Splitting of Fermi point of strongly interacting electrons in one dimension:
A nonlinear effect of spin-charge separation

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A system of one-dimensional electrons interacting via a short-range potential described by Hubbard model is considered in the regime of strong coupling using the Bethe ansatz approach. We study its momentum distribution function at zero temperature and find one additional singularity, at the $3k_F$ point. We identify that the second singularity is of the same Luttinger liquid type as the low-energy one at $k_F$. By calculating the spectral function simultaneously, we show that the second Luttinger liquid at $3k_F$ is formed by charge modes only, unlike the known one around $k_F$ consisting of both spin and charge modes. This result reveals the ability of the spin-charge separation effect to split the Fermi point of free electrons into two, demonstrating its robustness beyond the low-energy limit of Luttinger liquid where it was originally found.

Interactions have a dramatic effect on electrons in one dimension that has been attracting a significant interest in condensed-matter physics for a long time [1]. Their low-energy excitations become quantised density waves described by the Tomonaga-Luttinger liquid (TLL) theory based on linearisation of the spectrum around the Fermi points [2–4]. A hallmark prediction of this theory is separation of the spin and charge degrees of freedom of the underlying electrons into density waves of two distinct types with different velocities [4, 5]. Two linear dispersions originating from the Fermi point were observed in experiments on magnetotunneling spectroscopy in semiconductors [6, 7], on photoemission in organic [8] and strongly anisotropic [9] crystals, and on time-resolved microscopy in cold atoms [10], establishing firmly this phenomenon.

More recently, the theoretical interest was focused on spectral nonlinearity since it breaks construction of the TLL theory altogether [11] but, on the other hand, is unavoidable at any finite distance from the Fermi energy in a Fermi system. The Boltzmann equation approach to weakly interacting Fermi gas predicts a finite relaxation time due to nonlinearity [12–14], suggesting decay of the many-body modes. Application of the mobile impurity model to Luttinger liquids predicts survival of spin-charge separation at least in a weak sense, as a singularity–consisting of a mixture of spin and charge modes–at the spectral edge with nonlinear dispersion [15–17]. At the same time, the continuing experimental progress is starting to provide information on effects beyond the low-energy regime [18–22]. In one of these experiments [22], the spin-charge separated modes at low energy were observed to extend to the whole conduction band forming a pair of parabolic dispersions characterised by two incommensurate masses, raising the question if the spin-charge separation phenomenon manifests itself directly in other properties of the whole Fermi sea.

We explore such a possibility theoretically in this Letter by studying the momentum distribution function for a Fermi system with short-range interactions described by the Hubbard model, in which the spin-charge separation is well-established in the TLL limit [1]. Using the microscopic methods of Bethe ansatz in the strong coupling limit $(U = \infty)$ not restricted to low energy [23], we find (at $T = 0$) one extra divergence at $3k_F$ in addition to the usual Fermi point at $k_F$, see Fig. 1. Both singularities are of the same order, in the first derivative $dn_k/dk$, revealing the ability of spin-charge separation

![Figure 1](image-url)

**Figure 1.** (A) Momentum distribution function $n_k$ in the ground state of the model in Eq. (1) evaluated in the $U/t = \infty$ limit using Eqs. (6-9,11), where the two leading levels of the hierarchy of modes $l \leq 1$ were taken into account in the sum in Eq. (11), for $N = 200$ particles (solid line) and for free particles $U/t = 0$ (dashed line). Inset: Zoom-in around $3k_F$. (B), (C), and (D) First derivative $dn_k/dk$ around the $k_F$, $3k_F$, and $5k_F$ points respectively.
to split one Fermi point of free electrons into two [24]. It is a direct manifestation of this phenomenon in the whole Fermi sea, far away from the TLL limit. Around the second point, we find a power-law behaviour of $n_k$, $n_k \sim \cdots + \text{sgn}(k - 3k_F)|k - 3k_F|^{\alpha_{3k_F}}$, with a real exponent of the TLL type $\alpha_{3k_F} = 0.787 \pm 0.067$. However, this exponent does not correspond to the known exponents for spinful or spinless TLLs at $k_F$ [1]. By calculating simultaneously the spectral function we show that, out of the spin-charge separated linear modes around $k_F$, only the charge branch extends through the nonlinear region to form a TLL around $3k_F$, identifying it as a TLL of a new kind.

We analyse fermions with spin-1/2 interacting via a short-range potential that are described by the 1D Hubbard model,

$$H = -t \sum_{j,\alpha} (c_{j\alpha}^\dagger c_{j+1,\alpha} + c_{j\alpha}^\dagger c_{j-1,\alpha}) + U \sum_j n_{j\uparrow} n_{j\downarrow},$$

where $c_{j\alpha}$ are the Fermi operators at site $j$, $\alpha$ is the spin-1/2 index $\uparrow$ or $\downarrow$, $n_{j\alpha} = c_{j\alpha}^\dagger c_{j\alpha}$ is the local density operator of the spin species $\alpha$, $t$ is the hopping amplitude describing the kinetic energy, and $U > 0$ is the repulsive two-body interaction energy. Below, we consider the periodic boundary conditions, $c_{j+L} = c_j$, for a 1D lattice consisting of $L$ sites and for $N$-particle states we impose the constraint of low particle density, $N/L \ll 1$ [25]. In the strong-interaction limit, $U/t = \infty$, the spectrum of the model in Eq. (1) is given by the following Lieb-Wu equations [26, 27],

$$Lk_j - P_s = 2\pi I_j, \quad (2)$$

$$Nq_m = 2 \sum_{l \neq m}^{M} \varphi_{lm} = 2\pi J_m, \quad (3)$$

where $e^{i2\varphi_{lm}} = - (e^{i\epsilon q_l + i\epsilon m} + 1 - 2e^{i\epsilon m})/(e^{i\epsilon q_l + i\epsilon m} + 1 - 2e^{i\epsilon m})$ are the two-spin scattering phases, the total spin momentum $P_s = \sum_m q_m$ is defined in the interval of $-\pi..\pi$, and $N$ non-equal integers $I_j$ and $M$ non-equal integers $J_m$ define the solution for the charge $k_j$ and spin $q_m$ (quasi)momenta of the $N$-particle state. This solution gives the eigenenergy of the many-body state as $E = t \sum_j k_j^2/2$ and its momentum as $P = \sum_j k_j$.

In the same limit, the eigenstates are factorised, $|\Psi\rangle = |\Psi_c\rangle \otimes |\Psi_s\rangle$, into a Slater determinant (like for free particles) for the charge and a Bethe wave function (like that for a Heisenberg chain) for the spin degrees of freedom [27, 28],

$$|\Psi_c\rangle = \frac{1}{L^N} \sum_{Q,j}^{L} (-1)^Q e^{iQk_j a_j^\dagger \cdots a_{jN}^\dagger} |0\rangle \quad (4)$$

$$|\Psi_s\rangle = \frac{1}{Z} \sum_{R,x}^{N} e^{i \sum_{i < m} \varphi_{Rix} + iRq\cdot x} S_{x1}^+ \cdots S_{xM}^+ |\Psi\rangle \quad (5)$$

where $j$ are charge coordinates of $N$ particles on the original Hubbard chain of length $L$, $x$ are positions of say $M$ spins pointing up on the spin chain of $N$ spins forming the spin part of the wave function, and the sums over $Q$ and $R$ run over all possible permutations of $N$ momenta $k_j$ and $M$ momenta $q_m$ respectively. These wave functions are normalised to unity, with the non-trivial normalisation factor of the Bethe wave function being the determinant, $Z^2 = \text{det} Q$, of an $M \times M$ matrix with the following diagonal $Q_{aa} = N - \sum_{l \neq m} 4(1 - \cos q_l)/(e^{i\epsilon q_l} + e^{-i\epsilon q_l} - 2)/(e^{i\epsilon q_m} + e^{-i\epsilon q_m} - 2)$ and off-diagonal $Q_{ab} = 4(1 - \cos q_a)/(e^{i\epsilon q_a} + e^{-i\epsilon q_a} - 2)/(e^{i\epsilon q_b} + e^{-i\epsilon q_b} - 2)$, with $a \neq b$, elements [29]. Here, the spinless Fermi $a_j^\dagger$ and the purely spin $S_j^\dagger$ operators can be recombined in the original electron operators $c_{j\alpha}$ by introducing an insertion(deletion) of the spin-down state at a given position $x$ in the spin chain operator $I_x (D_x)$ as $c_{j\uparrow} = a_j^\dagger S_x^+ I_x$, $c_{j\downarrow} = a_j^\dagger I_x$, $c_{j\uparrow} = a_j^\dagger D_x S_x^-$, and $c_{j\downarrow} = a_j^\dagger D_x S_x^-$ [30].

