantitative description is available of the spectral densities at higher energies, where a significant part of the spectral weight is located [1,2]. Therefore, it has been suggested that fractional ($S = 1/2$ spinons) excitations play an important role in 2D [3] supporting the view that spinons and spin-charge separation are the basis of high-T_c superconductivity [4,5]. Spin ladders are similar to 2D planes in the range of higher energies. The importance of fractional excitations for the description of high energy excitations in 2D would hence imply their importance in spin ladders. Here we present a description of the spectral densities in unprecedented detail in terms of *integer* excitations. Our results show that the essential point is not the fractionality of the elementary excitations ("particles") but the proper description of multiparticle excitations.

Spectral densities provide information on the density of elementary excitations, on their interaction, and on how the particular excitation operator couples to them. For instance, the dynamic structure factor as measured by inelastic neutron scattering couples to excitations with total spin $S = 1$. Integer spin excitations induce a dominant so-called quasiparticle peak in the dynamic structure factor [6]. If the integer $S = 1$ excitation decays into two fractional $S = 1/2$ spinons, which move independently at large distances, the quasiparticle peak vanishes and an important continuum appears at higher energies. The generic example is found in spin chains for which spinons are the elementary excitations [7].

We address two-leg spin ladders, i.e., two chains with intrachain coupling $J_\parallel$ coupled by an exchange coupling $J_\perp$,

$$H = \sum_i [J_\parallel(\mathbf{S}_{1,i}\mathbf{S}_{1,i+1} + \mathbf{S}_{2,i}\mathbf{S}_{2,i+1}) + J_\perp \mathbf{S}_{1,i}\mathbf{S}_{2,i}], \quad (1)$$

where i denotes the rung and 1, 2 the leg. As far as the excitations at higher energies are concerned, spin ladders constitute an intermediate system between 1D chains and 2D square lattices. Additionally, they occur in a multitude of substances [8] comprising also superconducting systems [9].

What is the most effective way to describe the excitations? Two approaches are possible: (i) If the rung coupling $J_\perp$ dominates in (1), i.e., $H_0 := H|_{J_\parallel=0}$, the excitations are local triplets on each rung (rung triplets). When $J_\parallel$ is switched on they start to hop from rung to rung. On increasing $J_\parallel$ the excitations become more and more extended; they are rung triplets dressed by a magnetically polarized environment. (ii) If the rung coupling $J_\perp$ is weak, it can be treated as perturbation which acts on the elementary spinons in both chains. The rung coupling binds two spinons on either chain thereby binding two fractional $S = 1/2$ spinons to an integer $S = 1$ triplet. The size of this bound object tends to infinity for $J_\perp \to 0$.

For the value $J_\perp = J_\parallel$ needed to compare with the square lattice it is *a priori* unclear which picture is superior. Note that we are *not* aiming at the question which are the elementary excitations in the strict sense of the word since this question concerns only the lowest energies. But we ask which excitations describe the physics at all energies best. We show that approach (i) in terms of integral dressed excitations works excellently. It provides for the first time a quantitative description of the spectral densities on all energy scales.

Also previous investigations in gapped 1D systems were concerned with the nature of the excitations. For instance, Sushkov and Kotov compared quantum antiferromagnetism to quantum chromodynamics in the sense that the $S = 1/2$ spins correspond to quarks and integer triplets to (vector) mesons [10]. Zheng *et al.* described the deconfinement of fractional spinons in dimerized, gapped spin chains on decreasing dimerization in terms of integer triplet excitations [11].

