Spectral function of the spiral spin state in the trestle and ladder Hubbard model

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Eder and Ohta have found a violation of the Luttinger rule in the spectral function for the t-t’-J model, which was interpreted as a possible breakdown of the Tomonaga-Luttinger(TL) description in models where electrons can pass each other. Here we have computed the spin correlation along with the spectral function for the one-dimensional t-t’ Hubbard model and two-leg Hubbard ladder. By varying the Hubbard U, we have identified that such a phenomenon is in fact a spinless-fermion-like behavior of holes moving in a spiral spin configuration that has a spin correlation length of the system size.

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It is widely believed that the low-energy physics of a wide class of one-dimensional (1D) systems can be described as a Tomonaga-Luttinger(TL) liquid, which is an effective theory for electrons interacting in 1D. The ansatz has indeed been shown to be valid for exactly solvable 1D models such as the Hubbard model or the supersymmetric t-J model, and also for some other models numerically. However, recently, Eder and Ohta looked into the spectral function in 1D t-J model that has t’ (t-t’-J model), and made a very interesting observation that the density of electrons n and Fermi momentum k_F are related with k_F = πn in a certain parameter regime, which is incompatible with the Luttinger relation, k_F = πn/2, expected for a TL liquid, which they suggest to be an indication for a breakdown of the TL description.

In order to clarify the origin of such an curious behavior, here we study the t-t’ Hubbard model with finite values of U. The reason we have chosen the Hubbard model is that the magnetic phase diagram on the n-U plane has been obtained for the t-t’ Hubbard model by Daul and Noack (inset of Fig.2) so that we can identify the region on which we work. For the Hubbard model we find the same curious behavior of the spectral function. We further find that the state in question is a spiral spin state, in which the spin correlation has a wave length of the system size and thus has a local ferromagnetic nature. The curious behavior of the spectral function can be understood by a picture in which holes can hop almost freely in such a spin background as originally proposed by Doucot and Wen as a trial state for finite systems to prove the instability of Nagaoka’s ferromagnetism. The ferromagnetic-like state naturally explains the doubling of k_F into πn as a spinless-fermion-like behavior. The region over which the spiral behavior appears is indeed consistent with the phase diagram for the t-t’ Hubbard model. In order to see if the appearance of the spiral state extends to other quasi-1D systems, we have also studied the 2-leg Hubbard ladder with U = ∞, and have found similar features as in the t-t’ Hubbard model.

The t-t’ Hubbard Hamiltonian is given by

\[ H = -t \sum_{i=1}^{L} \sum_{\sigma} (c_{i\sigma}^d c_{i+1,\sigma} + H.c.) + t' \sum_{i=1}^{L} \sum_{\sigma} (c_{i\sigma}^d c_{i+2,\sigma} + H.c.) + U \sum_{n=1}^{L} n_{i\uparrow} n_{i\downarrow}, \]

in standard notations. Hereafter we set t = 1.

First we numerically calculate, with the continued fraction expansion, the single-particle spectral function given by

\[ A^\pm(k, \omega) = \frac{1}{\pi} \text{Im} \langle \Phi_G | \gamma_0^\pm | \omega \pm \left( E_0 - H \right) - i0 \rangle | \Phi_G \rangle \]

(1)

where \( A^+ (A^-) \) denote the electron addition (removal) spectrum with \( \gamma_{0}^\pm \equiv \gamma_{k\sigma}^\pm, \gamma_{k\sigma}^\pm \equiv (\gamma_{k\sigma}^\pm)^\dagger, | \Phi_G \rangle \) and \( E_0 \) the ground state and its energy, respectively. In Fig. (a) we show the results for the case of 10 electrons on a 12 site ring, \( U = 40(a) \) and \( U = 20(b) \) for \( t' = 0.2 \). We can see that for \( U = 20, k_F = \pi n/2 \) \( (n = 10/12) \) is satisfied, while the equality is violated in favor of \( k_F = \pi n \) for \( U = 40, \) which would be expected for spinless fermions. Such a behavior persists for larger values of \( U \). Thus this situation is indeed similar to the results for the t-t’-J model obtained by Eder and Ohta.

At this stage, let us recall the phase diagram of the t-t’ Hubbard model obtained by Daul and Noack with the density matrix renormalization group (DMRG) method in open boundary conditions. For \( t' = 0.2, n \sim 1 \) and large \( U \), they found a large ferromagnetic region in the
phase diagram. If the periodic boundary condition (PBC) is assumed, on the other hand, the ground state is \( S = 0 \) for any value of \( U \) at least for system sizes up to 12 sites as also pointed out by Daul and Noack. We find here that the region in the \( n-U \) plane over which the spinless-fermion-like behavior of \( A(k, \omega) \) is observed roughly coincides with the ferromagnetic region in the Daul-Noack phase diagram.

