The dynamic structure factor in impurity-doped spin chains

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The effects of impurities in spin-1/2 Heisenberg chains are recently experiencing a renewed interest due to experimental realizations in solid state systems and ultra-cold gases. The impurities effectively cut the chains into finite segments with a discrete spectrum and characteristic correlations, which have a distinct effect on the dynamic structure factor. Using bosonization and the numerical Density Matrix Renormalization Group we provide detailed quantitative predictions for the momentum and energy resolved structure factor in doped systems. Due to the impurities, spectral weight is shifted away from the antiferromagnetic wave-vector $k = \pi$ into regions which normally have no spectral weight in the thermodynamic limit. The effect can be quantitatively described in terms of scaling functions, which are derived from a recurrence relation based on bosonization.

Spin chains have been the center of attention as prototypical quantum many body systems ever since the early days of quantum mechanics \cite{1} and up to this day significant advances are made, e.g. in describing exact form factors \cite{2,3}, exact correlations \cite{4}, non-equilibrium states \cite{5,6}, and dynamic correlations in the regime of a non-linear spectrum \cite{7,8,9}. Recently, there has been renewed experimental interest in intentionally doped spin chain systems \cite{10,11} with new results on the Knight shift \cite{12,13}, magnetic ordering \cite{14}, and the dynamic structure factor \cite{15,16}. Doped spin chains are known to acquire characteristic boundary correlation functions \cite{17}, which lead to impurity induced changes in the Knight shift \cite{18,19}, the susceptibility \cite{20,21,22}, the static structure factor \cite{23}, and the ordering temperature \cite{24,25}. However, surprisingly a systematic analysis of the doping effects on the energy and momentum resolved dynamic structure factor is still missing so far. Previous research has taken into account the discrete spectrum of finite chains \cite{26,27,28}, which leads to an exponential suppression at low energies \cite{29,30}. The understanding of the momentum dependence is more involved, however, since characteristic correlations near the impurities play an important role and lead to a strong redistribution of spectral weight to higher momenta outside the dispersion relation as shown in this paper.

The underlying model is the well-known $xxz$-spin chain

\begin{equation}
H = J \sum_{i=1}^{L-1} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z) \tag{1}
\end{equation}

which represents a one-dimensional array of $L$ interacting spin-1/2 operators with open boundary conditions. This model can also be used to describe hard-core bosons \cite{31}, quantum dimer systems \cite{32}, or triplon excitations in ladder systems \cite{33}. The longitudinal dynamic structure factor is a key quantity, which can be measured by angle-resolved neutron scattering experiments \cite{34,35} and at the same time gives a deep insight into the spatial-temporal correlations. Impurities in the systems cut the spin chains \cite{36,37}, so we consider the structure factor for finite segments of length $L$

\begin{equation}
S(\omega, k) = \frac{1}{\pi} \sum_{j,j'} e^{-i k (j-j')} \int_{-\infty}^{\infty} dt \ e^{i \omega t} \langle S_j^z(t) S_{j'}^z(0) \rangle \tag{2}
\end{equation}

In recent years it was possible to calculate $S(\omega, k)$ to high accuracy from exact methods in the thermodynamic limit \cite{38,39}, which is nonzero only inside the bounds of the known dispersion \cite{40} as shown schematically in the bottom left panel of Fig. 1. Indicated in red are the dominant correlations near the antiferromagnetic wave-vector $k = \pi$ at low frequencies, which will be the topic of this paper. The low-energy behavior for infinite chains $L \to \infty$ has been known since the 1980s from bosonization \cite{41} and is described by powerlows as also derived in the appendix

\begin{equation}
S_\infty(\omega, q + \pi) = (2v)^{1-2K} \pi^2 A_1 \Gamma^{-4}(K) (\omega^2 - vq^2)^{K-1}, \tag{3}
\end{equation}

where $|q| = |k - \pi| < \omega/v$, $K = \pi/2(\pi - \theta)$ is the Luttinger parameter, $v = J \pi \sin \theta/2 \theta$ is the spinon velocity in terms of $\cos \theta = \Delta \xi$ and the overall amplitude $A_1$ is known from exact methods \cite{42}. Since $K < 1$ for $\Delta > 0$ the signal increases with $\omega^{2K-2}$ as the frequency is lowered and shows a divergence near the dispersion $\omega^2 - v^2 q^2 \to 0^+$, but vanishes for $|vq| > \omega$. A substantial amount of literature has been devoted to the analysis of the divergence at the dispersion in spin chains and quantum wires \cite{43}, which finds that it is not universal but depends on non-linear effects \cite{44,45} as well as the cut-off procedure \cite{46,47}. In this work we now consider finite chains, which show no divergence at all. Remarkably, at low energies bosonization nonetheless gives qualitatively accurate results for all $q = k - \pi$ and $L$. It is therefore possible to perform an efficient large-scale impurity averaging to predict the experimental signal.

