Boundary effects on one-particle spectra of Luttinger liquids

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We calculate one-particle spectra for a variety of models of Luttinger liquids with open boundary conditions. For the repulsive Hubbard model the spectral weight close to the boundary is enhanced in a large energy range around the chemical potential. A power law suppression, previously predicted by bosonization, only occurs after a crossover at energies very close to the chemical potential. Our comparison with exact spectra shows that the effects of boundaries can partly be understood within the Hartree-Fock approximation.

Interacting fermions in one spatial dimension do not obey Fermi liquid theory. It took about thirty years to fully understand the generic low-energy physics of one-dimensional (1D) fermions with repulsive interaction, now called Luttinger liquid (LL) behavior. For various correlation functions LL theory predicts anomalous power laws with interaction dependent exponents. Several systems were studied using different experimental techniques in order to verify these predictions. Photoemission or transport measurements seem to be most promising. While the basic understanding of LL behavior emerged in the study of 1D systems with periodic boundary conditions (PBC), it is obvious that in order to describe realistic geometries more realistic boundary conditions have to be used. Therefore hard walls, usually called “open” boundary conditions (OBC) were studied recently. For the translational invariant system standard renormalization group (RG) arguments can be used to show that for repulsive interactions the \(2K_F\)-scattering part (usually called “\(g_1\)-interaction”) scales to zero and the Tomonaga-Luttinger model (TLM) describes the generic low energy physics. In some of the previous publications on the open boundary problem it was tacitly assumed that similar RG arguments can also be applied to the system without translational invariance. Therefore a quadratic form in boson operators was used to describe the electron-electron interaction. Then it is straightforward to calculate correlation functions. It was shown that the local spectral density \(\rho(x, \omega)\) entering the description of angular integrated photoemission is strongly modified near the endpoints of a 1D chain. The algebraic vanishing of the spectral density with frequency \(\omega\) close to the chemical potential \(\mu\) was found to be governed by a coupling dependent boundary exponent \(\alpha_B\) which, for repulsive interaction, is larger than the bulk exponent. This result was used recently in the interpretation of photoemission experiments. In Ref. \(\alpha_B\) has been studied for a variety of integrable models using results of the Bethe ansatz (BA) and assuming conformal invariance.

Thus far only specialized methods (bosonization, the BA and conformal field theory) have been used to study the one-particle properties of LL’s with boundaries and assumptions were necessary to justify the applicability of these methods. Furthermore these methods do only provide the exponent which characterizes \(\rho(x, \omega)\) at asymptotically small energies. In this letter we study several models for LL’s with OBC using bosonization and the density matrix renormalization group (DMRG) method. By comparison with results obtained from these (numerically) exact methods we will show that the low energy behavior of \(\rho(x, \omega)\) can partly be understood within the (non-self-consistent) Hartree-Fock (HF) approximation for the self-energy, which already gives power law behavior. This is a very surprising observation as the HF approximation for the case of PBC does not capture any of the LL features. For the models considered we will explicitly demonstrate that \(\alpha_B\) can be expressed in terms of the bulk LL parameter \(K_F^\alpha = (K_F^{-1} - 1)/z\), where \(z = 1\) in the spinless case and \(z = 2\) for spin 1/2-fermions. For the TLM and the lattice model of spinless fermions (SF) with nearest neighbor interaction the exponent of the spectral weight at the endpoint \(\alpha_B\) found in HF agrees to leading order in the coupling with \(\alpha_B\) and for small couplings there is quantitative agreement between the exact local Green’s function and the HF approximation. We will show that for the Hubbard model (HM) with small or moderate Coulomb repulsion \(U\) the spectral weight at the endpoint of the chain is enhanced in a large energy range close to \(\mu\). A crossover to a power law decrease occurs in a surprisingly small energy range around \(\mu\). This crossover behavior cannot be obtained from bosonization or conformal field theory due to the limitation to asymptotically small energies. Because of the “flowing \(g_1\)-coupling” there is only qualitative agreement between DMRG and the HF approximation in case of the HM. Besides their relevance for LL’s with OBC our results are important for the investigation of LL’s with PBC including impurities, since such models are expected to scale to chains with OBC.
We first present a careful discussion of the interaction term of the Hamiltonian in the basis of the one-particle eigenstates \( \varphi_n(x) = \sqrt{2/L} \sin(k_n x) \) with \( k_n = n\pi/L, \ n \in \mathbb{N} \) for OBC, a continuum model, and an interaction with a spatial range \( R \). Here \( L \) denotes the length of the chain. Note that the \( k_n \) do not have the meaning of momenta. In terms of the creation and annihilation operators \( a_n(\dagger) \) of the eigenstates \( \varphi_n \), the two-body interaction takes the usual form

