Spectral function of one hole in several one-dimensional spin arrangements

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The spectral function of one hole in different magnetic states of the one-dimensional $t$-$J$ model including three-site term and frustration $J'$ is studied. In the strong coupling limit $J \rightarrow 0$ (corresponding to $U \rightarrow \infty$ of the Hubbard-model) a set of eigenoperators of the Liouvillian is found which allows to derive an exact expression for the one-particle Green’s function that is also applicable at finite temperature and in an arbitrary magnetic state. The spinon dispersion of the pure $t$-$J$ model with the ground-state of the Heisenberg model can be obtained by treating the corrections due to a small exchange term by means of the projection method. The spectral function for the special frustration $J' = J/2$ with the Majumdar-Ghosh wave function is discussed in detail. Besides the projection method, a variational ansatz with the set of eigenoperators of the $t$-term is used. We find a symmetric spinon dispersion around the momentum $k = \pi/(2\eta)$ and a strong damping of the holon branch. Below the continuum a bound state is obtained with finite spectral weight and a very small separation from the continuum. Furthermore, the spectral function of the ideal paramagnetic case at a temperature $k_B T \gg J$ is discussed.

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I. INTRODUCTION

The understanding of spin-charge separation is a central point in the physics of low-dimensional electronic systems. That issue is most clearly seen in one dimension where the exact solution of the 1D Hubbard model reveals that the low-energy physics is dominated by decoupled, collective charge and spin excitations (also called holon and spinon, respectively). The idea that the spin and charge degrees of freedom separate has also been proposed to explain the properties of 2D cuprate superconductors. However, even in one dimension, the Bethe ansatz solution did not yet give a complete answer for the spectral function $A(k, \omega)$. Only for $U \rightarrow \infty$ an exact expression for $A(k, \omega)$ was found due to the factorization property of the wave function according to Ogata and Shiba. The results for the insulating half-filled case could also be generalized to other filling factors.

The spin-charge separation was observed in ARPES measurements of the one dimensional, dielectric cuprate SrCuO$_2$. The spinon and holon branch of the spectral function were seen, in contrast to the analogous experiment of one hole in the CuO$_2$ plane where spin and charge are coupled and the spin polaron quasiparticle has a dispersion proportional to $J$ as proposed theoretically in Refs. [5,10]. The ARPES spectra in SrCuO$_2$ were analyzed using the pure $t$-$J$ model. On the other hand, many 1D compounds, like for instance CuGeO$_2$, are characterized by frustration in the magnetic subsystem which may lead to a gap in the spin excitation spectrum. For the special frustration $J' / J = 0.5$ and in the limit $J \rightarrow 0$ an analytic expression for $A(k, \omega)$ was derived recently under the assumption that the wave function factorizes. Besides the frustration, also temperature effects are important as it was observed in ARPES measurements on Na$_{0.96}$V$_2$O$_5$. So, there is a clear need to study the spectral function systematically under the influence of frustration and temperature and to derive analytic expressions.

The present work focuses mainly on the effect of frustration and temperature on the spectral function in the insulating case. For that, we rederive first the exact solution of Sorella and Parola in a straightforward way using Green’s function technique. That is possible due to our finding of a set of eigenoperators of the Liouvillian (Sec. III) in the strong coupling limit $J \rightarrow 0$. As a consequence, our derivation is applicable for any magnetic state and any temperature in that limit. Especially, one can show that the result which was derived in Ref. [12] does not depend on the assumption that the wave function factorizes. We present analytic expressions for the spectral function of one hole in several magnetic states: (i) the ground-state of the antiferromagnetic Heisenberg model, (ii) the Majumdar-Ghosh wave function at the special frustration $J' / J = 0.5$, and (iii) the ideal paramagnetic state at temperatures much larger than the exchange energy $k_B T \gg J$. 

For large finite coupling we compare two methods to account for corrections $J \propto (t^2/U)$, namely the projection method and a variational ansatz using the set of eigenoperators of the $t$-term. We show that the former method yields a reasonable description of the spinon dispersion in the pure $t$-$J$ model (Sec. IV) and an approximate result for the spectral function of the Majumdar-Ghosh model. For $J' = J/2$ it misses the bound state below the continuum which is obtained by the more accurate variational method (Sec. VB). The bound state has a finite spectral weight but a very small separation from the continuum. Both methods show in the Majumdar-Ghosh case that the low energy region for momenta $k$ between $\pi/2$ and $\pi$ (lattice constant $a = 1$) will be filled with states, that the spinon dispersion (i.e. that collective excitation corresponding to the lower edge of the continuum) becomes symmetric around $\pi/2$, and they indicate an overdamped holon branch. The damping of the holon branch is extremely large for very high temperatures (Sec. VI).

Before presenting our results let us shortly discuss the different understandings of the term “spin-charge separation” as it can be met in the literature. The naive picture means that the low energy effective Hamiltonian may be written as

$$\hat{H} = \hat{H}_h + \hat{H}_s, \quad [\hat{H}_h, \hat{H}_s] = 0,$$

and the electron operator is the product

$$c_{i\sigma} = s_{i\sigma} h_{i\sigma}^\dagger,$$

where spinon $s$ and holon $h$ can be basically regarded as free particles. Then the normalized (i.e. $\int A(k, \omega) d\omega = 1$) spectral function is

$$A(k, \omega) = \frac{1}{L} \sum_Q 2f(Q) \delta [\omega - \epsilon_h(k - Q) - \epsilon_s(Q)],$$

where $f(Q) = \theta(\frac{\pi}{2} - |Q|)$ is the Fermi distribution function of spinons, $\theta(x)$ is the Heaviside step function, $L$ is the number of sites, $\epsilon_h, \epsilon_s$ being holon and spinon energies, respectively.

However, the naive understanding is not that one which is realized in 1D electron systems There, it was found that the eigenstates factorize in the limit $U \to \infty$ in the form

$$\psi(x_1, \ldots, x_N, y_1 \ldots y_M) = \psi_{SF}(x_1, \ldots, x_N) \phi_H(y_1 \ldots y_M),$$

where $x_1, \ldots, x_N$ are the spatial coordinates of the $N$ electrons on a $L$-site ring, and the $y_1 \ldots y_M$ ‘coordinates’ label the position of the spin-up electrons on the squeezed Heisenberg ring, i.e. on the $N$ occupied sites. The $\psi_{SF}$ is a spinless fermion state, and $\phi_H$ is an eigenstate of an $N$-site Heisenberg Hamiltonian with periodic boundary conditions. The product form of equation (4) should not be interpreted as a trivial decoupling between charge and spin. In fact, the momentum of the spin wave function imposes a twisted boundary condition on the spinless fermion wave function. As a result, the Fermi distribution function $f(Q)$ in (3) will be replaced by a function $Z(Q)$ that is the expectation value of a chain of spin operators that has to be determined from the pure spin system (for the details see Sec. III). The singularity of $Z(Q)$ produces additional peaks in $A(k, \omega)$. This correct answer for the spectral function may be understood as a manifestation of the phase string effect. It means that spinon and holon interact with each other via a nonlocal phase-string. Instead of (4) we should write

$$c_{i\sigma} = s_{i\sigma} h_{i\sigma}^\dagger \exp \left[ \frac{\pi}{2} \sum_{l>1} h_{l\uparrow}^\dagger h_l + \frac{\pi}{2} \sum_{l>1} (s_{i\sigma}^\dagger s_{i\sigma} - 1) \right].$$