The low-energy spectrum of finite spin chains is well described by equally spaced energy levels $\omega_m \approx m \Delta \omega$ with $\Delta \omega = \pi/2L$ \cite{48}. Higher order corrections to this
with \( S = 100 \) averaged signal wave-vectors \( k \) to numerical DMRG calculations for \( \omega \) change the averaged signal. Because of the discrete presentation \( \Delta S \) as reviewed in the appendix. It is based on expressing the alternating part of the spin-operator in terms of a free bosonic field \( \phi \)

\[
S^z(x,t) \approx A(-1)^{\ell} \sin \sqrt{4\pi K} \phi(x,t),
\]

where the amplitude \( A^2 = A_z/2 \) is known from exact methods \([16]\). Long-distance correlations can then be calculated by expectation values of the form

\[
G^z(x,y,t) = \langle e^{i\sqrt{4\pi K} \phi(x,t)} e^{-i\sqrt{4\pi K} \phi(y,0)} \rangle.
\]

The main technical difficulty is the Fourier-transform over time in Eq. (2), which ordinarily requires a detailed analysis of the analytic structure and contour integrals with a cut-off procedure \([14, 47, 66]\). However, in our calculation we use finite systems, which provides an efficient way of calculating spectral weights, that can be summarized in a few lines as follows and is derived in the appendix. Due to the discrete energy spectrum, the Fourier-transform gives a sum over delta-functions

\[
\int_{-\infty}^{\infty} dt G^z(x,y,t) e^{i\omega t} = 2\pi \sum_{m} S_m^z(x,y) \delta(\omega - \omega_m).
\]

To evaluate the spectral weights \( S_m^z \) it is possible to use the mode expansion and an integration by parts of Eq. (8) to arrive at a recurrence relation \([53, 55]\)

\[
S_m^z(x,y) = \pm \frac{1}{m} \sum_{\ell=1}^{m} S_{m-\ell}^z(x,y) \gamma(x,y),
\]

which allows to express the \( S_m^z \) in Eq. (5) as a recursive sum of the ones with lower index \( m - \ell \) using starting values of

\[
S_0^z(x,y) = S_0^z(x,y) = c(x)c(y) = \left( \frac{4L^2}{\pi^2} \sin \frac{\pi x}{L} \sin \frac{\pi y}{L} \right)^{-K}
\]

and the coefficients

\[
\gamma(x,y) = 4K \sin \frac{\ell \pi x}{L} \sin \frac{\ell \pi y}{L}
\]

It is then straightforward to evaluate the spatial Fourier-transform

\[
S_m^z(k) = \frac{1}{L} \int_0^L dx \int_0^L dy e^{i(\pi - k)(x-y)} S_m^z(x,y),
\]

to obtain the spectral weights \( S_m^z \) in Eq. (5)

\[
S_m^z(k) = \frac{A_z L}{2v} \left( S_m^z(k) - S_m^z(k) \right).
\]
In the case of odd \( L \) the integrands \( S_m^\pm(x, y) \) acquire an additional factor of \( \cos \pi (x \pm y) / L \) from zero modes which reflects the parity symmetries of the wavefunctions. Note that the spatial Fourier transform in Eq. (12) dominates for antiferromagnetic wavevectors \( k \approx \pi \), i.e. small \( q = k - \pi \). The expression for \( S_m^\pm(x, y) \) from Eq. (9) contains products of different \( \gamma_k \) with the starting value \( S_0^\pm \), so the spatial integral in Eq. (12) can be evaluated exactly using known integrals as shown in the appendix.

In the following we use this procedure to efficiently calculate spectral weights \( S_L(\omega_m, k) \) for comparison to numerics, for impurity averaging, and for extracting the asymptotic behavior for long chains. However, it has been shown before that bosonization results can strongly depend on non-linear corrections \([10, 15]\) or the cut-off procedure \([18, 49]\), so we first critically examine if this approach gives correct results. To this end we use DMRG \([53]\) to calculate spectral weights in finite systems. Using the multi-targeting algorithm for spectral weights \([53]\) we can calculate the first 97 excitations, which captures all nearly-degenerate multiplets up to the energy level \( m = 9 \). Using \( M = 600 \) DMRG states gives an accuracy in the wavefunction of order \( 10^{-2} \) relative to exact results from the \( xx \)-model.

A direct comparison between bosonization \( S_L \) and numerics \( S_{\text{DMRG}} \) is shown in Fig. 1\( ^{1} \) for energy levels \( m = 8 \) and \( m = 9 \) in a finite system of \( L = 100 \) with \( K = 0.8 \). Without any fit the agreement is surprisingly accurate and even captures details like an alternating signal at \( k = \pi \) with even and odd \( m \) due to parity symmetry, which leads to overall oscillations. Due to the zero-mode prefactor the same alternation is observed between even and odd lengths \( L \). For a quantitative analysis we also compare the small error between DMRG \( S_{\text{DMRG}} \) and bosonization \( S_L \) with the finite size correction relative to the bulk behavior \( S_\infty \) in Eq. (3) by defining

\[
\Delta S = \frac{S_L - S_{\text{DMRG}}}{S_L - S_\infty}.
\]

Both the numerator and the denominator go to zero as \( L \to \infty \), but the error to the numerics vanishes quicker with \( 1/L \) as shown in the lower right panel of Fig. 1\( ^{1} \) for \( m = 4, K = 0.8 \) and selected \( k \)-values, for which the denominator tends to be small.

