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Local spectral properties of Luttinger liquids: scaling versus nonuniversal energy scales

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Abstract
Motivated by recent scanning tunneling and photoemission spectroscopy measurements on self-organized gold chains on a germanium surface, we reinvestigate the local single-particle spectral properties of Luttinger liquids. In the first part we use the bosonization approach to exactly compute the local spectral function of a simplified field theoretical low-energy model and take a closer look at scaling properties as a function of the ratio of energy and temperature. Translational-invariant Luttinger liquids as well as those with an open boundary (cut chain geometry) are considered. We explicitly show that the scaling functions of both set-ups have the same analytical form. The scaling behavior suggests a variety of consistency checks which can be performed on measured data to experimentally verify Luttinger liquid behavior. In the second part we approximately compute the local spectral function of a microscopic lattice model—the extended Hubbard model—close to an open boundary using the functional renormalization group. We show that it follows the field theoretical prediction in the low-energy regime as a function of energy and temperature, and point out the importance of nonuniversal energy scales inherent to any microscopic model. The spatial dependence of this spectral function is characterized by oscillatory behavior and an envelope function which follows a power law in accordance with the field theoretical continuum model. Interestingly, for the lattice model we find a phase shift which is proportional to the two-particle interaction and not accounted for in the standard bosonization approach to Luttinger liquids with an open boundary. We briefly comment on the effects of several one-dimensional branches cutting the Fermi energy and Rashba spin–orbit interaction.

(Some figures may appear in colour only in the online journal)

1. Introduction

For decades theoretical studies of the single-particle spectral properties of metallic one-dimensional (1d) correlated electron systems—so-called Luttinger liquids (LLs)—were ahead of the experimental attempts to find or synthesize appropriate quasi-1d materials and perform spectroscopy on them. In fact, while at the beginning of the 1990s a clear picture of the basic spectroscopic properties of translational-invariant LLs was established (for reviews see, e.g., [1–3]), this period witnessed the first serious attempts to experimentally verify the specific spectroscopic signatures of LLs. These are (i) the low-energy power-law suppression of the local spectral function \( \rho(\omega) \sim |\omega|^{\alpha} \) for energies \( \omega \) close to the chemical potential [5–7] with \( \alpha \) depending on the two-particle interaction, and (ii) the appearance of two dispersing features in the momentum-resolved spectral function \( \rho(k, \omega) \) (spin–charge separation) [8–10] instead of

³ For a review on the experimental status up to 2009 see: [4].
a single quasi-particle peak of a Fermi liquid. For finite temperatures $T$ the suppression of the spectral weight as a function of $\omega$ is cut off by $T$ and one finds the scaling behavior $\rho \sim T^\alpha \rho_0(\omega/T)$ with an $\alpha$-dependent scaling function $\rho_0$, in which the two energy scales $\omega$ and $T$ only enter via their ratio [$11$]. These results were exclusively obtained using bosonization within the Tomonaga–Luttinger (TL) model [$1–3$].

Using the modern language of renormalization group (RG) methods the (translational-invariant) TL model is the exactly solvable effective low-energy fixed-point model for a large class of metallic 1d correlated electron systems—the LLs [$12$]. It thus plays the same role as the free Fermi gas in Fermi liquid theory. The model has two strictly linear branches of right- and left-moving fermions and two-particle scattering is restricted to processes with small momentum transfer $|q| \ll k_F$, with the Fermi momentum $k_F$. These processes, as well as the kinetic energy, can be written as quadratic forms of the densities of right- and left-moving fermions which obey bosonic commutation relations. In most calculations in addition, the momentum dependence of the low-momentum scattering processes $g_2$ and $g_4$ are neglected and momentum integrals are regularized in the ultraviolet, introducing a cutoff ‘by hand’ (for an exception see [$9$]). One can extend the resulting scale-free, field theoretical model by allowing for additional two-particle scattering processes. These turn out to be RG irrelevant in a wide parameter regime [$13$]. The most important of these processes is the so-called $g_1$ process (in the g-ology classification [$13$]) with momentum transfer $2k_F$ between two scattering fermions of opposite spin.

In some of the early experiments on 1d chains these were obviously interrupted by local impurities (see footnote 3). A simple model of an inhomogeneous LL is the open boundary analog of the TL model. Interestingly, an LL is susceptible to single-particle perturbations with momentum transfer $2k_F$ [$7$], and on asymptotically low-energy scales even a single weak impurity has the same effects on the spectral properties as an open boundary [$14$]. Triggered by this theoretical insight and by early experiments, the spectral properties of the open boundary analog of the TL model were studied [$15$, $16$]. The local spectral function close to the boundary shows power-law behavior as a function of $\omega$ but with an exponent $\alpha_0$ different from the bulk one $\alpha$. As in the translational-invariant case in this model only those low-energy scattering terms which can be written as quadratic forms in bosonic densities are kept. Only recently was it shown that a large class of further two-particle processes appearing in a 1d system with an open boundary are indeed RG-irrelevant [$17$].

The latest scanning tunneling spectroscopy (STS) and photoemission spectroscopy (PES) measurements on different classes of 1d metallic systems [$18–22$] impressively demonstrated that experiment has caught up, and more refined questions must now be answered by theory. Important ones are: how do effects which are not captured by the low-energy fixed point model, such as the momentum dependence of the two-particle interaction and the nonlinearity of the single-particle dispersion, influence the spectral functions? What is the energy scale of a given microscopic model on which the low-energy LL physics sets in? What do scaling functions for lattice models look like in detail? Here we shed some light on the last two questions and briefly comment on the first one. It is widely believed that neglecting the momentum dependence of the interaction and regularizing momentum integrals in the ultraviolet ‘by hand’ has no effect on the low-energy physics of LLs. This is indeed correct if all energy scales are sent to zero, that is for $\rho(\omega)$ and $\rho(\pm k_F, \omega)$: at small $\omega$ the spectral properties are unaffected by the details of the momentum dependence of the $g$s. However, if $\rho(k, \omega)$ as a function of $\omega$ is studied at fixed $k \neq \pm k_F$, as is usually done in angular-resolved PES, details of the momentum dependence of the interaction do matter. This was investigated in [$23$]. An overview on the effects of the nonlinearity of the single-particle dispersion can be found in the very recent review [$24$].

