Exact Edge Singularities and Dynamical Correlations in Spin-1/2 Chains

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Exact formulas for the singularities of the dynamical structure factor, $S^{zz}(q, \omega)$, of the $S = 1/2$ *xxz* spin chain at all q and any anisotropy and magnetic field in the critical regime are derived, expressing the exponents in terms of the phase shifts which are known exactly from the Bethe ansatz solution. We also study the long-time asymptotics of the self-correlation function $\langle 0|S_j^z(t)S_j^z(0)|0\rangle$. Utilizing these results to supplement very accurate time-dependent density matrix renormalization group, for short to moderate times, we calculate $S^{zz}(q, \omega)$ to very high precision.

The "*xxz*" $S = 1/2$ spin chain, with Hamiltonian

$$H = J \sum_{j=1}^{L}[S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z - hS_j^z], \quad (1)$$

is one of the most studied models of strongly correlated systems. It is equivalent by a Jordan-Wigner transformation to a model of interacting spinless fermions, with the corresponding Fermi momentum $k_F = \pi(1/2 + \langle 0|S_j^z|0\rangle)$ [1]. The model with $\Delta = 1$ describes Heisenberg antiferromagnets. The regime $0 < \Delta < 1$ is also of experimental interest; for example, the model with $\Delta = 1/2$ can be realized in $S = 1/2$ spin ladders near the critical field [2]. In optical lattices, it should be even possible to tune the anisotropy Δ and explore the entire critical regime [3].

While some aspects of the model have been solved for exactly by Bethe ansatz [4], it has been very difficult to obtain correlation functions that way. Field theory (FT) methods give the low-energy behavior at wave vectors near 0 and $2k_F$ [1]. From the experimental viewpoint [5], a relevant quantity is the dynamical structure factor

$$S^{zz}(q, \omega) = \sum_{j=1}^{L} e^{-iqj} \int_{-\infty}^{+\infty} dt e^{i\omega t}\langle 0|S_j^z(t)S_0^z(0)|0\rangle. \quad (2)$$

This is the Fourier transform of the density correlation function in the fermionic model. For $\Delta = 1$ and $h = 0$, the exact two-spinon contribution to $S^{zz}(q, \omega)$ was obtained from the Bethe ansatz [6], partially agreeing with the Müller conjecture [7]. More recently a number of new methods have emerged which now make this problem much more accessible. These include time-dependent density matrix renormalization group (DMRG) [8–10], calculation of form factors from Bethe ansatz [11,12], and new field theory approaches which go beyond the Luttinger model [13,14]. The results point to a very nontrivial line shape at zero temperature for $S^{zz}(q, \omega)$ of the *xxz* model [14] and of one-dimensional models in general [13]. In the weak coupling limit $\Delta \ll 1$ and for small q, the singularities at the thresholds of the two-particle continuum have

been explained by analogy with the x-ray edge singularity in metals [13].

In this Letter we combine the methods of Ref. [13] with the Bethe ansatz to investigate the singularity exponents of $S^{zz}(q, \omega)$ for the *xxz* model for finite interaction strength Δ and general momentum q. In addition, we determine the exponents of the long-time asymptotics of the spin self-correlation function, which is *not* dominated by low-energy excitations. We check our predictions against high accuracy numerical results calculated by DMRG.

In the noninteracting, $\Delta = 0$ case, only excited states with a single particle-hole pair contribute to $S^{zz}(q, \omega)$. All the spectral weight is confined between the lower and upper thresholds $\omega_{L,U}(q)$ of the two-particle continuum. The choices of momenta corresponding to the thresholds depend on both k_F and q. For zero field, $k_F = \pi/2$, $\omega_L(q)$ for any $q > 0$ is defined by the excitation with a hole at $k_1 = \pi/2 - q$ and a particle right at the Fermi surface (or a hole at the Fermi surface and a particle at $k_2 = \pi/2 + q$), while ω_U is defined by the symmetric excitation with a hole at $k_1 = \pi/2 - q/2$ and a particle at $k_2 = \pi/2 + q/2$. For finite field and $q < |2k_F - \pi|$, $\omega_{L,U}(q)$ are defined by either a hole at k_F and a particle at $k_F + q$ or a hole at $k_F - q$ and a particle at $k_F + q$. For $h \neq 0$ and $q > |2k_F - \pi|$, there is even a third "threshold" between ω_L and ω_U, where $S^{zz}(q, \omega)$ has a step discontinuity (see [7]).