\[
\tilde{V} = \frac{1}{2} \sum_{n,n',m,m'} V_{nmn'} a_n^\dagger a_m^\dagger a_n a_{m'},
\]

with the matrix elements \( V_{nmn'} \). If we express products of the sine-functions \( \varphi_n \) in terms of cosine-functions they read

\[
v_{nmn'} = |F(k_n - k_m, k_m - k_m') - F(k_n + k_m', k_m - k_m') + F(k_n + k_m', k_m + k_m')| / L,
\]

with

\[
F(q,q') = \frac{1}{L} \int_0^L d x \int_0^L d x' \cos(q x) V(x - x') \cos(q' x').
\]

Due to the fact that \( k_n = n\pi/L \) (and not \( 2n\pi/L \)) in addition to terms involving Kronecker deltas a finite size correction appears for non-local interactions

\[
F(q,q') = \tilde{V}(q)/2 (\delta_{q,q'} + \delta_{-q,-q'}) + g(q,q')/L,
\]

where \( \tilde{V}(q) \) is the Fourier transform of the interaction \( V(x) \). The correction term \( g(q,q')/L \) does not contribute to \( \alpha_B \) and we thus neglect this term. For an interaction which is long range in real space, considered by Tomonaga for PBC, \( \tilde{V}(k) \) is different from zero for \( |k| < k_c \), where the cut-off \( k_c = 1/R \) is much smaller than the Fermi momentum \( k_F = n_F \pi/L \). Then only the first term on the right hand side (rhs) of Eq. (4) is important for the low energy physics and \( \tilde{V} \) can be written as a bilinear form in boson operators. Using bosonization correlation functions can then be calculated as discussed in Ref. 3 yielding \( \alpha_B = (K_p^{-1} - 1)/z \) with \( K_p = (1 + z \tilde{V}(0)/(\pi v_F))^{-1/2} \) and the Fermi velocity \( v_F \). The full \( \omega \) dependence of \( \rho(x,\omega) \) for the TLM has been presented in Fig. 1 of Ref. 5.

In contrast to the bulk exponential, which, for weak coupling, is quadratic in the interaction, \( \alpha_B \) has a contribution linear in the interaction. Thus signs of the non-analytic behavior of \( \rho(x,\omega) \) can already be obtained using the HF self-energy. The delta terms on the rhs of Eq. (2) yield

\[
(\Sigma^{HF})_{kk'} = \delta_{kk'} \left\{ \delta \mu - \frac{1}{2L} \sum_{k < k_F} [\tilde{V}(k - k) + \tilde{V}(k + k)] \right\}
\]

\[
+ \frac{1}{2L} \left\{ z(\tilde{V}(k + k') - \tilde{V}((k - k')/2)) f((k - k')/2) \right\}
\]

\[
- \frac{1}{2L} \left\{ z(\tilde{V}(k - k') - \tilde{V}((k + k')/2)) f((k - k')/2) \right\},
\]