This paper is organized as follows. In section 2 we compute the local spectral function of the translationally invariant and the open boundary continuum TL model using bosonization. We show that both display scaling in $\omega/T$ and that the scaling functions have the same analytical form. We next compute the spectral function of the extended Hubbard model on the lattice close to an open boundary as a function of energy, temperature and position in section 3. For this an approximate method is used which is based on the functional RG approach [$25$]. It is devised for weak to intermediate two-particle interactions. In particular, we concentrate on inhomogeneous LLs as the boundary exponent $\alpha_B$, characterizing the spectral function close to an open boundary as linear in the two-particle interaction, while the bulk exponent is quadratic (see below). By varying the microscopic parameters of the extended Hubbard model we can tune the strength of the different scattering processes and thus study the crossover between nonuniversal behavior and the low-energy LL physics. We perform a scaling analysis of the spectral function as a function of $\omega$ and $T$ and show that the spectral weight close to the boundary follows the bosonization prediction within the universal low-energy regime. The position dependence of the spectral function is characterized by oscillatory behavior and a power-law envelope function in accordance with the result for the TL. Interestingly, we additionally find a phase shift which is proportional to the two-particle interaction and not accounted for in the standard bosonization procedure. We summarize our results in section 4 and briefly comment on how spin–orbit interaction and several bands crossing the Fermi surface—both being potentially important effects in recent experiments—influence the single-particle spectral functions.

2. Scaling functions of the Tomonaga–Luttinger model

In this section we derive closed analytic expressions for the single-particle Green function and the related local spectral function of the TL model with and without an open boundary at finite $T$. We then closely inspect the scaling form of the spectral functions.
In field theoretical notation (see, e.g., [26]) the Hamiltonian density of the TL model in spin–charge-separated form is

\[ \mathcal{H}(x) = \sum_{\nu=\text{c,s}} \mathcal{H}_\nu(x), \]

\[ \mathcal{H}_\nu = \frac{v_{\nu c}}{16\pi} \left[ \frac{1}{K_c} (\partial_x \Phi_x)^2 + K_c (\partial_x \Theta_x)^2 \right], \]  

with the canonical Bose fields \( \Phi_x \) and their dual fields \( \Theta_x \). Within the TL model the charge and spin velocities \( v_{c,s} \) as well as the LL parameters \( K_{c,s} \) are free parameters. If the model is used to describe the low-energy physics of an underlying microscopic model they become functions of the corresponding model parameters and the band filling \([1–3]\). For spin-rotational-invariant models, on which we focus in this section and the next, \( K_c = 1 \). For repulsive interactions \( 0 < K_c < 1 \) while \( K_c > 1 \) in the attractive case. Here we exclusively consider the former. The field operator \( \Psi_\sigma(x) \) annihilating an electron with spin direction \( \sigma = \uparrow, \downarrow \) at position \( x \) is decomposed into a right- and a left-moving part:

\[ \Psi_\sigma(x) = e^{ik_s x} R_\sigma(x) + e^{-ik_s x} L_\sigma(x). \]

The imaginary time fields \( R_\sigma \) and \( L_\sigma \) are bosonized according to

\[ R_\sigma^\dagger(\tau, x) = \frac{\eta_\sigma}{\sqrt{2\pi}} \exp \left[ \frac{i}{2} \Phi_\sigma(\tau, x) \right] \exp \left[ \frac{i}{2} f_\sigma \Phi_\sigma(\tau, x) \right], \]

\[ L_\sigma^\dagger(\tau, x) = \frac{\eta_\sigma}{\sqrt{2\pi}} \exp \left[ -\frac{i}{2} \Phi_\sigma(\tau, x) \right] \exp \left[ -\frac{i}{2} f_\sigma \Phi_\sigma(\tau, x) \right], \]

where the Klein factors \( \eta_\sigma \) satisfy anticommutation rules \( \{ \eta_\sigma, \eta_\sigma' \} = 2\delta_{\sigma,\sigma'} \) and \( f_\uparrow = f_\downarrow = 1 \). The fields \( \Phi_\sigma \) and \( \Phi_\sigma^\dagger \) are the chiral components of \( \Phi_\nu \) and \( \Phi_\nu^\dagger \):

\[ \Phi_\nu = \Phi_\sigma + \Phi_\sigma^\dagger, \quad \Theta_\nu = \Phi_\sigma - \Phi_\sigma^\dagger, \quad \nu = \text{c,s}. \]

For the translational-invariant TL model the Hamiltonian follows by integrating the density equation (1) over \( R \). The TL model with an open boundary is obtained by integrating the density equation (1) over \( x \geq 0 \) and employing the boundary condition \( \Psi_\sigma(\tau = 0) = 0 \) for the fermionic and \( \Phi_{\text{c,s}}(x = 0) \equiv 0 \) for the bosonic fields, respectively.

Here we are interested in the imaginary time-ordered single-particle Green function

\[ G_{\sigma\sigma'}(\tau, x_1, x_2) = -\left[ T_\tau \Psi_{\sigma'}(\tau, x_1) \Psi_\sigma^\dagger(0, x_2) \right], \]

where \( \langle \cdots \rangle \) denotes the expectation value in the canonical ensemble. From the decomposition equation (2) it follows that

\[ G_{\sigma\sigma'} = e^{iK(x_1 - x_2)} G_{\sigma\sigma'}^{RR} + e^{-iK(x_1 - x_2)} G_{\sigma\sigma'}^{LL} + e^{iK(x_1 + x_2)} G_{\sigma\sigma'}^{RL} + e^{-iK(x_1 + x_2)} G_{\sigma\sigma'}^{LR}, \]

where, for example, \( G_{\sigma\sigma'}^{RL} = -\left[ T_\tau R_\sigma(\tau, x_1) L_{\sigma'}^\dagger(0, x_2) \right] \). As we are aiming at the local spectral function, we eventually set \( x_1 = x_2 = x \). For the translational-invariant TL model the left- and right-moving fermion fields are independent and thus \( G_{\sigma\sigma'}^{RL} = G_{\sigma\sigma'}^{LR} = 0 \). In the presence of an open boundary the above-mentioned boundary conditions imply \( R_\sigma(\tau, x) = -L_\sigma(\tau, -x) \). In this case and after setting \( x_1 = x_2 = x \) the cross-terms are characterized by a fast spatial oscillation with frequency \( 2K \).