The zero temperature Green function is expressed in terms of the expectation values of the ladder operators as [31] $G_{\alpha}(k,E) = \sum_{l \neq m} |\langle f| c_{l\alpha}^\dagger 0 \rangle|^2/(E - E_l + i\eta) + |\langle f| c_{l\alpha}^\dagger 0 \rangle|^2/(E + E_l - i\eta)$, where $c_{l\alpha}^\dagger = \sum_j e^{i\epsilon q_j} c_{j\alpha}^\dagger / \sqrt{L}$ is the Fourier transform and $\eta$ is an infinitesimally small real number. The factorisation of the wave functions makes this calculation easier since the matrix elements becomes a product of two factors, $\langle f| c_{l\alpha}^\dagger 0 \rangle = \langle f| c_{l\alpha}^\dagger 0 \rangle_c \cdot \langle f| c_{l\alpha}^\dagger 0 \rangle_s$, where $0 = (k^0, q^0)$ and $f = (k^f, q^f)$ the momenta of the ground and excited states. The model in Eq. (1) has the symmetry of swapping the spin indices $\uparrow \leftrightarrow \downarrow$, which its Green function also possesses, $G_{1}(k,E) = G_{\uparrow}(k,E)$. Therefore, we will consider only $\alpha = \uparrow$. The charge part of the matrix element is an expectation value with respect to the state in Eq. (4) that evaluates as an $N$-fold sum over coordinates $j$ producing a determinant of the Vandermonde type. Then, application of the generalised Cauchy formula gives the following result for the annihilation operator $c_{j\uparrow}$ [32, 33]

$$\langle f| c_{j\uparrow}^\dagger 0 \rangle_c = \frac{2^{N-1} \sin N^{-1} \left(\frac{p_f - p_0}{2}\right)}{L^{N-2}} e^{i(p_0 - p_f)j} \times \prod_{i<j}^{N-1} \left(k_i^j - k_j^i\right) \prod_{i,j}^{N-1} \left(k_i^j - k_0^j\right) \prod_{i,j}^{N-1} \left(k_j^i - k_0^i\right), \quad (6)$$

where $\langle f| c_{j\uparrow}^\dagger 0 \rangle_c \equiv \langle \Psi_c^f| a_j^\dagger |\Psi_c^f\rangle$ and the low-density limit, in which $k_i^j - k_j^i \ll 1$, is already taken.

The spin part of the matrix elements is an expectation value with respect to the states in Eq. (5) that is less straightforward to evaluate. A mathematical technique for dealing with these Bethe states analytically was invented in an algebraic form [34], leading to calculation of the correlation function for the non-iterarant quan-
tum magnets described by the Heisenberg model [35, 36]. However, this result cannot be used here directly since the operators of the Hubbard model \(c^\dagger_j\) change the length of the spin chain, making the constructions of [34] for the bra and ket states incompatible with each other. We resolve this problem by representing operators of one algebra (for the longer chain) through the other (for the shorter chain) and the spin operators of the extra site. Then, explicit evaluation of the expectation value in the spin subspace of the additional site restores applicability of the methods in [23], and we obtain the spin part of the matrix element in terms of the determinant of an \(M \times M\) matrix (see details of this calculation in [27]),

\[
\langle f | c_j^{\dagger} | 0 \rangle_s = \frac{\det R}{Z_0 Z_f} \prod_{i,j}^{M-1} \left( e^{i q_i^f} + e^{-i q_j^0} - 2 \right) \times \prod_{i \neq j}^{M-1} \left( e^{i q_i^f} + e^{-i q_j^0} - 2 \right)^{-\frac{1}{2}} \left( e^{i q_i^0} + e^{-i q_j^0} - 2 \right)^{-\frac{1}{2}},
\]

(7)

where \(\langle f | c_j^{\dagger} | 0 \rangle_s \equiv \langle \Psi_f | D_x S^{-1} | \Psi_0 \rangle\) and the elements of matrix \(R\) are

\[
R_{ab} = \frac{e^{i q_i^0(N-1)} \prod_{j \neq a}^{M-1} \left( e^{i q_i^f + i q_j^0 + 1 - 2e^{i q_j^0}} - 1 \right) (e^{-i q_i^f} - e^{-i q_j^0}) \left( e^{i q_i^f} + e^{-i q_j^0} - 2 \right)}{(e^{-i q_i^f} + e^{-i q_j^0} - 2)},
\]

(8)

\[
R_{Mb} = \frac{e^{i k_i^0} \prod_{j \neq b}^{M-1} \left( e^{i q_i^0} + e^{-i q_j^0} - 2 \right)}{(e^{i q_i^0} + e^{-i q_j^0} - 2)},
\]

(9)

for \(a < M\) and for \(a = M\) respectively. Together Eqs. (6-9) give the complete analytical expression for the matrix element for the 1D Hubbard model. Repeating the same calculation for the matrix element of the creation operator, \(\langle f | c_j^{\dagger} | 0 \rangle_s\), we obtain the same expressions as in Eqs. (6-9), in which the momenta are swapped, \(k_i^0, q_j^0 \leftrightarrow k_i^f, q_j^f\), and the particle (spin) quantum number is increased by one, \(N \rightarrow N + 1\) (\(M \rightarrow M + 1\)).

The response of a many-body system to a single-particle excitation at a given momentum and energy is described by the spectral function, making this observable particularly interesting for the experiments on spectroscopy. It is related to Green function as \(A_\alpha(k, E) = -\text{Im} G_\alpha(k, E) \text{sgn}(E - E_0)/\pi\) [31] giving

\[
A_\alpha(k, E) = \sum_f |\langle f | c_k^{\dagger} | 0 \rangle|^2 \delta(E - E_f + E_0) + \sum_f |\langle f | c_k^{\dagger} | 0 \rangle|^2 \delta(E + E_0 - E_f) + \sum_f |\langle f | c_k | 0 \rangle|^2 \delta(E - E_f),
\]

(10)

where the sum over the result in Eqs. (6-9) [37] needs to be evaluated over exponentially many final states \(f\).

Figure 2. (A) Spectral function \(A_\alpha(k, E)\) of the model in Eq. (1) evaluated in the \(U/t = \infty\) limit using Eqs. (6-9,10) for \(N = 500\) particles, where only the leading level of the hierarchy \(l = 0\) was taken into account in the sum in Eq. (10). The single particle dispersion of free particles \(U/t = 0\) is superimposed as dashed line. (B) Two sets of integer numbers, \(I_j\) for charge and \(J_m\) for spin degrees of freedom, defining the Lieb-Wu equations (2,3) for an excited state with momentum \(P\) and the total spin momentum \(P_s\); two “electron-hole” pairs are shown as examples of lowering the level of the hierarchy, see text. For a spin-unpolarised system, the number of spin degrees of freedom is \(M = N/2\) that makes the charges’ density twice larger than that of the spins.

It can be done based on emergence of the hierarchy of modes: Away from the low-energy regime around the Fermi points the many-body continuum splits itself into levels (consisting of a polynomial number of excitations on each of them) according to their spectral strength, which is proportional to integer powers of a small parameter \(1/L^2\) [38].

In the presence of spin and charge degrees of freedom this phenomenon manifests itself on the microscopic level in the following way. For the ground states, the charge and spin momenta form two Fermi seas that correspond to selecting the non-equal integer numbers in Eqs. (2,3) as \(I_j = -N/2 \ldots N/2\) and \(J_m = -(N - M)/2 \ldots (N + M)/2\) [26], see illustration in Fig. 2B. The charge part of the spectral amplitude for a
generic excitation above this ground state, \( |\langle f| c_{k \alpha}^\dagger |0\rangle_c|^2 \) given by Eq. (6), is vanishingly small in the thermodynamic limit since it is proportional to \( 1/L^{2N} \). However, the factor \( k_F^2 - k_0^2 \) in the denominator of Eq. (6) produces a singularity that is cut off by \( 1/L \) cancelling a power of \( 1/L^2 \) in the spectral amplitude each time a charge momentum of the excited state is equal to a momentum of the ground state. This property selects a specific set of the excitations, for which a charge is added above the ground–see the charge state in Fig. 2B–and for which the \( 1/L^{2N} \) factors is canceled altogether making \( |\langle f| c_{k \alpha}^\dagger |0\rangle_c|^2 \sim 1 \). Adding each “electron-hole” pairs of charges on top of these states multiplies the spectral amplitude by an extra small parameter \( 1/L^2 \) since some powers of the normalisation factor \( 1/L^{2N} \) remain uncanceled.

For the spin part of the spectral amplitude, \( |\langle f| c_{k \alpha}^\dagger |0\rangle_s|^2 \) given by Eq. (7), emergence of a small parameter is similar. The normalisation factor \( 1/(Z_0 Z_F) \) makes the amplitude proportional to a vanishing in the thermodynamic limit factor \( 1/N^{2M} \) and the singularity \( 1/(e^{-i\lambda k} - e^{-i\lambda k_0}) \) in the matrix elements in Eq. (8) cancels it altogether for a subset of states, for which only one spin is added on top of the spin ground states–see the spin state in Fig. 2B–making \( |\langle f| c_{k \alpha}^\dagger |0\rangle_s|^2 \sim 1 \). Adding each “electron-hole” pair of spins on top multiplies the spectral amplitude by an extra small parameter \( 1/N^2 \).