We are now in the position to efficiently calculate \( S_L \) for a large range of \( L, k, \) and \( \omega \) to average the signal in a randomly doped system. An impurity density \( p \) of non-magnetic sites gives a distribution of chain lengths \([35, 36]\) \( P(L) = p^2(1-p) L \) normalized so that \( \sum L P(L) = 1 \). The averaged signal \( \bar{S}_L \) for typical experimental doping values in Fig. 1\( ^{1} \) shows that the signal at the divergence is strongly reduced relative to the undoped case \( L \to \infty \) while significant spectral weight is observed just outside the dispersion \( |vq| > \omega \).

It must be emphasized that the finite-size bosonization is completely divergence free. For any finite or impurity-doped system we obtain a well-behaved finite signal even at \( |vq| = \omega \), so it is unclear in what situation the power-law divergence in Eq. (3) becomes relevant. To answer this question we analyze the impurity correction \( S_{\text{imp}} \) relative to the thermodynamic limit, which is defined as the first order in a \( 1/L \) expansion \([30]\)

\[
S_L(\omega, k) = S_\infty(\omega, k) + L^{-1} S_{\text{imp}}(\omega, k) + O(L^{-2}).
\]

Based on the efficient calculation of spectral weights from Eqs. (9)-(13) we can make a comprehensive finite-size scaling to determine \( S_\infty \) and \( S_{\text{imp}} \) for different \( \omega \) and \( k \). Due to the scale-invariance of the underlying bosonization the resulting contributions in Eq. (15) show perfect data collapse, so that \( \omega^2 S_\infty \) and \( \omega^3 S_{\text{imp}} \) are only functions of the scaling variable \( vq/\omega \) as shown in Fig. 2\( ^{1} \) for \( K = 0.7 \) and \( K = 0.9 \). While \( S_\infty \) is given by Eq. (3), we find that \( S_{\text{imp}} \propto \omega^{-2K-3} \) increases even faster with decreasing \( \omega \). This is reminiscent of quantum wires, which also show boundary dominated spectral functions at low energies \([56]\). Even more interesting is the strong divergence of the impurity part in Fig. 2\( ^{1} \) which goes as \( |vq| - \omega |^{-K-2} \) and implies a breakdown of the expansion in Eq. (15) as \( |vq| \to \omega \). In particular, summing over higher order corrections in \( 1/L \) in Eq. (15) would be required as \( |vq| \to \omega \) with more and more divergent power-laws, even though the final result must be finite at the corresponding length as shown above.

Nonetheless, the expansion in Eq. (15) is useful away from the divergences in order to estimate the length-averaged signal to lowest order in \( p \)

\[
S_p(\omega, k) \approx E_1 \left( \frac{p \pi v}{\omega} \right) S_\infty(\omega, k) + p E_2 \left( \frac{p \pi v}{\omega} \right) S_{\text{imp}}(\omega, k),
\]

in terms of the Einstein functions \( E_1 \) and \( E_2 \)

\[
E_1(x) = \frac{x^2 e^x}{(e^x - 1)^2} \quad \text{and} \quad E_2(x) = \frac{x}{e^x - 1}.
\]
that are derived in the appendix. Both $E_1$ and $E_2$ become exponentially small for energies below the average-length gap $\omega \ll \pi v/L \equiv p \pi v$. The suppression of bulk spectral weight with $E_1$ due to the finite size gaps was discussed and observed experimentally [24, 25], but we find that the additional redistribution of spectral weight becomes very important, which can be traced to the effect of boundary correlations. The rescaled average $\omega^{2-2K} \hat{S}_p$ from Eq. (10) is now a function of two scaling variables $vq/\omega$ and $vp/\omega$. The corresponding data collapse holds approximately also for the averages over all lengths shown in Fig. 1 above, so that the signal for a given $\omega$ can easily be generalized to other energies.

The averaged signal in Fig. 1 and the impurity correction in Fig. 2 show that the signal is strongly reduced for $|vq| < \omega$, while spectral weight is created for $|vq| > \omega$. This invites the question if the $k$-integrated signal $\hat{S}(\omega)$ at a given energy is overall increased or decreased or even unchanged due to the boundaries. This is relevant for neutron scattering experiments, which recently observed significant changes of the spectral weight around neutron scattering experiments, which recently observed unchanged due to the boundaries. This is relevant for at a given energy is overall increased or decreased or even unchanged due to the boundaries. This is relevant for neutron scattering experiments, which recently observed significant changes of the spectral weight around a given energy.