Using standard methods (see, e.g., [2]) one obtains for the Green function of a translational-invariant system \( (K_a = 1, \tau > 0, \beta = 1/T, r = x_1 - x_2, \, R = (x_1 + x_2)/2) \)

\[ G_{\sigma\sigma'}^{RR}(\tau, x_1, x_2) = \frac{\delta_{\sigma,\sigma'}}{\pi v_c} \left( \frac{\pi}{v_c} \right)^{1/2} \frac{1}{\sin^{1/2} \left( \frac{\pi}{v_c} (v_c \tau - ir) \right) \sin^{1/2} \left( \frac{\pi}{v_c} (v_c \tau + ir) \right)} \]

\[ \times \frac{1}{\sin^b \left( \frac{\pi}{v_c} (v_c \tau + ir) \right)}, \]

\[ G_{\sigma\sigma'}^{LL}(\tau, x_1, x_2) = \frac{\delta_{\sigma,\sigma'}}{\pi v_c} \left( \frac{\pi}{v_c} \right)^{1/2} \frac{1}{\sin^{1/2} \left( \frac{\pi}{v_c} (v_c \tau - ir) \right) \sin^{1/2} \left( \frac{\pi}{v_c} (v_c \tau + 2ir) \right)} \]

\[ \times \left\{ \frac{\sin \left( \frac{\pi}{v_c} x_1 \right) \sinh \left( \frac{\pi}{v_c} x_2 \right)}{\sin \left( \frac{\pi}{v_c} (v_c \tau + 2ir) \right) \sin \left( \frac{\pi}{v_c} (v_c \tau + 2ir) \right)} \right\}^c, \]

\[ G_{\sigma\sigma'}^{RL}(\tau, x_1, x_2) = G_{\sigma\sigma'}^{LL}(\tau, x_2, x_1). \]

The cross-terms \( G_{\sigma\sigma'}^{RL} \) and \( G_{\sigma\sigma'}^{RR} \) are equal to \( -G_{\sigma\sigma'}^{RR} \) and \( -G_{\sigma\sigma'}^{LL} \) after interchanging \( r \leftrightarrow 2R \). The appearing exponents are given by

\[ a = \frac{1}{8} \left( \sqrt{K_c} + \frac{1}{\sqrt{K_c}} \right)^2, \]

\[ b = \frac{1}{8} \left( \sqrt{K_c} - \frac{1}{\sqrt{K_c}} \right)^2, \]

\[ c = \frac{1}{8} \left( \frac{1}{K_c} - K_c \right). \]

The main steps to obtain the local spectral function from the imaginary time Green function are the analytic continuation \( \tau \rightarrow i\omega \) followed by Fourier transformation with respect to \( \omega \). Mathematically the real part \( \delta \) corresponds to the ultraviolet cutoff introduced to regularize momentum integrals. From an experimental perspective it can be considered as the resolution of the set-up (at \( T = 0 \)).

For the translational-invariant model one obtains \((x_1 = x_2 = x)\)

\[ \rho(\omega, x) = -\frac{1}{2\pi} \left( 1 + e^{-\beta\omega} \right) \times \sum_{\sigma,\sigma'} \int_{-\infty}^{\infty} d\tau e^{i\omega \tau} \left| G_{\sigma\sigma'}^{RR}(\tau, x, x) + G_{\sigma\sigma'}^{LL}(\tau, x, x) \right|_{\tau \rightarrow \omega + \delta} \]

\[ = \frac{1}{\pi^2} \left( 1 + e^{-\beta\omega} \right) \left( \frac{\pi}{v_c} \right)^{1/2} \left( \frac{\pi}{v_c} \right)^{1/2} \frac{1}{\sin^{1/2} \left( \frac{\pi}{v_c} (v_c \tau + 2ir) \right)} \]

\[ \times \int_{-\infty}^{\infty} d\tau e^{i\omega \tau} \left| \sin^{1/2} \frac{\pi}{v_c} (v_c \tau + 2ir) \right|_{\tau \rightarrow \omega + \delta} \]

\[ = \frac{4\pi^{a+b+1/2}}{\pi^2 v_c^{a+b+1/2}} T_s^{\delta} S_\delta(\omega/T), \]
with
\[ S_\gamma(u) = 2^{1+\gamma} \Gamma(-\gamma) \sin[\pi(1 + \gamma)] \cosh \left( \frac{u}{2} \right) \times \left| \Gamma \left( \frac{1 + \gamma}{2} + \frac{i}{2\pi} \right) \right|^2, \]
\[ \alpha = a + b - \frac{1}{2} = \frac{1}{4} \left( K_c + \frac{1}{K_c} - 2 \right). \]

The position-independent local spectral weight of the translational-invariant TL model thus shows scaling behavior: \( T^{-\alpha} \rho(\omega, x) \) is a function of \( \omega/T \) only. The amplitude of the scaling function depends on \( v_c/s \) and \( K_c \), which in turn are functions of the interaction strength, while its shape is given by \( K_c \) only. This result was first derived in [11]. A similar expression was later used to describe transport properties of LLs [27].