For $\Delta \neq 0$, $S^{zz}(q, \omega)$ exhibits a tail associated with multiple particle-hole excitations [14]. However, the thresholds of the two-particle continuum are expected to remain as special points at which power-law singularities develop [13]. In order to describe the interaction of the high-energy particle and/or hole with the Fermi surface modes, we integrate out all Fourier modes of the fermion field $\psi(x)$ except those near $\pm k_F$ and near the momentum of the hole, k_1, or particle, k_2, writing

$$\psi(x) \sim e^{ik_F x}\psi_R + e^{-ik_F x}\psi_L + e^{ik_1 x}d_1 + e^{ik_2 x}d_2. \quad (3)$$

Linearizing the dispersion relation about $\pm k_F$ we obtain relativistic fermion fields which we bosonize in the usual way [1]. We also expand the dispersion of the $d_{1,2}$ particles

around $k = k_{1,2}$ up to quadratic terms. This yields the effective Hamiltonian density

$$\mathcal{H} = \sum_{\alpha=1,2} d_\alpha^\dagger \left(\varepsilon_\alpha - iu_\alpha \partial_x - \frac{\partial_x^2}{2m_\alpha} \right) d_\alpha$$
$$+ \frac{v}{2}[(\partial_x \varphi_L)^2 + (\partial_x \varphi_R)^2] + V_{12} d_1^\dagger d_1 d_2^\dagger d_2$$
$$+ \frac{1}{\sqrt{2\pi K}} \sum_{\alpha=1,2} (\kappa_R^\alpha \partial_x \varphi_R + \kappa_L^\alpha \partial_x \varphi_L) d_\alpha^\dagger d_\alpha. \quad (4)$$

This Hamiltonian describes a Luttinger liquid coupled to one or two mobile impurities [15,16]. In the derivation of Eq. (4) from Eq. (1), we drop terms of the form $(d_\alpha^\dagger d_\alpha)^2$ because we only consider processes involving a single d_1 and/or a single d_2 particle. Here $\varphi_{R,L}$ are the right and left components of the rescaled bosonic field. The long wavelength fluctuation part of S_j^z is given by $S_j^z \sim \sqrt{K/2\pi}(\partial_x \varphi_R + \partial_x \varphi_L)$. The spin velocity v and Luttinger parameter K are known exactly from the Bethe ansatz [4]. For zero field, $v = (\pi/2)\sqrt{1 - \Delta^2}/\arccos\Delta$ and $K = [2 - 2\arccos(\Delta)/\pi)]^{-1}$ (we set $J = 1$). To first order in Δ, the coupling constants describing the scattering between the d particles and the bosons are $\kappa_{R,L}^\alpha = 2\Delta[1 - \cos(k_F \mp k_\alpha)]$. The direct d_1-d_2 interaction V_{12} is also of order Δ. The exact values of $\kappa_{R,L}$ play a crucial role in the singularities and will be determined below.

We may eliminate the interaction between the d particles and the bosonic modes by a unitary transformation

$$U = \exp\left\{ i \sum_\alpha \int \frac{dx}{\sqrt{2\pi K}} (\gamma_R^\alpha \varphi_R - \gamma_L^\alpha \varphi_L) d_\alpha^\dagger d_\alpha \right\}, \quad (5)$$

with parameters $\gamma_{R,L}^\alpha = \kappa_{R,L}^\alpha/(v \mp u_\alpha)$. In the resulting Hamiltonian $\tilde{H} = U^\dagger H U$, $\varphi_{R,L}$ are free up to irrelevant interaction terms [15]. As in the x-ray edge problem, $\gamma_{R,L}^\alpha$ may be related to the phase shifts at the Fermi points due to the creation of the high-energy d_α particle.

