Charge and spin fractionalization beyond the Luttinger-liquid paradigm

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It is well established that at low energies one-dimensional (1D) fermionic systems are described by the Luttinger-liquid (LL) theory, which predicts phenomena such as spin-charge separation and charge fractionalization into chiral modes. Here we show through the time evolution of an electron injected into a 1D t-J model, obtained with time-dependent density matrix renormalization group, that a further fractionalization of both charge and spin takes place beyond the hydrodynamic limit. Its dynamics can be understood at the supersymmetric point \( J = 2t \) in terms of the excitations of the Bethe-ansatz solution. Furthermore we show that fractionalization with similar characteristics extends to the whole region corresponding to a repulsive LL.

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I. INTRODUCTION

There is a sustained interest in the physics of one-dimensional (1D) quantum systems due to recent experimental advances that allow one to access exotic phenomena such as spin-charge separation and charge fractionalization. At low energies these systems are well described by the Luttinger-liquid (LL) theory, which predicts phenomena such as spin-charge separation and charge fractionalization into chiral modes. Experimental evidence of its existence has been observed in quasi-1D organic conductors, and spin-charge separation. Experimental evidence of its existence has been observed in quasi-1D organic conductors,3 semiconductor quantum wires,4 and quantum chains on semiconductor surfaces.5 The LL theory also predicts the fractionalization of injected charge into two chiral modes (left going and right going),6–10 a phenomenon recently confirmed experimentally.11 Along the experimental advances also theoretical progress was recently achieved pertaining to extensions beyond the LL limit by incorporating nonlinearity of the dispersion, leading to qualitative changes in the spectral function12–16 and relaxation processes of 1D electronic systems.17

Here we show that fractionalization of charge and spin beyond the forms described by LL theory takes place when a spin-1/2 fermion is injected into a strongly correlated 1D system, namely the t-J model. By studying the time evolution of the injected wave packet at different wave vectors \( k \), using time-dependent density matrix renormalization group (t-DMRG),18–23 different regimes are obtained. When \( k \) is close to the Fermi wave vector \( k_F \), the known features from LL theory such as spin-charge separation and fractionalization of charge into two chiral modes result. On increasing \( k \), a further fractionalization of charge and spin appears, in forms that depend on the strength of the exchange interaction \( J \) or the density \( n \). Their dynamics can be understood at the supersymmetric (SUSY) point \( J = 2t \) in terms of charge and spin excitations of the Bethe-ansatz solution.24–26 For the region of the phase diagram,27,28 where the ground state corresponds to a repulsive LL, two qualitatively different regimes are identified: one regime with \( v_s > v_c \) and another where \( v_s < v_c \). Here \( v_s(\tau) \) is the velocity of the excitations mainly carrying charge (spin). For \( v_s > v_c \) and \( k > k_F \) the spin excitation starts to carry a fraction of charge that increases with \( k \) while \( v_c \) corresponds to a wave packet carrying only charge. For \( v_s < v_c \) and \( k > k_F \) the situation is reversed and the fastest charge excitation carries a fraction of spin that increases with \( k \) while the wave packet with \( v_s \) carries almost no charge; i.e., in this case spin fractionalizes.29

The Hamiltonian of the 1D t-J model is as follows:

\[
H = -t \sum_{i,\sigma} (\tilde{c}_{i,\sigma}^{\dagger} \tilde{c}_{i+1,\sigma} + \text{H.c.}) + J \sum_i \left( \tilde{S}_i \cdot \tilde{S}_{i+1} - \frac{1}{4} n_i n_{i+1} \right),
\]

where the operator \( \tilde{c}_{i,\sigma}^{\dagger} \) (\( \tilde{c}_{i,\sigma} \)) creates (annihilates) a fermion with spin \( \sigma = \uparrow, \downarrow \) on the site \( i \). They are not canonical fermionic operators since they act on a restricted Hilbert space without double occupancy. \( \tilde{S}_i = \tilde{c}_{i,\sigma}^{\dagger} \sigma_{\alpha\beta} \tilde{c}_{i,\beta} \) is the spin operator and \( n_i = \tilde{c}_{i,\sigma}^{\dagger} \tilde{c}_{i,\sigma} \) is the density operator.