Such an observation has motivated us to look into the spin-spin correlation function, \( \langle \Phi_G | S_i^z S_j^z | \Phi_G \rangle \), to identify the nature of the \( S = 0 \) ground state in PBC. We show in Fig. 2 the result for 10 electrons in a 12-site ring with \( U = 20, 40 \). We can see that for \( U = 40 \), which belongs to the spinless-fermion-like region, the spin-spin correlation indeed indicates the spiral spin state with the spin correlation being as large as the system size. Such a spiral spin-spin correlation has also been encountered rather ubiquitously in 1D for Tasaki’s model, double exchange model, the Kondo lattice model, and also in the 2D Hubbard model with \( U = \infty \) for two holes.

Nature of such a spiral state has been discussed by Doucot and Wen (DW)[1], who studied the infinite-\( U \) Hubbard model with two holes, and found a trial state which gives an energy lower by inverse system size than the Na-gaoka’s ferromagnetic state. The key idea of DW is based on the following intuition. Holes behave as free fermions for on-site interactions when the background spin state is ferromagnetic (or nearly so). Then we have only to worry about the fermion statistics, i.e., the antisymmetry (node) in the wave function against the exchange of two holes. If we impose the node upon the spin part, the kinetic energy of holes can be lowered. This is accomplished by twisting the spin alignment in a full turn, but very slowly over the entire sample dimension to minimize the cost in energy and to maintain the ferromagnetic nature. Another way of saying is that the spiral spin texture generates a fictitious gauge flux which absorbs the frustration induced by the fermion statistics of the holes. Indeed the flux mimics an Aharonov-Bohm of half flux quantum to shift the k-points by half the k-point spacing to let an even number of spinless fermions take a closed shell configuration.

While these are conceived for the ordinary Hubbard model, it is intriguing to study whether the spinless-fermion-like behavior of \( A(k, \omega) \) found here for the quasi-1D system can be understood quantitatively in terms of the DW state. Although in the original paper DW considered the states in which the holes are dressed by spin waves as well, let us consider the state where holes hop in a rigid spin background for simplicity. The energy of the hole in the t-U Hubbard model is then given as

\[
\varepsilon = -2t \cos \left( \frac{\pi}{L} \right) \cos \left( \frac{2N \pi}{L} \pm \frac{\pi}{L} \right) + 2't \cos \left( \frac{2\pi}{L} \right) \cos \left( \frac{4N \pi}{L} \pm \frac{2\pi}{L} \right),
\]

where \( N \) is an integer with \( 0 < N < L \) and \( \pm \) corresponds to the sign of the fictitious flux. In Fig. 1(a), we plot the energy dispersion defined by the equation (2). We can see that the single-particle spectrum is reproduced remarkably well.

In the result for the addition spectrum an almost dispersionless band of low intensity peaks is seen (at around \( E = 2 \) in Fig. 1(a)). If the ground state were a fully spin-polarized ferromagnetic state, then such a band is trivially expected, since we can add an opposite spin at any k-point. Remnant of such a band again suggests the ferromagnetic nature of the present ground state.

A next question is whether the spiral state persists for more than two holes. In Fig. 3, we show the spin-spin correlation for 6 electrons on a 12-site lattice (\( n = 0.5 \); quarter filled) in PBC for \( U = 4, 6 \). We can see that for \( U = 6 \), the spin-spin correlation is again spiral. To investigate whether Doucot and Wen’s picture is valid for such an intermediate doping, we have calculated the single-particle spectrum for \( U = 6 \) in Fig. 3(a), \( U = 4 \) in Fig. 3(b). We can see that the nature of the spectrum also changes between \( U = 4 \) and \( U = 6 \). The spectrum for the spiral state is fitted well by the energy dispersion defined by the eq. (3)(dashed curves in Fig. 3(a)) even though the hole concentration is as large as \( n_h = 0.5 \). This is surprising, since the assumption that holes are nearly free would be valid only for infinitesimal doping. For detailed energetics the sample size dependence need be studied.