Combined, these two properties result in the hierarchy of modes for both types of the degrees of freedom, with the spectral power for the strongest excitations being of the order of \( |\langle f| c_{k \alpha}^\dagger |0\rangle_s|^2 \sim 1 \) and the subleading excitations being weak as \( |\langle f| c_{k \alpha}^\dagger |0\rangle_c|^2 \sim 1/(N^{2m}L^{2n}) \), where \( l = n + m > 0 \) and \( n \) and \( m \) are the numbers of extra “electron-hole” pairs in the charge and spin Fermi seas respectively. Close to the Fermi points this hierarchy of modes breaks down. The spectral amplitudes of all excitations become of the same order forming spin and charge density waves, and the spinful TLL theory becomes a better approach for calculating correlation functions [4, 5].

Analysing first the nonlinear regime away from the Fermi points, we evaluate the spectral function in Eq. (10) numerically taking into account only the top level of the hierarchy \( l = 0 \) in the sum over \( f \) [39]. The result is presented in Fig. 2A, where the Fermi momentum is defined by the free particle limit as \( k_F = \pi N/2 \) and the corresponding sum rule (which also includes the linear regime around the Fermi points) is already fulfilled as \( 2 \int_{-\infty}^{\infty} \alpha dE \alpha k_F^2 dE \alpha k \alpha /N \simeq 61\% \) even for a large number of particles \( N = 500 \). Unlike the case of spinless fermions [38], the excitations at the top level of the hierarchy form a continuum for fermions with spin-1/2 since adding an electron with spin-1/2 adds simultaneously both charge and spin with two different momenta \( P_0 \) and \( P_s \), see Fig. 2B. In this continuum, only two non-equivalent peaks emerge away from the Fermi points: One connects the \( \pm k_F \) points and the other connects the \( -k_F, 3k_F \) points (or equivalently, the \( -3k_F, k_F \) points) on the \( E = \mu \) line. Around the \( \pm k_F \) Fermi points, these nonlinear peaks become two linear peaks that are the manifestation of the collective spin (i.e. spinon) and charge (i.e holon) modes predicted by the spinful TLL model at low energy [4, 5]. This identifies the nonlinear modes as being collective spin and charge excitations as well (see more details in [27]), and shows that the spin-charge separation still manifests itself in observables beyond the linear TLL limit.

The line shapes of the peaks away from the low-energy region have the form of divergent power-laws, e.g. the particular momentum-dependent exponent was predicted for the spinon mode (which correspond to the spectral edge at finite \( U \)) in [15, 40] and experimentally confirmed in [29]. The nonlinear holon and spinon modes were observed directly in the momentum-energy resolved magnetotunneling experiments in semiconductor quantum wires at intermediate coupling strength [19, 22] that strongly suggests their robustness also for interactions with finite range and of finite strength, beyond the regime of the present calculation.

The momentum distribution function is another observable of interest in the many-body systems. It can be obtained from Green function as \( n_k = \int dE \Theta (E - \mu) \Im G_{\alpha} (k, E)/\pi \) [31] giving

\[
n_k = \sum_f |\langle f| c_{k \alpha} |0\rangle|^2. \tag{11}\n\]

One of the regions of particular interest for this quantity is proximity of the Fermi point, in which the infinite number the “electron-hole” pairs has to be included in the sum over \( f \). This can be, at least partially, accounted for by adding subleading levels of the hierarchy. The result of the numerical calculation for \( N = 200 \) and \( l \leq 1 \) is presented in Fig. 1A, where the sum rule already accounts for \( 2 \int dE n_k/N \simeq 86\% \) of the particles.

Singularities in \( n_k \) were introduced as the definition of a Fermi surface in many-body systems in the Luttinger theorem [41]. Here, we use this definition to interpret the result in Fig. 1. Due to the TLL physics, the singularity at \( k_F \) is weaker in 1D [42], e.g. instead of a discontinuity in \( n_k \) in \( D > 1 \) dimensions \( n_k \) is finite, with a divergence appearing in \( dn_k/dk \) in 1D, see Fig. 1B. Inspecting the result in Fig. 1A, we find a second singularity of same order at \( 3k_F \), see Fig. 1C. And we find no divergencies at any other points, e.g. see Fig. 1D. The second singularity can be interpreted as a direct manifestation of spin-charge separation beyond the low-energy regime, which facilitates appearance of two Fermi points at different momenta since the density of nonlinear holons twice larger than that of the nonlinear spinons in a spin-unpolarised system. Note that \( n_{k=0} \simeq 0.7 \) in Fig. 1A is still smaller than \( n_{k=0} = 1 \) for the free system so \( \sim 30\% \) of particles is
Figure 3. Momentum distribution function \( n_k \) around \( 3k_F \) on the log-log scale for \( N = 80 \) particles, where the three leading levels of the hierarchy of modes \( l \leq 2 \) were taken into account in the sum in Eq. (11). The dashed solid lines are power-law functions for \( k < 3k_F \) and for \( k > 3k_F \) giving the exponent as \( a_{3k_F} = 0.787 \pm 0.067 \), where the value is the average of the two and the error bars is the difference. Inset A: Finite size cutoff for \( n_k \) as the function of inverse system size \( 1/L \) on the log-log scale at \( 3k_F \). The solid line is a power-law fit giving \( a_{3k_F} = 0.838 \), within the accuracy of the fitting \( n_k \) directly. Inset B: The value of \( n_k \) at \( 3k_F \) as a function of the particle number \( N \). The solid line is a fit of finite size corrections, \( n_{3k_F} = C_{3k_F} + b/N \), giving \( C_{3k_F} = 0.027 \).

redistributed above \( k_F \) providing a significant amplitude around the \( 3k_F \) point.

The coinciding order of both singularities suggests that the states around \( 3k_F \) are also described by a TLL model, which predicts a power-law behaviour of the momentum distribution function [1],

\[
n_k = C_{(3)k_F} + \cdots \text{sgn} ((3)k_F - k) |k - (3)k_F|^{\alpha_{(3)k_F}}, \tag{12}
\]

where \( \alpha_{(3)k_F} \) is a real exponent and \( C_{(3)k_F} \) is the value of \( n_k \) exactly at \( (3)k_F \). Fitting a linear function on a log-log plot of \( n_k \) extracts the exponent around \( 3k_F \) directly, see Fig. 3. Alternatively, the same exponent can be extracted from the finite size cutoff at \( 3k_F \), see inset A in Fig. 3. Both methods give \( a_{3k_F} = 0.787 \pm 0.067 \). The scaling of \( n_{3k_F} \) with the system size gives a finite amplitude in the thermodynamic limit, \( C_{3k_F} = 0.027 \), see inset B in Fig. 3. In all of these numerical calculations the number of the levels \( l \) used in calculating Eq. (11) was increased until the next subleading level was giving only a small correction to the value of \( n_k \) at each point. Application of the same procedure around \( k_F \) gives \( C_{k_F} = 0.477 \) and \( a_{k_F} = 0.124 \pm 0.020 \) [27], which is the well-known result of the TLL theory \( a_{k_F} = 0.125 \) [43–45]. However, only one attempt of using the TLL approach at \( 3k_F \) was made in [46], in which \( a_{3k_F} = 1.125 \) was obtained, suggesting a lower order (in \( d^2 n_k/dk^2 \)) of the second singularity.

This discrepancy can be attributed to using both spinon and holon modes in [46], while the present microscopic calculation shows in Fig. 2A that only the holon modes can form a TLL at \( 3k_F \).

In conclusions, we have shown that spin-charge separation can split one Fermi surface into two. Together with the recent experimental observation of spin-charge splitting of the whole band in [22], it demonstrates that this phenomenon is more general than it was originally anticipated, and also that substantial features of the Fermi gas still survive in 1D despite formation of a genuine many-body continuum by the interactions.