It should be noted that the phenomenon of spin-charge separation is not restricted to the limit $U \to \infty$ in the 1D Hubbard model. At any finite $U$ the spin and charge fluctuations propagate with different velocities. That means that after some time the spin and charge degrees of freedom will be separated in space. But there is no analytic solution for the spectral function of the Hubbard model at arbitrary values of $U$ and also the present calculation treats terms of order $(t^2/U)$ as a perturbation. In that sense we will understand here spin-charge separation as a manifestation of the factorization property in the spectral density. Sharp maxima in the continuum correspond to collective excitations whereas possible bound states indicate special eigenfunctions with a strong coupling between spin and charge. Another possible effect of additional terms in the Hamiltonian is the broadening (i.e. the damping) of the collective excitations.
II. MODEL AND SPECTRAL DENSITY

To describe the low energy physics of compounds with a 1D electronic structure it is sufficient in most cases to take into account only that band which is closest to the Fermi energy (see for instance Ref. [17]). Treating the on-site Coulomb interaction explicitly, one obtains the well known 1D Hubbard model. In the present calculation we restrict ourselves to the strong coupling limit $U \gg t$ where we may project out the subspace of doubly occupied sites, and for the lower Hubbard band we obtain the effective Hamiltonian

$$\hat{H} = \hat{t} + \hat{J} + \hat{t}_3 ,$$

where

$$\hat{t} = -t \sum_{i,g,\alpha} X_{i}^{\alpha 0} X_{i+g}^{0\alpha} ,$$

$$\hat{J} = \frac{J}{2} \sum_{i,\alpha,\beta} X_{i}^{\alpha \beta} X_{i+1}^{\beta \alpha} ,$$

$$\hat{t}_3 = t_3 \sum_{i,g,\alpha,\beta} X_{i}^{\alpha 0} X_{i+g}^{\beta \alpha} X_{i+2g}^{0\beta} ,$$

and $\alpha, \beta = \uparrow, \downarrow$; $g$ are the nearest neighbors $g = \pm 1$. The Hamiltonian is valid near half filling ($X_{i}^{++} + X_{i}^{--} = 1$). The parameters $J$ and $t_3$ are connected with the original values of the Hubbard model by

$$J = 4t_3 = 4t^2/U ,$$

but the Hamiltonian (5) is more general, if we relax the condition (9). It may be derived directly from the more realistic three-band Hubbard model. Then, the $t_3$-term often becomes negligible and one obtains the $t$-$J$ model. The Hamiltonian (5) is written in terms of Hubbard projection operators that act in the subspace of on-site states

$$X_{i}^{\alpha \beta} \equiv |\alpha, i\rangle \langle \beta, i| , \quad \alpha, \beta = 0, \uparrow, \downarrow, 2 .$$

They are related with bare fermionic and spin operators through

$$X_{i}^{\alpha 0} = c_{i, \sigma}^\dagger (1 - n_{i, -\sigma}) , \quad X_{i}^{\sigma 2} = -\sigma c_{i, -\sigma} n_{i, \sigma} ,$$

$$X_{i}^{++} = s_{i}^\dagger = c_{i, \uparrow}^\dagger c_{i, \downarrow} , \quad X_{i}^{\sigma \sigma} = \frac{1}{2} + \sigma \left( c_{i, \uparrow}^\dagger c_{i, \uparrow} - c_{i, \downarrow}^\dagger c_{i, \downarrow} \right) = \frac{1}{2} + \sigma s_{i}^z ,$$

with $\sigma = \pm 1$. Other relations are easy to obtain with the use of the main property of Hubbard operator algebra

$$X_{i}^{\alpha \beta} X_{i}^{\gamma \lambda} = \delta_{\alpha \gamma} X_{i}^{\beta \lambda} ,$$

that follows immediately from the definition (10). The commutation relations for operators on different sites are fermionic for operators that change the number of particles by odd integers, like (11), and bosonic for others. In the presence of frustration in the magnetic system, which is discussed for instance for CuGeO$_3$, the $t$-$J$ Hamiltonian may be generalized by inclusion of the $J'$-term

$$\hat{J}' = \frac{J'}{2} \sum_{i,\alpha,\beta} X_{i}^{\alpha \beta} X_{i+2}^{\beta \alpha} .$$

Our aim is to calculate the one-particle two-time retarded Green’s function $G(k, \omega)$ and the spectral density of one hole in the magnetic state

$$A(k, \omega) = -\frac{1}{\pi} \text{Im} G(k, \omega + i0^+) ,$$

that is roughly proportional to the ARPES signal intensity. We define
\[ 2\pi \delta(k - k') G(k, \omega) = \langle \{X^0_k|X^0_{k'}\} \rangle \equiv -i \int_{t'}^{\infty} dt e^{i\omega(t-t')} \langle \{X^0_k(t), X^0_{k'}(t')\} \rangle, \]

where

\[
X^\sigma_m = \sqrt{2} \sum_{m=-\infty}^{+\infty} e^{-ikm} X^\sigma_m,
\]

\[
\langle \{X^\sigma_m, X^\sigma_{m'}\} \rangle = 2\pi \delta(k - k'),
\]

and where \{\ldots\} means the anticommutator. The expectation value denotes the thermal average over a grand canonical ensemble:

\[
\langle \ldots \rangle = Q^{-1} \text{Sp} [e^{-\beta(\hat{H} - \mu \hat{N})} \ldots], \quad Q = \text{Sp} e^{-\beta(\hat{H} - \mu \hat{N})}.
\]

Here \text{Sp} implies taking the trace of an operator, \hat{N} is the particle number operator, \( \beta = (kT)^{-1} \) is an inverse temperature, and \( \mu \) represents the chemical potential. The time dependence of the operator \( B(t) \) is given by \( B(t) = e^{it(\hat{H} - \mu \hat{N})} B e^{-it(\hat{H} - \mu \hat{N})} \).

