Tracking the effects of interactions in gapless Heisenberg chains

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We consider the effects of interactions on the nature of spinon excitations in Heisenberg spin-1/2 chains. We explicitly compute the two-spinon part of the longitudinal structure factor of the infinite chain in zero field for all values of anisotropy in the gapless antiferromagnetic regime, via an exact algebraic approach. Our results allow us to quantitatively describe the behaviour of these fundamental excitations for cases ranging from free to fully coupled chains, thereby explicitly mapping the effects of 'turning on the interactions' in a strongly-correlated system.

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I. INTRODUCTION

The effects of interactions in one-dimensional (1d) systems are known to be overwhelming, in that constituent particles lose their individual identity and become locked into a collective quantum liquid state. Low-energy excitations then typically take the form of hydrodynamic-like modes, the system falling in the Tomonaga-Luttinger liquid universality class [1] characterized by critical (massless) excitations with a linear spectrum.

While the 'universal' physics of 1d systems is by now phenomenologically well understood [2], it almost always remains impossible to precisely track the effects of 'turning on the interactions' on the constituent particles, as one does for Fermi liquids [3] (where bare fermions are adiabatically connected to Landau quasiparticles). On the other hand, 1d systems can sometimes be treated by nonperturbative methods based on the exact solution of the underlying microscopic model. One of the fundamental systems belonging to this category is the Heisenberg spin-1/2 anisotropic chain [4,5], whose Hamiltonian is

$$H = J\sum_{j=1}^{N}\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z\right). \qquad (1)$$

This system falls in the gapless Tomogana-Luttinger liquid universality class for anisotropy values Δ in the range $-1 < \Delta \leq 1$ (in zero field; we take $J > 0$). At the $\Delta = 0$ point, the model is equivalent to a theory of free fermions via the Jordan-Wigner transformation. At the isotropic point $\Delta = 1$, the fundamental excitations are spinons [6], spin-1/2 fractionalized objects which can be interpreted as domain walls dressed by quantum fluctuations.

A way to probe the nature of excitations is to determine how they carry observable correlations, an interesting example here being the longitudinal structure factor

$$S^{zz}(k,\omega) = \frac{1}{N}\sum_{j,j'} e^{-ik(j-j')}\int_{-\infty}^{\infty} dt e^{i\omega t}\langle S_j^z(t) S_{j'}^z(0)\rangle. \qquad (2)$$

At the $\Delta = 0$ point, this can simply be written as a density-density correlator for the Jordan-Wigner fermions. Only single particle-hole excitations contribute, and the exact structure factor becomes porportional to their density of states. For any $\Delta > 0$, this simple picture breaks down [7] and interactions lead to nonperturbative corrections.

It is the purpose of this paper to track in detail the effects of 'turning on' the interaction term on the spinon quasiparticles, throughout the gapless antiferromagnetic regime $0 \leq \Delta \leq 1$. We will do so exactly, and moreover directly in the thermodynamic limit $N \to \infty$. In this limit the model is amenable to the 'vertex operator approach' described in detail in [8]. This approach was developed originally for the case $\Delta \geq 1$ for which the Hamiltonian of the model commutes with the action of the quantum group $U_q(\widehat{sl}_2)$. The representation theory of this quantum group then leads to explicit expressions for states, physical operators and their matrix elements [8], providing the necessary building blocks for the reconstruction of correlations in terms of contributions from intermediate states made up of increasing numbers of pairs of spinon excitations, $S^{zz}(k,\omega) = \sum_{m=1}^{\infty} S^{zz}_{(2m)}(k,\omega)$.

The case of the isotropic XXX antiferromagnet is particularly interesting since it is the most readily realized experimentally (for recent experimental work on gapless XXX and XXZ systems, see *e.g.* [9,10]), but also because it sits at the boundary between the gapless and gapped regimes. It has been first treated within the vertex operator approach of [8] in [11] and [12], in which the two-spinon contribution to the structure factor was obtained, showing that almost three quarters of the correlation weight is carried by these states. The building blocks for the four-spinon contribution at the isotropic point were obtained in [13], and compiled into the actual four-spinon part of the structure factor in [14], the combination of two and four-spinon parts being shown to yield about 99% overall accuracy. The $\Delta > 1$ regime, in which spinons have a mass gap, in fact comes more naturally out of the vertex operator approach but was treated only later than the isotropic point in view of the latter's more common relevance to real compounds. In the anisotropic case, the two-spinon part of the transverse structure factor was considered in [15,16]. The gapless regime remains however largely unexplored by these exact thermodynamic methods.