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Supplementary material for
Splitting of Fermi point of strongly interacting electrons in one dimension:
A nonlinear effect of spin-charge separation

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I. LIEB-WU SOLUTION

The many-particle eigenstates of 1D Fermi-Hubbard model in Eq. (1) of the main text were constructed in [1]. In the representation of second quantisation, $|\Psi\rangle = \sum_{j,\alpha} \psi_{j\alpha} \phi_{j\alpha}^\dagger$ $|0\rangle$, they are described by the amplitude $\psi_{j\alpha}$ of finding all $N$ particles at a given set of sites $j_1, \ldots, j_N = j$ and with a given configuration of their spins $\alpha_1 \ldots \alpha_M = \alpha$. These amplitudes have the form of superposition of plane waves according to the Bethe’s hypothesis [2],

$$\psi_{j\alpha} = \sum_Q A_{Q\alpha} e^{iQkOj}, \quad (1)$$

where $O$ is the permutation that orders all $N$ coordinates such that

$$Oj_1 < \cdots < Oj_N, \quad (2)$$

the (charge) momenta of $N$ particles are $k = k_1, \ldots, k_N$, and $\sum_Q$ is the sum over all permutations of $N$ momenta $k_j$. The phase $A_{PQ\alpha}$ in this superposition is neither 1 nor $-1$, and it depends on the configuration of all $M$ spins $O\alpha$ explicitly. The algebraic method of constructing it was proposed in [3, 4] in the form of Bethe ansatz, producing another “nested” Bethe-ansatz wave function for the 1D Fermi Hubbard model,

$$A_{QO\alpha} = (-1)^{QO} \sum_R \left( \prod_{1 \leq l < m \leq M} R_{\lambda_l} - R_{\lambda_m} - \frac{iU}{2t} \right) \left( \prod_I R_{\lambda_l} - \sin Q\lambda_l - \frac{iU}{2t} \right) \sum_{j=1}^{x_I-1} R_{\lambda_l} - \sin Q\lambda_j - \frac{iU}{2t} \right), \quad (3)$$

where $x_1, \ldots, x_M = x$ are the coordinates of $M$ spins $\uparrow$ in the configuration $O\alpha$ of all spins of $N$ particles, $\lambda_1, \ldots, \lambda_M = \lambda$ are the spin momenta associated with these $M$ spins $\uparrow$, and $\sum_R$ is the sum over all permutations of these spin momenta.

The momenta are quantised by boundary conditions. Application of the periodic boundary condition to the many-particle wave function in Eq. (1) gives the Lieb-Wu equations [1],

$$k_jL - \sum_{m=1}^M \varphi(\lambda_m - \sin k_j) = 2\pi I_j, \quad (4)$$

$$\sum_{j=1}^N \varphi(\lambda_m - \sin k_j) - \sum_{l=1}^M \varphi(\lambda_m/2 - \lambda_l/2) = 2\pi J_m, \quad (5)$$

with $\varphi(x) = -2 \arctan\left(\frac{4tx}{U}\right)$, \quad (6)

where $N$ non-equal integers $I_j$ and $M$ non-equal integers $J_m$ define the solution for the charge $k_j$ and the spin $\lambda_j$ momenta for a given value of the interaction strength $U/t$. This solution gives the eigenenergy of the many-particle state as $E = t \sum_{j=1}^N \cos k_j$ and its momentum as $P = \sum_{j=1}^N k_j$. These simultaneous quantisation conditions for all spin and charge degrees of freedom are a system of $N + M$ connected equations for any finite $U$.

A. $U = \infty$ limit

In the regime of strong coupling $U/t \gg 1$, it was noted in [5] that the spin momenta $q_m$ in the solutions of Eqs. (4,5) become large (growing with $U/t$ without constraint for large $U$) while the charge momenta $k_j$ remain finite in the limit. This property allows to decouple the system of the $N + M$ connected equations into, at least, some disconnected
parts by means of \( t/U \ll 1 \) expansion, simplifying the solution in this \( U = \infty \) limit. It is convenient to perform such an expansion by introducing the following mapping for the spin degrees of freedom,

\[
\lambda_l = -\frac{iU}{4t} e^{i q_l} + 1 \quad \frac{4t}{e^{i q_l} - 1},
\]

(7)

where, in addition to the rescaling by \( U/t \), the parameterisation of the spin momenta is changed from Orbach [6] to coordinate so the representation for the charge and spin momenta is the same.

Under substitution of the mapping in Eq. (7) the leading \( t/U \) order term in the Taylor expansion of Eqs. (8,9) becomes

\[
L k_j - \sum_m q_m = 2\pi I_j,
\]

(8)

\[
N q_m - 2 \sum_{l \neq m}^M \phi_{lm} = 2\pi J_m,
\]

(9)

where

\[
e^{i 2\phi_{lm}} = \frac{e^{i q_l + i q_m} + 1 - 2e^{i q_l}}{e^{i q_l + i q_m} + 1 - 2e^{i q_m}},
\]

(10)

are the two-spinon scattering phases. Note that the mapping in Eq. (7) is chosen such so the resulting two-spinon scattering phases above correspond to the antiferromagnetic case since the Hubbard model in the strong coupling regime is well-approximated by the \( t - J \) model [7], with its antiferromagnetic correlations for the spin degrees of freedom making this choice the most natural. Taking additionally the low density limit, \( N/L \ll 1 \), leaves the Lieb-Wu equations in Eqs. (8,9) unchanged but simplifies the eigenenergy of the many-particle state as \( E = t \sum_{j=1}^N k_j^2 / 2 \).

As a result of taking this limit, the spin part of the Lieb-Wu equations decouples completely in Eq. (9) becoming a self-contained set of \( M \) nonlinear equations, which are exactly the Bethe equations for the antiferromagnetic Heisenberg chain [2]. Once this system of \( M \) equations for \( q_m \) is solved, each equation for \( k_j \) in Eq. (8) becomes just an independent single-particle quantisation condition.

The form of the Lieb-Wu eigenstates in Eq. (1) also simplifies in the \( U = \infty \) limit. Under the substitution of the mapping in Eq. (7) into the phase factor \( A_{QO} \alpha \) in Eq. (3), the leading order term of the Taylor expansion in \( t/U \) of the resulting expression is

\[
A_{QO} \alpha = (-1)^O \sum_R e^{i \sum_{l<m}^M \varphi_{R_l,R_m} + \sum_{l=1}^M q_{R_l} x_l}.
\]

(11)

Here a factor that depends only on the spin momenta \( q_j \) but not on any permutation \( Q \) or \( R \) was ignored since it can be absorbed by the normalisation of the whole wave function \( |\Psi\rangle \).

The resulting expression under the sum over \( R \) in Eq. (11) depends only on the spin momenta \( q_j \) and spin coordinates \( x_l \), which allows to factorise the wave function in Eq. (1) as \([5]\]

\[
\psi_j \alpha = \psi^s_j \cdot \psi^c_\alpha,
\]

(12)

where the spin part is

\[
\psi^s_j = \sum_R e^{i \sum_{l<m} \varphi_{R_l,R_m} + \sum_{l=1}^M q_{R_l} x_l}
\]

(13)

and the charge part,

\[
\psi^c_j = \sum_Q (-1)^Q e^{i Q k_j},
\]

(14)

depends only on the charge momenta \( k_j \) and charge coordinates \( j_l \). The ordering permutation \( O \) disappears from this limiting expression since the sum over \( Q \) in Eq. (14) is a Slater determinant, under which exchange of the rows corresponding to the charge coordinates \( x_j \) cancels the \((-1)^O\) factor altogether.

The expressions in Eqs. (8,9) and in Eqs. (13,14) are presented in Eqs. (2-5) of the main text as the starting point for the calculation in this work.
II. ALGEBRAIC REPRESENTATION OF BETHE ANSATZ

The Bethe states for the spin part of the wave function in Eq. (13) are the eigenstates of the antiferromagnetic Heisenberg model [2]. In Eq. (13) these many-body states are written in the so-called coordinate representation, in which they are not factorisable, making calculations of scalar products and expectation values almost intractable. Another, the so-called algebraic representation of Bethe ansatz was invented [8] as a way for solving this kind of problems. In the algebraic representation the Bethe states are factorised in terms of operators with given commutation relations, which can be used to perform practical calculations.

It is more convenient to construct such an algebraic representation for a bit more general spin model, the XXZ model

\[ H = \sum_{j=1}^{N} \left( \frac{S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+}{2} + \Delta S_j^z S_{j+1}^z \right). \]

The eigenstates of this model are the same as in Eq. (13) where the \( M \) spin momenta \( q_j \) satisfying the spin part of Lieb-Wu equation (9) with the two-spinon scattering phase

\[ e^{i2\varphi_{1m}} = \frac{e^{iq_1 + iq_m} + 1 - 2\Delta e^{iq_1}}{e^{iq_1 + iq_m} + 1 - 2\Delta e^{iq_m}}. \]

For \( \Delta = 1 \) Eqs. (15,16) are the antiferromagnetic Heisenberg model, \( H = \sum_i S_i \cdot S_{i+1} \), and its two-spinon scattering phase in Eq. (10).

Following the notations of the book in [9], the many-body wave function of the XXZ model can be written using (Bethe ansatz) operators that satisfy an algebra generated by the Yang-Baxter equation as

\[ |\mathbf{u}\rangle = \prod_{j=1}^{M} C(u_j) |\downarrow\rangle, \]

where \( u_j \) are \( M \) complex parameters corresponding to \( M \) spin momenta \( q_j \), \( |\downarrow\rangle \) is the “vacuum” state (associated with all the \( N \) spins on the chain are in the down state configuration), and \( C(u) \) is one of the four matrix elements of the transition (monodromy) matrix

\[ T(u) = \left( \begin{array}{cc} A(u) & B(u) \\ C(u) & D(u) \end{array} \right). \]

This matrix is defined in an auxiliary \( 2 \times 2 \) space and is a function of the parameter \( u \) that can be arbitrary complex number. This \( T \)-matrix is a solution of the Yang-Baxter equation

\[ R(u - v) (T(u) \otimes T(v)) = (T(v) \otimes T(u)) R(u - v), \]

ensuring that any more than two-body scattering matrix factorises into a product of only two-body scattering matrices.