### III. EIGENOPERATOR AND HOLON DISPERSION

Let us consider first the limit \( U \to \infty \) in the Hubbard model or \( J, t_3 \to 0 \) in (3). Then only the \( t \)-term

\[
\hat{t} = -t \sum_{i,g,\alpha} X^\sigma_{i\alpha} X^\sigma_{i+g},
\]

is nonzero. Note that it is a true many-body Hamiltonian due to the constraint of no double occupancy, as we see from Eq. (11). We introduce the set of operators

\[
v_{m,r} = \sum_{\alpha_1, \ldots, \alpha_r} X^\sigma_{m1} X^\sigma_{m+g \alpha_1} \cdots X^\sigma_{m+r-g \alpha_r} X^\sigma_{m+r}, \quad g = \text{sign}(r),
\]

for which

\[
[v_{m,r}, \hat{t}] = t (v_{m,r-1} + v_{m,r+1})
\]

holds at half filling. Any operator (18) can be considered as a string operator of a certain length consisting of a hole and an attached string of spin flips. Such a string can be produced by creating a hole in the Néel state and applying several times the kinetic energy (17) which creates misaligned spins. Similar string operators were used to describe the spin polaron quasiparticle in the 2D case (\textsuperscript{4,14}). We make double Fourier transform

\[
v_{k,q} = \sqrt{2} \sum_{m,r=-\infty}^{+\infty} e^{-ikm-iqr} v_{m,r},
\]

and see that

\[
[v_{k,q}, \hat{t}] = 2tv_{k,q} \cos q.
\]

The interpretation in terms of the string operator (18) is quite easy. We see that only the right end of the operator (18) was influenced by the \( t \)-term. Therefore, we may identify the right end of \( v_{m,r} \) with the holon excitation. In the next Section, it will become clear that the left end of \( v_{m,r} \) may be connected with the spinon.

The operators \( v_{k,q} \) (20) are eigenoperators of the Liouvillian \( \mathcal{L} \) of the problem, where \( \mathcal{L} \hat{A} \equiv [\hat{H}, \hat{A}] \). Note that it is one of the rarest, if not the unique case in many-body physics that the explicit form for a set of eigenoperators can be given. From (21) we see that the equation of motion for the corresponding string operator Green’s function closes and it has a simple pole form

\[
\langle \{v_{k,q}^\dagger v_{k',q'}^\dagger\} \rangle = \frac{\langle \{v_{k,q}^\dagger v_{k',q'}^\dagger\} \rangle}{\omega - 2t \cos q}, \quad \langle \{v_{k,q}^\dagger v_{k',q'}^\dagger\} \rangle = 8\pi^2 \delta(k - k') \delta(q - q') Z(k - q + \pi),
\]

\[{}^{(22)}\]
where the spectral weight is the expectation value

\[ Z(q + \pi) = \frac{1}{2} \sum_{r = -\infty}^{+\infty} e^{-ir} \langle \Omega_r \rangle , \]  

(23)

of a chain of *X*-operators

\[ \Omega_r = \sum_{\alpha_1, \ldots, \alpha_r, \sigma} X_{m}^{\alpha_1 \sigma} X_{m+g}^{\alpha_2 \sigma} \cdots X_{m+r-g}^{\alpha_r \sigma} X_{m+r}^{\alpha_r \sigma} \]

\[ = \langle 2S_m S_{m+g} + \frac{1}{2} \rangle \langle 2S_{m+g} S_{m+2g} + \frac{1}{2} \cdots \rangle \langle 2S_{m+r-g} S_{m+r} + \frac{1}{2} \rangle , \]  

(24)

to be calculated for the pure spin-system without any hole. The expectation value \( \langle \Omega_r \rangle \) of \( (24) \) cannot depend on the starting point \( m \) due to the translational symmetry of the problem. The operator \( (24) \) was introduced in Ref. 4 and explicit values on a 26-site Heisenberg ring were given for \( T = 0 \), when \( \langle \ldots \rangle \) becomes the average over the ground-state. Asymptotically, the following behavior was found

\[ \langle \Omega_l \rangle \to \frac{1}{\sqrt{l}} \Re \left[ A e^{i\pi l/2} \right] \]  

(25)

which leads to a square root singularity of \( Z(Q) \). Using additionally the exact values \( \langle \Omega_0 \rangle = 1 \) and \( \langle \Omega_1 \rangle = 1 - 2 \ln 2 \) the following formula may be derived

\[ Z(Q) = \left( -0.393 + 0.835/\sqrt{\cos Q} \right) \theta \left( \frac{\pi}{2} - |Q| \right) . \]  

(26)

For the hole Green’s function \( (14) \) we have

\[ \langle \langle X_k^0 | X_{k'}^0 \rangle \rangle = \int_{-\pi}^{+\pi} \frac{dq}{2\pi} \int_{-\pi}^{+\pi} \frac{dq'}{2\pi} \langle \langle v_{k,q} | v_{k',q'} \rangle \rangle = 2\pi \delta(k - k') \int_{-\pi}^{+\pi} \frac{dq}{\pi} \frac{Z(k - q + \pi)}{\omega - 2t \cos q} , \]  

(27)

and the spectral density is obtained in the way

\[ A(k, \omega) = \int_{-\pi}^{+\pi} \frac{dQ}{\pi} Z(Q) \delta [\omega + 2t \cos (k - Q)] . \]  

(28)

That gives the exact answer in the strong coupling limit \( (J \to 0) \) where only the holon dispersion \( \epsilon_h(q) = -2t \cos q \) is important. But the ratio \( J'/J \) may be arbitrary and \( (28) \) is not only exact in the Heisenberg case with \( Z(Q) \) from \( (24) \). Instead, from our derivation follows its validity for arbitrary magnetic states and it is not restricted to zero temperature. Then, however, \( Z(Q) \) is different. In the following we will give exact results for i) the Majumdar-Ghosh wave function at the special frustration \( J'/J = 0.5 \), and ii) the ideal paramagnetic case at \( k_BT \gg J \). Two cases are quite trivial, namely the saturated ferromagnetic case and the classical Néel state. The former one leads to \( Z(Q + \pi) \propto \delta(Q) \) and a spectral function like for free fermions, whereas the latter case leads to the Brinkmann-Rice continuum \( (Z(Q) = 1/2) \). A magnetic state inbetween the classical Néel and the Heisenberg case could, in principle, also be considered, for which the one-hole spectral function was derived in Ref. 20 treating the spin-fluctuations as perturbation.

### IV. SPINON DISPERSION

In real systems the ratio \( J/t \) is roughly 0.3. It means that they are in the regime of strong coupling and the above consideration correctly describe the largest energy scale \( \propto t \). Now, we want to estimate the corrections that arise from other terms of the Hamiltonian \( (3) \). First we note that \( v_{k,q} \) are eigenoperators for the \( t_3 \)-term

\[ [v_{k,q}, \hat{t}_3] = -2t_3 v_{k,q} \cos 2q , \]  

(29)

which leads to the replacement \( \epsilon_h(q) \to \epsilon_h(q) + 2t_3 \cos 2q \) in the denominator of \( (23) \). The commutation with \( \hat{J} \) gives (see Appendix A for the details)
\[ [v_{k,q}, J] = -J \cos(k - q)v_{k,q} + \frac{J}{2}(v'_{k,q} + v''_{k,q}), \] (30)

where \( v'_{k,q} \) and \( v''_{k,q} \) are Fourier transforms of the operators

\[ v'_{m,r} = \sum_{\gamma, \alpha_1, \ldots, \alpha_r} X_m^{\sigma_\gamma} X_{m-g}^{\alpha_1 \alpha_2} \cdots X_{m-r+1}^{\alpha_r} X_{m+r}^{0}, \] (31)

\[ v''_{m,r} = -\sum_{\gamma, \alpha_1, \ldots, \alpha_r} X_m^{\sigma_\gamma} X_{m+g}^{\alpha_1} \cdots X_{m+r-g}^{\alpha_r} X_{m+r}^{0}. \] (32)