Spinon excitations – The ground state of the gapless XXZ antiferromagnet supports basic excitations in the form of spinons [6]. The dispersion relation of a spinon is exactly given at zero field by

$$e(p) = v_F |\sin p|, \qquad p \in [-\pi, 0], \tag{3}$$

where the Fermi velocity is in this case

$$v_F(\Delta) = \frac{\pi J}{2} \frac{\sqrt{1-\Delta^2}}{\text{acos}\Delta}. \tag{4}$$

Spinons however always appear in pairs, so the simplest set of excitations over the ground state which contribute to the structure factor are made of 2 spinons. Parametrizing their momentum by p_1 and p_2, momentum and energy conservation constraints impose that

$$k = -p_1 - p_2, \qquad \omega = e(p_1) + e(p_2). \tag{5}$$

The two-spinon states therefore form a continuum in the k-ω plane defined by the lower and upper boundaries

$$\omega_{2,l}(k) = v_F |\sin k|, \qquad \omega_{2,u}(k) = 2 v_F \sin k/2. \tag{6}$$

Matrix elements via vertex operator approach – The vertex operator approach is also applicable, albeit indirectly, to the gapless region $0 \leq \Delta \leq 1$. The strategy [17,18] is to first generalize the problem to the completely anisotropic Heisenberg model $\sum_j (J_x S_j^x S_{j+1}^x + J_y S_j^y S_{j+1}^y + J_z S_j^z S_{j+1}^z)$ in the so called principal regime $|J_y| \leq J_x \leq J_z$ [19] for which matrix elements of local operators between the vacuum and excited states can be computed exactly using the variant of the vertex operator approach developed in [20–23]. These results can then be mapped to the disordered regime $|J_z| \leq J_y \leq J_x$ [18,24] before taking the $J_x \to J_y$ limit to reconstruct the matrix elements for the gapless Hamiltonian (1) with $0 \leq \Delta \leq 1$. In this way we find (details will be published elsewhere) the following exact expression for the two-spinon contribution to $S^{zz}(k, w)$:

$$S_2^{zz}(k,\omega) = \frac{\Theta(\omega_{2,u}(k) - \omega)\Theta(\omega - \omega_{2,l}(k))}{\sqrt{\omega_{2,u}^2(k) - \omega^2}} \times (1 + 1/\xi)^2 \frac{e^{-I_\xi(\rho(k,\omega))}}{\cosh \frac{2\pi\rho(k,\omega)}{\xi} + \cos\frac{\pi}{\xi}} \tag{7}$$

in which $\xi = \frac{\pi}{\text{acos}\Delta} - 1$, Θ is the Heaviside function, and

$$I_\xi(\rho) \equiv \int_0^\infty \frac{dt}{t} \frac{\sinh(\xi+1)t}{\sinh \xi t} \frac{\cosh(2t)\cos(4\rho t) - 1}{\cosh t \sinh(2t)} \tag{8}$$

in which the parameter ρ is defined as

$$\cosh(\pi\rho(k,\omega)) = \sqrt{\frac{\omega_{2,u}^2(k) - \omega_{2,l}^2(k)}{\omega^2 - \omega_{2,l}^2(k)}}. \tag{9}$$

II. RESULTS

In Fig. 1, we give plots of the two-spinon part of the longitudinal structure factor (7) for values of anisotropy interpolating between weak and strong coupling. A few striking things are worth mentioning when observing how increasing interactions influence the two-spinon part of the correlations. Most noticeably, the divergence at the upper threshold disappears immediately upon turning interactions on. Also, the correlation weight starts flowing around the edges of the continuum, mostly via the wings at $k \simeq 0, 2\pi$ (see the $\Delta = 0.2$ plot), and thereafter starts accumulating at the antiferromagnetic point $k = \pi$ (see the $\Delta = 0.4$ plot). The divergence at the lower threshold starts carrying more correlation weight from $\Delta \simeq 0.5$ onwards, and becomes increasingly sharp as one moves towards the isotropic point.

Within the two-spinon continuum, so away from the thresholds, two things can be noticed. First of all, the weight within the bulk of this continuum quickly changes shape as Δ is turned on: from a pure $[\omega_{2,u}(k) - \omega]^{-1/2}$ form at $\Delta = 0$, it becomes almost uniform in frequency for $\Delta \simeq 0.2$, and then becomes a rapidly decreasing function of frequency for higher interactions. Turning interactions on therefore leads to a remarkable collapse of correlation weight from *high* to *low* energies.

