Excitations in One-Dimensional $S = \frac{1}{2}$ Quantum Antiferromagnets

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The transition from dimerized to uniform phases is studied in terms of spectral weights for spin chains using continuous unitary transformations. The spectral weights in the $S = 1$ channel are computed perturbatively around the limit of strong dimerization. We find that the spectral weight is concentrated mainly in the subspaces with a small number of elementary triplets (triplons), even for vanishing dimerization. So, besides spinons, triplons may be used as elementary excitations in spin chains. We conclude that there is no necessity to use fractional excitations in low-dimensional, undoped, or doped quantum antiferromagnets.

The determination of elementary excitations is a fundamental issue in condensed matter physics. Especially in the context of high-temperature superconductivity, the role of magnetic excitations in two-dimensional quantum antiferromagnets is strongly debated [1–5]. The bottom line of the debate is whether or not it is possible and/or necessary to consider fractional excitations, so-called spinons with $S = 1/2$, or whether integer excitations, magnons, or elementary triplets, triplons [6], with $S = 1$, can equally be used. Here we provide clear indication that, even in one-dimensional spin chains where spinons are a valid description, an alternative description by triplons is possible. Hence, the necessity to resort to fractional excitations is quite generally questioned.

The spinon concept comes from 1D spin chains ($\delta = 0$)

$$H' = J_0 \sum_i [1 + \delta(-1)^i]\mathbf{S}_i\mathbf{S}_{i+1}, \tag{1}$$

where spinons with $S = 1/2$ are established as the elementary excitations [7,8]. For any finite dimerization $\delta \neq 0$, however, the spin chain can be described by massive triplets with $S = 1$. They can be viewed as bound states of two spinons [9–12] which are, however, not free due to their confining interaction. Starting from strong dimerization, where a description with triplons is certainly appropriate, the question arises as to what happens to the triplons for vanishing dimerization. Besides its academic interest, this question is of great practical importance since in recent years triplon-based techniques have been advanced considerably [13–19]. Our recent progress has rendered even the computation of spectral *densities* possible [13,19–22].

In this work, we investigate to what extent a triplon-based description is possible by computing spectral weights of multi-triplon contributions for dimerized spin chains. Two scenarios are conceivable for $\delta \to 0$: (i) The spectral weight is distributed rather evenly over the multi-triplon channels implying that the weight of a particular channel is small and that a large number of channels must be taken into account; see discussion in Ref. [12]. This scenario would make an approach in terms

of triplons difficult to use, hence inappropriate. (ii) The spectral weight is found mainly in the channels with a *small* number of triplons, implying that a triplon approach is very useful and appropriate because spectral properties can be computed from the dynamics of a small number of excitations in a small number of channels.

Scenario (i).—Let us look at a field theoretic description for indications for this scenario. Using Abelian bosonization [10,23–25] the low-lying states of an anisotropic spin chain are described by the Hamiltonian

$$H_{\text{FT}} = \frac{v}{2\pi} \int_{-\infty}^{\infty} [K(\pi\Pi(x))^2 + K^{-1}(\partial_x\Phi(x))^2]dx, \tag{2}$$

where $v \propto J_0$ is the spin-wave velocity and K is the interaction parameter, e.g., $K = 1$ for the XY model, equivalent to free fermions, and $K = 1/2$ for the isotropic case. A local operator is

$$S_j^z = (2\pi)^{-1}\partial_x\Phi(j) + A(-1)^j \cos[2\Phi(j)], \tag{3}$$

where the lattice constant is unity, and A is a nonuniversal constant. The undimerized Hamiltonian (1) corresponds essentially to free bosons (2). A finite dimerization is accounted for by an additional term proportional to $\delta \int_{-\infty}^{\infty} \cos[2\Phi(x)]dx$ leading to a sine-Gordon model. For $K < 2$ the system is massive with a gap $\Delta \propto \delta^{1/(2-K)}$ ($= \delta^{2/3}$ for the isotropic chain).

