

Recursive Method for the Density of States in One Dimension

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We derive a powerful yet simple method for analyzing the local density of states (DOS) in gapless one-dimensional fermionic systems, including extensions such as momentum dependent interaction parameters and hard-wall boundaries. We study the crossover of the local DOS from individual density waves to the well-known asymptotic power laws and identify characteristic signs of spin charge separation in possible STM experiments. For semi-infinite systems a closed analytic expression is found in terms of hypergeometric functions.

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The density of states (DOS) is a central quantity in the study of electronic condensed matter systems. The corresponding expression for the local DOS

$$\begin{aligned} \rho(\omega, x) &= \sum_m |\langle \omega_m | \Psi^\dagger(x) | 0 \rangle|^2 \delta(\omega - \omega_m) \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} \langle \Psi(x, t) \Psi^\dagger(x, 0) \rangle dt \end{aligned} \quad (1)$$

describes the probability of inserting an electron at a given energy ω and can be probed in tunneling experiments or, averaged over a range x , in photoemission experiments. In two or more dimensions the DOS is typically peaked at renormalized single particle excitation energies. In one-dimensional systems, however, interaction effects are enhanced, so that the DOS is determined by collective many-body states instead [1]. Accordingly, there has been considerable theoretical interest in analyzing the one-dimensional DOS for several decades [1–7]. Typical features that have been predicted are separate spin and charge density excitations and a characteristic depletion of the DOS at low energies and near boundaries, which have been seen experimentally in some special cases, such as cleaved edge overgrowth wires [8], superstructures on surfaces [9], and carbon nanotubes [10]. Recent theoretical activities in the field have produced notable advances in the areas of nonlinear corrections [11], numerical simulations [12,13], and applications of exact methods [14].

On the other hand, there remain a number of open questions, especially in regards to the applicability of typical effective low energy theories such as the Luttinger liquid formalism to more realistic systems and models. In fact a number of energy and length scales can affect the behavior, including perturbations from other degrees of freedom, longer-range electron-electron interactions, impurities, and finite system sizes, so that realistic systems are never truly scale invariant. The renormalization due to higher order perturbing operators leads to an energy and momentum dependence of the interaction parameters, so that a description in terms of a single constant Luttinger liquid parameter is in general *not* adequate.

Accordingly, the low energy theory is altered substantially and the generically predicted power law behavior with energy, momentum, and position is changed into a more complicated behavior of the DOS.

In this Letter, we address the question of how to generally calculate the local DOS including complications which make the central interaction parameters effectively energy and momentum dependent. The calculation is based on the Fourier transform in Eq. (1) for vertex correlation functions in finite systems, which yields an expansion in delta functions for the discrete DOS with coefficients that follow a recursion relation for arbitrary momentum dependent interaction parameters. It is shown that boundaries cause a natural scale dependence in the description of the local DOS, which leads to the crossover from boundary to bulk behavior. Using a continuous description, we obtain a closed analytic expression of the local DOS as a function of energy and position. In order to identify spin and charge separation by scanning tunneling microscopy (STM) it is useful to analyze the spatial Fourier transform of the local DOS.

The starting point is the general expression of chiral fermionic fields in terms of vertex operators in the normal ordered form

$$O^\dagger(x, t) := c e^i \sum_{\ell=1}^{\infty} e^{i\ell\Delta\omega t} A_\ell^\dagger(x)/\sqrt{\ell} e^{i\sum_{\ell=1}^{\infty} e^{-i\ell\Delta\omega t} A_\ell(x)/\sqrt{\ell}}, \quad (2)$$

where A_ℓ are linear combinations of bosonic annihilation operators, e.g., of the form $A_\ell(x) = \alpha_\ell e^{ik_\ell x} b_\ell^R + \beta_\ell e^{-ik_\ell x} b_\ell^L$ for a periodic system with length L , energy spacing $\Delta\omega = \frac{2\pi v}{L}$, and $k_\ell = \frac{2\pi\ell}{L}$ [15]. Such operators O^\dagger are used to represent left- or right-moving fermion operators $\psi_{L/R}^\dagger$. In the case of several fermion channels (e.g., spin and charge) the chiral fermion field will be the product of operators $O^\dagger(x, t)$ for each channel separately, all of which have the form in Eq. (2), but with different energy spacings $\Delta\omega$. The magnitude of the prefactor c is typically unknown unless a comparison with exact results can be made. Zero mode terms have been omitted in Eq. (2) since they only shift the spectrum of the DOS.