Taking the \( T \to 0 \) limit of equation (13) one obtains the well-known power-law suppression of the spectral weight [5–7]
\[ T = 0 : \quad \rho(\omega, x) \sim |\omega|^\alpha, \]
for \( |\omega| \to 0 \). For fixed small \( T > 0 \) this is cut off by temperature and \( \rho \) saturates for \( |\omega| \ll T \). For the energy set to the chemical potential, that is \( \omega = 0 \), one finds a power-law suppression of \( \rho \) for \( T \to 0 \) (see equation (13)); \( \alpha \sim T^\alpha \). From studies of microscopic models it is known that (see, e.g., [3])
\[ K_c = 1 - \frac{U}{U_m} + \mathcal{O} \left( \frac{U}{U_m} \right)^2, \]
where \( U \) is a measure of the two-particle interaction and \( U_m \) is a scale which depends on the other model parameters. Using equation (15) one thus obtains
\[ \alpha \sim U^2, \]
for the exponent characterizing the low-energy behavior of the local spectral function of the translational-invariant TL model.

Verifying the power-law suppression of the spectral weight as a function of \( T \) and \( \omega \) with the same exponent \( \alpha \), as well as the scaling property of measured STS and/or PES data provides a strong indication that the system under investigation is indeed an LL [22]. It was very recently argued that these characteristics are still not unique to LLs as mechanisms other than 1d electronic correlations might lead to similar behavior [28]. We therefore suggest further consistency checks by, in addition, measuring spectra close to the end points of cut 1d chains.

The local spectral function becomes position-dependent when considering a chain with an open boundary. In this case \( \rho(\omega, x) \) has three contributions:
\[ \rho_B(\omega, x) = \rho_0(\omega, x) + e^{2i k_F x} \rho_{2k_F}(\omega, x) + e^{-2i k_F x} \rho_{-2k_F}(\omega, x), \]
where the first follows from Fourier-transforming \( G^{RR} + G^{LL} \) and the last two from transforming \( G^{RL} \) and \( G^{LR} \), respectively (\( x_1 = x_2 = x \)). Following the same steps as above we obtain
\[ \rho_0(\omega, x) = \frac{\pi^{a+b+1/2}}{\pi^2 v_c^{a+b} v_s^{b-1/2}} T^{a+b-1/2} F(\omega/T, xT/v_c), \]
with
\[ F(u, v) = \int_{-\infty}^{\infty} d\xi \frac{e^{iux}(1 + e^{-u})}{\sin^{1/2}(\pi s - 2\pi ivc/v_c + \delta)} \times \left( \frac{\sin^2(\pi s - 2\pi iv + \delta)}{\sin(\pi s + 2\pi iv + \delta)} \right)^c \]
and
\[ \rho_{2k_F}(\omega, x) = \rho_{-2k_F}(\omega, x) = -\frac{\pi^{a+b+1/2}}{2\pi^2 v_c^{a+b} v_s^{b}} \times T^{a+b-1/2} G(\omega/T, xT/v_c), \]
where
\[ G(\omega, v) = \int_{-\infty}^{\infty} d\xi \frac{e^{iux}(1 + e^{-u})}{\sin^{1/2}(\pi s - 2\pi ivc/v_c + \delta)} \times \left( \frac{\sin^2(\pi s - 2\pi iv + \delta)}{\sin(\pi s + 2\pi iv + \delta)} \right)^c. \]

In the limit \( T \to 0 \) these expressions simplify to the ones given in [16] and [29].

For distances from the boundary beyond the thermal length \( \sim 1/T \), that is \( xT/v_c = v \ll 1 \), we expect \( \rho_B(\omega, x) \) to become equal to \( \rho(\omega, x) \) of equation (13) (exponentially fast). That this is indeed the case follows from
\[ \frac{xT}{v_c} \gg 1 : \quad F(\omega/T, xT/v_c) \approx 4\pi x T^{a+b}/\pi s + 2\pi iv + \delta, \]
\[ G(\omega/T, xT/v_c) \approx 0, \]
equations (19), (20), (22) and (14). We thus end up with
\[ \frac{xT}{v_c} \gg 1 : \quad \rho_B(\omega, x) \approx \rho(\omega, x). \]

We next consider the limit \( xT/v_c = v \ll 1 \), that is the local spectral function close to the open boundary. Then
\[ F(u, v) \approx (2\pi)^{2c} v_c^{2c}(1 + e^{-u}) \times \int_{-\infty}^{\infty} d\xi \frac{e^{iux}}{\sin^{a+b+c+1/2}(\pi s + \delta)}. \]

Interistingly the remaining integral has the same form as the one appearing in the second line of equation (13) but with \( a+b+1/2 \) replaced by \( a+b+c+1/2 \). For fixed \( x \) close to the boundary \( \rho_B(x, \omega) \) thus displays scaling with the same scaling function as the one found in the bulk but with \( \alpha \) replaced by
\[ \alpha_B = a + b + 2c - 1/2 = \frac{1}{2} \left( \frac{1}{K_c} - 1 \right). \]

Explicitly one obtains
\[ \frac{xT}{v_c} \ll 1 : \quad \rho_B(x, \omega) \sim x^{2c} T^{\alpha_B} S_{\alpha_B}(\omega/T). \]

With equation (17) the boundary exponent \( \alpha_B \) equation (27) has, in contrast to the bulk one \( \alpha \), a contribution linear in the interaction
\[ \alpha_B \sim U. \]
and one finds \( \Theta_B > \alpha \). To show that for fixed \( x \) close to the boundary \( T^{-a_B} \rho_B \) indeed follows the same scaling function as in the bulk (with \( \alpha \rightarrow \Theta_B \)) we still have to analyze \( \rho_{2k_F} \), for \( xT/v_c = \nu \ll 1 \). In the simplest approximation we neglect the \( \nu \) dependence in the integral equation (23) and obtain

\[
\frac{xT}{v_c} \ll 1 : \quad \rho_{2k_F}(\omega, x) = \frac{1}{2} \rho_0(\omega, x). \tag{30}
\]

Using equation (19) this completes our proof that for fixed \( x \) in the bulk:

\[
T^{-\alpha} \rho(\omega, x) = T^{-\alpha} \rho_B(\omega, x) \sim S_\rho(\omega/T), \tag{31}
\]

close to the boundary:

\[
T^{-a_B} \rho_B(\omega, x) \sim S_\rho(\omega/T), \tag{32}
\]

with \( S_\rho \) given in equation (14).