A single bosonic mode of (2) is created by

$$b_k^\dagger = 1/\sqrt{2}[\tilde{\Phi}(k)/N_k - iN_k\tilde{\Pi}(k)], \tag{4}$$

where $N_k = \sqrt{\pi K/|k|}$. The quantities with tilde are the Fourier transforms of the real-space fields. We expand the excited state $S_j^z|0\rangle$ in states of various numbers of bosons with focus on the vicinity of momentum π where most of the weight in the dynamic structure factor is found: $S_j^z \propto \cos[2\Phi(j)]$. The coefficients of one- and two-boson states are

$$c_k = \langle 0|b_k \cos(2\Phi)|0\rangle = \langle 0|[b_k, \cos(2\Phi)]|0\rangle, \tag{5a}$$

$$c_{k,q} = \langle 0|b_k b_q \cos(2\Phi)|0\rangle = \langle 0|[b_k[b_q, \cos(2\Phi)]]|0\rangle. \tag{5b}$$

We make use of

$$[b_k, 2\Phi(j)] = \sqrt{K/|k|}\sqrt{2\pi/L}\exp(ikj), \qquad (6)$$

where the momenta are discretized by a finite system size L to ensure normalizability. This yields $c_k = 0$ and

$$c_{k,q} \propto \frac{K}{\sqrt{|k||q|}}\frac{2\pi}{L}\exp[i(k+q)j]\Delta^K, \qquad (7)$$

where $\langle\sin(2\Phi)\rangle = 0$ and $\langle\cos(2\Phi)\rangle \propto \Delta^K$ are used. So the total weight W_1^z in the one-boson channel is always zero. The total weight W_2^z in the two-boson channel is

$$W_2^z \propto \sum_{k,q}|c_{k,q}|^2 \propto \Delta^{2K}\int_{v|k|,v|q|>\Delta}\frac{K^2}{|k||q|}dkdq$$
$$\propto \Delta^{2K}\ln(\Delta)^2 \propto \delta^{2K/(2-K)}\ln(\delta)^2 \qquad (8)$$

in leading order in $\ln(\delta)$. Generally, all channels with an odd number of bosons carry no weight (at momentum π), whereas channels with $2n$ bosons have

$$W_{2n}^z \propto \delta^{2K/(2-K)}\ln(\delta)^{2n}, \qquad (9)$$

whence we conclude that *any* single channel becomes *irrelevant* on $\delta \to 0$. Only the consideration of an infinite number allows one to treat vanishing dimerization correctly. This appears to be sound evidence for scenario (i).

Scenario (ii).—Our main argument is an explicit calculation of spectral weights for the first triplon channels. First, however, we challenge the *general* validity of the previous argument by four basic considerations.

(a) Considering free fermions ($K = 1$) we know that the operator $S_j^z = n_j - 1/2$ excites a particle-hole continuum at all wave vectors. So the dynamic correlations of this operator are exhaustively described by *two* elementary excitations, a particle and a hole, independent of the dimerization δ.

(b) Considering the isotropic spin chain ($K = 1/2$) it was shown that 72.89% of the total weight (sum over all wave vectors) of the dynamic structure factor is described by the *two*-spinon continuum [26].

(c) It is undisputed that the dimerized isotropic spin chain displays a *single*-mode peak with finite spectral weight at all wave vectors as long as $\delta \neq 0$ [11,12].

(d) By construction, the bosonic modes of the field theory (4) exist at *small* momenta $k \approx 0$ [23,25,27]. The dynamics at momenta close to π are captured by the superposition of an infinite number of these modes as becomes evident from Eqs. (3) and (9).

The above arguments prove that there can be several, rather different looking descriptions for the *same* physics. One may *not* conclude from the validity of a particular description, e.g., in terms of a multitude of modes, that another description, e.g., in terms of only a few modes, is not valid.