Fortunately, we have access to the high-energy spectrum of the xxz model by means of the Bethe ansatz. Following the formalism of Ref. [16], we calculate the finite size spectrum from the Bethe ansatz equations with an impurity term corresponding to removing (adding) a particle with dressed momentum $k_1 = k(\lambda_1)$ [$k_2 = k(\lambda_2)$], where $\lambda_{1,2}$ are the corresponding rapidities. The term of $O(1)$ yields $\varepsilon_\alpha = \epsilon(k_\alpha)$, the dressed energy of the particle. For zero field, we have the explicit formula $\epsilon(k) = -v \cos k$. The excitation spectrum for a single impurity to $O(1/L)$ reads

$$\Delta E = \frac{2\pi v}{L} \left[\frac{1}{4K}(\Delta N - n_{imp}^\alpha)^2 + K(D - d_{imp}^\alpha)^2 + n_+ + n_- \right], \quad (6)$$

with a conventional notation for ΔN, D, and $n_\pm$ [4]. The phase shifts n_{imp}^α and d_{imp}^α are given by

$$n_{imp}^\alpha = \int_{-B}^{+B} d\lambda \rho_{imp}^\alpha(\lambda), \quad (7)$$

$$d_{imp}^\alpha = \int_{-\infty}^{-B} d\lambda \frac{\rho_{imp}^\alpha(\lambda)}{2} - \int_B^{+\infty} d\lambda \frac{\rho_{imp}^\alpha(\lambda)}{2}, \quad (8)$$

where B is the Fermi boundary and $\rho_{imp}^\alpha(\lambda)$ is the solution to the integral equation

$$\rho_{imp}^\alpha(\lambda) - \int_{-B}^{+B} \frac{d\lambda'}{2\pi} \rho_{imp}^\alpha(\lambda') \frac{d\Theta(\lambda - \lambda')}{d\lambda} = \frac{\Phi^\alpha(\lambda)}{2\pi}, \quad (9)$$

where $\Theta(\lambda) = i\log[\sinh(i\zeta + \lambda)/\sinh(i\zeta - \lambda)]$, with $\Delta = -\cos\zeta$, is the two-particle scattering phase [4], and $\Phi^{1,2}(\lambda) = \mp d\Theta(\lambda - \lambda_{1,2})/d\lambda$. The spectrum of Eq. (6) describes a shifted $c = 1$ conformal field theory. The scaling dimensions of the various operators can then be expressed in terms of K, n_{imp}^α, and d_{imp}^α. In the effective model (4), the shift is introduced by the unitary transformation of Eq. (5), which changes the boundary conditions of the bosonic fields. The equivalence of the two approaches allows us to identify

$$\gamma_{R,L}^\alpha/\pi = n_{imp}^\alpha \pm 2K d_{imp}^\alpha. \quad (10)$$

The phase shifts can be determined analytically for zero magnetic field. In this case, $B \to \infty$ and we have $d_{imp}^\alpha = 0$. Moreover, by integrating Eq. (9) over λ we find

$$n_{imp}^{1,2} = \mp \Theta(\infty)/(\pi - \Theta(\infty)) = \pm(1 - K). \quad (11)$$

Once the exact phase shifts are known, the exponent for the (lower or upper) threshold determined by a single high-energy particle can be calculated straightforwardly. For example, for a lower threshold defined by a deep hole, $\omega_L(q) = -\epsilon(k_F - q)$, the correlation function $\langle d_1^\dagger \psi_R(t, x) \psi_R^\dagger d_1(0, 0) \rangle$ can be factorized into a free d_1 propagator and correlations of exponentials of $\varphi_{R,L}$. After Fourier transforming, we find that near the lower edge $S^{zz}(q, \omega) \sim [\omega - \omega_L(q)]^{-\mu}$ with exponent [17]

$$\mu = 1 - (1 - n_{imp}^1)^2/2K - 2K(1/2 - d_{imp}^1)^2. \quad (12)$$

For $h \to 0$, we use Eq. (11) and obtain

$$\mu = 1 - K, \quad (h \to 0) \quad (13)$$

independent of the momentum of the hole. This form for the lower edge exponent had been conjectured long ago by Müller *et al.* [7]. It agrees (up to logarithmic corrections) with the exponent of the two-spinon contribution to $S^{zz}(q, \omega)$ for the Heisenberg point ($K = 1/2$) [6].