We study the time evolution of a wave packet, corresponding to a fermion with spin-up injected into the ground state, by means of t-DMRG.18–23 The state of a Gaussian wave packet \( |\psi\rangle \) centered at \( x_0 \), with width \( \Delta_x \) and average momentum \( k_0 \), is created by the operator \( \psi^\dagger_{x_0} \) applied onto the ground state \( |G\rangle \):

\[
|\psi\rangle \equiv |\psi^\dagger_{x_0} G\rangle = \sum_i \psi_i |\psi^\dagger_i| |G\rangle,
\]

with

\[
\psi_i = A e^{-(x_i - x_0)^2/2\Delta_x} e^{i k_0 x_i}.
\]

A is fixed by normalization. The time-evolved state \( |\psi(\tau)\rangle \) by the Hamiltonian (1) determines the spin \( s \) and charge \( c \) density relative to the ground state as a function of time \( \tau \) measured in units of \( 1/t \) (\( \hbar = 1 \)),

\[
\rho_{sc}(x_i, \tau) \equiv \langle \psi(\tau)| n_{i\sigma} |\psi(\tau)\rangle - \langle G| n_{i\sigma} |G\rangle,
\]

where \( \alpha = s, c \), \( n_{i\sigma} = n_{i\uparrow} + n_{i\downarrow} \), and \( n_{is} = n_{i\uparrow} - n_{i\downarrow} \). Most of the numerical results were carried out on systems with \( L = 160 \) lattice sites, using 600 DMRG vectors (this translates into errors of the order of \( 10^{-4} \) in the spin and charge density up
to times of 50/\tau and $\Delta_\tau = 5$ lattice sites (which corresponds to a width $\Delta_\tau \sim 0.06\pi$ in momentum space).

**II. BETHE-ANSATZ SOLUTION**

At the supersymmetric (SUSY) point $J = 2\tau$ the 1D $t-J$ model can be solved exactly using the Bethe ansatz.\textsuperscript{25,26} We consider here only the case of zero magnetization. The solution is expressed in terms of two independent degrees of freedom, $c$ and $s$, related to two different kinds of pseudoparticles, with dispersion relations determined by

\begin{equation}
\epsilon_c(q) = 4t \int_B^B dq \frac{\phi_{c,c}(r,qs) - \phi_{c,c}(r,Q)}{1 + (2q)^2}
\end{equation}

\begin{equation}
\epsilon_s(q) = -\frac{4t}{1 + [2qs(q)]^2}
\end{equation}

where $q \in [-(\pi - k_F), (\pi - k_F)]$, with $\alpha = c$ or $s$, $k_F = \pi n/2$, $n = N/L$, $N$ the number of electrons, and $L$ that of lattice sites. The range of momenta for the excitations is later restricted to the occupied states for electron addition processes according to the pseudo-Fermi momenta given below, Eq. (11). The ground-state rapidities $r_{\alpha}(q)$ (with $\alpha = c,s$) are defined in terms of their inverse functions

\begin{equation}
q_{\alpha}(r) = 4t \int_B^B dq \phi_{c,c}(r,qs) \frac{1 + (2q)^2}{1 + (2qs)^2}
\end{equation}

\begin{equation}
c_r = 2 \arctan(2r)
\end{equation}

\begin{equation}
s_r = \frac{4t}{1 + (2r)^2}
\end{equation}

The functions $\phi_{c,c}(r,qs)$ are the phase shifts defined by the following self-consistent integral equations:

\begin{equation}
\phi_{c,c}(r,qs) = -\frac{1}{\pi} \arctan(2r - r')
\end{equation}

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\end{equation}

The kernel $G(r,r')$ reads

\begin{equation}
G(r,r') = -\frac{1}{\pi} \frac{1}{1 + (r - r')^2}
\end{equation}

\begin{equation}
+ \frac{4}{\pi} \int_n^0 \frac{dr'}{1 + (2[r - r']^2) 1 + (2[r' - r]^2)}
\end{equation}

\begin{equation}
- \frac{f(r,r')}{\pi} \frac{1}{1 + (r - r')^2},
\end{equation}

where

\begin{equation}
f(r,r') = 1 - \frac{1}{2} \left( t(r) + t(r') + \frac{l(r) - l(r')}{2(r - r')} \right),
\end{equation}

\begin{equation}
t(r) = \frac{1}{\pi} \sum_j \arctan(2[r + j Q]),
\end{equation}

\begin{equation}
l(r) = \frac{1}{\pi} \sum_j \arctan(2[r + j Q]).
\end{equation}

In the thermodynamic limit the ground state corresponds to symmetrical compact occupancies of both $\alpha = c,s$ momentum bands (5) with Fermi momentum $q_{F\alpha}$ given by