To calculate the integrated antiferromagnetic spectral weight $\hat{S}$ as a function of $L$, we use the fact that an integration over $k$ of Eq. (12) leads to delta-functions $2\pi \delta(x-y)$, so it is possible to apply the recurrence relation in Eq. (3) for $S^\omega_m(x,x)$, which is inserted into the corresponding spatial integral. Finite size scaling gives a bulk part $\hat{S}_\infty(\omega) \propto \omega^{2K-1}$ which now decreases with decreasing $\omega$ corresponding to the integral of Eq. (3). However, the impurity part $\hat{S}_{\text{imp}}(\omega) \propto \omega^{2K-2}$ increases with decreasing $\omega$, so we define the energy independent ratio $\omega \hat{S}_{\text{imp}}/\omega S_\infty(\omega)$, which is only dependent on $K$ (i.e. $\Delta$) as shown in the inset of Fig. 6. Note that due to the alternation $m=L$ is even or odd, but the experimentally relevant average gives a finite and relatively small value. Therefore, the corresponding expansion and averaging in Eqs. (15) and (16) work well to calculate the doping and energy dependence using the $k$-integrated data in Fig. 2 (inset). The impurity part becomes negative at $K \lesssim 0.7$ i.e. larger $\Delta$, which may in part explain an additional depletion of spectral weight at low energies, but the experimentally observed changes with different impurity types [26] require more refined models beyond simple chain breaks.

Last but not least it is instructive to consider finite systems with periodic boundary conditions. The starting values in Eq. (11) are now independent of position $c = (2\pi \ell)^K$, so all integrals can be done directly. As shown in the appendix the recurrence relation leads to an analytical result for all energies, lengths, and momenta

$$S_L(\omega_m,k_l) = \frac{A}{4\ell^2 \Gamma} \Gamma \left( \frac{m+1}{2} + K \right) \Gamma \left( \frac{m-1}{2} + K \right)$$

$$\propto \frac{\Gamma \left( \frac{m+1}{2} + K \right) \Gamma \left( \frac{m-1}{2} + K \right)}{\Gamma \left( \frac{m+1}{2} + 1 \right) \Gamma \left( \frac{m-1}{2} + 1 \right)}$$

where now $\omega_m = 2\pi v m/L$ and also $k_l = \pi = 2\pi l/L$ is quantized due to periodicity with the condition that $l$ and $m$ are either both even or both odd integers and $|l| \leq m$. Therefore, there is no spectral weight for $|v|k - \pi| > \omega_m$ in strong contrast to open boundary condition discussed above.

In summary we have analyzed the structure factor of doped spin chain systems. Using bosonization and numerical DMRG, we see that doping leads to a significant shift of spectral weight from lower momenta to regions $|v|k - \pi| > \omega$ in neutron scattering experiments, which would not show any signal for infinite or periodic systems. The relative change from doping near the dispersion $|vq| \rightarrow \omega$ is infinitely large, so that the first order impurity contribution diverges near the dispersion $|vq| \rightarrow \omega$ with a stronger powerlaw than the bulk and a $1/L$ expansion from the thermodynamic limit always breaks down. Previous studies also found that the divergence in the thermodynamic limit is not universal, but instead strongly dependent on either the cut-off procedure [18] or higher order terms and non-linear effects [10]. Naively, it could have been expected that bosonization works particularly well in the thermodynamic limit, but instead it turns out that the finite-size theory is much better controlled and quantitatively accurate even for $|vq| \rightarrow \omega$ as shown in Fig. 1. From a technical point of view, the mode expansion for finite systems leads to finite sums, which can be efficiently evaluated using a recurrence relation without the need for contour integral, asymptotic limits, non-linearities, or cut-off procedures.

It is fair to say that in one dimension it is always important to consider boundaries, since physical systems only contain finite chains even in the absence of doping [60]. This is especially also true for artificially created spin chains using surface structures [61, 62], ion-traps [63], or ultra-cold gases [64–66] as quantum simulators, where measurements of energy and space resolved correlations are in principle possible [67].

Finally we would also like to discuss the limitations and open questions which remain. It is known that for higher energies than considered in Fig. 1 higher order operators play a role, which lead to systematic corrections [28, 50, 51, 54]. In particular, in the limit $\Delta \rightarrow 1$ it is well known that logarithmic corrections lead to strong quantitative changes [50]. Those log-corrections have not yet been fully understood for open boundary systems [51, 54] and are beyond the scope of this paper. Nonetheless, preliminary DMRG simulations at $\Delta = 1$ show that the strong transfer of spectral weight to $|v|k - \pi| > \omega$ is a robust feature.
Here we review the bosonization and calculation of correlation functions for finite spin-1/2 $XXZ$-chains

$$H = J \sum_i \left( S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \right) \quad (19)$$

with $L$ sites and open or periodic boundary conditions. Using the correlation functions we want to calculate the dynamic structure factor at low frequencies and near the antiferromagnetic wave-vector $k \approx \pi$, which is given by

$$S(\omega, k) = \frac{1}{L} \sum_{j,j'} e^{-ik(j-j')} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle S_j^z(t) S_{j'}^z(0) \rangle \quad (20)$$

where in the last line we have used the Lehmann representation using individual spectral weights

$$S_L(\omega_m, k) = \frac{2\pi}{\Delta \omega} |\langle \omega_m | S_k^z | 0 \rangle|^2 \quad (21)$$

at discrete energies $\omega_m = m\Delta \omega$.