The general result of Eq. (12) is consistent with the weak coupling expression for μ [13]. To first order in Δ, Eq. (12) reduces to

$$\mu \approx \frac{\kappa_R^1}{\pi(v - u_1)} \approx \frac{2\Delta(1 - \cos q)}{\pi[\sin k_F - \sin(k_F - q)]}. \quad (14)$$

For $k_F \neq \pi/2$, we expand for $q \ll k_F$ and get $\mu \approx m\Delta q/\pi$, where $m = (\cos k_F)^{-1}$ (cf. [13]). For $k_F = \pi/2$, we obtain $\mu \approx 2\Delta/\pi$, which is $1 - K$ to $O(\Delta)$. Note the cancellation of the q dependence of κ_R^1 and $v - u_1$ in the

latter case. Momentum-independent exponents have also been derived for the Calogero-Sutherland model [18].

We now consider a threshold defined by high-energy particle and hole at $k_{1,2} = \pi/2 \mp q/2$. The relevant correlation function is the propagator of the transformed $d_2^\dagger d_1$. For simplicity, here we focus on the zero field case, in which $\varepsilon_2 = -\varepsilon_1 = v \sin(q/2)$, $u_2 = u_1$, and $-m_2 = m_1 = [v \sin(q/2)]^{-1}$. Particle-hole symmetry then implies that $\gamma_{R,L}^1 = \gamma_{R,L}^2$ and $d_2^\dagger d_1$ is invariant under the unitary transformation of Eq. (5). In the noninteracting case, there is a square-root singularity at the upper threshold due to the divergence of the joint density of states: $S^{zz}(q, \omega) \propto \sqrt{m_1/[\omega_U(q) - \omega]}$ for $\omega \approx \omega_U(q) = 2v \sin(q/2)$ [7]. For $\Delta \neq 0$, we need to treat the direct interaction V_{12} between the particle and the hole, which is not modified by U. This problem is analogous to the effect of Wannier excitons on the optical absorption rate of semiconductors [19,20]. This simple two-body problem can be solved exactly for a delta function interaction. The result is that the upper edge exponent changes discontinuously for $\Delta \neq 0$: the square-root divergence turns into a universal (for any q and Δ) square-root cusp, $S^{zz}(q, \omega) \propto \sqrt{\omega_U(q) - \omega}$. This behavior contradicts the Müller ansatz [7], but is consistent with the analytic two-spinon result for $\Delta = 1$ [6]. Unlike the original exciton problem, a bound state only appears for $V_{12} < 0$ ($\Delta < 0$) [21], because the particle and hole have a negative effective mass. For $\Delta \neq 0$, the upper edge cusp should intersect a high-frequency tail dominated by four-spinon excitations as proposed in [22]. This picture must be modified for $h \neq 0$, since then $\gamma_{R,L}^1 \neq \gamma_{R,L}^2$ and one needs to include the bosonic exponentials. The upper edge singularity then becomes Δ and q dependent. The general finite field case, including the middle singularity [7] for $q > |2k_F - \pi|$, will be discussed elsewhere.

