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Dynamics of the 1D Heisenberg model and optical absorption of spinons in cuprate antiferromagnetic chains.

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We use numerical and analytical results to construct a simple ansatz for the energy dynamical correlation function of the 1D antiferromagnetic Heisenberg model. This is applied to compute the phonon assisted absorption spectra of magnetic excitations (spinons) in quasi-one dimensional spin 1/2 insulators and show to reproduce very well recent infrared measurements in Sr_2CuO_3.

75.40.Gb,78.30.Hv,75.50.Ee,75.10.Jm

After the solution by Bethe and many years of intense research, the spin 1/2 Heisenberg chain is one of the most studied many-body problems. In spite of this little is known on its dynamical properties. This is because the extreme complexity of Bethe's wave functions makes it too hard to compute dynamical correlations. Much of the progress came from numerical studies which inspired an ansatz for the dynamical structure factor [1,2], a recent analytical evaluation of the exact two-spinon contribution [3] and low energy bosonization studies [4–6].

In this letter we use numerical and known analytical results to obtain a simple ansatz for the energy dynamical correlation function defined below. This correlation function is important when considering the problem of coupling with phonons [6] and in optical properties [7,8]. As an application we compute the line shape for optical absorption of magnetic excitations assisted by phonons [7,8] and show how spinon physics appears naturally in the spectra. This is shown to reproduce very well recent measurements of the line shape by Tokura *et al.* [9,10] in quasi-one dimensional cuprates (See Fig. 3).

We will consider the 1-dimensional (1D) Hamiltonian,

$$H = \sum_i^N J B_i \tag{1}$$

where

$$B_i = S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \tag{2}$$

is the bond-energy operator, Δ measures the anisotropy and we take periodic boundary conditions. We will consider $\Delta = 0$ (the XY model) and $\Delta = 1$ (the antiferromagnetic Heisenberg model).

The energy correlation function is defined as [6], $G(p,\omega) = \langle\langle \delta B_p; \delta B_{-p} \rangle\rangle(\omega)$ (in Zubarev's notation [11]) where δB_p is the Fourier transform of $\delta B_i \equiv B_i - \langle B_i \rangle$.

To warm-up we will compute $G(\omega, p)$ for $\Delta = 0$. This is trivially done by using a Jordan-Wigner transformation [12] to map the problem to a noninteracting 1D free fermion gas. Excitations are free fermions and $G(p,\omega)$ becomes a Lindhard like response describing density like fluctuations. We get for the imaginary part,

$$-2\,\mathrm{Im}\, G_{XY}(p, \omega > 0) = D_{XY}(p,\omega) M_{XY}(p,\omega) \tag{3}$$

where following the approach of Ref. [2] we defined a density of states $D(p,\omega)$ and a matrix element $M(p,\omega)$.

$$D_{XY}(p,\omega) = \frac{N}{2\pi} \frac{\theta(\omega - \omega_1^{XY}(p))\theta(\omega_2^{XY}(p) - \omega)}{\sqrt{\left[\omega_2^{XY}(p)\right]^2 - \omega^2}} \tag{4}$$

with $\omega_1^{XY}(p) = J\sin(p)$, $\omega_2^{XY}(p) = 2J\sin(p/2)$ and

$$M_{XY}(p,\omega) = 2\frac{\left[\omega_2^{XY}(p)\right]^2 - \omega^2}{N^2\left[\omega_2^{XY}(p)\right]^2} \tag{5}$$

Two-fold degenerate states are counted once in Eq. (4) and this is taken into account by the factor of 2 in the matrix element (See Ref. [2]).

Notice that $\mathrm{Im}\, G_{XY}(p,\omega)$ is only different from zero between ω_1^{XY} and ω_2^{XY} . For a finite system the spectrum is given by a two-parameter set of discrete states with energy and pole strength given for $p > 0$ by,

$$\begin{array}{l} \omega_{XY}(p,q) = \omega_2^{XY}(p)\cos(q - p/2) \\ M_{XY}(p,q) = \frac{2}{N^2}\sin^2(q - p/2) \end{array} \tag{6}$$

where $0 < q \leq p/2$. Eq. (6) corresponds to particle-hole excitations around the $-\frac{\pi}{2}$ Fermi point.

When we switch to the isotropic limit ($\Delta = 1$) a simple analytic way of computing $G(p,\omega)$ is not available. Next we will follow Ref. [2] and use numerical results in finite chains, known low energy bosonization results and Bethe

ansatz results to construct a phenomenological ansatz for $\mathrm{Im}\, G(p,\omega)$.