\begin{equation}
q_{F\alpha} = (\pi - 2k_F), \quad q_{F\alpha} = (\pi - k_F),
\end{equation}

respectively. The momenta of the states occupied in the ground state $q_c \in [-q_{Fc}, q_{Fc}]$ and $q_s \in [-q_{Fs}, q_{Fs}]$ refer to rapidity ranges $r \in [-Q, Q]$ and $r \in [-B, B]$, respectively, such that

\begin{equation}
r_c(\pm q_{Fc}) = \pm Q; \quad r_s(\pm q_{Fs}) = \pm B,
\end{equation}

where $Q$ and $B$ are obtained by solving self-consistently the normalization conditions given by the following integral equations:

\begin{equation}
\begin{align*}
\pi - 2k_F &= 4 \int_B^B dq \phi_{c,c}(r,Q) \frac{1}{1 + (2q)^2}, \\
\pi - k_F &= 2 \arctan(2B) + 4 \int_B^B dq \phi_{c,c}(r,B) \frac{1}{1 + (2q)^2}.
\end{align*}
\end{equation}

We proceed by solving Eqs. (7) and (8) assuming that $Q$ and $B$ are known and then we use Eqs. (13) and $k_F = \frac{\pi n}{2}$ to find the corresponding electronic density $n$. In Fig. 1 we show the resulting dispersion relations for different values of $n$. The ground state energy reference is defined such that $\epsilon_c(\pm q_{Fc}) = 0$. The dispersions plotted in Fig. 1 are the ones entering the calculation of velocities discussed in the next section.

**III. SIMULATIONS AT THE SUSY POINT**

We discuss first the time evolution of a wave packet at the SUSY point $J = 2\tau$, since here we will be able to identify the different portions in which the wave packet splits on the basis of the Bethe-ansatz solution. Figure 2 shows the time evolution of $\rho_c(x,\tau)$ for a density of $n = 0.6$. The momentum of the injected fermion is $k = 0.7\pi$, i.e., midway between $k_F = 0.3\pi$ and the zone boundary. The charge (i.e., $\rho_c$) splits into four fractions, one portion traveling to the left and the rest doing so to the right. A splitting into chiral modes is expected in the frame of LL theory,\textsuperscript{8} where for an injected right-going fermion, a splitting $Q^{\text{chiral}} = (1 \pm K_\alpha)/2$ [where $K_\alpha$ is the so-called LL parameter and “+” (“−”) corresponds to the right (left) propagating part] is predicted. The amount of charge (i.e., the integral of the wave packet over its extension) corresponding to the portion denoted $P_1$ is $Q^{\text{chiral}} \sim 0.1$. This value is independent of the momentum of the injected fermion and agrees well with the prediction of LL theory, since for the parameters in this case, $K_c \sim 0.8.\textsuperscript{25}$ However, at long enough times, a further splitting of the right-going charge is observed.
FIG. 1. (Color online) Solution of the dispersion relations (5) for different electronic density \( n \). The ground state energy reference is defined such that \( \varepsilon_\alpha(\pm q_{F\alpha}) = 0 \). (a) \( \alpha = c \) and (b) \( \alpha = s \). The momentum range is given by \( q \in \left[ -\left( \pi - k_F \right), \left( \pi - k_F \right) \right] \).

FIG. 2. (Color online) Time evolution of \( \rho_c(x, \tau) \) for a wave packet initially at \( x = 0 \), with momentum \( k = 0.7\pi \), at density \( n = 0.6 \), and \( J = 2t \). Charge fractionalizes into four wave packets, one to the left(\( P_1 \)) and the rest(\( P_2, P_3, P_4 \)) to the right. \( P_1 \) and \( P_3 \) have the same charge and speed but opposite velocities.

FIG. 3. (Color online) Charge [\( \rho_c(x, \tau) \); full line] and spin [\( \rho_s(x, \tau) \); dashed line] densities for \( J = 2t, n = 0.6 \), at time \( \tau = 40 \), for different values of the momentum of the injected fermion. \( Q^{(\pm)}_c \) denotes the charge of the left-going wave packet. Its value (~0.1) remains unchanged in all three panels.