The so-called \( R \)-matrix here acts on a \( 4 \times 4 \) tensor product \( V_1 \otimes V_2 \) space, where \( V_1 \) and \( V_2 \) are two-element subspaces, each of which consists of two spin states \( |\downarrow\rangle \) and \( |\uparrow\rangle \). For the model in Eq. (15) the \( R \)-matrix is [9]

\[ R(u) = \left( \begin{array}{cc} 1 & b(u) & c(u) \\ b(u) & c(u) & b(u) \\ c(u) & b(u) & 1 \end{array} \right), \]

where

\[ b(u) = \frac{\sinh(u)}{\sinh(u + 2\eta)}, \quad c(u) = \frac{\sinh(2\eta)}{\sinh(u + 2\eta)}, \]

and \( \eta \) is a real number corresponding to the interaction strength. Note that this \( R \)-matrix also satisfies the Yang-Baxter equation, \( R_{12}(u_1 - u_2) R_{13}(u_1) R_{23}(u_2) = R_{23}(u_2) R_{13}(u_1) R_{12}(u_1 - u_2) \).
A two-element subspace of the $R$-matrix can be identified with the two-state spin subspace on the lattice site $j$ in the model in Eq. (15). Then, the quantum version of the so-called Lax matrix ($L$-matrix) for a single spin site $j$ can be defined as $L_j = R_{ij}$ [8], where the subspace 1 plays the role of the auxiliary $2 \times 2$ space, in which the $T$-matrix in Eq. (18) is defined. In this auxiliary space the matrix form of the Lax operator is

$$L_j (u) = \begin{pmatrix} \cosh(u+\eta 2S^+_j) & -i \sinh(2\eta)S^+_j \\ i \sinh(2\eta)S^-_j & -i \cosh(u+\eta 2S^-_j) \end{pmatrix}. \quad (22)$$

The prefactor in front of $L_j (u)$, and the matrix elements of the $R$-matrix in Eq. (20), are chosen such that in the non-interacting limit $\eta = 0$ the $L$-operator is a unit matrix. Lastly, the transition matrix $T (u)$ for a chain consisting of $N$ spin sites can be constructed similarly to the Lax method for classical systems as

$$T (u) = \sum_{j=1}^N L_j (u), \quad (23)$$

providing a definition of the algebraic Bethe ansatz operators in terms of the spin operators of the model in Eq. (15).

Note that starting from the $L$-matrix in Eq. (22), which satisfy the Yang-Baxter equation by construction, it can be shown explicitly that the $T$-matrix defined in Eq. (23) also satisfies the same Yang-Baxter equation, e.g. see proof in [9].

The 16 entries (in the $4 \times 4$ space) of Yang-Baxter equation (19) with the $R$-matrix in Eq. (20) give the commutation relations between all four Bethe ansatz operators $A (u), B (u), C (u),$ and $D (u)$, which are the the matrix elements of $T$-matrix. The explicit from for the four of them that will be needed later is

$$[B_u, C_v] = \frac{c (u-v)}{b (u-v)} (A_u D_v - A_v D_u), \quad (24)$$

$$A_u C_v = \frac{1}{b (u-v)} C_v A_u - \frac{c (u-v)}{b (u-v)} C_u A_v, \quad (25)$$

$$D_u C_v = \frac{1}{b (v-u)} C_v D_u - \frac{c (v-u)}{b (v-u)} C_u D_v, \quad (26)$$

$$[A_u, D_v] = \frac{c (u-v)}{b (u-v)} (C_u B_v - C_v B_u), \quad (27)$$

where the subscript for $u$ and $v$ was introduced as a shorthand for the argument, e.g. $A_u \equiv A (u)$.

Within the algebraic approach the transfer matrix is given by the trace of the transition matrix as

$$\tau (u) = \text{Tr} T (u) = A (u) + D (u). \quad (28)$$

This operator gives a family of commuting matrices, $[\tau (u), \tau (v)] = 0$ for all pairs of $u$ and $v$, which contain all the conserved quantities of the model in Eq. (15) including the Hamiltonian itself. Thus, if $|u\rangle$ is an eigenstate of $\tau (u)$, then it is also an eigenstate of the Hamiltonian. Therefore, the eigenstate equation can be written down as

$$\tau (u) |u\rangle = \tau_u |u\rangle, \quad (29)$$

where $\tau_u$ is a scalar quantity—the corresponding eigenvalue of the transition matrix.

The diagonalisation problem in Eq. (29) can be solved using the commutation relation in Eqs. (24-27). The results of acting with the $A_u$ and $D_u$ operators on the state $|u\rangle$ in Eq. (17) are obtained by commuting them from left to right through the product of $C (u_j)$ operators,

$$A_u \prod_{j=1}^M C (u_j) |\psi\rangle = a_u \prod_{j=1}^M \frac{1}{b_{u_j}} C (u_j) |\psi\rangle + \sum_{j=1}^M a_j \frac{c_{u_j}}{b_{u_j}} C (u) \prod_{l=1 \neq j}^M \frac{1}{b_{l_j}} C (u_l) |\psi\rangle, \quad (30)$$

$$D_u \prod_{j=1}^M C (u_j) |\psi\rangle = d_u \prod_{j=1}^M \frac{1}{b_{j u}} C (u_j) |\psi\rangle - \sum_{j=1}^M d_j \frac{c_{u_j}}{b_{u_j}} C (u) \prod_{l=1 \neq j}^M \frac{1}{b_{l_j}} C (u_l) |\psi\rangle, \quad (31)$$

where the vacuum eigenvalues of the operators \( A_u |\downarrow\rangle = a_u |\downarrow\rangle \) and \( D_u |\downarrow\rangle = d_u |\downarrow\rangle \) are obtained explicitly using of
the construction in Eqs. (22,23) as
\[
a_u = \frac{\cosh^N (u - \eta)}{\cosh^N (u + \eta)} \quad \text{and} \quad d_u = 1,
\]
and shorthand notations with the subscripts were introduced as \( a_j \equiv a (u_j), b_jl \equiv b (u_j - u_l), \) and \( b_ju \equiv b (u_j - u) \).

Since the right-hand sides of Eqs. (30,31) contain terms that are not proportional to the original state multiplied
by a scalar, an arbitrary algebraic Bethe state with arbitrary set of parameters \( u_j \) is not an eigenstate of the transfer
matrix \( \tau (u) \). However, the sum of the two second terms in Eqs. (30,31), appearing in definition of the transition
matrix in Eq. (28), can be made zero by selecting particular sets of \( u_j \) that satisfy the following set of \( M \) equations,
\[
\frac{a_j}{d_j} = \prod_{l=1, l \neq j}^M \frac{b_jl}{b_jl}.
\]
Substitution of the expressions for \( a_j \) and \( d_j \) from Eq. (32) and for \( b_jl \) from Eq. (21) gives the set of equations for the
diagonalisation problem of the transition matrix as
\[
\frac{\cosh^N (u_j - \eta)}{\cosh^N (u_j + \eta)} = \prod_{l=1, l \neq j}^M \frac{\sinh (u_j - u_l - 2\eta)}{\sinh (u_j - u_l + 2\eta)}
\]
and its corresponding eigenvalue as
\[
\mathcal{T}_u = \frac{\cosh^N (u - \eta)}{\cosh^N (u + \eta)} \prod_{j=1}^M \frac{\sinh (u - u_j + 2\eta)}{\sinh (u - u_j)} + \prod_{j=1}^M \frac{\sinh (u_j - u + 2\eta)}{\sinh (u_j - u)}.
\]

The set of equations (34) are the Bethe equations for the XXZ model in Eq. (15). Noting that the spin momenta in
the set of equations (34) are written in Orbach parametrisation [6], their mapping back to the coordinate representation
is given by
\[
\begin{align*}
    u_j &= \frac{1}{2} \ln \left( \frac{1 - e^{i\eta_j - 2\eta}}{1 - e^{-i\eta_j - 2\eta}} \right) - \frac{i\eta_j}{2}, \\
    \eta &= \frac{1}{2} \cosh \Delta.
\end{align*}
\]
Substitution of this mapping into Eq. (34) gives the Bethe ansatz equations (9) with the scattering phases for the
XXZ model in Eq. (16).

### A. Scalar product of Bethe states

A straightforward example of the advantage that the algebraic representation of Bethe ansatz provides over the
coordinate representation is calculation of the scalar product between two Bethe states \( \langle \nu | u \rangle \) given in the
algebraic representation by Eq. (17). It can be evaluated directly with the help of the commutation relations in
Eqs. (24-27).