In the isotropic limit there is no upper bound for the support of $\mathrm{Im}\, G(p,\omega)$ however the dominant contribution to $\mathrm{Im}\, G(p,\omega)$ comes from singlet states between $\omega_1(p)$ (the des Cloizeaux-Pearson [13] dispersion relation) and $\omega_2(p)$ which are obtained from $\omega_1^{XY}(p)$ and $\omega_2^{XY}(p)$ by changing J according to

$$J_{XY} \to J\pi/2 \tag{7}$$

and we attached an XY subindex to avoid confusion latter. This is analogous to the scenario found for the dynamical structure factor [2] and corroborated by a recent analytical evaluation which retains only two-spinon excited states [3]. We illustrate the analogous behavior for the energy correlation function for a finite system in Fig. 1.

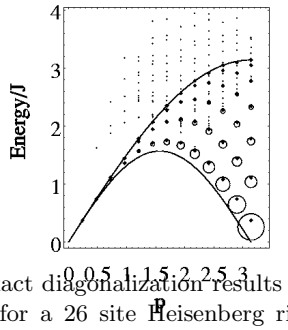

FIG. 1. Exact diagonalization results for $\mathrm{Im}\, G(p,\omega)$ in the $\omega - p$ plane for a 26 site Heisenberg ring. Excitations are given by the position of the circles and matrix elements by the radius. The dots are the XY energies with the renormalization of Eq. (7). The lines are $\omega_1(p)$ (lower) and $\omega_2(p)$ (upper).

In the thermodynamic limit these states form a two-parameter continuum degenerate with the triplet states that dominate the dynamical correlation function and have a density of states, $D(p,\omega) = D_{XY}^{J_{XY}\to J\pi/2}(p,\omega)$ [2].

To construct an ansatz for the energy correlation function of the Heisenberg model we put

$$-2\,\mathrm{Im}\, G(p,\omega>0) = D(p,\omega)M(p,\omega). \tag{8}$$

Our ansatz for $M(p,\omega)$ is given by,

$$M(p,\omega) = M_{XY}^{J_{XY}\to J\pi/2}(p,\omega)(A\frac{\sqrt{J}}{\sqrt{\omega}} + B\frac{J}{\sqrt{\omega^2-\omega_1(p)^2}}) \tag{9}$$

For a finite system we use Eq 's (6) to construct $M(p,q)$ in the same manner. In Fig. 2 we plot the matrix elements of Fig. 1 as a function of p together with the best fit of $M(p,q)$ from the ansatz. The agreement is very good for all branches with significant spectral weight.

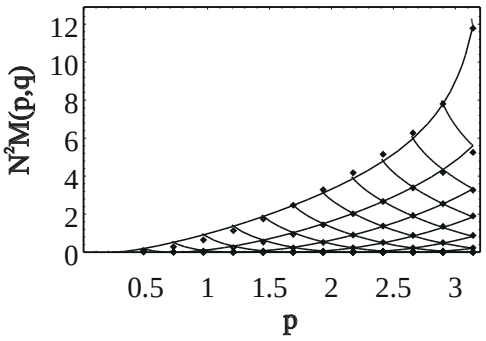

FIG. 2. The dots are the matrix elements (times N^2) vs. p from exact diagonalization of a 26 site Heisenberg ring. We had plotted the fit of $N^2M(p,q)$ (the ansatz) as continuous functions of p for each allowed q in the 26-site chain. The intersection of the continuous curves gives the actual values for the finite chain.

It is interesting that one can fit all branches except the upper one with $A \simeq 3$ and $B = 0$. The upper branch corresponds to the states closer to $\omega_1(p)$ where the square root becomes important. i.e. the dominant correction to the XY matrix elements in most of the (p,ω) plane is given by the p independent $1/\sqrt{\omega}$ factor.

To determine A and B for an infinite system we have made a finite size scaling study and used the sum rule $\sum_p \int d\omega(-2)\,\mathrm{Im}\, G(p,\omega) = \ln 2 - (\ln 2)^2$ to get $A = 2.4$, $B = 0.6$.

Bosonization studies predict [4–6] a divergence for $-\,\mathrm{Im}\, G(p=\pi,\omega)$ like ω^{-1} which becomes $(\omega-\omega_1(p))^{-1/2}$ close but not at $p = \pi$. The term proportional to B in $M(p,\omega)$ ensures this behavior and is analogous to the form introduced by Muller *et al.* [2] for the dynamic structure factor . As mentioned before its importance here is quantitatively minor in most of the (p,ω) plane whereas in the case of the dynamic structure factor it was the dominant contribution.