Sum rules – To quantify the importance of the two-spinon contribution to the full structure factor, we use two useful sum rules, namely the integrated intensity

$$I^{zz} = \int_0^{2\pi} \frac{dk}{2\pi} \int_0^\infty \frac{d\omega}{2\pi} S(k,\omega) = 1/4, \tag{10}$$

and the f-sumrule (at fixed momentum) [25],

$$I_1^{zz}(k) = \int_0^{2\pi} \frac{d\omega}{2\pi} \omega S(k,\omega) = -2X^x(1 - \cos k) \tag{11}$$

where $X^x \equiv \langle S_j^x S_{j+1}^x \rangle$ is the ground state expectation value of the in-plane exchange term. This can be obtained from the ground-state energy density e_0 [26] and its derivative, namely $X^x = \frac{1}{2J}(1 - \Delta\frac{\partial}{\partial\Delta})e_0$, with

$$e_0 = \frac{-J(\xi+1)}{2\pi} \sin\left[\frac{\pi}{\xi+1}\right] \int_{-\infty}^\infty dt \left(1 - \frac{\tanh t}{\tanh[(\xi+1)t]}\right). \tag{12}$$

We provide the explicit values of the sum rule saturations coming from two-spinon contributions in Table I (for the f-sumrule, the saturation is the same at all momenta). The two-spinon states carry the totality of the correlation at $\Delta = 0$, and this remains approximately true up to surprisingly large values of interactions $\Delta \sim 0.8$, above which four, six, ... spinon states become noticeable.

Threshold behaviour – The behaviour of the longitudinal structure factor in the vicinity of the excitation thresholds can be determined from the analytic expressions we have obtained.