The form of the vertex operators in Eq. (2) is believed to apply to gapless interacting fermion systems in one dimension. However, it is important to note that the expression (2) already implies that the possible energy levels are assumed to be evenly spaced at $\omega = \ell\Delta\omega$ relative to the Fermi energy ϵ_F , which is generally *not* exactly justified in realistic systems and is also explicitly violated in any finite lattice model. The reason why bosonization remains useful is that the central information about the electron-electron interactions is encoded in the Bogoliubov rotations, i.e., the exact form of the linear combinations of bosons $A_\ell(x)$ in Eq. (2). These do not crucially depend on the assumption of an equally spaced spectrum, since they are derived in momentum space. Therefore, the typical bosonization theory does not describe the exact energy locations of the levels very accurately, but it appears to predict the spectral weights surprisingly well, as can also be seen by numerical studies [13].

The general time correlation function can be calculated from Eq. (2),

$$\langle O(x, t)O^\dagger(x, 0) \rangle = |c|^2 \exp\left(\sum_{\ell=1}^{\infty} \frac{1}{\ell} e^{-i\ell\Delta\omega t} \gamma_\ell(x)\right), \quad (3)$$

where $\gamma_\ell(x) = [A_\ell(x), A_\ell^\dagger(x)]$. In accordance with the periodicity in time, the Fourier transform in Eq. (1) yields an expansion in delta functions for the DOS

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle O(t)O^\dagger(0) \rangle = \sum_m \rho_m \delta(\omega - m\Delta\omega). \quad (4)$$

By partial integration a recursion formula for the individual spectral weights ρ_m is obtained,

$$\rho_m = \frac{1}{m} (\rho_{m-1}\gamma_1 + \rho_{m-2}\gamma_2 + \cdots + \rho_0\gamma_m) \quad (5)$$

with $\rho_0 = |c|^2$. This simple but central result is the main instrument for analyzing the DOS in what follows. Besides the obvious simplicity of calculating the DOS with Eq. (5), it has the major advantage of being free from divergences and regularization schemes. Moreover, it is possible to analyze a dependence of the γ_ℓ on the principle energy quantum number ℓ which will be especially useful for boundaries and long-range interactions.

Let us first reexamine the simplest example of a Luttinger liquid, which is a short-range interacting single channel system with periodic boundary conditions. The commutator $\gamma = [A_\ell, A_\ell^\dagger] = \frac{1}{2}(\frac{1}{K} + K)$ is then given in terms of the Luttinger parameter K independent of ℓ . In this case, Eq. (5) is solved analytically by

$$\rho_m = |c|^2 \frac{\Gamma(m + \gamma)}{\Gamma(\gamma)\Gamma(m + 1)} \approx |c|^2 \frac{1}{\Gamma(\gamma)} m^{\gamma-1}. \quad (6)$$

This is a well-known result [3], which will be useful later. However, many states can potentially contribute to each spectral weight ρ_m , the number of which increases with the partitions of m . As mentioned above, those states are in

general not exactly degenerate at the energy $m\Delta\omega$. Therefore, the weights ρ_m are spread in energy [16], which is also the case in all examples that follow. However, the total value of ρ_m is expected to be rather accurate [13].

Next, we consider fermions in a finite system with hard-wall boundary conditions $\Psi(0) = \Psi(L) = 0$. In this case, the operators in Eq. (2) are of the form $A_\ell(x) = (\alpha_\ell e^{ik_\ell x} + \beta_\ell e^{-ik_\ell x})b_\ell^R$ with $k_\ell = \frac{\pi\ell}{L}$ [17]. The Green's function splits into a uniform and a $2k_F x$ oscillating part $\langle \Psi(x, t)\Psi^\dagger(x, 0) \rangle = (G_R(x, x, t) - e^{i2k_F x} G_R(x, -x, t)) + \text{c.c.}$, where $G_R(x, y, t) = \langle \psi_R(x, t)\psi_R^\dagger(y, 0) \rangle$ [5–7, 17]. For spinful fermions those correlation functions have the form of Eq. (3) for the spin factor (K_s, v_s) and the charge factor (K_c, v_c) separately

$$G_R(x, x, t) = |c_x|^2 \prod_{\nu=c,s} e^{\sum_{\ell=1}^{\infty} e^{-i\ell\Delta\omega_\nu t} \gamma_{\nu,\ell}^{\text{uni}}(x)/\ell} \quad (7)$$

$$G_R(x, -x, t) = |c_x|^2 \prod_{\nu=c,s} e^{\sum_{\ell=1}^{\infty} e^{-i\ell\Delta\omega_\nu t} \gamma_{\nu,\ell}^{\text{osc}}(x)/\ell},$$