**BOSONIZATION AND CORRELATIONS FOR OPEN BOUNDARY CONDITIONS**

The low-energy theory for the model in Eq. (19) is well described in the continuum limit by bosonic fields, which are rescaled by the square-root of the Luttinger parameter $K = \pi/2(\pi - \theta)$ where $\cos \theta = \Delta$ [45]. The free Hamiltonian is given by

$$H = v \frac{2}{\pi} \int_0^L dx \left[ \Pi(x)^2 + (\partial_x \phi(x))^2 \right]. \quad (22)$$

where $v = J \pi \sin \theta/2\theta$ is the spinon velocity and $\Pi$ is the momentum density conjugate to $\phi$, $[\phi(x), \Pi(y)] = i \delta(x-y)$. Higher order corrections are well understood [28, 50–52], but are irrelevant for low energies and long chains.

We are interested in the local $S^z$-operators, which can be expressed in terms of the bosons

$$S^z(x, t) = \sqrt{\frac{K}{\pi}} \partial_x \phi(x, t) + A(-1)^x \sin \left( \sqrt{4\pi K} \phi(x, t) \right), \quad (23)$$

where $A^2 = A_z/2$ is related to the amplitude of the asymptotic correlation functions, that is known from exact methods [46].

Open boundaries lead to the following mode expansion of the bosonic fields [28, 45]

$$\phi(x, t) = \hat{Q} \frac{2x}{L} + \phi_{osc}(x, t) \quad (24)$$

with

$$\phi_{osc}(x, t) = \sum_{\ell=1}^{\infty} \frac{1}{\sqrt{\pi \ell}} \sin \frac{\pi \ell x}{L} \left( e^{-i\frac{\pi \ell}{L} b_{\ell} + e^{i\frac{\pi \ell}{L}} b_{\ell}^\dagger} \right). \quad (25)$$

The zero mode $\hat{Q}$ is given in terms of the total magnetization

$$S^z = \int_0^L \sqrt{\frac{K}{\pi}} \partial_x \phi = 2\sqrt{\frac{K}{\pi}} \hat{Q}. \quad (26)$$

Note that those expressions agree with previous works [28, 45], up to an overall phase shift $\phi_0$ in the boson, which is of no consequence.
For the dynamical structure factor near \( k \approx \pi \) we are interested in the alternating part of the \( S^z S^z \)-correlation function

\[
\langle \sin(\sqrt{4\pi K} \phi(x,t)) \sin(\sqrt{4\pi K} \phi(y,0)) \rangle = \frac{1}{2} \left( G^+(x,y,t) - G^-(x,y,t) \right)
\]  
(27)

with

\[
G^\pm(x,y,t) = \langle e^{\pm 2i\pi S^z(x+y)/L} \rangle \langle e^{i\sqrt{4\pi K} \phi_{\text{vac}}(x,t)} e^{\mp i\sqrt{4\pi K} \phi_{\text{vac}}(y,0)} \rangle.
\]
(28)

The first factor gives different results for even chains \( S^z = 0 \) and for odd chains \( S^z = \pm 1/2 \)

\[
\langle e^{i2\pi S^z(x\pm y)/L} \rangle = \begin{cases} 
1, & L \text{ even} \\
\cos(\frac{\pi(x \pm y)}{L}), & L \text{ odd}
\end{cases}
\]
(29)

which reflects the different parity symmetry of the wavefunctions in even and odd chains. For the second factor in Eq. (28) it is useful to apply normal ordering

\[
\exp \left( i\sqrt{4\pi K} \phi_{\text{vac}}(x,t) \right) = c(x) \exp \left( i \sum_\ell e^{i\omega_\ell t} A_\ell(x) \right) \exp \left( i \sum_\ell e^{-i\omega_\ell t} A_\ell(x) \right)
\]
(30)

where \( \omega_\ell = \ell \Delta \omega \) with \( \Delta \omega = \frac{\pi v}{T} \) and operators

\[
A_\ell(x) = 2\sqrt{K} \sin \frac{\pi \ell x}{L} b_\ell.
\]
(31)

The prefactor is given via the Baker-Campbell-Hausdorff formula by

\[
c(x) = \exp \left( - \sum_\ell \frac{2K}{\ell} \sin^2 \frac{\pi \ell x}{L} \right),
\]
(32)

which is divergent. However, using

\[
\sum_{\ell=1}^\infty \frac{q^\ell}{\ell} = -\log(1-q)
\]
(33)

it is possible to capture the dependence on \( L \) and \( x \) correctly, so that only an overall factor is dependent on the regularization, which we choose to be finite by setting

\[
c(x) = \left( \frac{2L}{\pi} \sin \frac{\pi x}{L} \right)^{-K}.
\]
(34)

Therefore, upon using Baker-Campbell-Hausdorff again, the correlation functions in Eq. (28) becomes

\[
G^\pm(x,y,t) = c(x)c(y) \exp \left( \sum_{\ell=1}^\infty \frac{(-1)^{\ell-1}}{\ell} e^{-i\omega_\ell t} \gamma_\ell(x,y) \right)
\]
(35)

where we introduced the commutator

\[
\gamma_\ell(x,y) = [A_\ell(x), A_\ell^\dagger(y)] = 4K \sin \frac{\ell \pi x}{L} \sin \frac{\ell \pi y}{L}.
\]
(36)

For odd chains, the additional factor in Eq. (29) must also be inserted.