The multiplication of the bra and ket states is the vacuum expectation value of a product of the Bethe ansatz
operators \( B (v_j) \) and \( C (u_j) \), in which all the \( B (v_j) \) operators appear to the left from all the \( C (u_j) \) operators. Under
such an expectation value, each \( B (v_j) \) operator can be commuted all the way from left to right through the product
of \( C (u_j) \) operators using the commutation relation in Eq. (24), which generates all the \( A \) and \( D \) operators with
arguments that all possible values of \( u_j \) and \( v_j \). They, in turn, also have to be commuted to the right through the
remaining product of \( C (u_j) \) operators. Finally, the \( B (v_j) \) operators acting upon the vacuum state give 0 and the
products of \( A \) and \( D \) operators give products of their vacuum eigenvalues \( a (u_j) \) and \( d (v_j) \) given in Eq. (32). When
at least one set of the parameters, say \( u_j \), is a solution of the Bethe equations (34) the result of all the commutations
can be written in a compact form as a determinant of an \( M \times M \) matrix—the so-called Slavnov’s formula [10],
\begin{equation}
\langle v | u \rangle = \prod_{i<j}^{M} \sinh (v_j - u_j) / \prod_{i<j}^{M} \sinh (v_i - v_j) \prod_{i<j}^{M} \sinh (u_i - u_j) \det \hat{C},
\end{equation}

where the matrix elements of the $M \times M$ matrix $\hat{C}$ are $C_{ab} = \partial_{u_a} T(v_b)$. Under substitution of the eigenvalue of the transition matrix $T(u)$ from Eq. (35), these matrix elements read in explicit form as

\begin{equation}
C_{ab} = \frac{\cosh^N (v_b - \eta)}{\cosh^N (v_b + \eta) \sinh^2 (v_b - u_a)} \prod_{j=1 \neq a}^M \frac{\sinh (v_b - u_j + 2\eta)}{\sinh (v_b - u_j)} - \frac{\sinh (2\eta)}{\sinh^2 (u_a - v_b)} \prod_{j=1 \neq a}^M \frac{\sinh (u_j - v_b + 2\eta)}{\sinh (u_j - v_b)}.
\end{equation}

### B. Normalisation factor of Bethe state

The normalisation factor of the Bethe states in the algebraic form in Eq. (17) can be evaluated by taking the limit of $v \to u$ in the scalar product in Eq. (38) giving [11, 12]

\begin{equation}
Z^2 = \langle u | u \rangle = \sinh^M (2\eta) \prod_{i \neq j}^M \frac{\sinh (u_j - u_i + 2\eta)}{\sinh (u_j - u_i)} \det \hat{F},
\end{equation}

where the matrix elements of $\hat{F}$ are

\begin{equation}
F_{ab} = \begin{cases} 
-N \frac{\sinh(2\eta)}{\cosh(\eta) \sinh(4\eta)} - \sum_{j=1 \neq a}^M \frac{\sinh(u_a - u_j - 2\eta)}{\sinh(u_a - u_j + 2\eta)}, & a = b, \\
\frac{\sinh(4\eta)}{\sinh(u_b - u_a - 2\eta) \sinh(u_b - u_a + 2\eta)}, & a \neq b.
\end{cases}
\end{equation}

Let us map this result back into the coordinate representation by substituting Eqs. (36,37) for the Heisenberg model $\Delta = 1$, which is a part of the original problem for the spin part of the wave function in this work. For $\Delta = 1$ the interaction parameter in the algebraic representation in Eq. (37) is $\eta = 0$ making the mapping for spin momenta in Eq. (36) degenerate, $u_j = i\pi/2$ for any $q_j$. Therefore, the proper limit needs to be taken by expanding Eq. (36) in Taylor series up to the linear order in $\eta$,

\begin{equation}
u_j = \frac{i\pi}{2} + i\eta \cot \frac{q_j}{2},
\end{equation}

substituting this expansion in the normalisation factor in Eq. (40), and taking the limit of $\eta \to 0$ for the whole expression. Implementation of this procedure,

\begin{equation}
\lim_{\eta \to 0} Z^2 \bigg|_{u_j = \frac{i\pi}{2} + i\eta \cot \frac{q_j}{2}},
\end{equation}

gives

\begin{equation}
Z^2 = (-4)^M \prod_{i \neq j=1}^M \frac{(\cot \frac{q_j}{2} - \cot \frac{q_j}{2} - 2i)}{(\cot \frac{q_j}{2} - \cot \frac{q_j}{2})} \prod_{j}^M \sin^2 \frac{q_j}{2} \det \hat{Q},
\end{equation}

where the matrix under the determinant is

\begin{equation}
Q_{ab} = \begin{cases} 
N - \sum_{j=1 \neq a}^M \frac{4(1 - \cos q_j)}{4(1 - \cos k_b)} \left( e^{i\eta q_j} + e^{-i\eta q_j} - 2 \right), & a = b, \\
\frac{e^{i\eta q_a} + e^{-i\eta q_a} - 2}{(e^{i\eta q_a} + e^{-i\eta q_a} - 2)} \left( e^{i\eta q_j} + e^{-i\eta q_j} - 2 \right), & a \neq b.
\end{cases}
\end{equation}

This is the determinant of the same matrix as was obtained for the normalisation of the Bethe state in the coordinate representation in [11], which is quoted after Eq. (5) in the main paper. However, the prefactor in front of this determinant is not 1 but a function of spin momenta, see Eq. (44), demonstrating that normalisation of the wave functions in two different representations in Eq. (13) and in Eq. (17) is different. Since the algebraic representation is used for the calculation of the correlation functions in this work, Eq. (44) will be used as the normalisation factor for the relevant spin matrix elements, although the final result, Eqs. (63-65) below and Eqs. (7-9) of the main paper, is presented in the coordinate representation.
III. SPIN MATRIX ELEMENT

Evaluation of the spin part, $\langle f|c_1\uparrow|0\rangle_s$, of the matrix element, needed for the correlation functions in the main paper, requires the use of algebraic representation of Bethe ansatz introduced in the previous section. Since the spin part of the wave function does not contain any change degree of freedom, the explicit form of this matrix elements is

$$
\langle f|c_1\uparrow|0\rangle_s = Z_f^{-1}Z_0^{-1}\langle f|D_1S_1^-|0\rangle_s,
$$

(46)

were $Z$ are the normalisation factor of the Bethe wave function in the algebraic representation in Eq. (40). Note that the charge part of the $c_1\uparrow$ operator, $a_1$, acts only on the charge degrees of freedom giving the result quoted in Eq. (6) of the main text [13].

There are two problems in calculating the spin matrix element in Eq. (46). One is representation of the local spin operator $S_1^-$ in terms of the delocalised along the chain Bethe operators in Eq. (18) so the commutation relations in Eqs. (24-27) can be used. And the other problem is dealing with the $D_1$ operator that makes the spin chain shorter by one site and, therefore, the Bethe operators in the algebraic representation for the states $|0\rangle_s$ and $\langle f|_s$ in Eq. (17) are different according to the construction in Eq. (23) so the commutation relations between them are not defined. We will address these two problems one by one.

The first problem of expressing the local spin operators in terms of Bethe operators was solved by means of Drinfeld twist [14]. It allows to construct a representation for the transition matrix in which it becomes quasi-local, obtaining a relatively simple expression for the original spin operators. For instance, for the $S_j^-$ operator, appearing in matrix element in Eq. (46), it reads [15]

$$
S_j^- = \tau_\xi^{-j}B_\xi\tau_\xi^{j-1}
$$

(47)

where $\xi = -i\pi/2 + \eta$.

Note that this expression is not identical to the one presented in [15]. The correctness of the above expression can be check explicitly by expressing the $B_\xi$ and $\tau_\xi$ operators in terms of the local spin operators for a chain of small length $N = 3$, by means of the construction in Eq. (23). As a result, it can be checked explicitly that the transfer matrix $\tau_\xi$ shifts the chain by one site to the left and the Bethe operator $B_\xi$ removes the last spin in the chain. The discrepancy between Eq. (47) and [15] makes no difference for the pure Heisenberg model since the same periodic boundary condition for the bra and the ket states ensures a change only in the irrelevant phase factor in the matrix elements there. But using one or the other expression strongly affects the correlation function of the Hubbard model, in which the relevant ladder operators simultaneously change the length of the spin chain, leading to different amplitudes in the resulting matrix elements—not just different phase factors.

Still in the coordinate representation, the spin chain can be shifted $N - 1$ times to the right. Under such a shift, the matrix element in Eq. (46) acquires only an irrelevant phase factor,

$$
\langle f|D_1S_1^-|0\rangle_s = e^{i(P_0^j-P_f^j)(N-1)} \langle f|D_NS_N^-|0\rangle_s.
$$

(48)

However, it will help to avoid the need to commute the operators $\tau_\xi$ and $B_\xi$ explicitly, simplifying the algebra in the calculation below.