We next question whether the antiferromagnetic state is connected adiabatically to the spiral state as we increase the Hubbard \( U \). We show the ground-state energy as a function of \( U \) for 6 electrons on a 12-site ring in Fig. 4. We can clearly identify a level crossing appearing as a cusp around \( U \sim 5 \), which indicates that a transition occurs within the \( S = 0 \) space from the antiferromagnetic phase (low-\( U \) side) to the spiral phase (high-\( U \) side).

Finally, we move on to the 2-leg Hubbard ladder. Ferromagnetic behavior is also found in the ladders where \( U \) is infinite[4], so it is intriguing to study whether a spiral state appears in this system as well, and if so, whether \( A(k, \omega) \) exhibits a DW-like behavior. The Hamiltonian is given by

\[
\mathcal{H} = -t \sum_{i=1}^{L} \sum_{\alpha, \sigma} (c_{i\alpha \sigma}^\dagger c_{i+1 \alpha \sigma} + \text{H.c.}) -t \sum_{i=1}^{L} \sum_{\sigma} (c_{i1 \sigma}^\dagger c_{i2 \sigma} + \text{H.c.}) + U \sum_{n=1}^{L} \sum_{\alpha} n_{i\alpha \uparrow} n_{i\alpha \downarrow},
\]

where \( \alpha = (1, 2) \) labels the two legs of the ladder. We set \( t = 1 \), \( U = \infty \) and we consider only the case of two holes.

We have calculated the spin-spin correlation \( \langle S_{i\alpha}^z \rangle \langle S_{j\alpha}^z \rangle \) (not shown), and found that the ground state is indeed spiral. We have also calculated the single-particle excitation, eq. (4), where we now take \( \gamma_{k\sigma}^+ = c_{k1\sigma}^\dagger + c_{k2\sigma}^\dagger \) (bonding states) or \( \gamma_{k\sigma}^+ = c_{k1\sigma}^\dagger - c_{k2\sigma}^\dagger \) (antibonding states). In
Fig. 6, we show the result for two holes (14 electrons on a 8 × 2 ladder). We fit the spectrum by a two-band extension of eq.(2),
\[ \varepsilon = -2t \cos \left( \frac{\pi}{L} \right) \cos \left( \frac{2N\pi}{L} \pm \frac{\pi}{T} \right) \pm t. \]  
(3)

Fig. 3 shows that the picture of two holes hopping in a twisted spin background is surprisingly accurate.

To summarize, we have pointed out that the behavior of the spectral function found by Eder and Ohta for the t-t’-J model can be understood as a realization of the spiral spin state. As mentioned above, the fully polarized ferromagnetic state is the ground state for the open-boundary t-t’ Hubbard ladder. This is also the case with the open-boundary Hubbard ladder (Figs. 1, 2) and their spin stiffness.

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**FIG. 1.** Full single particle spectral function for 10 electrons on a 12 site t-t’ lattice, U=40 (a) and U=20 (b). Solid line denotes the electron removal spectrum, while dotted line the electron addition spectrum. Dashed curves in (a) indicate the energy dispersion defined by eq.(2).

**FIG. 2.** The spin-spin correlation function for 10 electrons on a 12 site lattice, \(U=20\) (solid line) and \(40\) (dashed line) with the periodic boundary condition. The inset shows the phase boundary of the ferromagnetic phase (solid curve) due to Daul and Noack\(^2,3\) on which the present identification of the spiral phase (solid straight lines) is indicated for \(n=10/12\) (Figs. 1,2) and \(n=6/12\) (Figs. 3,4).

**FIG. 3.** A plot similar to Fig. 2 for 6 electrons on a 12 site t-t’ lattice, \(U=4\) (solid line) and 6 (dashed line).

**FIG. 4.** A similar plot to Fig. 1 for 6 electrons on a 12 site t-t’ lattice, \(U=6\) (a) and \(U=4\) (b).

**FIG. 5.** The ground state energy for 6 electrons on a 12 site t-t’ lattice as a function of 1/\(U\).

**FIG. 6.** A similar plot to Fig. 1 for 14 electrons on a 8 × 2 ladder. Dashed curves indicate the dispersion defined by eq.(3).
Fig. 1(a)

R. Arita et al, Phys. Rev. B
Fig. 1 (b)

R. Arita et al, Phys. Rev. B
Fig. 2

R. Arita et al, Phys. Rev. B
Fig. 3

R. Arita et al, Phys. Rev. B
Fig. 4(a)

R. Arita et al, Phys. Rev. B
Fig. 4(b)

R. Arita et al, Phys. Rev. B
Fig. 5

R. Arita et al, Phys. Rev. B
Fig. 6

R. Arita et al, Phys. Rev. B