We construct a mapping by a continuous unitary transformation (CUT) [12] of the Hamiltonian in (1) to an effective H_{eff} conserving the number of rung triplets:

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$[H_0, H_{\rm eff}] = 0$. The ground state of $H_{\rm eff}$ is the rung triplet vacuum [13]. In this way a tremendously complicated many-body problem is reduced to a tractable few-body problem. The mapping needs an auxiliary variable ℓ running between 0 and ∞. The Hamiltonian $H(\ell)$ is transformed from $\ell = 0$ $[H(0) = H]$ to $\ell = \infty$ $[H(\infty) = H_{\rm eff}]$ by

$$dH/d\ell = [\eta(\ell), H(\ell)], \tag{2}$$

$$\eta_{i,j}(\ell) = {\rm sgn}(Q_{i,i} - Q_{j,j})H_{i,j}(\ell), \tag{3}$$

where η defines the mapping. The matrix elements $\eta_{i,j}$ and $H_{i,j}$ are given in an eigenbasis of the number of rung triplets $Q = H_0$. Equations (2) and (3) constitute a general, versatile prescription for any many-body problem to obtain an effective model in terms of elementary excitations, the number of which is counted by Q. The choice (3) eliminates all parts of H changing the number of triplets while retaining a certain simplicity in $H(\ell)$ for intermediate values of ℓ [13,14], namely, that the number of rung triplets is changed at most by ± 2. For details on the form of $H_{\rm eff}$ the reader is referred to Ref. [13]. To determine response functions the physical observable under study must be subject to the same unitary transformation (2) as the Hamiltonian. Hence the CUTs are based on a very clear-cut concept. Indeed, this concept rendered the computation of bound states in higher order possible [15,16]. Conventional cluster techniques [17] allow equally to determine the energies of bound states very accurately if they are supplemented by similarity transformations substituting the unitary transformation [18,19]. A diagrammatic approach with hard-core bosons [10,20] describes the excitations equally in terms of triplets with qualitatively similar results deviating, however, quantitatively for $x \gtrapprox 0.5$.

We were able to keep terms in $H(\ell)$ up to order 14 in $x := J_\parallel/J_\perp$ for the kinetic energy (triplet hopping) and up to order 13 for the triplet-triplet interaction. Observables were transformed up to order 10 allowing for the first time to determine true multiparticle *continua,* i.e., spectral densities, not only spectral weights, from a nonsimulation approach. Our perturbative approach is supplemented by standard extrapolations and optimizations of the resulting series. It turned out that it is possible to determine the spectral densities within about 5% accuracy for $x \approx 1$. For lower values of x, the accuracy improves rapidly so that the results at $x \lessapprox 0.6$ can be considered exact. The results are not plagued by any finite size nor by any finite resolution effects thereby providing for the first time predictions in great detail.

For experimental relevance [21] and for comparison to the square lattice we present results for $J_\parallel = J_\perp$. For orientation Fig. 1 depicts the dispersion of the gapped elementary triplets [22–24], the resulting lower and upper edge of the 2-triplet continuum, and the bound states in the $S = 0$ and the $S = 1$ channel [10,18,19,21,25,26]. The spectral densities $I(\omega)$ are computed for the resolvent

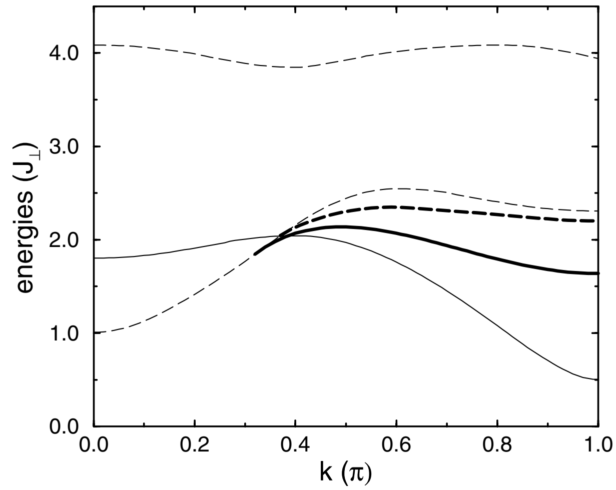

FIG. 1. Dispersions at $J_\parallel = J_\perp$. Elementary triplet (thin solid line), lower and upper 2-triplet continuum edge (thin dashed line), bound 2-triplet states with $S = 0$ (thick solid line), and $S = 1$ (thick dashed line).