where the commutators are dependent on position x and mode ℓ in this case $\gamma_{\nu,\ell}^{\text{uni}}(x) = \frac{1}{4K_\nu} + \frac{K_\nu}{4} + (\frac{1}{4K_\nu} - \frac{K_\nu}{4}) \times \cos(2k_\ell x)$ and $\gamma_{\nu,\ell}^{\text{osc}}(x) = (\frac{1}{4K_\nu} - \frac{K_\nu}{4}) + (\frac{1}{4K_\nu} + \frac{K_\nu}{4}) \times \cos(2k_\ell x) + \frac{i}{2} \sin(2k_\ell x)$ with $\Delta\omega_\nu = v_\nu \frac{\pi}{L}$ for $\nu = s, c$. Also the prefactor is position dependent $|c_x|^2 \propto \prod_\nu (\sin \frac{\pi x}{L})^{(1/4K_\nu) - (K_\nu/4)}$ from normal ordering. Using Eq. (5) for the uniform (oscillating) and spin (charge) parts separately $\rho_{\nu,m}^{\text{uni}/\text{osc}} = \frac{1}{m} \sum_{\ell=1}^m \rho_{\nu,m-\ell}^{\text{uni}/\text{osc}} \gamma_{\nu,\ell}^{\text{uni}/\text{osc}}$, it is possible to solve the Fourier transform (1) even for this more complicated case. The local DOS at the energy $\omega = m_c \Delta\omega_c + m_s \Delta\omega_s$ is then simply the folded product of spin and charge, i.e.,

$$\rho_{u/o} = \sum_{m_c, m_s} \rho_{c, m_c}^{\text{uni}/\text{osc}} \rho_{s, m_s}^{\text{uni}/\text{osc}} \delta(\omega - m_c \Delta\omega_c - m_s \Delta\omega_s) \quad (8)$$

and $\rho(\omega, x) = (\rho_u(\omega, x) - e^{i2k_F x} \rho_o(\omega, x)) + \text{c.c.}$

Equations (5) and (8) can be evaluated very quickly with a few lines of code for a large number of levels and different parameters. The analytic expressions for each level are superpositions of density waves up to wave numbers corresponding to m_s and m_c . The level density increases with ω , according to the number of ways of choosing m_s and m_c for a given energy interval in Eq. (8). It is therefore useful to average over a small energy window, which results in a typical local DOS as a function of x and ω as shown in Fig. 1 for $K_c = 0.531$, $K_s = 0.618$, and $v_c/v_s = 1.618$, where the oscillating part has been omitted. The solid lines in Fig. 1 show the characteristic standing density waves with higher wave numbers as the energy increases, with scaling of features along hyperbolas with $\omega = mv_c/x$, while v_s plays a lesser role. In contrast, for noninteracting systems $K_c = K_s = 1$ Fig. 1 is completely flat.

In order to get clear evidence of the spin and charge separation it is necessary to consider the oscillating part,

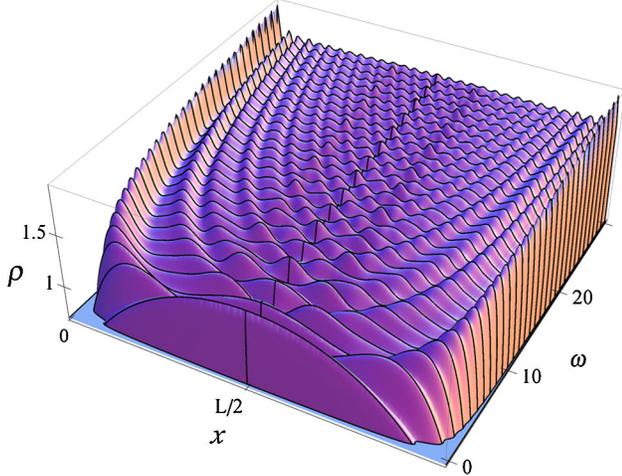


FIG. 1 (color online). $\rho_u(\omega, x)$ in units of $|c_{x=L/2}|^2$ for $K_c = 0.531$, $K_s = 0.618$, and $v_c/v_s = 1.618$ averaged over an energy interval of 0.3 in units of $\Delta\omega_c$.

which is best analyzed by a Fourier transform as first considered in Ref. [7]. In Fig. 2 we have plotted the absolute value of the Fourier transform in space of the local DOS including uniform and oscillating parts. It is possible to identify separately dispersing spin and charge features starting at $2k_F$. In addition there is a third maximum at $2k_F$ for all energies. The uniform DOS at $k = 0$ shows the typical power law increase. For spin-independent interactions $K_s = 1$, $K_c < 1$ the results for Figs. 1 and 2 look qualitatively very similar (not shown), except for a missing slowly dispersing maxima which can barely be detected in Fig. 2 starting from $k = 0$.