where \( f(k_m) \) is the Fermi function, which is equal to one if \( m \) is integer and \( m \leq n_F \) and zero otherwise, and \( \delta \mu = z \tilde{V}(0)n_F/L \). The calculation of \( \rho^{HF} \) requires a matrix inversion. The leading non-analytic behavior in the HF approximation can be traced to the term in \( \Sigma^{HF} \) which is proportional to \( f((k + k')/2) \). To leading order in \( \tilde{V} \) the term in the second line of Eq. (2) gives a contribution to \( \rho^{HF} \) proportional to \( \tilde{V}(0)/(2\pi v_F) \) \log(\omega - \mu^{HF}) \). For a long range repulsive interaction \( \tilde{V}(2k_F) = 0 \) and the prefactor of the logarithm is positive. This indicates the suppression of spectral weight close to \( \mu^{HF} \). Note that the logarithmic divergence is not due to a singular frequency behavior of \( \Sigma^{HF} \), as it occurs in second order perturbation theory for PBC, but emerges in the process of the matrix inversion. For finite systems it is numerically straightforward to perform the matrix inversion and calculate \( \rho^{HF} \). Instead of comparing \( \rho^{HF} \) and the exact spectral function \( \rho \) obtained from bosonization as a function of \( \omega \) we have studied the spectral weight at the chemical potential and position \( x \), denoted \( \rho_0(x,n_F,\tilde{V}) \), for a given \( k_F \) as a function of \( n_F \). The ratio \( \rho_0(x,n_F;\tilde{V})/\rho_0(0,n_F;0) \) as a function of \( 1/n_F \) displays the same kind of power law behavior as does \( \rho(x,\omega) \) as a function of \( \omega \). For the lattice models considered later we will only be able to exactly determine the spectral weight at the chemical potential on a lattice site \( i \) as a function of the system size. In Fig. 4 we compare the \( 1/n_F \) dependence of \( w_i(x,n_F;\tilde{V})/w_i(0,x,n_F;0) \) for the exact solution and the HF approximation. Already the HF approximation displays power law behavior, which shows that the leading logarithmic divergence of \( \rho^{HF} \) discussed above can be resummed to give a power law. A detailed study shows that \( \alpha_B^{HF} = \tilde{V}(0)/(2\pi v_F) \) with \( v_F = \tilde{V}(0)/(2\pi) \) is the Fermi velocity in the HF approximation and thus \( \alpha_B^{HF} \) and \( \alpha_B \) do agree up to leading order in \( \tilde{V}(0)/(2\pi v_F) \). Quantitative agreement between exact results and HF can be reached for \( \tilde{V}(0)/(2\pi v_F) \ll 1 \).

For the lattice models (SF, HM) considered next even the case with OBC can be solved exactly by the BA, but as for PBC not much about correlation functions can be learned directly from the BA. Information about boundary excitations can be obtained if conformal invariance is assumed [1]. First we will discuss the local spectral function at site \( i = 1 \) in a lattice model of SF with lattice constant \( a = 1 \), hopping matrix element \( t = 1 \), nearest neighbor interaction \( U \), and OBC. We have performed a DMRG study [10] for chains of up to \( N = 512 \) sites calculating matrix elements \( w_i(n_F;U) = |\langle E^{n_F-1}|c_i|E^{n_F}\rangle|^2 \), i.e. the spectral weight at the chemical potential and the boundary site. Here \( |E^{n_F}\rangle \) denotes the exact \( n_F \)-particle groundstate and \( c_i \) destroys a fermion at site \( i \).
cal data for \( w_0(n_F; U)/w_0(n_F; 0) \) at quarter filling and for \( U = 1 \) are shown in Fig. 1. For these parameters \( K_F = 0.8447 \) as can be found in Ref. [4]. For large \( n_F \) the numerical data nicely follow the solid line, which is proportional to a power law with exponent \( \alpha_B = 0.1838 \) and we can thus conclude, that for SF the suppression is described by \( \alpha_B \).