At this point all information for the asymptotic behavior of the correlation function is known, which in fact can be expressed in closed form using Eq. (29), so that the normalization in Eqs. (34) and (35) is simply a matter of convenience.
FOURIER TRANSFORM AND RECURSIVE FORMULA

To calculate the dynamical structure factor it is useful to go back to Eq. (35) in order to obtain the Fourier transformation in time. In accordance with the periodicity in $t$ this yields an expansion in delta functions

$$
\int_{-\infty}^{\infty} dt \ e^{i\omega t} G^\pm(x, y, t) = 2\pi \sum_m S^\pm_m(x, y) \delta(\omega - \omega_m).
$$

(39)

where the discrete spectral weight for $\omega_m = m\Delta\omega = m\pi/L$ is determined by the functions $\gamma_l$ in a recursive way $53$,

$$
S^\pm_m(x, y) = \frac{1}{m} \sum_{\ell=1}^{m} S^\pm_{m-\ell}(x, y) \gamma_\ell(x, y).
$$

(40)

which simply follows from partial integration. This equation defines the recursion formula, which allows to calculate any individual spectral weight as a sum of the previous ones from starting values $S^\pm_m(x, y) = c(x)c(y)$ (and including Eq. (29) for odd $L$). Note that this is much easier than an integration over Eq. (37) which would require a small imaginary cutoff for the time and a complicated contour integration.

For the spatial Fourier transform we define

$$
S^\pm_m(k) = \frac{1}{L} \int_0^L dx \int_0^L dy \ e^{i(\pi-k)(x-y)} S^\pm_m(x, y)
$$

(41)

where the shift of the wavevector by $\pi$ follows from the alternating factor in Eq. (29). Using $S_m(k) = \frac{1}{L} (S^+_m(k) - S^-_m(k))$ we obtain

$$
S(\omega, k) = 2\pi \sum_m S_m(k) \delta(\omega - \omega_m).
$$

(42)

Since the integrand $S_m^\pm(x, y)$ in Eq. (41) only involves a sum of exponentials $\exp(i\ell_x \pi x/L)$ and $\exp(i\ell_y \pi y/L)$ according to Eqs. (39) and (40), it is possible to perform the integral for each such term analytically together with the prefactor $c(x)$ in Eq. (35) by using

$$
\int_0^L \frac{dx}{\sin \left( \frac{\pi x}{L} \right)^K} = \frac{\pi e^{i\pi/2} 2^K L \csc(\pi K)}{\Gamma(K) \Gamma(q/2 - K/2 + 1)) \Gamma(-q/2 - K/2 + 1)}
$$

(43)

for $K < 1$ and analogously for the integration over $y$. In the summation of Eq. (40) we therefore keep track of the prefactors for each pair ($\ell_x, \ell_y$) for each level $m$ and then add up the exactly known integrals as a function of $k$ in Eq. (43) in the end.

PERIODIC BOUNDARY CONDITIONS

The recursive approach is particularly simple for periodic boundary conditions. In this case the system is translationally invariant, so that $G^+(x, y, t)$ is a function of $x - y$ and $t$ only and $G^-(x, y, t)$ vanishes. The prefactor is constant $c(x) = c = (2\pi)^K$. It is then convenient to introduce light-cone coordinates $z = vt-(x-y)$ and $\bar{z} = vt+x-y$ such that the correlation function factorizes

$$
e^{-ik(x-y)}e^{i\omega t}G^+(x, y, t) = e^{iz}e^{i\bar{z}}G(z)G(\bar{z})
$$

(44)

where $k$ is measured relative to $\pi$ and

$$
G(z) = c \exp \left( \sum_\ell \frac{1}{L} e^{-\ell_\ell^2 \gamma} \right)
$$

(45)

with $\gamma = K$. The double Fourier transform in $z$ and $\bar{z}$ with frequencies $u = \frac{1}{L}(\ell_\ell + k)$ and $\bar{u} = \frac{1}{L}(\ell_\ell - k)$, respectively, can then be performed directly by applying the recursion formula in Eq. (40) to the contributions of right-movers and left-movers separately. Due to periodicity with $L$ in $z$ and $\bar{z}$, the values for both $u$ and $\bar{u}$ are quantized

$$
u = \frac{2\pi}{L} u \quad \bar{u} = \frac{2\pi}{L} \bar{u}
$$

(46)
The boundaries of the integrals transform as follows:

\[
\frac{1}{L} \int_0^L dx \int_0^L dy \to \frac{1}{L} \int_0^L dy \int_{-y}^{L-y} dx = \int_0^L dr
\]