Now, the whole the whole spin matrix element can be written in the algebraic representation by substituting the expression in Eq. (47) for $S_N^-$ and the Bethe wave function in Eq. (17) for the eigenstates into the matrix element in the right-hand side of Eq. (48) as

$$
\langle f|D_NS_N^-|0\rangle_s = \langle \downarrow | \prod_{j=1}^{M-1} B^{N-1}(u_j) B_\xi^N \prod_{j=1}^{M} C^N(u_j) | \downarrow \rangle,
$$

(49)

where the set of $u_j$ and the set of $v_j$ are two solutions of the Bethe equations (34) and $\tau_\xi^{N-1}$ acting upon an eigenstate, see Eq. (29), gives just its eigenvalue in Eq. (35), which for $u = \xi$ becomes just an irrelevant phase shift $T^{N-1}_\xi|0\rangle = e^{iP_0(N-1)|0\rangle}$. Here the $D_N$ operator removes the $N^{th}$ spin from the chain, reducing its length by one. Therefore, the Bethe ansatz operators before the position of this operators are constructed, see Eq. (23), out of the spin operators for the $1^{st}$ to $N^{th}$ site, which is marked by the superscript $N$, e.g. $C^N(u_j)$. The Bethe ansatz operators after the position of the $D_N$ operator are constructed out of the spin operators for the $1^{st}$ to $N - 1^{st}$ site, which is marked by the superscript $N - 1$, e.g. $B^{-1}(v_j)$. 

$$
\langle f|D_1S_1^-|0\rangle_s = \langle \downarrow | \prod_{j=1}^{M-1} B^{N-1}(u_j) B_\xi^N \prod_{j=1}^{M} C^N(u_j) | \downarrow \rangle,
$$

(49)

where the set of $u_j$ and the set of $v_j$ are two solutions of the Bethe equations (34) and $\tau_\xi^{N-1}$ acting upon an eigenstate, see Eq. (29), gives just its eigenvalue in Eq. (35), which for $u = \xi$ becomes just an irrelevant phase shift $T^{N-1}_\xi|0\rangle = e^{iP_0(N-1)|0\rangle}$. Here the $D_N$ operator removes the $N^{th}$ spin from the chain, reducing its length by one. Therefore, the Bethe ansatz operators before the position of this operators are constructed, see Eq. (23), out of the spin operators for the $1^{st}$ to $N^{th}$ site, which is marked by the superscript $N$, e.g. $C^N(u_j)$. The Bethe ansatz operators after the position of the $D_N$ operator are constructed out of the spin operators for the $1^{st}$ to $N - 1^{st}$ site, which is marked by the superscript $N - 1$, e.g. $B^{-1}(v_j)$. 

$$
\langle f|D_1S_1^-|0\rangle_s = \langle \downarrow | \prod_{j=1}^{M-1} B^{N-1}(u_j) B_\xi^N \prod_{j=1}^{M} C^N(u_j) | \downarrow \rangle,
$$

(49)

where the set of $u_j$ and the set of $v_j$ are two solutions of the Bethe equations (34) and $\tau_\xi^{N-1}$ acting upon an eigenstate, see Eq. (29), gives just its eigenvalue in Eq. (35), which for $u = \xi$ becomes just an irrelevant phase shift $T^{N-1}_\xi|0\rangle = e^{iP_0(N-1)|0\rangle}$. Here the $D_N$ operator removes the $N^{th}$ spin from the chain, reducing its length by one. Therefore, the Bethe ansatz operators before the position of this operators are constructed, see Eq. (23), out of the spin operators for the $1^{st}$ to $N^{th}$ site, which is marked by the superscript $N$, e.g. $C^N(u_j)$. The Bethe ansatz operators after the position of the $D_N$ operator are constructed out of the spin operators for the $1^{st}$ to $N - 1^{st}$ site, which is marked by the superscript $N - 1$, e.g. $B^{-1}(v_j)$. 

$$
\langle f|D_1S_1^-|0\rangle_s = \langle \downarrow | \prod_{j=1}^{M-1} B^{N-1}(u_j) B_\xi^N \prod_{j=1}^{M} C^N(u_j) | \downarrow \rangle,
$$

(49)

where the set of $u_j$ and the set of $v_j$ are two solutions of the Bethe equations (34) and $\tau_\xi^{N-1}$ acting upon an eigenstate, see Eq. (29), gives just its eigenvalue in Eq. (35), which for $u = \xi$ becomes just an irrelevant phase shift $T^{N-1}_\xi|0\rangle = e^{iP_0(N-1)|0\rangle}$. Here the $D_N$ operator removes the $N^{th}$ spin from the chain, reducing its length by one. Therefore, the Bethe ansatz operators before the position of this operators are constructed, see Eq. (23), out of the spin operators for the $1^{st}$ to $N^{th}$ site, which is marked by the superscript $N$, e.g. $C^N(u_j)$. The Bethe ansatz operators after the position of the $D_N$ operator are constructed out of the spin operators for the $1^{st}$ to $N - 1^{st}$ site, which is marked by the superscript $N - 1$, e.g. $B^{-1}(v_j)$. 

The operators with the superscript $N$ in Eq. (49) obey the same commutation relations in Eqs. (24-27). Thus, commuting $B^N$ through a product of $C^N$, a procedure similar to what was used in deriving Eqs. (30-31), gives

$$B^N (\xi) \prod_{j=1}^{M} C^N (u_j) |\psi\rangle = \prod_{x=1}^{M} a_x c_{\xi} \prod_{i=1\neq x}^{M+1} \frac{1}{b_{xi}} \prod_{y=1\neq x}^{M+1} d_{xy} c_{\xi y} \prod_{j=1\neq x,y}^{M+1} \frac{1}{b_{jxy}} \prod_{j=1\neq x,y}^{M+1} C^N (u_j) |\psi\rangle,$$

(50)

where the notation of $u_{x+1} \equiv \xi$ was introduced and all the vacuum eigenvalues and the matrix element of the $R$-matrix are given only for $u_j$, e.g. $d_{xy} = d (u_x)$ or $c_{\xi} = c (u_x - \xi)$. After substitution of this result back into Eq. (49), the remaining structure in terms of Bethe ansatz operators is that of a scalar product, which can, in principle, be evaluated in terms of a determinant expression, see Eq. (38). However, before the formula in Eq. (38) can be used both the bra and ket states have to be expressed in terms of the Bethe ansatz operators for a spin chain of the same length satisfying the same commutation relations.

We resolve this problem by expressing the Bethe ansatz operators for the longer chain in terms of the Bethe ansatz operators from the shorter chain and the local spin operator for the $N^{th}$ spin. The last ($N^{th}$) spin in the product in the construction in Eq. (23) can be singled out giving

$$\left( \begin{array}{cc}
A^N_u & B^N_u \\
C^N_u & D^N_u
\end{array} \right) = \left( \begin{array}{cc}
A^{N-1}_u & B^{N-1}_u \\
C^{N-1}_u & D^{N-1}_u
\end{array} \right) \left( \begin{array}{cc}
\frac{\cosh (u + \eta 2 S^+_N)}{\cosh (u + \eta)} & -i \frac{\sinh 2 \eta S^+_N}{\cosh (u + \eta)} \\
i \frac{\sinh 2 \eta S^+_N}{\cosh (u + \eta)} & \frac{\cosh (u + \eta)}{\cosh (u + \eta)}
\end{array} \right),$$

(51)

where the transition matrix for the shorter chain of $N - 1$ spins, $T^{N-1} (u) = \prod_{j=1}^{N-1} L_j (u)$, gives the corresponding Bethe operators in the right-hand side. The bottom-left matrix elements in both sides of this equation gives representation of the $C^N_u$ operator needed for calculating the element in Eq. (49) through Bethe operators of the shorter chain,

$$C^N = \frac{\cosh (u + \eta 2 S^+_N)}{\cosh (u + \eta)} C^{N-1} - i \frac{\sinh 2 \eta S^+_N}{\cosh (u + \eta)} D^{N-1}.$$  

(52)

Substituting the result of the commutation in Eq. (50) and this expression above into Eq. (49), we obtain a vacuum expectation value with respect to the ferromagnetic states of the chain of $N$ spins, $|\psi\rangle^N = \prod_{j=1}^{N} |\psi\rangle_j$. In this expression, the contribution of all terms containing $S^+_N$ at least in the first power is zero since the product of $B^{N-1}$ contains no $S^+_N$ operators so that such terms has a factor

$$\langle \downarrow | \left[ \frac{\sinh 2 \eta S^+_N}{\cosh (u + \eta)} \right]^k | \downarrow \rangle_N = 0$$

(53)

for $k > 0$. The other terms containing only $S^-_N$ operators give a non-zero contribution,

$$\langle \downarrow | \left[ \frac{\cosh (u + \eta 2 S^-_N)}{\cosh (u + \eta)} \right]^k | \downarrow \rangle_N = \frac{\cosh^k (u - \eta)}{\cosh^k (u + \eta)},$$

(54)