The HF self-energy for SF is best studied in the site representation. Due to the OBC the site occupancies \( \langle n_i \rangle \) and the renormalization of the hopping amplitudes \( \langle c_{i+1}^\dagger c_i \rangle \) depend on \( i \) and in order to obtain the site diagonal Green’s function one numerically has to invert a tridiagonal matrix. Fig. 1 presents HF data for \( w_0(n_F; U)/w_0(n_F; 0) \) and the same parameters as above. The HF approximation shows power law behavior with exponent \( \alpha_B^{HF} = \tilde{V}_{\text{eff}}/(2\pi\nu_{HF}) \) which has the same form as for the TLM if one replaces \( \tilde{V}(0) \) by the effective interaction \( \tilde{V}_{\text{eff}} = \tilde{V}(0) - \tilde{V}(2k_F) = 2U[1 - \cos (2k_F)] \). Again \( \alpha_B \) and \( \alpha_B^{HF} \) do agree up to order \( \tilde{V}_{\text{eff}}/(2\pi\nu_{HF}) \) and both curves show quantitative agreement for \( \tilde{V}_{\text{eff}}/(2\pi\nu_{HF}) \ll 1 \).

Next we will consider the HM and first discuss the results of the Hartree approximation (the Fock term vanishes). To obtain the site diagonal Green’s function one again has to invert a tridiagonal matrix which we have done numerically for systems of up to \( N = 10^6 \) lattice sites. The corresponding spectral function \( \rho_H(\omega) \) at the boundary site \( i = 1 \) is shown in Fig. 2 for various values of the onsite interaction \( U \) and fixed filling \( n_F/N = 0.4 \). We have connected the individual weights of the finite system to a continuous line. In contrast to the expectation from the general statement in previous work the spectral weight near \( \mu^H \) is strongly enhanced. This could have been expected already from Eq. (3). The prefactor \( \tilde{V}(0) - z\tilde{V}(2k_F) \) of the leading logarithmic correction to \( \rho \) is given by \( (1 - z)\tilde{V}(0) \) for a \( k \)-dependent delta interaction, i.e. in a model with spin it has the opposite sign as in the case of a long range interaction. As long as \( [U/(2\pi\nu_{HF})]\log (N) \ll 1 \) this indicates a logarithmic increase of the weight close to \( \mu^H \). If we go to larger values of \( [U/(2\pi\nu_{HF})]\log (N) \), i.e. larger \( N \) (or \( U \)), as in Fig. 3, we observe a crossover to a power law decay for energies extremely close to \( \mu^H \). It can be shown that the crossover occurs at energies which are exponentially (in \(-1/U\)) close to \( \mu^H \). In Fig. 2 the crossover cannot be observed as the energy resolution \( \Delta \omega \simeq 1/N \) is too low. In the inset of Fig. 3 the spectral weight of the occupied states is shown on a log-log scale. The increase of weight close to \( \mu^H \) is given by a power law with exponent \(-U/(2\pi\nu_{HF})\) which is cut off at the crossover energy. This shows that the logarithmic divergence obtained in leading order in \( U \) can be resummed to produce a power

![Fig. 1. Spectral weight at \( \mu \) and close to the boundary. The circles show the exact results for the spinless TLM at \( x = 3R \) with a long range interaction \( \tilde{V}(q) = U\Theta(k_c - |q|) \), \( U/(2\pi\nu_{HF}) = 0.1 \) and \( k_F = 4k_c \). The dashed line presents the HF approximation. The squares show the exact results for the lattice model of SF at site \( i = 1 \) for \( n_F/N = 0.25 \) and \( U = 1 \). The respective HF approximation is given by the long dashed line. The solid line displays a power law with exponent \( \alpha_B = 0.1838 \). The error of the DMRG data is of the order of the symbol size.](image1)

![Fig. 2. Spectral density at the boundary site for the HM with \( N = 800 \) sites and \( n_F = 320 \) in the Hartree approximation and for different values of \( U \).](image2)

![Fig. 3. The same as in Fig. 2, but for \( U = 3 \), \( N = 10^6 \), and \( n_F = 4 \cdot 10^5 \). The inset shows the spectral weight for the occupied states \( \omega < \mu^H \) on a log-log scale (solid line). The dashed lines display power laws with exponents \( \pm U/(2\pi\nu_{HF}) \).](image3)
law in a large energy range close to $\mu^H$. The exponent of the subsequent power law suppression is given by $U/(2\pi v_F)$.