Bearing these considerations in mind, we turn to a continuous unitary transformation (CUT) of the

Hamiltonian (1) onto an effective Hamiltonian in terms of triplons. To proceed perturbatively we transform (1) into

$$H = H'/J = \sum_i[\mathbf{S}_{2i}\mathbf{S}_{2i+1} + \lambda\mathbf{S}_{2i}\mathbf{S}_{2i-1}], \qquad (10)$$

where $J = J_0(1 + \delta)$ and $\lambda = (1 - \delta)/(1 + \delta)$. We expand about isolated dimers at $\lambda = 0$. A CUT is used to map the Hamiltonian H to an effective Hamiltonian H_{eff} which conserves the number of triplets on the strong bonds, i.e., $[H_0, H_{\text{eff}}] = 0$ where $H_0 := H|_{\lambda=0}$ [15]. Hence these triplets become the elementary excitations, triplons, of the effective Hamiltonian. The ground state of H_{eff} is the triplon vacuum. An infinitesimal anti-Hermitian generator η induces the flow $dH/dl = [\eta(l), H(l)]$ [28], where l is an auxiliary variable, $H(0) = H$, $H(\infty) = H_{\text{eff}}$. An appropriate choice for η is

$$\eta_{i,j}(l) = \text{sgn}([H_0]_{i,i} - [H_0]_{j,j})H_{i,j}(l), \qquad (11)$$

where the matrix elements $\eta_{i,j}$ and $H_{i,j}$ are given in an eigenbasis of H_0. The choice (11) retains only triplon conserving processes eliminating all parts of H changing the number of triplons [15].

In order to determine spectral weights corresponding to a given observable R this observable is transformed in the same way as the Hamiltonian

$$dR/dl = [\eta(l), R(l)] \qquad (12)$$

leading for $l \to \infty$ to the effective observable R_{eff}. After the transformation, i.e., at $l = \infty$, the subspaces with different numbers of triplons are disentangled: the Hamiltonian conserves the number of triplons and does not mix subspaces with different numbers of triplons. Given this property, it makes sense to define the spectral weight of each of these subspaces by

$$I_n = \langle 0|R_{\text{eff}}^\dagger P_n R_{\text{eff}}|0\rangle, \qquad n \in \{0, 1, 2, 3, \ldots\}, \qquad (13)$$

where P_n projects onto the subspace with n triplons [13,19–21]. This requires only explicit counting since the ground state $|0\rangle$ after the transformation is the triplon vacuum, i.e., it is the product state of singlets on all strong bonds. The technically involved explicit definition of "reduced exclusive matrix elements" is avoided [29]. Note that the definition of spectral weights such as I_n is useless if the triplon number is not conserved. Only the triplon conservation ensures that the total correlation splits into additive contributions from the various subspaces.

The CUT cannot be carried out completely. Perturbatively, the differential equations are truncated when terms of a certain order in λ arise [15]. The local spin component S_j^z is the observable R. The effective observable R_{eff} is calculated until order 7 in the one-, two-, and three-triplon sector. The four-triplon sector is transformed until order 6.

The total weight $I_{\text{tot}} = \sum_0^\infty I_n$ is given by the sum rule $I_{\text{tot}} = \langle R^\dagger R \rangle = \langle (S_j^z)^2 \rangle = 1/4$, which serves as a sensitive check for the validity of the results. In the following we will discuss the relative weights $I_{n,\text{rel}} = I_n/I_{\text{tot}} = 4I_n$.

For isolated dimers ($\lambda = 0$), the total spectral weight lies in the one-triplon channel $I_{1,\text{rel}} = 1$. As λ increases $I_{1,\text{rel}}$ decreases and the weight flows into the multi-triplon sectors. In Table I, the results for unbiased dlogPadé approximants indicate a singularity at $\lambda \approx 1$. From the physics of the Hamiltonian (1) we know that the singularity is located at $\lambda = 1$, where the system becomes critical. Thus it is advised to investigate approximants biased to display the singularity at unity: $I_1 \propto (1 - \lambda)^\gamma$ (last column in Table I). The exponent is found to be $\gamma = 0.325 \pm 0.016$, which leads us to conjecture that it takes exactly the value $\gamma = 1/3$. More generally, we presume that any single mode, which vanishes due to mixing with a continuum with square-root singularities at the band edges, looses its weight as $I_{\text{mode}} \propto \sqrt{\Delta \omega}$, where $\Delta \omega$ is the distance of the mode to the band edge of the continuum. The weight in the continuum is assumed to be constant.