It is impressive that terms, which come from the commutation of “inner” \( X_n \) operators in \( v_{m,r} \) with \( n \) between the points \( m \) and \( m + r \) cancel each other and only the terms coming from the ends remain. The term \( v''_{m,r} \) presents a distortion of the right end of \( v_{m,r} \) by means of the exchange part and may be interpreted as the loss of magnetic energy due to the presence of a holon. On the other hand, the term \( v'_{m,r} \), with a distorted left end will be shown to give rise to the spinon dispersion. We really observe the “separate” motion of the holon that is represented by the right end of \( v_{m,r} \) and of the spinon that is the left end of \( v_{m,r} \). The holon motion is governed by the \( t \)-term and the spinon motion by the \( J \)-term. We put the word “separate” in quotes because the motion remains correlated due to the set of “inner” \( X_n \) operators, connecting the ends of \( v_{m,r} \).

We need an approximate approach to account for \( v'_{k,q} + v''_{k,q} \). For this purpose we use the projection technique

\[ v'_{k,q} + v''_{k,q} \approx \frac{\{v'_{k,q} + v''_{k,q}, v_{k,q}\}}{\{v_{k,q}, v_{k,q}\}} v_{k,q}. \] (33)

Now, the Green’s function for the string operator has the form

\[ \langle \langle v_{k,q} | v_{k,q} \rangle \rangle = \frac{8\pi^2 \delta(k - k') \delta(q - q') Z(k - q + \pi)}{\omega - 2t \cos q + 2t_3 \cos 2q - \epsilon_s(k - q)}, \] (34)

where \( \epsilon_s(k - q) \) is defined by the equation

\[ \langle \{v_{k,q}, J\}, v_{k',q'}\rangle \equiv 8\pi^2 \delta(k - k') \delta(q - q') \epsilon_s(k - q) Z(k - q + \pi). \] (35)

The contribution of the \( v''_{m,r} \) term to the spinon dispersion is determined by an expression of the form

\[ \langle \langle v''_{m,r}, v''_{m',r'} \rangle \rangle = \frac{1}{2} \delta_{m+r,m'+r'} \langle \Omega''_{r,r'} \rangle, \] (36)

where the precise order of the \( X \)-operators in \( \Omega''_{r,r'} \) can be easily inferred from (32) and is given in the Appendix A. There, it is also shown that for slowly decaying spin correlation functions (as in the present case, see (25)) the correlation functions \( \langle \Omega''_{r,r'} \rangle \) can be approximated to be a function of \( r - r' \) only, in the way:

\[ \langle \Omega''_{r,r'} \rangle \approx \langle \Omega''_{r-r',0} \rangle \approx \langle \Omega_1 \rangle \langle \Omega_{r-r'} \rangle. \] (37)

That leads to a constant shift of the energy \( \epsilon_s \) as the only effect of \( v''_{m,r} \) which will be neglected further on. The contribution of the \( v'_{m,r} \) term can be written analogously to (33), defining the spin correlation functions \( \langle \Omega'_{r,r'} \rangle = \langle \Omega'_{r-r',0} \rangle \). The correlation functions \( \langle \Omega'_{l,0} \rangle \) differ from \( \langle \Omega_{l+1} \rangle \) only by the exchange of two \( X \)-operators. Therefore, for large \( l \), we may expect that

\[ \langle \Omega'_{l,0} \rangle \approx \langle \Omega_{l+1} \rangle. \] (38)

That leads after Fourier transformation to the contribution of the \( v'_{m,r} \) term to the spinon dispersion (Appendix A). Together with the contribution of \( v_{k,q} \) we obtain for the spinon dispersion

\[ \epsilon_s(Q - \pi)Z(Q) = \frac{J}{2} \left\{ \cos Q \left[ Z(Q) + \frac{1}{2} \right] + \frac{1}{2} \langle \Omega_{l,0} \rangle - \langle \Omega_1 \rangle - \frac{1}{2} \sin Q \int_0^{2\pi} \frac{d\kappa}{2\pi} Z(\kappa) \left( \cot \frac{Q - \kappa}{2} + \cot \frac{Q + \kappa}{2} \right) \right\}, \] (39)

and the hole spectral function becomes
\begin{equation}
A(k, \omega) = \int_{-\pi}^{+\pi} \frac{dQ}{\pi} Z(Q) \delta [\omega + 2t \cos(k - Q) - 2t_3 \cos 2(k - Q) - \epsilon_s(Q - \pi)].
\end{equation}

The curve that we obtained for $\epsilon_s$ with the formula (39) is close to
\begin{equation}
\epsilon_s(Q - \pi) \approx \alpha J \cos Q , \quad \alpha \approx 2. \tag{41}
\end{equation}
as shown in Fig. 1. The functional form (41) is consistent with Bethe-ansatz and field-theoretical considerations. (Sorella and Parola derived a contribution $J\pi/2 \cos Q \approx 1.6 J \cos Q$.) We tested it also by comparing the first two terms of Fourier expansion of the product $\cos Q Z(Q)$ with $(\Omega_{0,0})$ and $(\Omega'_{1,0})$ that give values for $\alpha$ in (11) of 2.1 or 1.8, respectively (for the pair correlation functions we took the data of Ref. 4). Therefore, we are using the simplified formula (41) instead of (39) in the following analysis of the spectral density. We have checked that the differences are negligible.

The spectral density (for $t_3 = 0$) is shown in Fig. 2. One can clearly distinguish between the spinon and holon features at the lower edge of the spectral density dispersing at an energy scale $\propto J$ (from $k = 0$ to $k = \pi/2$) or $\propto t$ (from $k = \pi/2$ to $k = \pi$). At $k = k^*$, which is determined by $t \cos k^* = J$, another holon branch splits off the lower edge of the spectrum and disperses towards $k = 0$ at an energy scale of $t$ (and a corresponding holon branch splits off the upper edge of the spectrum). For $k$ values inbetween 0 and $k^*$ one has three peaks in the spectral function (one spinon and lower and upper holon branch). One can easily imagine the situation in the doped case. Then the spinon and holon branches start at the Fermi energy with two different velocities.

In contrast to the 2D case there is no separate bound state at the lower edge of the spectrum indicating that there are only collective spin and charge excitations. Most of those features were also observed in the ARPES experiment. In the naive picture of spin-charge separation the spectral density would have square root singularities only either at the lower or at the upper edge of the spectrum. In Fig. 2, however, there are additional holon branches due to the square root singularity in $Z(Q)$ (see also Ref. 13). For $J \rightarrow 0$ the spinon feature in the spectral density, i.e. the lower edge of the spectrum, becomes completely flat between 0 and $\pi/2$. The corresponding pictures were already given in Ref. 11. Fig. 2 agrees also qualitatively with the finite cluster results.