In order to demonstrate that the crossover behavior found in the Hartree approximation is present also in the exact spectral function we again have calculated matrix elements $w_0(n_F;U)$ using DMRG for chains of up to $N = 256$ sites. In Fig. 4 $w_0(n_F;U)/w_0(n_F;0)$ is presented for $n_F/N = 0.25$, $U = 0.5$, $2.5$ and $U = 8$. For small $N$ and $U$ the DMRG and the Hartree results do approach each other as expected. A detailed study shows that the difference between the weights for fixed $N$ goes like $U^2$. If one goes from small to large $N$ the Hartree result for $U = 2.5$ displays the power law increase with exponent $-U/(2\pi v_F)$, the crossover, and the subsequent decrease with exponent $U/(2\pi v_F)$ similar to $\rho_1(\omega)$ as a function of $\omega$. For $U = 0.5$ only the increase can be seen as the crossover occurs at much longer chain length not shown in Fig. 4. The exact weight obtained from the DMRG also increases for increasing $N$. From the $U = 2.5$ data it is clear that the crossover occurs at smaller $N$ and the maximum is less pronounced compared to the Hartree result. For $U = 8$ the weight already decreases even for the smallest system sizes available. The dashed-dotted line displays a power law with exponent $\alpha_B$. The bulk LL parameter $K_\rho$ for a given $U$ and $n_F/N$ can be found in Ref. [4]. The DMRG data are consistent with the conclusion that the final power law suppression near the boundary is given by the boundary exponent $\alpha_B$. The increase of weight in the $U = 0.5$ DMRG data follows a line which is proportional to a power law with exponent $-\alpha_B$. The leading behavior of the boundary exponent is $\alpha_B \approx U/(4\pi v_F)$ which is one-half of the exponent $U/(2\pi v_F)$ found in the Hartree approximation. This kind of discrepancy between exponents obtained in perturbation theory and the leading behavior of exact exponents is known from the HM with PBC and occurs because a fixed point is reached only when backscattering has scaled to zero. For $U = 2.5$ the crossover length is too small to observe a well defined power law increase. We can conclude that analogous to the Hartree solution the DMRG results are consistent with an increase of spectral weight for small $|U/(2\pi v_F)|\log(N)$, a crossover and a subsequent power law decrease.

In conclusion for the models studied we have explicitly confirmed the expression for the boundary exponent $\alpha_B$ in terms of the bulk LL parameter $K_\rho$ obtained from bosonization and the BA. This exponent characterizes the one-particle spectral weight for asymptotically small energies and close to the boundary. Investigating the spectral function at higher energies we have found a quite unexpected behavior for the HM. For small and moderate positive $U$ the spectral weight close to the boundary first increases when the energy approaches the chemical potential from below and only in a narrow energy range the power law decrease with exponent $\alpha_B$ sets in. Whether LL behavior has convincingly been demonstrated in photoemission experiments is still a matter of debate [3]. Nonetheless the above scenario has to be taken into consideration in any discussion of the influence which boundaries (open ends or impurities) might have on the photoemission spectra of quasi-one-dimensional conductors. We have furthermore demonstrated that the influence of boundaries on one-particle spectra of LL’s can partly be understood within the HF approximation.

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FIG. 4. Spectral weight at $\mu$ and the boundary site for the quarter filled HM. The symbols show the results obtained from DMRG. The dashed curves display the weight in the Hartree approximation. The solid line shows a power law proportional to $(1/N)^{-\alpha_B}$ for $U = 0.5$ and the dashed-dotted line is proportional to $(1/N)^{\alpha_B}$ for $U = 8$. The error of the DMRG data is of the order of the symbol size.

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