We support our claim by considering a generic resolvent $I(\omega) = 1/[\omega - a - \Sigma(\omega)]$ with $\Sigma(\omega) = [\omega + \sqrt{\omega^2 - 4}]/2$ for $\omega \leq -2$. Such a resolvent appears for instance in the dynamics of two hard-core particles hopping from site to site in one dimension at given total momentum [12]. The constant a allows one to tune a nearest-neighbor interaction ($a < 0$: attraction; $a > 0$: repulsion) whereas $\Sigma(\omega)$ incorporates the kinetic energy of the relative motion. For $a \leq -1$ a bound state emerges from the continuum. It is separated from the continuum by the energy $\Delta \omega = -(2 + a + 1/a)$. Its weight I_{mode} is $1/[1 - \partial_\omega \Sigma(-2 - \Delta \omega)]$ implying $I_{\text{mode}} \propto \sqrt{\Delta \omega}$ for $\Delta \omega \to 0$.

For dimerized spin chains, the single triplon mode is separated from the continuum by an energy $\Delta \omega$ of the order of the energy gap Δ [12]. Using $I_{\text{mode}} \propto \sqrt{\Delta \omega}$ for each total momentum and integrating then over all momenta to obtain the local weights we find that the single mode looses its weight as $\sqrt{\Delta} \propto \delta^{1/3}$, which agrees excellently with the extrapolations.

In the two-triplon channel, there is no indication for a zero of I_2 at $\lambda = 1$. On the contrary, Padé approximants indicate significant weight at criticality. The weight in the two-triplon channel is the weight transferred from the one-triplon channel minus the weight transferred further to channels with three and more triplons. Hence it is natural to assume the existence of a singularity with exponent $1/3$ in I_2. But if this singularity is not linked to a zero, dlogPadé approximants cannot detect it. Hence we investigate the derivative $\partial_\lambda I_2$, which should be governed by a divergence with exponent $-2/3$. Indeed, Padé (not shown) and dlogPadé approximants (Table II) indicate a singularity at $\lambda \approx 1$. Approximants biased to a singularity of $\partial_\lambda I_2$ at $\lambda = 1$ yield exponents $\gamma_2 \approx -0.76$. The corresponding value of $I_{2,\text{rel}}$ found from integrating $\partial_\lambda I_2$ is 1.25. Since this value overestimates the sum rule by at least 25%, we conclude that the exponent $\gamma_2 \approx -0.76$ is too large in absolute value. Thus, we bias the approximants to the expected behavior $\partial_\lambda I_2 \propto (1 - \lambda)^{-2/3}$. In the last column of Table II the ensuing values for $I_{2,\text{rel}}$ are given. Quite unexpectedly, the results conclusively point to a spectral weight very close to unity. Since diagonal approximants usually yield the most reliable results, we retain the value $I_{2,\text{rel}} \approx 0.998$, keeping a possible error of a few percent in mind.

The sum rule corroborates the above result strongly. Padé and unbiased dlogPadé approximants consistently show that $I_{3,\text{rel}}$ is not larger than about 3×10^{-4}, which agrees perfectly with the value close to unity for $I_{2,\text{rel}}$. The inclusion of a singularity does not enhance $I_{3,\text{rel}}$. The biased approximants for $\partial_\lambda I_3$ (position $\lambda = 1$ and exponent $-2/3$) yield also only a contribution of about 2×10^{-4} ([2, 2]). Finally, the Padé and dlogPadé approximants for the four-triplon contribution $I_{4,\text{rel}}$ consistently indicate values well below 10^{-4}. The biased approximants for $\partial_\lambda I_4$ (position $\lambda = 1$ and exponent $-2/3$) even yield values below 10^{-5}. Therefore, we conclude that the contributions of channels with four and more triplons can be safely neglected.