Showing the consistency of the scaling of spectra measured in the two spatial regimes is within reach of the latest STS experiments [22]. Combined with a consistency check of the two exponents \( \alpha \) and \( \Theta_B \), which both depend on \( K_c \) only and which was already achieved in [22] (see also section 4), this would provide a stringent experimental verification of LL physics.

One can improve the analysis of \( \rho_{2k_F} \) close to the boundary by keeping the phase factor \( \exp(\im \omega u) \) of the integral equation (23).\(^4\) A numerical evaluation of the integral shows that \( \kappa \) is a function of \( K_c \) and \( v_c/v_s \) with \( \kappa(K_c = 1, v_c/v_s = 1) = 2 \). Taking all terms together we find

\[
\frac{xT}{v_c} \ll 1 : \quad T^{-a_B} \rho_B(\omega, x) = A x^{2c} \cos \left( \frac{\omega}{2T} \right) \\
\times \Gamma \left( \frac{1+\Theta_B}{2} + i \frac{\omega}{2\pi T} \right)^2 \\
\times \left\{ 1 - \cos \left( \frac{2k_F + \kappa \omega}{v_c} x \right) \right\}, \tag{33}
\]

where the overall amplitude \( A \) depends on \( K_c \), \( v_c \) and \( v_s \) but \textit{not} on the variables \( \omega \), \( x \) and \( T \).

In the \( T \rightarrow 0 \) limit equations (19)–(23) give close to the boundary

\[
T = 0, \quad \frac{x|\omega|}{v_c} \ll 1 : \quad \rho_B(\omega, x) \sim x^{2c} |\omega|^{\Theta_B} \\
\times \left\{ 1 - \cos \left( \frac{2k_F + \kappa \omega}{v_c} x \right) \right\}. \tag{34}
\]

At fixed \( x \), \( \rho_B \) thus vanishes \( \sim |\omega|^{\Theta_B} \). As in the translational-invariant case this power law is cut off by a finite temperature and \( \rho_B \) saturates for \( |\omega| \lesssim T \). For fixed \( x \) close to the boundary and \( \omega = 0 \) equation (32) gives \( \rho_B \sim T^{-\alpha_B} \) for \( T \rightarrow 0 \). At \( T = 0 \) and deep in the bulk, that is for \( x|\omega|/v_c \gg 1 \), \( \rho_{2k_F} \) can be written as a sum of terms which vanish algebraically in \( x \) [16, 29]. They show a power-law dependence on \( |\omega| \) in general, each with a different exponent. The contribution \( \rho_0 \) to \( \rho_B \) becomes position-independent and goes as \( \rho_0 \sim |\omega|^{\alpha_B} \) (instead of \( \alpha_B \) close to the boundary). For sufficiently large \( x|\omega|/v_c \) (such that algebraically decaying terms can be neglected) one thus finds (\( \omega \rightarrow 0 \))

\[
T = 0, \quad \frac{x|\omega|}{v_c} \gg 1 : \quad \rho_B(\omega, x) \sim |\omega|^{\alpha_B}. \tag{35}
\]

For \( T = 0 \) and in the \textit{noninteracting} limit \( \rho^0_{\pm 2k_F} \) does not decay and one obtains

\[
T = 0 : \quad \rho^0_B(\omega, x) = \frac{2}{\pi v_F} \left\{ 1 - \cos \left[ 2 \left( \frac{k_F + \kappa \omega}{v_F} \right) x \right] \right\}, \tag{36}
\]

for all \( x \) and \( \omega \).

It is often argued that the contribution \( \rho_{2k_F} \) to \( \rho_B \) can be neglected when comparing to experiments. The electrons in PES and STS do not come from a specific location \( x \) but rather from an extended spatial range. If this is large enough compared to the characteristic length \( 1/k_F, 2k_F \) averages out due to the fast spatial oscillations with frequency \( 2k_F \). It is not obvious that the criterion for neglecting \( \rho_{2k_F} \) is fulfilled in the latest STS experiments [22] (see section 4).

Equation (33) (or equation (34) for \( T = 0 \)) allows for another consistency check of LL behavior. It predicts a spatial power-law dependence of \( \rho_B \) close to the boundary with exponent \( 2x = (1/K_c - K_c)/4 \) superimposed by oscillations. If it is possible to measure the envelope function of the spatial dependence of the spectral weight close to a boundary and extract the power-law exponent it would allow us to relate the resulting \( K_c \) to the ones obtained from \( \alpha \) and/or \( \Theta_B \).

We note in passing that performing a spatial Fourier transform of \( \rho_B(\omega, x) \) reveals characteristic information of the bulk state of an LL including its elementary excitations (see [26] and references therein).

In section 3 we show that the spectral function of microscopic lattice models of interacting 1d electrons, in our case the extended Hubbard model, indeed shows scaling behavior as a function of \( \omega/T \). Up to a subtlety in the spatial dependence, namely an interaction-dependent phase shift in the oscillatory factor, the lattice spectral function falls on top of the above-computed scaling function of the TL model. This holds in the low-energy regime. We discuss the crossover between this universal behavior and the nonuniversal regime at higher energies. The crossover scale \( \Delta \) depends on the parameters of the microscopic model.

### 3. Spectral properties of the extended Hubbard model

Parity aiming at the low-energy LL physics of microscopic lattice models of interacting electrons, different groups computed the local spectral function [30, 31] as well as the momentum-resolved one [32, 33] for such models using very accurate numerical methods (often denoted as 'numerically exact'). Quantum Monte Carlo (QMC) [30, 33] and (dynamical) density-matrix renormalization group (DMRG) [32, 31] methods were used. The results obtained by these methods turned out to be very useful for understanding the spectral features of the models studied over the entire
For a very recent attempt to observe power-law behavior of the spectral function in a spinless lattice model using DMRG, see [34].