The sum of all such uch non-zero terms gives the matrix element in Eq. (49) as

$$\langle f | D_N S^-_N | 0 \rangle = \sum_{x=1}^{N} a_x c_{\xi} \prod_{i=1\neq x}^{N} \frac{1}{b_{xi}} \sum_{y=1\neq x}^{N} c_{\xi y} \cosh (\xi - \eta) \prod_{j=1\neq x,y}^{N} \frac{1}{b_{jy}} \cosh (u_j - \eta) \langle v | u_{x-1}, u_{x+1}, u_{y-1}, u_{y+1}, \xi \rangle$$

(55)

$$+ \sum_{x=1}^{N} a_x c_{\xi} \prod_{i=1\neq x}^{N} \frac{1}{b_{xi}} \prod_{j=1\neq x}^{N} \frac{1}{b_{jy}} \cosh (u_j - \eta) \langle v | u_{x-1}, u_{x+1} \rangle,$$

(56)

$$= \sum_{j=1}^{N} \frac{\cosh (u_j - \eta)}{\cosh (u + \eta)} \sum_{x=1}^{N} a_x c_{\xi} \prod_{i=1\neq x}^{N} \frac{1}{b_{xi}} \cosh (u_x + \eta) \prod_{j=1\neq x}^{N} \frac{1}{b_{jy}} \langle v | u_{x-1}, u_{x+1} \rangle.$$  

(57)
where the factor \( \cosh(\xi - \eta) / \cosh(\xi + \eta) = 0 \) makes the line (55) zero. Here the scalar factors can be taken out of the vacuum expectation value, leaving only a product of \( M - 1 \) operators for all \( N^{-1} \) and \( C N^{-1} \) under it, in which all the \( B N^{-1} \) operators occur to the left of all the \( C N^{-1} \) operators, \( \langle \psi \mid u_{x-1}, u_{x+1} \rangle \). The latter is evaluated using the determinant formula for scalar product in Eq. (38), where the elements of the matrix under the determinant are \( \mathcal{C}_{ab} = \partial_{\nu_a} \mathcal{T}(u_b) \) since \( v_1, \ldots, v_{M-1} \) is a solution of Bethe equations for the shorter chain but the set of \( M - 1 \) parameters \( u_1, \ldots, u_{x-1}, u_{x+1}, \ldots, u_M \) is not a solution of any Bethe equation.

The remaining sum over determinants of \( M - 1 \times M - 1 \) matrices in Eq. (57) can be expressed as a single determinant of an \( M \times M \) matrix since the sum has the form of a Laplace expansion of a matrix through the sum of minors over one of its columns,

\[
\det \mathcal{T} = \sum_{x=1}^{M} T_{Mx} (-1)^{x+M} \text{minor}_{Mx}.
\] (58)

where \( T_{Mx} \) is the entry of \( M \)th row and \( x \)th column of the matrix \( \mathcal{T} \) and minor \( Mx \) is the determinant of the submatrix obtained by removing the \( M \)th row and \( x \)th column of \( \mathcal{T} \). Applying this formula Eq. (57) in reverse, and rearranging various factors for compactness, we obtain the following expression for the matrix element

\[
\langle f \mid D_N S_N^{-1} \rangle = \frac{\prod_{i<j=1}^{M} \sinh(u_j - v_i)}{\prod_{j<i} \sinh(v_j - v_i) \prod_{j<i} \sinh(u_j - u_i)} \det \mathcal{R},
\] (59)

where the elements of the \( M \times M \) matrix \( \mathcal{R} \) are

\[
R_{ab} = \frac{\sinh(2\eta)}{\sinh^2(\eta(b - a))} \left[ \frac{\cosh(\xi - \eta)^{(N-1)} \prod_{j=1 \neq a}^{M-1} \sinh(u_j - v_j + 2\eta)}{\cosh(\xi + \eta)^{(N-1)} \prod_{j=1 \neq a}^{M-1} \sinh(u_j - v_j - 2\eta)} \right],
\] (60)

for \( a < M \) and

\[
R_{M \theta} = \frac{\prod_{1 \neq a}^{M} \sinh(u_j - u_i - 2\eta)}{\cosh(\xi - \eta) \prod_{1 \neq a}^{M-1} \sinh(u_j - v_i)}
\] (61)

for \( a = M \). Calculation of the the same matrix element in the coordinate representation for a small number of spin excitations \( M = 1, 2, 3 \), using the Bethe wave function in Eqs. (13,16) and evaluating the \( M \)-fold integrals numerically, give the same result as Eq. (59).

Finally, Eq. (59) needs to be substituted back into Eqs. (48,46) and the Heisenberg limit of \( \Delta = 1 \) has to be taken. The latter is done by substituting the Taylor expansion for the \( u_j \) and \( v_j \) in small \( \eta \) from Eq. (42) and taking the limit of the resulting expression

\[
\langle f \mid c_{j \uparrow} \rangle_{s} = \lim_{\eta \to 0} \frac{\langle f \mid D_N S_N^{-1} \rangle}{Z_f Z_f},
\] (62)

giving

\[
\langle f \mid c_{j \uparrow} \rangle_{s} = \frac{1}{\sqrt{\det Q_0 \det Q_f}} \prod_{j \neq a}^{M-1} \left( e^{iq_j^0} + e^{-iq_j^0} - 2 \right) \left( e^{iq_j^0} + e^{-iq_j^0} - 2 \right) \det \mathcal{R},
\] (63)

where the elements of the \( M \times M \) matrix \( \mathcal{R} \) are

\[
R_{ab} = \frac{e^{iq_a^0(N-1)} \prod_{j \neq a}^{M-1} \left( e^{-iq_j^0} + e^{-iq_j^0} + 2e^{iq_j^0} \right) - 1}{\left( e^{-iq_j^0} - e^{-iq_j^0} \right) \left( e^{iq_j^0} + e^{-iq_j^0} - 2 \right)},
\] (64)

\[
R_{M \theta} = \frac{e^{iq_a^0} \prod_{j \neq a}^{M} \left( e^{iq_j^0} + e^{-iq_j^0} - 2 \right)}{\prod_{1 \neq a}^{M-1} \left( e^{iq_j^0} + e^{-iq_j^0} - 2 \right)},
\] (65)
and the matrices $\hat{Q}_0$ and $\hat{Q}_f$ are given by Eq. (45) for the spin momenta of the initial 0 and the final state $f$ respectively. Repetition of the same calculation for $\langle f | c^{\dagger}_{i,j} | 0 \rangle_s$ gives the same expression as in Eqs. (63-65), in which the spin momenta are swapped, $\mathbf{q}^0 \leftrightarrow \mathbf{q}^f$, and the spin and particle quantum numbers are increased by one, $N \rightarrow N+1$ and $M \rightarrow M+1$.

The result in Eqs. (63-65) is presented in Eq. (7-9) of the main paper.

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Figure 1. Momentum distribution function $n_k$ around the $k_F$ point on the log-log scale for $N = 80$ particles, where the three leading levels of the hierarchy of modes $l \leq 2$ were taken into account in the sum in Eq. (11) of the main text. The dashed solid lines are power-law functions for $k < k_F$ and for $k > k_F$ giving the exponent as $a_{k_F} = 0.124 \pm 0.020$, where the value is the average of the two and the error bars is the difference. Inset A: Finite size cutoff for $n_k$ as the function of inverse system size $1/L$ on the log-log scale at the $k_F$ point. The solid solid line is a power-law fit giving $a_{k_F} = 0.13384$, within the accuracy of the fitting $n_k$ directly. Inset B: The value of $n_k$ at the $k_F$ point as a function of the particle number $N$. The solid line is a finite size a fit with finite size corrections, $n_{k_F} = C_{k_F} + b/N$ giving $C_{k_F} = 0.477$. 
Figure 2. (A) Spectral function $A_\alpha(k, E)$ of the Hubbard model in Eq. (1) of the main text evaluated in the $U/t = \infty$ limit using Eqs. (6-10) of the main text for $N = 500$ particles, where only the leading level $l = 0$ of the hierarchy of modes was taken into account in the sum in Eq. (10) of the main text. The nonlinear holon dispersions for the states in (B) and (C) are the two green dashed lines. The nonlinear spinon dispersion for the states in (D) is the blue dashed lines. Around the $\pm k_F$ points the slopes of these dispersions are the spinon $v_s = 0$ (labelled as $v_s$) and the holon $v_c = 2v_F$ (labelled as $v_c$) velocity, phenomenological parameters of the linear TLL model; $v_F$ is the Fermi velocity of the free particles. (B) and (C) Two sets of integer numbers, $I_j$ for charge and $J_m$ for spin degrees of freedom, defining the Lieb-Wu for the pure holon excitations in the particle sector. (D) Two sets of integer numbers, $I_j$ for charge and $J_m$ for spin degrees of freedom, defining the Lieb-Wu for the pure spinon excitations in the particle sector. The excitations in the hole sector are constructed analogously.