We can apply the Hamiltonian of Eq. (4) to study the self-correlation function $G(t) \equiv \langle 0|S_j^z(t)S_j^z(0)|0\rangle$. Even in the noninteracting case, the long-time asymptotics is a *high-energy* property, since it is dominated by a saddle point contribution with a hole at the bottom and a particle at the top of the band [23]. In this case, $k_1 = 0$ and $k_2 = \pi$ and $d_{\text{imp}}^{1,2}$ vanish by symmetry ($\gamma_R^\alpha = \gamma_L^\alpha$). Here we restrict to zero field, but the method can be easily generalized. For $h = 0$ and $\Delta \geq 0$, $G(t)$ takes the form

$$G(t) \sim B_1 \frac{e^{-iWt}}{t^\eta} + B_2 \frac{e^{-i2Wt}}{t^{\eta_2}} + \frac{B_3}{t^\sigma} + \frac{B_4}{t^2}, \quad (15)$$

where $W = -\epsilon(0) = v$. The last two terms are the standard low-energy contributions, with $\sigma = 2K$. The amplitudes B_3 and B_4 are known [24]. The first term is the contribution from the hole at the bottom of the band and the particle at $k_F = \pi/2$, with exponent

$$\eta = (1 + K)/2 + (1 - n_{\text{imp}}^1)^2/2K = K + 1/2. \quad (16)$$

The term oscillating at $2W$ comes from a hole at $k = 0$ and a particle at $k = \pi$. For $\Delta = 0$, we have $\eta_2 = 1$. The

exponent η_2 is connected with the singularity at the upper threshold of $S^{zz}(q, \omega)$ by $G(t) \sim \int d\omega e^{i\omega t} \int dq S^{zz}(q, \omega)$ for $q \approx \pi$ and $\omega \approx \omega_U(\pi) = 2v$. Because of the discontinuity of the exponent at ω_U, η_2 jumps from $\eta_2 = 1$ to $\eta_2 = 2$ for any nonzero Δ. This behavior should be observed for $t \gg 1/(m_1 V_{12}^2) \sim 1/\Delta^2$. As a result, the asymptotics of $G(t)$ is governed by the exponent $\eta < 3/2$ for $0 < \Delta < 1$. For $\Delta < 0$, we must add to Eq. (15) the contribution from the bound state.

We can also study $S^{zz}(q, \omega)$ with time-dependent DMRG (tDMRG) [8,9]. The tDMRG methods directly produce $S^{zz}(x, t)$ and its spatial Fourier transform $S^{zz}(q, t)$ for short to moderate times. This information nicely complements the asymptotic information available analytically. The DMRG calculation begins with the standard finite system calculation of the ground state $\phi(t = 0)$ on a finite lattice of typical length $L = 200$–400, where a few hundred states are kept for a truncation error less than 10^{-10}. One of the sites at the center of the lattice is selected as the origin, and the operator S_0^z is applied to the ground state to obtain a state $\psi(t = 0)$. Subsequently, the time evolution operator for a time step τ, $\exp[i(H - E_0)\tau]$, where E_0 is the ground state energy, is applied via a fourth order Trotter decomposition [10] to evolve both $\phi(t)$ and $\psi(t)$. At each DMRG step centered on site j we obtain a data point for the Green's function $G(t, j)$ by evaluating $\langle \phi(t)|S_j^z|\psi(t)\rangle$. As the time evolution progresses, the truncation error accumulates. The integrated truncation error provides a useful estimate of the error, and so longer times require smaller truncation errors at each step, attained by increasing the number of states kept m. The truncation error grows with time for fixed m, and is largest near the center where the spin operator was applied. We specify the desired truncation error at each step and choose m to achieve it, within a specified range. Typically for later times we have $m \approx 1000$. Finite size effects are small for times less than $(L/2)/v$. We are able to obtain very accurate results for $G(t, j)$, with errors between 10^{-4} and 10^{-5}, for times up to $Jt \sim 30$–60.