5 For a very recent attempt to observe power-law behavior of the spectral function in a spinless lattice model using DMRG, see [34].

Under the assumption that a given microscopic model is a LL (at low-energy scales) one can use general relations between the exact ground state energy $E_0$ and $K_c$ [12, 1–3] to extract the dependence of the LL parameter $K_c$ on the parameters of the model considered. In general, however, $E_0$ of a many-body system is not known analytically. The translational-invariant Hubbard model constitutes one of the rare exceptions and closed expressions for $E_0$ in the form of integral equations can be determined using a Bethe ansatz [37]. The integral equations can easily be solved numerically which gives access to the dependence of $K_c$ on the parameters $U/t$ and the band filling $n$ ($n$ can vary between 0 and 2) [38]. We emphasize that this only implies that on asymptotically small scales one can expect power-law behavior with $\alpha$ (bulk) or $\alpha_B$ (close to the boundary), while no information on the crossover scale $\Delta$ from nonuniversal to universal LL behavior can be extracted this way. Furthermore, this expectation holds under the assumption that the Hubbard model is an LL, which away from half-filling $n = 1$—for which it is a Mott insulator [37]—is not in serious doubt, but is also not rigorously proven. For the (translational-invariant) extended Hubbard model $K_c(U/t, V/t, n)$ can only be computed numerically along similar lines [39]. The exponents $\alpha$ and $\alpha_B$ for the Hubbard [38] cannot become large enough to match the exponents inferred from experiments on different systems [18–22] or, putting it differently, $K_c$ cannot become small enough. For the extended Hubbard model $K_c$s of roughly the correct order can be achieved for $U$ and $V$ of the order of the bandwidth or larger. This part of the parameter space lies very close to the Mott transition of the model [39]. One can expect that this affects the spectral properties. When aiming at a typical LL spectral function with $\alpha$ and $\alpha_B$ of experimental size it is thus advisable to study models with interactions of longer spatial range. We note that within our approximate approach $U$ and $V$ are bound to be sufficiently smaller than the bandwidth. The extended Hubbard model is spin-rotational-invariant which implies $K_c = 1$.

For the Hubbard model with an open boundary the scale $\Delta$ was earlier computed in the small $U$ limit and was estimated to be exponentially small [40]

$$\frac{\Delta}{v_F k_F} = \exp \left\{ -\frac{\pi v_F}{U} \ln \frac{1 + \frac{[U/(8\pi v_F)]^2}{[U/(8\pi v_F)]^2}} \right\}. \quad (38)$$

In fact, approaching the chemical potential $\omega \to 0$ the local spectral weight first increases before the LL power-law suppression sets in for $|\omega| \lesssim \Delta$ (see the solid line in figure 1 which does not look ‘LL-like’ around $\omega = 0$; the power-law suppression is beyond the energy resolution). This is consistent with the observation of a small crossover scale and a peak close to $\omega = 0$ in the local spectra of the translational-invariant Hubbard model obtained numerically by QMC and DMRG [30, 31].

To compute the finite-temperature $\rho_B(\omega,j)$ (here the continuous position $x$ is replaced by the discrete lattice site index $j$) of the extended Hubbard model we consider a chain of $N$ lattice sites described by equation (37). For this the
spectrum is discrete and the spectral function consists of δ peaks. Due to even–odd effects the spectral weight might vary quickly from one eigenvalue to the next. A smooth function of ω is obtained by averaging the weight over neighboring eigenvalues\textsuperscript{6}. To obtain the local spectral function as defined in the continuum one has to furthermore divide the weights by the level spacing between eigenvalues. The energy scale δN = πvF/N associated with the chain length becomes irrelevant as we always consider sufficiently large systems with T ≥ δN for fixed T. Our results are thus not influenced by finite-size effects (for an exception, see the discussion of figure 4).

Typical experimental temperatures are in the few to a few tens of Kelvin range which corresponds to T ≈ 10\(^{-4}\) – 10\(^{-3}\) for our model.

In figure 1 \(\rho_B(ω, j)\) is shown for filling \(n = 3/4\), lattice site \(j = 1\) next to the boundary, \(U/t = 0.5\), \(N = 2^{14}\), \(T/t = 10^{-3}\) and different \(V/t\). For the Hubbard model with \(V/t = 0\) no suppression of the spectral weight is observable as \(\Delta\) is much smaller than temperature. Obviously, \(\Delta\) increases with increasing \(V/t\) and the LL suppression at \(ω = 0\) becomes apparent. This can be understood as follows. The crossover scale \(\Delta\) is strongly affected by the size of the open boundary analog of a \(g_{1, \perp}\) two-particle scattering process \([17, 36, 40]\) which cannot be written quadratically in the bosonic densities. Its initial value (with respect to a RG flow) in the extended Hubbard model is given by \(g_{1, \perp} = U + 2V \cos(2kF)\) with \(kF = nπ/2\). It is large for \(V = 0\). At \(V_0 = −U/[2 \cos(2kF)]\) it vanishes (see the dashed–dotted line in figure 1). Under an RG procedure this ‘non-LL term’ flows to zero and is thus RG-irrelevant. However, the flow is only logarithmic. This implies that for sizable initial \(g_{1, \perp}\) LL physics sets in on exponentially small scales consistent with equation (38) for the Hubbard model [40]. For small initial \(g_{1, \perp}\) \(\rho_B\) appears LL-like with the characteristic power-law behavior of the spectral weight close to \(ω = 0\). In figure 1 the spectral weight at \(ω = 0\) remains finite due to the finite temperature. We conclude that to observe LL physics on moderate scales in the present model the interaction should not be too local. In particular, to demonstrate power-law behavior and obtain an estimate of the exponent by fitting \(ρ_B\) for fixed \(j\) close to the boundary) and \(T ≪ t\) as a function of \(ω\) (in the range \(T ≪ |ω| ≪ t\) one should consider fine-tuned parameters with \(V = V_0\). The spectral functions of figure 1 show another ‘high-energy’ nonanalyticity. A similar feature was observed for a model of spinless fermions in [41] and was explained there as a lattice effect.