$$I(\omega) = -\pi^{-1}\Im\langle 0|R(\omega + E_0 - H)^{-1}R|0\rangle_{\rm retarded} \tag{4}$$

for various operators R connecting the ground state to excited states of different spin and parity. Odd (even) parity with respect to reflection about the centerline of the ladder implies an odd (even) number of rung triplets. In Fig. 2 the distribution of spectral weight among the sectors of a different number of rung triplets is depicted. For local (i.e., k-integrated) excitations the relative intensities $I_n^{\rm r} = I_n/I_{\rm tot}$ are plotted where the intensity I_n stands for the ω-integrated spectral densities $I(\omega)$ in the sector of n rung triplets. Recall that by our transformation the number of rung triplets has become a good quantum number. The total intensities $I_{\rm tot} = \int_{0+}^{\infty} I(\omega)\, d\omega = \sum_{n=1}^{\infty} I_n$ are accessible through the sum rule $I_{\rm tot} = \langle 0|R^2|0\rangle - \langle 0|R|0\rangle^2$.

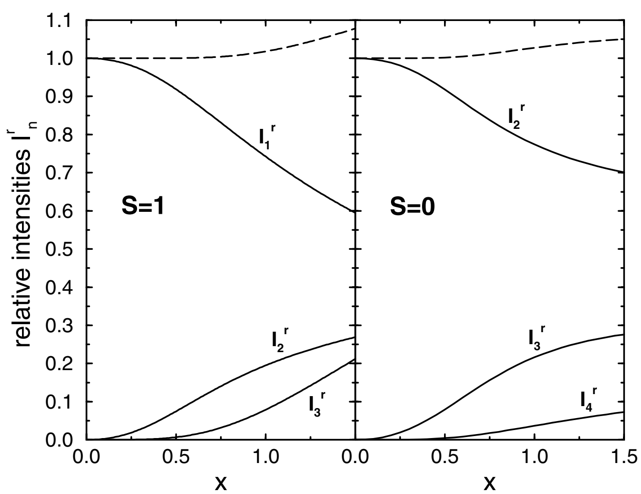

FIG. 2. Relative intensities $I_n^{\rm r}$ of subsectors of a different number n of triplets and their sum (dashed line) for local excitations R_i as a function of $x = J_\parallel/J_\perp$. Left panel $S = 1$: $R_i = \mathbf{S}_{1,i}^z$; right panel $S = 0$: $R_i = \mathbf{S}_{1,i}\mathbf{S}_{1,i+1}$.

For $x = 0$, the excitation of a local rung triplet exhausts the entire spectral weight for $S = 1$, i.e., $I_1^r(x = 0) = 1$. On increasing x the triplet becomes dressed and the quasiparticle weight decreases. The sum of all relative intensities must be unity. Up to $x \approx 1$ our result (dashed lines) deviates from the sum rule less than 3% giving evidence for the reliability of the extrapolations. For larger x the weight is overestimated increasingly. For $x = 1$ the I_1 and I_2 contributions exhaust $74\% + 19\% = 93\%$ for $S = 1$ and 77% for $S = 0$ of the total weight. The neglect of contributions from more triplets is hence well justified. A description in terms of 1, 2, or 3 integer excitations works perfectly without need to resort to spinons.

In Figs. 3 and 4 the k-resolved spectra are shown for $n = 1$ (Fig. 3a) and $n = 2$ (other panels). In both spin channels the 2-triplet spectral densities display important and fine-structured continua bounded by square-root edges. Generally the interaction shifts weight down to lower energies. For momenta not too far away from π, bound states (grey lines in Figs. 3b and 4) leave the continua. These bound states carry a large fraction of the 2-triplet weight. The differences between Figs. 4a and 4b result from the different parity of the two excitation operators at $k = \pi$