FIG. 4. (Color online) Time evolution of \( \rho_s(x, \tau) \) for a wave packet with the same parameters as Fig. 2. The small depressions in spin density (red) have a slope in a time-space diagram corresponding to the Fermi velocity \( v_Fs \). \( v_s \) denotes the velocity of the wave packet \( P_4 \) in Fig. 3, that contains most of the spin density.
this small depression in spin-density moves with the Fermi velocity \( v_{Fc} \approx 2t_a \), where \( a \) is the lattice constant set to one, at the pseudo-Fermi sea in Fig. 1(b). Moreover, part of the charge \( (P_t) \) is accompanying the spin, such that spin-charge separation does not appear to be complete. The amount of charge accompanying the spin increases as the momentum of the injected fermion approaches the zone boundary. These results make already evident that injecting a fermion at a finite distance from the Fermi energy leads to fractionalization of charge beyond the expectations from the LL theory.

In order to understand the new forms of fractionalization that go beyond the LL frame, we consider the excitations corresponding to one-particle addition processes, whose energies can be obtained from the Bethe-ansatz solution. \(^{16,30}\) When adding an electron with momentum \( k \), the single-particle excitation energy is given by \( \omega(k) = -\epsilon_c(q_c) - \epsilon_s(q_s) \), where \( \epsilon_c(q_c) \) and \( \epsilon_s(q_s) \) are the dispersion relations \(^{5}\) of the excitations for charge and spin, respectively, and the momenta are related to the momentum of the incoming particle as follows: \( k = \pm 2k_F - q_c - q_s \), where \( q_c \in [-q_{Fc}, q_{Fc}] \), and \( q_s \in [-q_{Fs}, q_{Fs}] \), with \( q_{Fc} \) and \( q_{Fs} \) the pseudo-Fermi momenta for the excitations for charge and spin, given in Eqs. \((11)\), respectively. \(^{26}\)

Figure 5 displays the velocities obtained from t-DMRG for the different wave packets (symbols) compared to those obtained from Bethe ansatz (full lines), as a function of the momentum of the injected fermion. The velocity of each \( P_i \) is extracted by measuring the position of the maximum of the packet at the most convenient time, i.e., at that time where we can resolve \( P_i \) and the spreading of one packet does not destroy the other packets. The wave packets \( P_1 \) (triangles) and \( P_3 \) (squares) have opposite directions, but the same speed and charges \( Q_{1}^{-1}c \approx Q_{3}^{+} \), where the charges for the (+) branch are labeled by an index corresponding to the respective wave packets. The velocity of the wave packet \( P_t \) (circles) agrees almost perfectly with the one corresponding to spin excitations. Its determination is best since it is the fastest wave packet, such that it can be easily discerned from the rest. The velocity of the remaining wave packet, \( P_2 \) (diamonds), is more difficult to assess, since it overlaps at the beginning with other ones. Nevertheless, its velocity closely follows the one of charge excitations. The wave packets just described deliver a direct visualization of the excitations appearing in the Bethe-ansatz solution, where only two different kinds of particles are involved: the \( c \) and \( s \) pseudoparticles with their associated bands. The excitation associated with spin involves one hole in the \( c \) band with fixed momentum \( q_{Fc} \), and one hole in the \( s \) band with momentum \( q_s \), where \( q_s = \pm 2k_F - q_{Fc} - k \). \(^{26}\) In fact, the velocities of \( P_1 \) and \( P_3 \) correspond to the group velocity at both pseudo-Fermi momenta \( \pm q_{Fc} \), indicating that these wave packets correspond to low-energy excitations. This explains the fact that \( Q_{i}^{-1} \) is well described by LL theory in spite of the fermion being injected at high energy, and supports the assumption that the same applies to a left-going wave packet for spin (see Fig. 4). Furthermore, as shown in Fig. 5, the velocity of those fractions is independent of the momentum of the injected fermion, in agreement with the picture given by Bethe ansatz. The dispersion of the hole in the \( s \) band gives rise to the velocity displayed by the red line in Fig. 5. Similarly, the \( c \) line (black line in Fig. 5) involves one hole in the \( s \) band with fixed momentum \( q_{Fs} \) and one hole in the \( c \) band with momentum \( q_c \) determined in terms of \( k \) by \( q_c = \pm 2k_F - q_{Fs} - k \). Using the same argument as for the \( s \) line we can associate the \( P_2 \) packet (diamonds) with the \( c \) pseudoparticle. However, in this case we cannot observe wave packets associated with spin and velocities corresponding to the group velocity at the pseudo-Fermi momenta \( \pm q_{Fc} \). We understand this as due to the fact that \( K = 1 \), by analogy to what we observe in the \( K = 1 \) case. On the SUSY point this case is reached in the limit of vanishing density, where the system can be described by a Fermi gas. Hence, fractionalization is absent in this limit. In Fig. 6 we show finally a comparison of dispersions with highest weight in the spectral function obtained from quantum Monte Carlo (QMC) simulations for the one-dimensional \( t-J \) model.\(^{32}\)
and the energies obtained from t-DMRG by integrating the velocities between $k_F$ and $k$ with the zero of energy at $k_F$. While the dispersions obtained in QMC simulations can be well reproduced by the velocities obtained from the wave packets $P_2$ and $P_3$ from t-DMRG, given the discretization errors in integrating the velocities, and uncertainties from the analytic continuation in QMC, no direct access to the wave packets $P_1$ and $P_3$ is possible from the spectral function. Their contribution to the spectral function is contained in the intensities of the spectrum, but no distinct feature allows to extract them from it.