In figure 2 the low-energy regime of \(\rho_B\) is shown for the same parameters as in figure 1 but ‘optimal’ \(V = V_0 = U/\sqrt{2}\) for \(n = 3/4\), which allows for the largest low-energy regime, and varying position \(j\) close to the boundary \(j = 1\). For fixed \(ω\) we observe strong variations of the weight with \(j\) and pronounced \(ω \leftrightarrow −ω\) asymmetries which is consistent with the result from the TL model equation (33). Below we return to the spatial dependence of \(\rho_B\).

To confirm scaling in \(ω/T\) at fixed \(j\) as predicted in equation (33) we computed \(ρ_B\) for the parameters of figure 2 but with \(j = 1\) and for different \(T\). By fitting \(ρ_B(ω, j = 1)\) as a function of \(ω\) for the smallest \(T\) in the range \(T ≪ |ω| ≪ t\) we can extract a functional RG estimate of the boundary exponent \(α_R^B\). For the given parameters we obtain \(α_R^B = 0.089\) in good agreement with the DMRG result \(α_R^{DMRG} = 0.095\) obtained from equation (27) and \(K_B^{DMRG} = 0.840\) derived as explained above [39]. The scaling obtained with this \(α_R^B\) is shown in figure 3. In the inset the unscaled data are displayed. The thick solid line is the prediction equation (33) of the TL model with an open boundary, where we replaced \(α_R^B \rightarrow α_R^B\). The data nicely collapse on the TL model curve in the low-energy regime.

We next take a closer look at the \(j\) dependence of \(ρ_B\) at fixed \(ω\). As emphasized in the last section, measuring the local spectral weight as a function of \(j\) offers another possibility for a consistency check that the system under consideration

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\textsuperscript{6} A similar energy averaging is inherent to any STS or PES experiment due to the finite energy resolution of these techniques.
is an LL: equation (33) predicts power-law behavior of the envelope with exponent $2c = (1/K_1 - K_2)/4$. Figure 4 shows $\rho_B$ for $n = 3/4$, $U/t = 0.5$, $N = 2^{14}$, $T/t = 10^{-3}$ and $\omega \approx 0$ as a function of $j$ (filled circles). Here $\omega \approx 0$ refers to taking the eigenvalue of the finite system closest to $\omega = 0$, which might be of order $1/N$ away from zero. We again tune $V$ to the optimal value $V_0 = U/\sqrt{2}$ (for $n = 3/4$) providing the largest $\Delta$. The spatial oscillations with frequency $2k_F = 3\pi/4$ are apparent. We fitted the envelope to a power law $\sim j^{2c}$ and obtained $2c_{\text{fRG}} = 0.087$ in excellent agreement with $2c_{\text{DMRG}} = (1/K_{c,\text{DMRG}} - K_{c,\text{DMRG}})/4 = 0.088$. The power-law fit is shown as a thick solid line in figure 4. As mentioned above, we control the different exponents only to leading order in the interaction. To this order the analytic expressions for $\alpha_B$ and $c_B$ agree, as is apparent from equations (12), (27) and (17). The numerical values for $2c_{\text{fRG}}$ and $c_{\text{RG}}$ differ by roughly 2% as the RG produces higher than linear order terms in the different exponents as well. We emphasize that for $V = 0$, that is for the Hubbard model, in a similar plot no spatial suppression of the envelope of the spectral weight at small $j$ is visible. In fact, the envelope of the spectral weight at $\omega \approx 0$ even increases for $j$ approaching the boundary site $j = 1$.

A comparison of the data for $U/t = 0.5$ (filled circles) and for $U/t = 0$ (crosses) additionally presented in figure 4 shows that a phase shift $\xi$ of the spatial $2k_F$ oscillations appears which is not captured by the result for the TL model equation (33). The latter was derived using standard bosonization with the boundary conditions on the continuum fields given after equations (5). The deviation of the $U/t = 0$ curve from equations (36) for $j \gtrsim 20$ (splitting of degenerate values of the spectral weight) is a finite-size effect; $\omega$ is not exactly zero but of order $1/N$ (eigenvalue closest to zero). The phase shift can be most easily identified from the observation that $\rho_B$ vanishes on every eighth lattice site for $U/t = 0$ (crosses), as it is supposed to according to equation (36) with $\omega = 0$ and $2k_F = 3\pi/4$, but is not so for $U/t = 0.5$ (filled circles), where the same should hold according to equation (33). The phase $\xi$ turns out to be linearly dependent on $U$ (for small $U/t$ and $V = V_0(U)$). As our functional RG approximation scheme is controlled to this order, the appearance of $\xi$ is a reliable finding. Considering $T = 0$ at different system sizes $N$ we furthermore verified that $\xi$ does not vanish for decreasing $1/N$. The phase shift is thus not a finite-size effect. A phase shift as observed in the extended Hubbard model (with $V = V_0(U)$) can be accounted for in bosonization by adding a local single-particle forward scattering term $W_0(\omega)\delta_0\Phi(x)$ to the Hamiltonian density equation (1). The phase shift is then given by $2\pi K_0 W_0/\nu c$. To match the result of the extended Hubbard model (with $V = V_0(U)$) $W_0$ has to be chosen as $U$-dependent, in particular $W_0 \sim U$ for small $U/t$. The STS and PES experiments always imply a spatial averaging. As the phase shift becomes illusive even after averaging over only a few lattice sites, and as the main focus of the present paper is on relating theoretical spectral functions to experimental ones, we do not further investigate this issue here.