V. MAJUMDAR-GHOSH MODEL

We have shown that our approach is applicable for any magnetic state for $J \rightarrow 0$. Now, we are going to present the spectral function of one hole in the $t$-$J$-$J'$ model with the special frustration $J' = J/2$ (called here Majumdar-Ghosh (MG) model for simplicity). In that case rigorous analytic results may be obtained since the ground-state wave function of the MG spin Hamiltonian is exactly known. It is the combination of two simple dimer states
\begin{equation}
\Psi_{MG} = (\Phi_1 + \Phi_2)/\sqrt{2}, \tag{42}
\end{equation}
where
\begin{equation}
\Phi_1 = \prod_{n = -\infty}^{+\infty} \left[ 2n, 2n + 1 \right] , \quad \Phi_2 = \prod_{n = -\infty}^{+\infty} \left[ 2n - 1, 2n \right],
\end{equation}
and the singlet bond is denoted as
\begin{equation}
[l, m] = \frac{1}{\sqrt{2}} \sum_\sigma \sigma X_l^{\sigma0} X_m^{-\sigma0} \langle \text{vac} \rangle.
\end{equation}

We are considering the MG model as a representative example for the case that there is a gap in the spin excitation spectrum (and also in the charge channel). To give the result for the spectral density in the strong coupling limit $J \rightarrow 0$ one has to find the modified quasiparticle residue $Z(Q)$ in (28). It can be simply derived from the correlation functions (see also Ref. 12)
\begin{equation}
\langle \Omega_i \rangle = \frac{1}{2} [\langle \Phi_1 | \Omega_i | \Phi_1 \rangle + \langle \Phi_2 | \Omega_i | \Phi_2 \rangle]
\end{equation}
\begin{equation}
\langle \Omega_{2n} \rangle = \left( -\frac{1}{2} \right)^n, \quad \langle \Omega_{2n+1} \rangle = \frac{1}{2} \left( -\frac{1}{2} \right)^{n+1}, \quad n \geq 0, \tag{43}
\end{equation}
in the following way.
\[
Z(Q) = \frac{1}{2} + \sum_{n=1}^{\infty} \left[ \left( \frac{1}{2} - \frac{e^{-iQ}}{4} \right) \left( -\frac{e^{2iQ}}{2} \right)^n + h.c. \right] = \frac{3}{2} \frac{1 + \cos Q}{5 + 4 \cos 2Q} .
\] (44)

The corrections for small \( J \ll t \) may only be derived approximatively and we present two methods, projection method and variational procedure having different accuracy.

A. Projection method

First we calculate the spinon dispersion \( \epsilon_s \) in the same way as it was done in the Heisenberg case in Sec. IV. But we should keep in mind that its applicability is less justified for the MG model than for the pure \( t-J \) model due to the much faster decay of spin correlation functions (compare (43) with (25)). As before, we approximate

\[
\langle \Omega''_{r,r'} \rangle \approx \langle \Omega_1 \rangle \langle \Omega_{r-r'} \rangle
\]

which results in a constant energy shift from the \( v''_{k,q} \) term. Therefore, the first contribution to \( \epsilon_s \) coming from \( \hat{J} \) is merely determined by

\[
\epsilon_{s,0}(Q - \pi) = 2J \cos Q .
\] (45)

We have a second contribution to \( \epsilon_s \) from \( \hat{J}' \)

\[
\epsilon_{s,J'}(Q - \pi) = J' \left[ -4 \cos Q + \frac{5}{4} + \cos 2Q \right] .
\] (46)

We see that for \( J' = J/2 \) the terms proportional \( \cos Q \) cancel and we find

\[
\epsilon_s(Q - \pi) = J \left[ \frac{5}{8} + \frac{1}{2} \cos 2Q \right] ,
\] (47)

which is symmetric around \( \pi/2 \).

The spectral density is presented in Fig. 3. We see that in contrast to the \( t-J \) model the structures coming from \( Z(Q) \) (the holon branches) are much less pronounced, whereas square root singularities exist at the lower and upper edges of the spectrum. Their intensities are proportional to \( Z(k) \) or \( Z(k - \pi) \) at the lower and upper edges, respectively. Therefore, the square root singularity vanishes for \( k = \pi \) at the lower edge. Furthermore, one can see that the low energy region for \( k \) between \( \pi/2 \) and \( \pi \) being empty in Fig. 2 is now filled with states. The spectrum becomes more symmetric around \( \pi/2 \) and the low-energy edge is given by the spinon dispersion \( \epsilon_s(Q) \). The strong damping of the holon branch is due to the suppression of the singularity at the spinon Fermi edge (at \( Q = \pi/2 \) in \( Z(Q) \)). It is a universal feature for any 1D magnetic state having a gap in the spin excitation spectrum. The suppression of holon weight was also found by Voit for the Luther-Emery phase in the Luttinger liquid. The form of the spectral density in Fig. 3 resembles also roughly the exact diagonalization study in Ref. 12. But a single bound state with a finite spectral weight that was obtained there, is missing in Fig. 3. That deficiency is due to the special projection procedure which can only result in a continuous spectral density. Therefore, one has to go beyond the projection method.

B. Variational ansatz

Here we will use the set of string operators \( \{v_{k,r}\} \) as a set defining a variational wave function for the whole Hamiltonian. Due to the knowledge of the exact ground-state \( \Omega_1 \) all necessary matrix elements can be calculated without any further approximation. More precisely, we will diagonalize the Hamiltonian \( \hat{H} = \hat{t} + \hat{J} + \hat{J}' \) in the space spanned by the set of basis operators

\[
v_{k,r} = \frac{1}{\sqrt{L}} \sum_{m=-\infty}^{\infty} e^{ik(m+r)}v_{m,r} ,
\] (48)

where \( L \) is the number of lattice sites and \( v_{m,r} \) was defined in (18). For that purpose one has to calculate the overlap matrix resulting in

\[
S_{r,r'} = \langle \{v_{k,r}, v_{k,r'}^\dagger\} \rangle = \frac{1}{2} \langle \Omega_{r-r'} \rangle .
\] (49)
The kinetic energy part of the Hamilton matrix is given by:

\[
\frac{t}{2} E_{r,r'}^k = \left\{ v_{k,r} \hat{t}, v_{k,r'}^\dagger \right\} = \frac{t}{2} \left( e^{ik \Omega_{r-r'-1}} + e^{-ik \Omega_{r-r'+1}} \right).
\]

(50)

The calculation of the exchange part of the Hamilton matrix is quite lengthy but straightforward. It shall not be given here in detail. To present the results we define a matrix \( E_x \):

\[
\frac{J}{4} E_{r,r'}^x = \left\{ v_{k,r} \hat{J} + \hat{J}', v_{k,r'}^\dagger \right\},
\]

(51)

whose matrix elements are listed in Appendix C. The Hamilton matrix is then given by

\[
E = \frac{t}{2} E^k + \frac{J}{4} E^x,
\]

(52)

and the matrix GF

\[
G_{r,r'} = \langle \langle v_{k,r} | v_{k,r'}^\dagger \rangle \rangle
\]

(53)

can be found by solving the equation

\[
(\omega + i\Gamma + -E S^{-1}) G = S, \quad \Gamma > 0.
\]

(54)

Finally, the GF \( G(k,\omega) = 2G_{0,0} \).