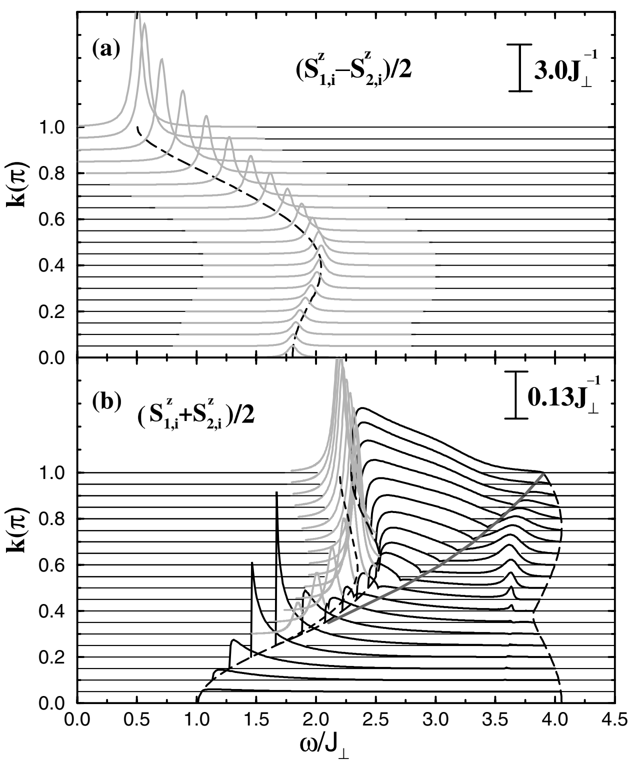

FIG. 3. k-resolved spectral densities for operators indicated ($S = 1$); δ-peaks (grey lines) broadened for visualization by $J_\perp/20$ and inserted in front of the unbroadened continua. The bound state energies and the continuum edges are also shown (dashed lines). (a) 1-triplet peak; (b) 2-triplet continuum (multiplied by 4 to show details) and bound state. The dark grey line is a guide to the eye linking the midband square-root singularities.

with respect to reflection about the rung direction; see also Ref. [21].

A very intriguing feature is the line of square-root singularities seen within the continuum in Figs. 3b (dark grey line) and 4b. It increases from $k \approx \pi/3$ to $k = \pi$ being particularly clearly visible above $k = \pi/2$. Below this line the larger part of the spectral weight is found. The momentum dependence of these midband square-root singularities is strongly reminiscent of the upper edge of the 2-spinon continuum in single chains [7], to which it will evolve for $J_\perp \to 0$. The striking fact that a 2-triplet description is capable to yield 2-spinon features leads us to the conjecture that the important point is *not* the fractionality of the excitations *but* the correct description of multiparticle excitations. Support for our conjecture is provided by the computation of bound states of two spinons [27,28] in terms of two triplets [11,25] in dimerized spin chains.

In Fig. 4 for small values of k a second upper peak occurs which is due to density-of-states effects resulting from the shallow dip that the 1-triplet dispersion (thin solid line in Fig. 1) displays at $k = 0$. This local minimum in the dispersion induces a Van Hove singularity which is smeared out by the interaction to the additional peak. It appears that the two parts of the dispersion from $k = 0$ to $k \approx 0.4\pi$ and from $k = \pi$ to $k \approx \pi/2$ act as rather independent bands. With the help of this picture, the rather sharp resonance at about $k = \pi/2$ in Fig. 4 is interpreted as a bound state of the part of the dispersion