For $Jt > 10$–20, we find the behavior of $S^{zz}(q, t)$ and $G(t)$ is well approximated by asymptotic expressions, determined by the singular features of $S^{zz}(q, \omega)$ and $G(\omega)$. By utilizing the leading and subleading terms for each singularity, we have been able to fit with a typical error in $S^{zz}(q, t)$ or $G(t)$ for $Jt \sim 20$–30 between 10^{-4} and 10^{-5}. We can fit with the decay exponents determined analytically or as free parameters to check the analytic expressions. Table I shows the comparison between the exponents for $G(t)$ extracted independently from the DMRG data and the FT predictions. In all cases the agreement is very good. By smoothly transitioning from the tDMRG data to the fit as t increases, we obtain accurate results for all times. A straightforward time Fourier transform with a very long-time window yields very accurate high resolution spectra. Examples of line shapes for $S^{zz}(q, \omega)$ obtained this way are shown in Fig. 1. We also did DMRG for the hole Green's

TABLE I. Exponents for the spin self-correlation function $G(t)$
for $h = 0$. The parameters W, η, η_2, and σ were obtained
numerically by fitting the DMRG data according to Eq. (15).
These are compared with the corresponding FT predictions (with
v and K taken from the Bethe ansatz).

Δ	W	v	η	$\frac{1}{2} + K$	σ	$2K$	η_2	
0	1	1	1.5	1.5	2	2	1	1
0.125	1.078	1.078	1.451	1.426	1.954	1.852	1.761	2
0.25	1.153	1.154	1.366	1.361	1.811	1.723	2.034	2
0.375	1.226	1.227	1.313	1.303	1.694	1.607	2.000	2
0.5	1.299	1.299	1.287	1.25	1.491	1.5	2.120	2
0.75	1.439	1.438	1.102	1.149	1.324	1.299	2.226	2

function for the fermionic model corresponding to Eq. (1),
obtaining good agreement with the predicted singularities
from the x-ray edge picture.

We have not seen any exponential damping of the η_2
term in $G(t)$ for $\Delta > 0$. This suggests that the singularity at
the upper edge is not smoothed out in the integrable *xxz*
model, even when the stability of the excitation is not
guaranteed by kinematic constraints [25]. Integrability
also protects the singularity at ω_U for finite field, as
implied by the conformal field theory form of the spectrum
in Eq. (6).

In conclusion, we presented a method to calculate the
singularities of $S^{zz}(q, \omega)$ for the *xxz* model. The exponents
for general anisotropy, magnetic field and momentum can
be obtained by solving the Bethe ansatz equations which
determine the exact phase shifts. For the particle-hole
symmetric zero field case, we showed that the lower edge
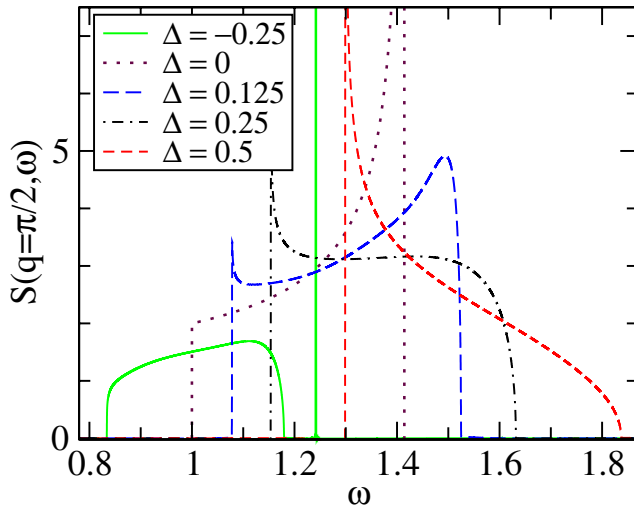exponent is q independent and the ("excitonlike") upper
edge has a universal square-root singularity. The combina-
tion of analytic methods with the tDMRG overcomes the
finite t limitation on the resolution of the tDMRG and can
be used to study dynamics of other one-dimensional sys-
tems (integrable or not).

FIG. 1 (color online).   DMRG results for $S^{zz}(q, \omega)$ vs ω for
$q = \pi/2$, $h = 0$, and several values of anisotropy Δ. The line
shapes for $\Delta > 0$ show a divergent x-ray type lower edge and a
universal square-root cusp at the upper edge. The curve for $\Delta <
0$ shows a bound state above the upper edge. The width of the
peak is very small for small $|\Delta|$.

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