TABLE I. Relative weight $I_{1,\text{rel}}$ of the one-triplon channel. (a) Position of the singularity from unbiased approximants, (b) exponent at the unbiased positions, (c) exponents in the biased approximants. (Blank cells: approximants without singularity.)

dlogPadé	(a) Zero λ_0	(b) $\gamma\|_{\lambda=\lambda_0}$	(c) $\gamma\|_{\lambda=1}$
[4, 2]			0.325 24
[3, 3]	1.025 03	0.367 98	0.328 91
[2, 4]	1.098 17	0.581 84	0.341 10
[1, 5]	1.098 17	0.581 84	0.314 57
[0, 6]			0.314 58

TABLE II. Relative weight $I_{2,\text{rel}}$ of the two-triplon channel. (a) Position of the singularity from unbiased approximants for $\partial_\lambda I_{2,\text{rel}}$, (b) exponent at the unbiased positions, (c) exponents in the biased approximants, (d) $I_{2,\text{rel}}\|_{\lambda=1}$ integrated from the biased (position $\lambda = 1$ and exponent $-2/3$) approximants. (Blank cells: approximants without singularity; stars: approximants with spurious poles.)

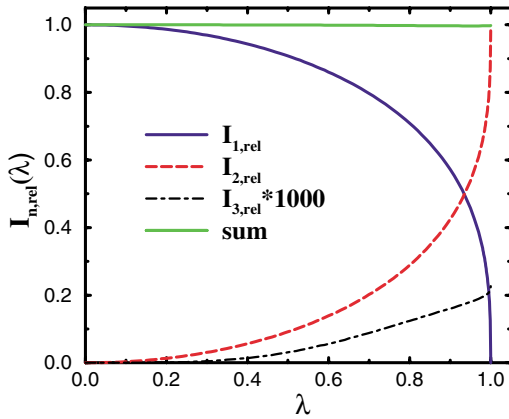| dlogPadé	(a) Zero λ_0	(b) $\gamma_2\|_{\lambda=\lambda_0}$	(c) $\gamma_2\|_{\lambda=1}$	(d) $I_{2,\text{rel}}$
[5, 0]			⋆	1.0618
[4, 1]			⋆	0.9818
[3, 2]			−0.7601	0.9976
[2, 3]	0.9908	−0.7323	−0.7603	⋆
[1, 4]			⋆	0.9895

FIG. 1 (color online). Relative spectral weights $I_{n,rel}(\lambda)$ of the dynamic structure factor in the dimerized chain. Depicted are biased approximants with singularity at $\lambda = 1$ and exponent $1/3$ for $I_{1,rel}$ ([4, 2], black solid line); exponent $-2/3$ in the derivative of $I_{2,rel}$ ([3, 2], dashed line) and similarly for $1000 \times I_{3,rel}$ ([2,2], dash-dotted line). The solid line toward the top is the sum $\sum_{n=1}^{3} I_{n,rel}$.

Figure 1 shows the final results for $I_{1,rel}$, $I_{2,rel}$, and $I_{3,rel}$; the tiny four and more triplon contributions are neglected. The sum rule is excellently fulfilled to within ≈ 0.003 for all values of λ supporting the above analysis.

In conclusion, we have found that even the dynamic structure factor of the critical uniform spin chain can be described to about 99% by two elementary triplets (triplons). This shows that scenario (ii) is correct for spin chains. A description in terms of a few triplons is possible. This lays the foundation for a new route to spectral densities in many models (first results in [13,30]).

Since the spin chain is the archetype of a gapless critical model described by spinons, we conclude that neither the occurrence of fractional excitations nor the vanishing of the gap precludes the applicability of an approach in terms of integer triplons. Even a larger part of the spectral weight is covered by two-triplon states than is covered by two-spinon states (72.89%) [26], which calls for further investigations of the relation between spinon and transformed triplon states. Since these results hold in spin chains, the home field of spinons, we conclude that a large class of low-dimensional quantum antiferromagnets is accessible by calculations based on integer excitations. If this is true for undoped antiferromagnets there is no necessity either to resort to fractional excitations for doped antiferromagnets. Hence our finding embodies an important message for potential theories for high-temperature superconductors.

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