(47)

for integrands independent of \( y \) and \( L \)-periodic in \( r \). Furthermore we use

\[
\int_0^L dr \int_{-\infty}^\infty dt \to \frac{1}{2v} \int_{-\infty}^\infty dz \int_{-z}^{2L-z} \bar{dz} = \frac{1}{2v} \int_{-\infty}^\infty dz \int_{0}^{2L} \bar{dz}
\]

(48)

for integrands invariant under \( \bar{z} \to \bar{z} + L \). Since \( \gamma = K \) is independent of \( \ell \) in Eq. (15), the recursion can be solved exactly to give a ratio of gamma functions [58], i.e.

\[
\int_{-\infty}^\infty e^{iaz}G(z)dz = \frac{2\pi c}{\Gamma(K)} \sum_n \frac{\Gamma(n + K)}{\Gamma(n + 1)} \delta \left( u - \frac{2\pi}{L} n \right)
\]

(49)

and

\[
\int_0^{2L} e^{ia\bar{z}}G(\bar{z})d\bar{z} = \frac{2Lc}{\Gamma(K)} \sum_n \frac{\Gamma(n + K)}{\Gamma(n + 1)} \delta_{n,\bar{a}L/2\pi}
\]

(50)

for the integration over \( \bar{z} \). Now using the exact result for the asymptotic amplitude of the alternating correlation functions \( A_z \) from Ref. [46] we obtain

\[
S(\omega, k) = \frac{\pi A_z L c^2}{2v\Gamma^2(K)} \sum_{n, \bar{n}} \frac{\Gamma(n + K)}{\Gamma(n + 1)} \frac{\Gamma(\bar{n} + K)}{\Gamma(\bar{n} + 1)} \delta \left( u - \frac{2\pi}{L} n \right) \delta_{\bar{a}2\pi n/L}
\]

(51)

\[
= \frac{\pi A_z L c^2}{2^2\Gamma^2(K)} \sum_m \sum_{l=-m}^m \frac{\Gamma(\frac{m+1}{2} + K)}{\Gamma(\frac{m+1}{2} + 1)} \frac{\Gamma(\frac{m+1}{2} + K)}{\Gamma(\frac{m+1}{2} + 1)} \delta \left( \omega - \frac{2\pi vm}{L} \right) \delta_{k,2\pi l/L}
\]

(52)

where the sum over \( l \) goes in steps of two, so that \( l = n - \bar{n} \) and \( m = n + \bar{n} \) are either both even or both odd and \( |l| \leq m \). Comparing with Eq. (20) we can write for quantized frequencies \( \omega_m = m\Delta\omega = m\frac{2\pi}{L} \) and momenta \( k_l = \frac{l\pi}{L} \)

\[
S_L(\omega_m, k_l) = \frac{A_z L^2 c^2}{4\pi^2(K)} \frac{\Gamma(\frac{m+1}{2} + K)}{\Gamma(\frac{m+1}{2} + 1)} \frac{\Gamma(\frac{m+1}{2} + K)}{\Gamma(\frac{m+1}{2} + 1)}
\]

(53)

Stirling’s formula for large arguments \( \Lambda \) gives

\[
\frac{\Gamma(\Lambda + K)}{\Gamma(\Lambda + 1)} \approx \Lambda^{K-1} \left( 1 + \frac{K(\Lambda - 1)}{2\Lambda} + \mathcal{O} \left( \frac{1}{\Lambda^2} \right) \right)
\]

(54)

so that to leading order we find the bulk behavior in the thermodynamic limit

\[
S_\infty(\omega, q + \pi) = \frac{\pi^2 A_z}{2e\Gamma^2(K)} q^{2-2K} \left( \frac{\omega^2}{v^2} - q^2 \right)^{K-1} \quad \text{for } v|q| < \omega,
\]

(55)

where we get a factor of 2 due to the fact that the quantization of \( k_l \) jumps in steps of two at a given \( m \). The analogous analysis can be made for odd \( L \) where the prefactor in Eq. (29) basically gives the sum of two contributions with the \( k \)-quantization changed by one \( l \to l \pm 1 \).