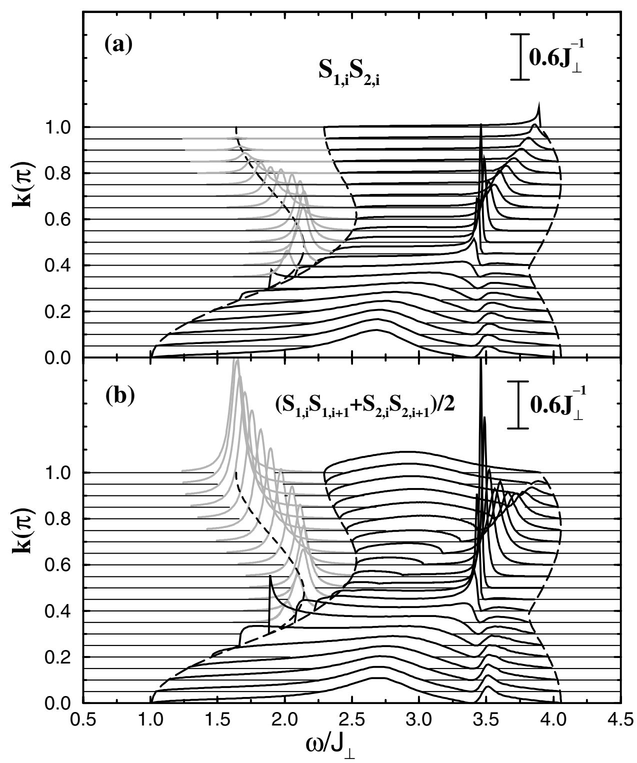

FIG. 4. Same as in Fig. 3 for $S = 0$; (a),(b) 2-triplet continuum and bound state. In (b) continuum multiplied by 4 to show details.

for $|k| \in [0, 0.4\pi]$. It is not an absolutely stable state, i.e., not a δ peak of zero width, because it may still decay into states with $|k| \in [0.4\pi, \pi]$. To be more specific, the dispersion for small values of k can be described approximately by $\omega(k) \approx J_\perp[1.9 - 0.1\cos(k/0.4)]$ (see Fig. 1) so that the two-particle kinetic energy $\Omega(k, q)$ at total momentum k and relative momentum q given by $\Omega(k, q) = \omega(k/2 + q) + \omega(k/2 - q)$ becomes dispersionless for $k = 0.4\pi$: $\Omega(0.4\pi, q) \approx 3.8J_\perp$ for values of $k/2 \pm q$ in the range of the shallow dip. This implies that the relative kinetic energy is negligible and interaction effects dominate. Indeed, Fig. 4 shows that the resonance is shifted by an attractive interaction from $3.8J_\perp$ to $\approx 3.5J_\perp$.

Our results predict many features in experiment. By inelastic neutron scattering the 2-triplet $S = 1$ response (Fig. 3b) is detectable if the momentum along the rungs can be tuned to zero so that only the symmetric combination $(S^z_{1,i} + S^z_{2,i})/2$ leads to excitations. Then the 2-triplet response (Fig. 3b) is separated clearly from the stronger 1-triplet response (Fig. 3a). To gain further insight in the 2-triplet interaction in the $S = 1$ channel we strongly suggest such experiments.

Optical spectroscopy in terms of bimagnon-plus-phonon absorption detects a weighted superposition of the curves in Fig. 4 providing the first experimental verification of the existence of the bound state in the $S = 0$ sector [21]. Raman spectroscopy measures in leading order [29] the curves at $k = 0$ in Fig. 4 [30]. The theoretical results agree very well with experiment [31] though some deviations remain. These are most probably due to the general presence of non-negligible cyclic exchange terms in the cuprates [21,32–36].

Our findings on the distribution of spectral weight show that large weight at high energies does not imply the necessity to resort to fractional excitations contrary to a frequently used line of argument; see, e.g., Ref. [3]. Integer excitations allow one to describe spectral densities of spin ladders in great detail on all energy scales. It turns out to be essential to describe multiparticle excitations adequately. We find also that this task is tractable since the sectors of low particle number dominate clearly.

We expect that a similar approach with integer excitations will also allow one to describe undoped 2D cuprates quantitatively. Continuous unitary transformations proved to be a very powerful concept to deal with dressed excitations. The above findings call for a renewed discussion of the importance of fractional excitations in low-dimensional strongly correlated electron systems such as doped and undoped high-T_c superconductors.

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