The numerical results for \( J = 0 \) and \( J = 0.4 \) at three different momenta are presented in Fig. 4. The curves for \( J = 0 \) coincide with the analytic expression \( \epsilon_s(Q) \). A number of 400 basis functions and a broadening of \( \Gamma = 0.05 \) are sufficient to reach the thermodynamic limit in contrast to the exact diagonalization method yielding only a sequence of \( \delta \)-peaks. For \( J = 0.4 \) we can confirm the features found by the projection method, i.e. the low energy intensity between \( \pi/2 \) and \( \pi \), the symmetric spinon dispersion and the overdamped holon branch. In addition, the exchange terms produce two new features not present in Sec. VA: a resonance peak near zero energy and a bound state below the continuum. The resonance peak is visible near \( k = \pi \) and becomes an antiresonance near \( k = 0 \). Careful inspection of the exact diagonalization data indicates also a very high peak at the resonance position for \( k = \pi \) and a small gap at \( k = 0 \), but a better understanding of the resonance/antiresonance feature is still required.

The bound state is not visible in Fig. 4 due to the broadening \( \Gamma \) which is too large. Instead, we present in Fig. 5 the spectral weight of the lowest eigenstate \( \epsilon_1 \) for \( k = \pi/2 \) and \( J = 0.4 \) in dependence on the number of basis functions. It is clearly seen that the weight tends to a constant value \( \epsilon_1 \approx 0.1 \) in difference to the weight \( \epsilon_3 \) of the third eigenstate.\( \epsilon_3 \) At the same time, the separation \( \epsilon_1 = E_3 - E_1 \) between the first and the third eigenvalues \( E_1/3 \) stays finite for \( N \to \infty \) but the separation is very small \( (\epsilon_1 \approx 0.02 \text{ in units of } t) \). For \( J = 0 \), both \( \epsilon_1 \) and \( \epsilon_1 \) tend to zero for \( N \to \infty \). That means that the bound state is connected with the presence of a gap in the spin excitation spectrum.

VI. IDEAL PARAMAGNETIC STATE

Such a state is realized for very high temperatures \( T \), much larger than the exchange energy \( k_B T \gg J \). In that case spins at neighboring sites are completely uncorrelated. But the temperature is assumed to be lower than the Hubbard \( U \) such that the constraint of no double occupancy is preserved. Then the correlation functions become simply

\[
\langle \Omega_l \rangle = \left( \frac{1}{2} \right)^l,
\]

which results in

\[
Z(Q) = 3 \frac{1}{8^{1/4} + \cos Q}.
\]

(55)

The calculation of the spinon part (without frustration) gives

\[
\epsilon_s(Q - \pi) = \frac{J}{2} \left[ 2 \cos Q + \frac{1}{2} \right].
\]

(56)
To calculate it one has to note that (38) is no approximation in the present case. The effect of the \( \langle \Omega''_{r,r'} \rangle \) terms can only be treated approximatively (see (37)) but it was checked by the variational method that its influence on the spectral function can be neglected.

The information on \( Z(Q) \) and \( \epsilon_s \) is sufficient to calculate the spectral function (Fig. 6). It is surprising that the strong singularities at the band edges survive despite the large temperature. The lower edge disperses according to the dispersion of the spinon (56) with a width proportional to \( J \) and has its minimum at \( k = \pi \) (in contrast to the frustrated case Fig. 3 with a minimum at \( k = \pi/2 \)). But a peak connected with the holon dispersion proportional to \( t \) is not seen in Fig. 6. Such a peak appears in the finite temperature spectral function of the 2D \( t-J \) model and it can be expected since the first moment of the spectral function disperses according to \( t \cos k \). Its absence in 1D is a nontrivial and unexpected result. It can be understood in the present context since the holon branch is strongly damped due to the suppression of the singularity in \( Z(Q) \) at \( Q = \pi/2 \). Apparently, that suppression is more strong in (55) than in the frustrated case (44) such that the holon branch is still visible in Fig. 3 but it disappears nearly in Fig. 6. One should note that the above result holds only in the region \( J \ll k_B T \ll U \). One may speculate that a further increase of the temperature such that the constraint of no double occupancy is lifted should lead to drastic changes in the spectral function. The strong singularities at the lower or upper band edges should disappear and a free dispersion should become visible.

**VII. CONCLUSION**

In conclusion we could derive analytic expressions for the spectral function of one hole in several magnetic states. The expressions are rigorous in the limit \( J \to 0 \), but our approach allows also to calculate the small \( J \) corrections. We analyzed the frustration and temperature effects. Results were given for the special frustration \( J' = J/2 \) with a gap in the spin excitation spectrum and for the ideal paramagnetic case. Both effects, frustration and temperature, lead to low-energy excitations between \( \pi/2 \) and \( \pi \), and to a strong damping of the holon branches in the spectral function caused by the suppression of the singularity at the Fermi edge of spinons. The exchange terms in the MG model were found to be responsible for the finite weight of the lowest eigenstate and its finite, but small, energy separation from the rest of the spectrum, i.e. the bound state. The proposed scenario of holon branch damping seems to be a universal feature of frustration and temperature. Therefore, our results are of direct importance for photoemission experiments on strongly frustrated 1D compounds like CuGeO\(_3\), for instance. However, edge-shared cuprate chains have a smaller energy scale and less ideal 1D behavior in comparison with corner-shared compounds, which hinders direct comparison with experiment. But it cannot be excluded that a small frustration is also present in SrCuO\(_2\) such that our study gives one possible reason, why no real, separate holon branch could be observed in the experimental spectra of SrCuO\(_2\) between \( k = 0 \) and \( \pi/2 \). In the spin gap case we found a very small energy separation of the bound state from the continuum such that it is nearly impossible to detect it in a photoemission experiment.