We next apply our results to the computation of the line shape for phonon assisted optical absorption of magnetic excitations for a 1D spin 1/2 isotropic Heisenberg chain. The absorption coefficient is given by [7,8],

$$\alpha(\omega) = \alpha_0 \omega I(\omega - \omega_\parallel)\,, \tag{10}$$

where α_0 determines the oscillator strength and is given by

$$\alpha_0 = \frac{4\pi^2 q_{\mathrm{A}}^2}{c\sqrt{\epsilon_1} M V_{\mathrm{Cu}} \omega_\parallel}\,, \tag{11}$$

M is the O mass, V_{Cu} is the volume associated with a Cu ion, $\omega_\parallel$ is the frequency of the Cu-O stretching mode phonons, ϵ_1 is the real part of the dielectric constant, q_{A} is an effective charge associated with this process and is of order $|q_{\mathrm{A}}| \sim e\beta a J/(S\Delta^2)$, where β is the rate of

change of the Cu on-site energy due to a nearby O-ion displacement, a is the lattice constant, $S = 1/2$ is the magnitude of the spin and Δ the on-site energy difference between Cu and O.

The function I is given by

$$I(\omega) = -16 \sum_p \sin^4(p/2)\, \mathrm{Im}\, G(p,\omega). \qquad (12)$$

$I(\omega)$ has a logarithmic singularity at $\omega = J\pi/2$ which will be convoyed to the optical absorption. The position of the singularity is a very robust feature which comes from the saddle point at $p = \pi/2$ in the *exact* des Cloizeaux-Pearson [13] dispersion relation (See Fig. 1). The distance between $\omega_\parallel$ and the singularity in the data provides a quick way to obtain the microscopic parameter J directly from experiments.

The two-dimensional version of this theory [7,8] within an interacting spin-wave approach was recently applied to explain related mid-IR bands measured by Perkins *et al.* in spin 1/2 [14] and spin 1 [15] insulating materials. Unlike estimations done in higher dimension [7,8,16] the J obtained from the position of the singularity in 1D is "exact" since the location of the singularity is known exactly. Here the only approximation is the Heisenberg model itself.

In Fig. 3 we compare the calculated optical absorption line shape to recent optical data by Tokura and collaborators [9,10] in Sr_2CuO_3. The agreement is excellent. We mention that the agreement, specially close to the singularity is not so good if B is set to zero. This suggest (in accordance with the numerical evidence) that the exponent predicted by bosonization at low energies persist up to energies quite far from its range of applicability.

$J = 0.246$eV was adjusted and found to compare very well with the value obtained in susceptibility measurements [17].

The value of α_0 which was fitted to the observed spectral weight, can be used to estimate the effective charge q_{A}. We find $|q_{\mathrm{A}}| \simeq 0.4e$ whereas in the 2D cuprates $|q_{\mathrm{A}|} \simeq 0.1e$ was found. This is not surprising since the processes that give rise to q_{A} are quite similar to the ones that give rise to J and the latter is found to be a factor of 2 larger in the 1D compounds.

Both the singularity and the cutoff at $\omega_2(\pi) + \omega_\parallel$ reflect the dominance of the spectra by two-spinon states analogous to the two-spinon states considered in Ref. [3] for the dynamical structure factor.

In conclusion we presented a simple ansatz for the energy dynamical correlation function of the Heisenberg model. The ansatz reproduces very well numerical data and the low energy behavior predicted by bosonization studies and provides new insight on the dynamical properties of the 1D Heisenberg

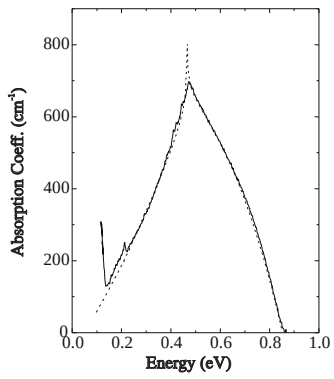

FIG. 3. Experimental absorption coefficient from Ref. [9] (solid line) and theoretical line shape (dashed line) in Sr_2CuO_3. Parameters are $J = 0.246$ eV, $\omega_\parallel = 0.08$ eV and $\alpha_0 = 132\mathrm{cm}^{-1}$. $\omega_\parallel$ was taken similar to the value in the 2D materials. A linear background was subtracted from the experimental data.

After this work was completed we became aware of Ref. [10] which contains the experimental data and a theoretical analysis of the line shape *qualitatively* similar to ours. They predicted the same position for the singularity however their matrix elements where computed in the XY limit. Although at first glance the theoretical line shape resembles the experiment they have missed the factor ω in Eq. (10) and the p-dependent form factor in Eq. (12). When they are included the resemblance is partially lost. Additionally they get a cusp singularity instead of a logarithmic singularity.

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