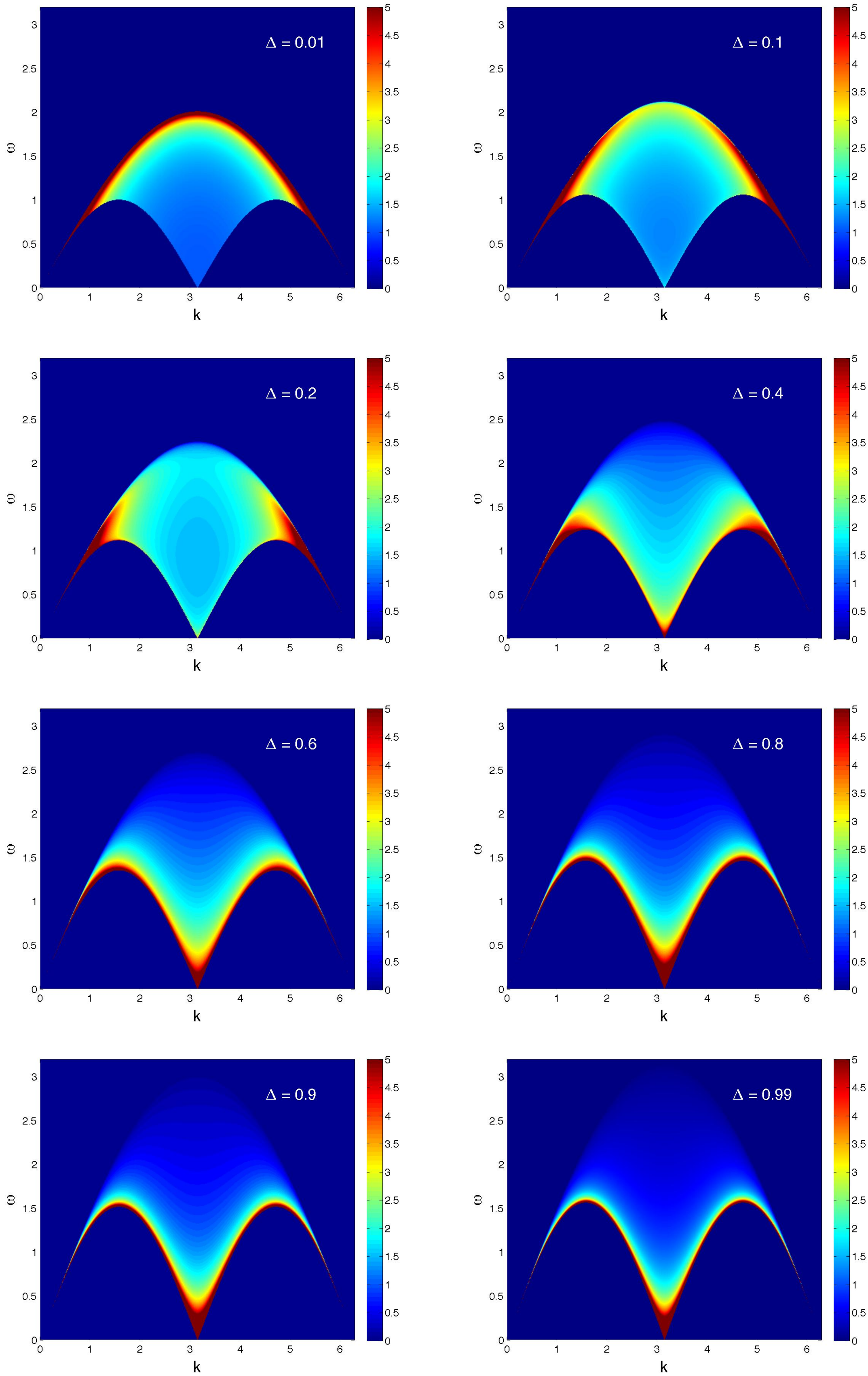

FIG. 1: Two-spinon part of the longitudinal structure factor of the infinite Heisenberg chain, for different values of the anisotropy parameter Δ. For $\Delta \to 0$, the correlation follows the density of states, and has a square root singularity at the upper threshold for all values of momenta. Increasing the anisotropy shifts the weight progressively towards the lower boundary. The lower boundary becomes increasingly sharp as the $\Delta \to 1$ limit is approached.

Δ	I^{zz}_{2sp}/I^{zz}	$I^{zz}_{1,2sp}/I^{zz}_1$	Δ	I^{zz}_{2sp}/I^{zz}	$I^{zz}_{1,2sp}/I^{zz}_1$
0	1	1	0.6	0.9778	0.9743
0.1	0.9997	0.9997	0.7	0.9637	0.9578
0.2	0.9986	9.9984	0.8	0.9406	0.9314
0.3	0.9964	9.9959	0.9	0.8980	0.8844
0.4	0.9927	0.9917	0.99	0.7918	0.7748
0.5	0.9869	0.9849	0.999	0.7494	0.7331

TABLE I: Sum rule saturations as a function of anisotropy: two-spinon contribution to the integrated intensity I^{zz} (10) and first frequency moment I^{zz}_1 (11).

a. The structure factor near the upper threshold. The upper threshold $\omega \to \omega_{2,u}(k)$ is approached by the limit $\rho \to 0$ as can be seen from (9). A careful evaluation shows that the integral (8) then behaves according to

$$I_\xi(\rho) \xrightarrow[\rho\to 0]{} -2\ln\rho + \mathrm{O}(1). \tag{13}$$

We thus have (using $\rho \sim \sqrt{\omega_{2,u}(k) - \omega}$ from (9)) that the structure factor vanishes as a square root,

$$S^{zz}_2(k,\omega) \xrightarrow[\omega\to\omega_{2,u}(k)]{} O(1)\ \sqrt{\omega_{2,u}(k) - \omega}. \tag{14}$$

This anisotropy-independent result (for $0 < \Delta \leq 1$) matches the same limit known to apply for the XXX case [12]. For the $\Delta \to 0$ limit (so $\xi \to 1$) however, we have to work more carefully, since the $\cosh\frac{2\pi\rho}{\xi} + \cos\frac{\pi}{\xi}$ in the denominator of the structure factor (7) now vanishes when $\rho \to 0$. Overall, in this case one rather obtains a square-root divergence,

$$S^{zz}_2(k,\omega) \xrightarrow[\omega\to\omega_{2,u}(k)]{} \frac{O(1)}{\sqrt{\omega_{2,u}(k) - \omega}}, \qquad \Delta = 0 \tag{15}$$

which follows the singularity of the density of states since the matrix elements are then energy independent.

b. The structure factor near the lower threshold. The lower threshold $\omega \to \omega_{2,l}(k)$ is obtained by taking $\rho \to \infty$. A careful evaluation of (8) in this limit yields

$$I_\xi(\rho) \xrightarrow[\rho\to\infty]{} -\pi\left(1 + \frac{1}{\xi}\right)\rho + \mathrm{O}(1). \tag{16}$$

We thus have (using $\rho \sim \frac{1}{2\pi}\ln(\frac{1}{\omega-\omega_{2,l}(k)})$ from (9)) that the structure factor obeys a nontrivial power law,

$$S^{zz}_2(k,\omega) \xrightarrow[\omega\to\omega_{2,l}(k)]{} \frac{O(1)}{[\omega - \omega_{2,l}(k)]^{\frac{1}{2}(1-1/\xi)}}, \tag{17}$$

as expected from the detailed asymptotic conformal field theory predictions (see [2,24] and references therein). Once again, the $\Delta \to 0$ limit (so $\xi \to 1$) yields the expected behaviour,

$$S^{zz}_2(k,\omega) \xrightarrow[\omega\to\omega_{2,l}(k)]{} O(1), \qquad \Delta = 0. \tag{18}$$