IV. AWAY FROM THE SUSY POINT

Next we depart from the SUSY point and examine how fractionalization takes place in the region of the phase diagram where the ground state corresponds to a LL with $K_c < 1$. Figure 7 shows the velocity of the different fractions at $J = 1.75t$, where a slight decrease (increase) in the velocity of the spin (charge) fraction can be observed. As shown in Fig. 8,

essentially the same features are observed as at the SUSY point both for $J > 2t$ and $J < 2t$. In all the cases shown in Fig. 8, where the velocity of spin excitations ($v_s$) remains higher than that of charge excitations ($v_c$) in most parts of the Brillouin zone, spin does not fractionalize, as opposed to charge, so that the interpretation derived from Bethe ansatz remains valid over an extended region of the phase diagram: Charge splits into four portions of which one travels with the spin wave packet, and two have the same speed but opposite group velocity which does not depend on the momentum of the injected fermion. It is tempting to assign those excitations to states at a pseudo-Fermi surface for charge excitations. For smaller values of $J/t$ than those in Fig. 8, $v_s$ becomes smaller than $v_c$. Figure 9 shows that for $v_s < v_c$ the role of spin and charge wave packets experience a change with respect to fractionalization. In this case it is the spin density that splits into two fractions, one attached to the fastest fraction of charge, an another one left behind. Again, this new feature is not predicted by LL theory. However, no left propagating fraction of spin could be observed (excepting the small depression due to finite-size effects). We therefore

FIG. 7. (Color online) As in Fig. 5 but for $J = 1.75t$. The full lines correspond to the SUSY Bethe ansatz.

FIG. 8. (Color online) Fractionalized wave packets for different values of $J/t$ away from the SUSY point, at a density $n = 0.6$. As in the SUSY case, charge fractionalizes into four pieces, while spin does not, and carries an appreciable amount of charge.

FIG. 9. (Color online) Fractionalized wave packets at $J/t = 1$, $n = 0.5$, $\tau = 50$, and $L = 200$. In this case, where $v_s < v_c$, fractionalization of the spin density is observed.

FIG. 10. Free expansion of noninteracting spinless fermions at different times, where the wave packet disperses for increasing time. The momentum of the injected fermion is $k = 0.7\pi$ and $n = 0.5$. 

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In summary, we have shown through the time evolution of an injected spinfull fermion onto the \( t-J \) model, that charge and spin fractionalization occurs beyond the predictions of the Luttinger-liquid theory. A comparison with results from Bethe ansatz allowed us to identify charge and spin excitations that split into components at high and low energies. The components at high energy reveal the dispersion \( \epsilon_c \) and \( \epsilon_s \) of charge and spin excitations, respectively. The components at low energy have a velocity that does not depend on the momentum of the injected fermion and are very well described by states at the pseudo-Fermi momenta of the charge excitation. This picture can be extended to a wide region in the phase diagram of the \( t-J \) model as long as the ground state corresponds to \( K_c \approx 1 \) and \( v_c < v_s \). In this region fractionalization is observed only in the charge channel. However, for \( v_c > v_s \), a region that develops for \( J/t \) below \( \approx 1.5 \), the spin density shows fractionalization. All over, the fastest excitation is accompanied by the complementary one, such that spin-charge separation is for them only partial. The other fractions present an almost complete spin-charge separation. Finally, we would like to remark that the time evolution leads to a direct visualization of all fractions stemming from an injected fermion in contrast to the one-particle spectral function, where only the fractions \( P_2 \) and \( P_3 \) can be identified, but not those propagating at the pseudo-Fermi points.

V. CONCLUSIONS

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