**INTEGRATED SPECTRAL WEIGHT**

For the total spectral weight near the antiferromagnetic wave vector, we can integrate the contribution from the alternating correlation function

\[
\tilde{S}(\omega) = \int dk S(\omega, k)
\]

(56)
where the integral is taken in the vicinity of \( k = \pi \). Let us also define the integrated spectral weight at discrete energies by

\[
\hat{S}(\omega) = 2\pi \sum_m \hat{S}_m \delta(\omega - \omega_m). \tag{57}
\]

with \( \hat{S}_m = \frac{4}{\pi} (\hat{S}_m^+ - \hat{S}_m^-) \). Integrating Eq. (11) over \( k \) generates a delta function \( 2\pi \delta(x - y) \) such that one spatial integration can be trivially performed and \( \hat{S}_m \) simplifies to

\[
\hat{S}_m = \frac{\pi A_z^4}{2L} \int_0^L dx \left( \hat{S}_m^+(x,x) - \hat{S}_m^-(x,x) \right). \tag{58}
\]

The functions \( \hat{S}_m^+(x,x) \) are generated recursively via Eq. (40). In case of periodic boundary conditions – since \( \gamma_l(x,x) = 2K \) is independent of \( l \) – the recursion can again be solved exactly. From Eq. (19) we find

\[
\hat{S}_m = \pi A_z^2 \frac{\Gamma(m + 2K)}{2\Gamma(2K)} \frac{\Gamma(m + 1)}{\Gamma(m + 1)}. \tag{59}
\]

The bulk power law for the \( k \)-integrated structure factor is

\[
\hat{S}_\infty(\omega) = \frac{\pi^2 A_z^2}{v(2K)} \left( \frac{\omega}{v} \right)^{2K-1}. \tag{60}
\]

Note that this result can also be obtained by directly integrating Eq. (55).

**AVERAGING OVER CHAIN LENGTHS**

For a doping density of \( p = N_{imp}/N \) missing sites, the probability of finding a linear segment of length \( L \) is

\[
P(L) = p^2(1-p)^L \approx p^2 \exp(-Lp), \tag{61}
\]

which is normalized so \( N \sum P(L) = N_{imp} \). The probability of a single site to belong to a segment of length \( L \) is \( LP(L) \) which is normalized so that \( N \sum LP(L) = N - N_{imp} \), which excludes the missing sites. In the limit of large chains or small doping, the sums can be converted to integrals since the signal does not change significantly as a function of length so that \( \int dL P(L) = p \) and \( \int dL LP(L) = 1 \).

For a segment of length \( L \) we use the Lehmann representation in Eq. (11) in order to define the average signal

\[
\bar{S}(\omega, k) = \sum_L P(L)LS(\omega, k) \approx \int dL P(L) \sum_m \pi v S_L(\omega_m, k) \delta(\omega - \omega_m) \tag{62}
\]

which allows us to average separately over the bulk and impurity contributions in the \( 1/L \) expansion from the thermodynamic limit

\[
S_L(\omega_m, k) \approx S_\infty(\omega_m,k) + \frac{1}{L} S_{\text{corr}}(\omega_m,k) + O \left( \frac{1}{L^2} \right). \tag{63}
\]

For the bulk average we find

\[
\bar{S}_\infty = \int_0^\infty dL \pi vp^2 \exp(-Lp) \sum_m S_\infty(\omega_m) \delta \left( \omega - \frac{\pi v}{L} \right) \tag{64}
\]

\[
= \sum_m \int_0^{\infty} d\nu \frac{m \pi^2 v^2}{\nu^2} \exp(-mp\pi v/\nu) S_\infty(\omega) \delta(\omega - \nu) \tag{65}
\]

\[
= \sum_m \frac{mp^2 \pi^2 v^2}{\omega^2} \exp(-mp\pi v/\omega) S_\infty(\omega) \tag{66}
\]

\[
= E_1(\pi v p/\omega) S_\infty(\omega). \tag{67}
\]
upon using the substitution $L = \frac{\pi v y}{\nu}$ and $dL = -d\nu \frac{m v y}{\pi v}$. Here

$$E_1(y) = \sum_m m y^2 e^{-my} = \frac{y^2 e^y}{(e^y - 1)^2}$$

is the Einstein function of the scaling variable $y = p\pi v/\omega$ which measures the "average-length" gap $\nu/\bar{L}$ compared to $\omega$ [24, 25]. For the average impurity correction we use the same substitution $L = \frac{\pi v L}{\nu}$ and $dL = -d\nu \frac{\pi v L}{\nu}$

$$\bar{S}_{\text{imp}} = \int_0^\infty dL \frac{\pi v y^2 e^{-L\nu}}{L} \sum_m \bar{S}_{\text{imp}}(\omega_m) \delta \left( \omega - m \frac{\pi v}{L} \right)$$

$$= \sum_m \int_0^\infty d\nu \frac{p^2 \pi v}{\nu} e^{-p\pi v/\nu} \bar{S}_{\text{imp}}(\omega) \delta (\omega - \nu)$$

$$= \sum_m \frac{p^2 \pi v}{\omega} e^{-p\pi v/\omega} \bar{S}_{\text{imp}}(\omega)$$

$$= pE_2(\pi v \nu/\omega) \bar{S}_{\text{imp}}(\omega).$$

which is proportional to $p$ and the scaling function

$$E_2(y) = \sum_m y e^{-my} = \frac{y}{e^y - 1}.$$

This work was supported by the Deutsche Forschungsgemeinschaft (DFG) via the research centers SFB/TR49 and SFB/TR185 and by the Studienstiftung des deutschen Volkes.

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