Conclusions – In this paper, we have tracked how the spinon excitations in Heisenberg antiferromagnets contribute to a fundamental observable, namely the longitudinal spin structure factor (2), as a function of anisotropy (*i.e.* interaction). We have obtained the two-spinon part of this correlator exactly in the zero-field, infinite-size chain throughout the gapless antiferromagnetic regime, by exploiting the vertex operator approach to express states and correlators in a purely algebraic language. This has allowed us to track in detail how the correlations carried by these excitations are affected by interactions. Our results show that while the correlation function behaves at first glance smoothly as the anisotropy is tuned from zero to its full value at the boundary of the gapless regime, detailed features including the threshold behaviour display remarkable modifications highlighting the nonperturbative nature of interaction effects in this one-dimensional system. Our results provide an accurate characterization of these effects, which should be observable in *e.g.* inelastic neutron scattering experiments.

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[1] F. D. M. Haldane, J. Phys C: Sol. St. Phys. **14**, 2585 (1981).
[2] T. Giamarchi, *Quantum Physics in One Dimension* (Oxford University Press, 2004).
[3] L. D. Landau, Sov. Phys. JETP **3**, 920 (1957).
[4] W. Heisenberg, Z. Phys. **49**, 619 (1928).
[5] R. Orbach, Phys. Rev. **112**, 309 (1958).
[6] L. D. Faddeev and L. A. Takhtajan, Phys. Lett. A **85**, 375 (1981).
[7] G. Müller, H. Thomas, M. W. Puga, and H. Beck, J. Phys. C: Sol. St. Phys. **14**, 3399 (1981).
[8] M. Jimbo and T. Miwa, *Algebraic Analysis of Solvable Lattice Models* (American Mathematical Society, Providence, RI, 1995).
[9] A. C. Walters, T. G. Perring, J.-S. Caux, A. T. Savici, G. D. Gu, C.-C. Lee, W. Ku, and I. A. Zaliznyak, Nature Physics **5**, 867 (2009).
[10] B. Thielemann, C. Rüegg, H. M. Rønnow, A. M. Läuchli,

J.-S. Caux, B. Normand, D. Biner, K. W. Krämer, H.-U. Güdel, J. Stahn, et al., Phys. Rev. Lett. **102**, 107204 (2009).
[11] A. H. Bougourzi, M. Couture, and M. Kacir, Phys. Rev. B **54**, R12669 (1996).
[12] M. Karbach, G. Müller, A. H. Bougourzi, A. Fledderjohann, and K.-H. Mütter, Phys. Rev. B **55**, 12510 (1997).
[13] A. Abada, A. H. Bougourzi, and B. Si-Lakhal, Nucl. Phys. B **497**, 733 (1997).
[14] J.-S. Caux and R. Hagemans, J. Stat. Mech: Th. Exp. p. P12013 (2006).
[15] A. H. Bougourzi, M. Karbach, and G. Müller, Phys. Rev. B **57**, 11429 (1998).
[16] J.-S. Caux, J. Mossel, and I. P. Castillo, J. Stat. Mech.: Th. Exp. **2008**, P08006 (2008).
[17] M. Jimbo and T. Miwa, J. Phys. A: Math. Gen. **29**, 2923 (1996).
[18] M. Jimbo, H. Konno, and T. Miwa, in *Deformation theory and symplectic geometry*, edited by D. Sternheimer, J. Rawnsley and S. Gutt (1997), no. 20 in Math. Phys. Studies, pp. 117 – 138, proceedings of the Ascona Meeting, June 1996.
[19] R. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic Press, 1982).
[20] M. Lashkevich and Y. Pugai, Nucl. Phys. B **516**, 623 (1998).
[21] M. Lashkevich and Y. Pugai, JETP Letters **68**, 257 (1998).
[22] M. Lashkevich, Nucl. Phys. B **621**, 587 (2002).
[23] T. Kojima, H. Konno, and R. Weston, Nucl. Phys. B **720**, 348 (2005).
[24] S. Lukyanov and V. Terras, Nucl. Phys. B **654**, 323 (2003).
[25] P. C. Hohenberg and W. F. Brinkman, Phys. Rev. B **10**, 128 (1974).
[26] C. N. Yang and C. P. Yang, Phys. Rev. **150**, 327 (1966).