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Appendix A: Spinon dispersion of the Heisenberg case

In this Appendix we outline the main steps to derive the spinon dispersion of the pure t-J model using the projection method. For long chains of X-operators it is convenient to introduce the notations:

\[ \sum_{\alpha_1, \ldots, \alpha_r} X_{n_1}^{\alpha_1} \cdots X_{n_r}^{\alpha_r} \equiv (n_1|n_2| \cdots |n_r) \]

and

\[ \sum_{\sigma, \alpha_1, \ldots, \alpha_r} X_{n_1}^{\alpha_1 \sigma} \cdots X_{n_r}^{\alpha_r \sigma} \equiv (n_1|n_2| \cdots |n_r) . \]

which means especially that (18) may be rewritten as \( v_{m,r} \equiv (m|m + g|m + 2g) \cdots |m + r) \). In such a notation we obtain for the commutation with the Heisenberg Hamiltonian

\[ \left[ X_m^{\sigma 0}, \hat{J} \right] = -\frac{J}{2} \sum_{g, \gamma} X_m^{\sigma \gamma} X_m^{\gamma 0} = -\frac{J}{2} \sum_{g} (m + g|m) , \]

(A.1)

and

\[ \left[ X_m^{\alpha \beta}, \hat{J} \right] = \frac{J}{2} \sum_{g, \gamma} (X_m^{\gamma \alpha} X_{m+g}^{\gamma \beta} - X_m^{\alpha \gamma} X_{m+g}^{\gamma \beta}) = \frac{J}{2} \sum_{g} \{(m|m + g| - (m + g|m) \} , \]

(A.2)

and then

\[ \left[ v_{m,r}, \hat{J} \right] = \frac{J}{2} \{(m|m - g|m + g|m + 2g) \cdots |m + r) - (m - g|m + g|m + 2g) \cdots |m + r) \]

\[ -(m + g|m + 2g) \cdots |m + r) - (m|m + r - g|m + r + g|m + r) \} , \]

(A.3)

where \( g = \text{sign}(r) \). In deriving (A.3) it is important that the commutation of the ”inner” operators \( X_{m+l}^{\alpha \beta} \) with \( l < r \) do not give rise to additional terms since the corresponding sums cancel each other. That is a direct consequence of one-dimensionality.

Now, we consider the holon contribution to \( \epsilon_s \) coming from \( v_{k,q}^{\prime} \)

\[ \left\langle \left\{ v_{k,q}^{\prime}, v_{k',q'}^{\dagger} \right\} \right\rangle = 2\pi \delta(k - k') \sum_{r,r'} e^{i q(r'-r) + i q r} \Omega_{r,r'}^{\prime} \]

(A.4)

with

\[ \Omega_{r,r'}^{\prime} = (m|m + r - g|m + r + g|m + r + g'| \cdots |m + r - r') , \]

(A.5)

and \( g = \text{sign}(r) \), \( g' = \text{sign}(r') \). We see that in general \( \Omega_{r,r'}^{\prime} \) depends both on \( r \) and \( r' \). Eqn. (A.4) can also be written as

\[ \left\langle \left\{ v_{k,q}^{\prime}, v_{k',q'}^{\dagger} \right\} \right\rangle = 2\pi \delta(k - k') \sum_{l} e^{i(k-q)l} S_l \]

(A.6)

with

\[ S_l = \sum_{r=-\infty}^{+\infty} e^{-i(q-q')r} \Omega_{r,r-l}^{\prime} . \]

Due to the slow decay of spin correlation functions in the 1D Heisenberg state, one can expect that the main contribution to \( S_l \) comes from regions where \( |r| \gg |l| \). There holds \( g = g' \) and we may rewrite and approximate (A.5) by

\[ \langle \Omega_{r,r-l}^{\prime} \rangle = \langle 0| \cdots |l)(r + g|r) \approx \langle \Omega_l \rangle \]

(A.6)

Then, the explicit dependence on \( r \) drops out and we obtain
\[ \langle \{ v_{k,q}', v_{k',q}' \} \rangle = 8\pi^2 \delta(k-k')\delta(q-q')Z(k-q+\pi)\langle \Omega_1 \rangle , \quad (A.8) \]

i.e. a simple constant shift of the energy \( \epsilon_s \).

The contribution of the \( v_{k,q}' \) term to the spinon dispersion is determined by the sequence of spin operators

\[ \Omega'_{r,r'} = (m|m-g|m+g|\ldots|m+r|m+r-g'|\ldots|m+r-r'|) \quad (A.9) \]

instead of (A.5). The expectation value of that term has to be calculated for the magnetic system without holes. In difference to \( \langle \Omega''_{r,r'} \rangle \), it depends only on \( r-r' \) without further approximation

\[ \langle \Omega'_{r,r} \rangle = \langle \Omega'_{l,0} \rangle = \langle 0 \mid -1 \mid 1 \mid \ldots \mid l \rangle , \quad (l > 0) , \quad (A.10) \]

and \( \langle \Omega'_{-l,0} \rangle = \langle \Omega'_{l,0} \rangle \). For \( l = 0, 1 \) it can be expressed through pair correlation functions

\[ \langle \Omega'_{0,0} \rangle = \frac{1}{2} + 2\langle S_0 S_2 \rangle , \]

\[ \langle \Omega'_{1,0} \rangle = \frac{1}{4} + 2\langle S_0 S_1 \rangle + \langle S_0 S_2 \rangle . \]

For large \( l > 0 \) we may expect

\[ \langle \Omega'_{l,0} \rangle \approx \langle \Omega_{l+1} \rangle . \quad (A.11) \]

Using this approximation we obtain the following contribution to the spinon dispersion \( \epsilon_s \) which stems from the \( v_{k,q}' \) term

\[ \frac{J}{2} \langle \{ v_{k,q}', v_{k',q}' \} \rangle = 8\pi^2 \delta(q-q')\delta(k-k')\epsilon_s'(k-q)Z(k-q+\pi) \quad (A.12) \]

with

\[ \epsilon_s'(k)Z(k+\pi) = \frac{J}{4} \sum_{l=-\infty}^{+\infty} e^{-ikl} \langle \Omega'_{l,0} \rangle . \quad (A.13) \]

After some algebra we find

\[ 4\epsilon_s'(Q-\pi)Z(Q)/J = \langle \Omega'_{0,0} \rangle - 2\langle \Omega_1 \rangle - 2 \cos Q \left[ Z(Q) - \frac{1}{2} \right] - \sin QY(Q) , \quad (A.14) \]

where

\[ Y(Q) = \sum_{l=1}^{+\infty} 2(-1)^l \sin(Ql)\langle \Omega_l \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\kappa Z(\kappa) \left[ \cot \frac{Q-\kappa}{2} + \cot \frac{Q+\kappa}{2} \right] . \quad (A.15) \]

The complete expression for the spinon dispersion follows from

\[ \epsilon_s(Q-\pi) = J \cos Q + \epsilon_s'(Q-\pi) + \text{const} , \]

and is given in Eqn. (39) neglecting the constant energy shift.
Appendix B: Majumdar-Ghosh model with projection method

The commutation with the frustration Hamiltonian \([14]\) is very similar to \([A.3]\). It gives

\[
\left[ v_{m,r}, \hat{J} \right] = \frac{J'}{2} \left\{ v_{m,r}^{(3)} + v_{m,r}^{(4)} \right\}
\]

(B.1)

where

\[
v_{m,r}^{(3)} = \{(m|m - 2g|m + g| \ldots |m + r| - (m - 2g|m + g| \ldots |m + r|)
- (m|m + g|m + 2g| \ldots |m + r| + (m|m + g|m - g|m + 2g| \ldots |m + r|)
- (m|m - g|m + g| \ldots |m + r|) \},
\]

\[
v_{m,r}^{(4)} = \{- (m| \ldots |m + r - g|m + r + 2g|m + r|)
- (m| \ldots |m + r - 2g|m + r + g|m + r - g|m + r|
+ (m| \ldots |m + r - g|m + r + g|m + r) \} .
\]

(B.2)

Again we see that all terms coming from commutations at “inner” operators cancel. But now the motion of spinons becomes more complicated. The same considerations that show the absence of dispersion from the \(v_{m,r}''\) term are applicable to \(v_{m,r}^{(4)}\).