Finally we compare the spatial dependence of $\rho_B$ for two different $\omega$ in figure 5. Apparently the frequency of the spatial oscillations depends on $\omega$ which is consistent with equation (33). As this is more transparent for a ‘more commensurable’ filling, the parameters of this figure are $n = 2/3$, $U/t = 0.5$, $V = V_0(U)$ (for $n = 2/3$), $N = 2^{14}$ and $T/t = 10^{-3}$.

### 4. Summary

In the first part of this paper we derived analytical expressions for the power-law behavior of the local spectral weight $\rho$ of the translational-invariant TL model as well as that with an open boundary $\rho_B$ as a function of $\omega$, $T$ and $x$. The results provide a variety of possibilities for consistency checks of experimental STS and PES data on 1d electron systems. The first is to show scaling of the data for different $\omega$ and $T$ taken in the bulk or at fixed position close to the boundary onto the bosonization predictions equations (13) and (15).
(bulk) or equation (33) (boundary). Scaling of bulk spectra was demonstrated in, for example, [22]. If the same could be achieved for boundary spectra the same scaling function with $\alpha$ replaced by $\alpha_B$ should appear if the system is an LL. Experimentally showing this together with the required consistency of $\alpha$ and $\alpha_B$ (for a spin-rotational-invariant model with $K_s = 1$ both given by a single number $K_c$; see equations (15) and (27)) would constitute a second highly nontrivial check that the studied system is indeed an LL. A consistency of bulk and boundary exponents within the experimental error bars (but not the entire scaling function) was achieved in [27, 22] (also see below). A third consistency check is provided by the predicted spatial power-law behavior with the exponent $2c$, which again can be expressed solely in terms of $K_c$ (see equations (12)).

It is often argued that the spatially oscillating contributions $\rho_{2k_F}$ and $\rho_{-2k_F}$ to $\rho_B$ with frequency $2k_F$ can be neglected when comparing to experimental spectra due to spatial averaging effects. Taking the numbers from [22] this is not apparent. In this experiment $k_F \approx 5 \times 10^9$ m$^{-1}$ while the range of spatial averaging is estimated as $\Delta x \approx 5 \times 10^{-9}$ m, leading to $2k_F \Delta x = 5$. This is not a very large number and one would thus conclude that $\rho_{2k_F}$ and $\rho_{-2k_F}$ cannot be dropped. A quantitative picture of the averaging effects can easily be obtained by integrating equation (19) over an appropriate spatial range. We have explicitly verified that averaging over $\Delta x \approx 5 \times 10^{-9}$ m does not significantly smear out the boundary $(\omega_0/\omega_c < 1)$ and bulk $(\omega_0/\omega_c \gg 1)$ exponents in $\omega$ at low temperatures (here $T = 0$). In particular, this shows that the spatial resolution of the experiment is high enough to detect $\alpha_B$ (as is implicit in the analysis presented in [22]).

In connection with the comparison of the experimental results on gold chains on a germanium surface of [22] to the LL predictions, one might be concerned about two effects which are not included in the TL model of section 2. One is the Rashba spin–orbit interaction (SOI), which in a surface set-up can become sizable. Along the lines of [42, 43] one can bosonize the 1d electron gas with Rashba SOI. An important effect is the appearance of two different Fermi velocities $v_F(1 \pm \xi)$ due to subband mixing and the SOI splitting [42, 43]. Here $\xi$ is a measure of the strength of the SOI. The local spectral function (with and without an open boundary) shows the same characteristics as a function of $\omega$ as discussed in section 2, but with modified exponents

$$\alpha^{\text{SOI}} = \alpha - \frac{(K_c - 1)^2}{2(1 + K_c)} \xi + \mathcal{O}(\xi^2),$$

$$\alpha_B^{\text{SOI}} = \alpha_B + \frac{K_c - 1}{K_c + 1} \xi + \mathcal{O}(\xi^2).$$

Taking realistic numbers for the velocities it turns out that $\xi \ll 1$ and the effects of Rashba SOI on the exponents are negligible. We note also in passing that the momentum-resolved spectral function of a translational-invariant LL is barely modified by SOI of realistic size [44].

The other issue is the observation of four electron branches (instead of two in the TL model) crossing the Fermi surface in PES measurements on the gold chains [45]. The four-branch situation can also be accounted for in bosonization [46, 47]. One then has to introduce even and odd pairs of charge and spin density bosons as well as the related $K$s and velocities. Under the plausible assumption that only the even-charge channel LL parameter is different from the noninteracting value 1, that is $K_{c,e} = K_c < 1$, one finds the same power-law behavior for the local spectral functions as a function of $\omega$ as the ones given in section 2 but with

$$\alpha = \frac{1}{8} \left( K_c + 1 \frac{1}{K_c} - 2 \right),$$

$$\alpha_B = \frac{1}{4} \left( \frac{1}{K_c} - 1 \right).$$

Interestingly taking these expressions would significantly improve the consistency of the experimentally determined $\alpha$ and $\alpha_B$ [22]. From the measured value $\alpha = 0.53$ of the bulk spectra one finds $\alpha_B = 1.27$ which agrees nicely with the measured value $\alpha_B = 1.20$. In particular, the agreement is improved compared to taking the two-branch expressions in equations (15) and (27) which gives $\alpha_B = 1.43$ [22].

In the second part of our paper we showed that the behavior of $\rho_B$ as a function of $\omega$, $T$ and $j$ close to an open boundary predicted by the bosonization solution of the TL model can indeed be found in an example of a microscopic lattice model, namely the extended Hubbard model. Interestingly, a linear-in-$U$ phase shift $\xi$ not captured by standard open boundary bosonization appears in the spatial oscillations of the spectral weight of the extended Hubbard model. The energy resolution required to access the low-energy LL regime strongly depends on the model parameters. Even for the fairly high-energy resolution we can achieve within our approximate method, convincingly demonstrating LL power-law behavior and reliably extracting exponents requires fine-tuning of the parameters. Roughly speaking, the crossover scale becomes small if the two-particle interaction becomes too local. This suggests that to access the low-energy LL regime at a given experimental energy resolution one should consider systems with poor screening properties.
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