Taking into account that

\[
\langle \Omega_{0,0}' \rangle = \frac{1}{2}, \quad \langle \Omega_{2n,0}' \rangle = - \frac{1}{4} \left( - \frac{1}{2} \right)^n, \quad \langle \Omega_{2n-1,0}' \rangle = \left( - \frac{1}{2} \right)^n, \quad n > 0,
\]

we obtain the following contributions to \(\epsilon_s = \epsilon_{s,J} + \epsilon_{s,J'}\) (we drop dispersionless terms). From \(\hat{J}'\) comes

\[
\epsilon_{s,J}(Q - \pi)Z(Q) = \frac{J'}{2} \left[ 2 \cos QZ(Q) + Z'(Q) \right],
\]

\[
Z'(Q) = \frac{3(-1 + \cos Q)}{5 + 4 \cos 2Q} + \frac{1}{4} + \frac{1}{8} = Z(Q)2 \cos Q .
\]

(B.3)

Thus

\[
\epsilon_{s,J}(Q - \pi) = 2J \cos Q
\]

(B.4)

has the same form \([14]\) that we have assumed for the \(t-J\) model.

For the term that comes from the left distorted end of \(v_{m,r}\) due to \(\hat{J}'\) we have

\[
\langle \left\{ v_{m,r_1}^{(3)}, v_{m+r_1-r_2,r_2}^{(3)} \right\} \rangle = \frac{1}{2} \langle \Omega_{r_1-r_2}'^{(3)} \rangle,
\]

\[
\langle \Omega_{2n}^{(3)} \rangle = \left( - \frac{1}{2} \right)^n, \quad \langle \Omega_{2n-1}^{(3)} \rangle = -4 \left( - \frac{1}{2} \right)^n, \quad n > 1,
\]

\[
\langle \Omega_{0}^{(3)} \rangle = \left( - \frac{1}{2} \right), \quad \langle \Omega_{1}^{(3)} \rangle = \frac{5}{4}.
\]

The contribution from \(\hat{J}'\) is

\[
\epsilon_{s,J'}(Q - \pi)Z(Q) = \frac{J'}{2} \left[ -4Z'(Q) + \frac{3}{4} + \frac{6}{8} \cos Q \right]
\]

\[
= Z(Q)\frac{J'}{2} \left[ -8 \cos Q + 2 \left( \frac{5}{4} + \cos 2Q \right) \right]
\]

(B.5)

and we obtain \([14]\).
Appendix C: Matrix elements of the variational basis set

The matrix elements of $E_{r,r'}^x$ in the neighborhood of $r, r' = 0$ are given by:

| $r'$ | -3 | -2 | -1 | 0 | 2 | 3 |
|------|----|----|----|---|---|---|
| -3   | 3/8| 0  | 3/16| -3/32| -9/32| 3/32| 3/16 |
| -2   | 0  | 3/8| -9/16| 3/8 | 0  | -3/8| 3/32 |
| -1   | 3/16| -9/16| 3/8 | -3/16| 3/8 | 0  | -9/32|
| 0    | -3/32| 3/8 | -3/16| 0  | -3/16| 3/8 | -3/32|
| 1    | -9/32| 0  | 3/8 | -3/16| 3/8 | -9/16| 3/16 |
| 2    | 3/32| -3/8| 0  | 3/8 | -9/16| 3/8 | 0  |
| 3    | 3/16| 3/32| -9/32| 3/32| 3/16| 0  | 3/8 |

One has two different regions in the matrix. The first one is defined for $r > 0$, $r' > 0$ and $r \geq r' + 2$ where we have

$$E_{r,r'}^x = \frac{3}{8} \left( \frac{-1}{2} \right)^{n-m}, \quad E_{r,r'}^x = \frac{3}{8} \left( \frac{-1}{2} \right)^{n-m},$$

and the second one for $r' \leq -2$, $r \geq 2$ with

$$E_{r,r'}^x = -\frac{3}{2} \langle \Omega_{r-r'} \rangle.$$

There are special matrix elements along the diagonal (3/8) and along the side diagonal (alternatively -9/16 or 0) and also for the two lines ($n \geq 1$):

$$E_{2n,0}^x = -\frac{3}{4} \left( \frac{-1}{2} \right)^n, \quad E_{2n+1,0}^x = \frac{3}{16} \left( \frac{-1}{2} \right)^n,$$

$$E_{2n,-1}^x = 0, \quad E_{2n+1,-1}^x = \frac{9}{16} \left( \frac{-1}{2} \right)^n.$$

The matrix is filled by

$$E_{r',-r'}^x = E_{r',r}^x = E_{r',r}^x.$$
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Figures

Fig. 1: Comparison of the spinon dispersion $\epsilon_s(Q - \pi)$ as calculated from the projection method (broken line, $J = 0.4$) with $2J \cos Q$ (full line).
Fig. 2: Spectral density of the $t$-$J$ model for $J = 0.4$ and $t = 1$.
Fig. 3: Spectral density of the frustrated $t$-$J$ model ($J = 0.4$ and $t = 1$) at the special frustration $J' = 0.5J$ (using the Majumdar-Ghosh wave function) within the projection method.
Fig. 4: Spectral density of the Majumdar-Ghosh model $A(k, \omega)$ for three different momenta $k/\pi$ and $t = 1$, $J = 0.4$ (full lines) or $J = 0$ (dashed lines) with a variational set of 400 basis functions and a broadening of $\Gamma = 0.05$.
Fig. 5: Weight $w_1$ and energy separation $\epsilon_1 = E_3 - E_1$ of the lowest eigenvalue $E_1$ at $k/\pi = 0.5$, $t = 1$, $J = 0.4$ (full lines) as a function of the inverse number of basis functions $1/N$. The dashed lines are the weights $w_3$ and the energy separation $\epsilon_3 = E_5 - E_3$ of the third eigenvalue $E_3$.
Fig. 6: Spectral density of the $t$-$J$ model ($J = 0.4$ and $t = 1$) in the ideal paramagnetic state.
The graph shows the spectral density as a function of energy for different values of $k/\pi$. The energy is plotted on the x-axis, and the spectral density is plotted on the y-axis. The values of $k/\pi$ range from 0 to 5/6.