A further analytical analysis of the local DOS is possible in the continuous limit of the level spacing $xm_v \gg L$. In this case, Eq. (5) becomes an integral equation

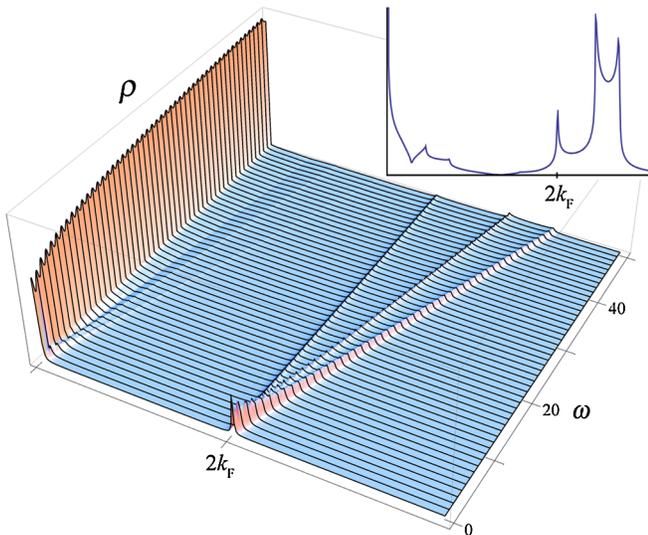


FIG. 2 (color online). Spatial Fourier transform of the local DOS with parameters as in Fig. 1 in arbitrary units. Inset: Cut at fixed energy.

$$\omega\rho(\omega, x) = \int_0^\omega \rho(\omega', x)\gamma(\omega - \omega', x)d\omega', \quad (9)$$

which again holds for the oscillating (uniform) and spin (charge) parts separately, where $\gamma(\omega, x)$ are the corresponding continuous functions. Let us focus on the uniform charge part close to a single edge, i.e., $\gamma(\omega, x) = \frac{1}{4K_c} + \frac{K_c}{4} + (\frac{1}{4K_c} - \frac{K_c}{4})\cos(\frac{2\omega x}{v_c})$ from above. After rewriting Eq. (9) in terms of the dimensionless variable $y = \omega x/v_c$, differentiating three times, and using the fact that $\gamma'' = 4(\frac{1}{4K_c} + \frac{K_c}{4} - \gamma)$, it is possible to obtain a third order differential equation, which in turn can be solved by the following hypergeometric function

$$\rho_c^{\text{uni}}(y) = y^{(1/2K_c)-1} {}_1F_2\left(\frac{1}{8K_c} - \frac{K_c}{8}; \frac{1}{4K_c}, \frac{1}{4K_c} + \frac{1}{2}, -y^2\right), \quad (10)$$

where ${}_1F_2(a; b_1, b_2, z) = \frac{\Gamma(b_1)\Gamma(b_2)}{\Gamma(a)} \sum_{k=0}^{\infty} \frac{\Gamma(a+k)}{\Gamma(b_1+k)\Gamma(b_2+k)} \frac{z^k}{k!}$. The dependence on position is not yet specified. The full local DOS from several channels can then be obtained by folding according to the continuous version of Eq. (8) which for $K_s = 1$ again results in a hypergeometric function

$$\begin{aligned} \rho_u &= f(x) \frac{v_c}{v_s} \int_0^y \rho_c^{\text{uni}}(y') \rho_s^{\text{uni}}\left(\frac{v_c}{v_s}(y - y')\right) dy' \\ &= \sqrt{\frac{v_c}{v_s}} \frac{|c_x|^2}{\Gamma(1/2 + 1/2K_c)} \left(\frac{\omega}{\Delta\omega_c}\right)^{1/2K_c-1/2} \\ &\quad \times {}_1F_2\left(\frac{1}{8K_c} - \frac{K_c}{8}; \frac{1}{4K_c} + \frac{1}{4}, \frac{1}{4K_c} + \frac{3}{4}, -\left(\frac{\omega x}{v_c}\right)^2\right) \end{aligned} \quad (11)$$

as shown in Fig. 3. The x dependence $f(x)$ is fixed by the asymptotic behavior near $x = 0$ which yields the expression (6) with $\gamma = \frac{1}{2K_c} + \frac{1}{2}$. Therefore an exact analytic formula (11) has been derived without the need to evaluate the Fourier transform of correlation functions in Eq. (1), which involves a complicated contour integration [5] and has so far not been possible analytically. Figure 3 also shows the DOS for all m_s and m_c quantum numbers from the discrete recursion formula (5). Clearly, the individual weights *drop* with increasing ω , but the averaged behavior follows the analytical prediction (11). The boundary and bulk exponents of the effective power laws $\rho \propto \omega^\alpha$ are given by $\alpha \sim \sum_\nu \gamma_\nu^{\text{uni/osc}} - 1$ expanded for small x or averaged over large x , respectively, which are, however, only rough approximations compared to the analytic expressions above.

So far, we have considered a constant Luttinger parameter K , where the scale dependence of the DOS stems only from the boundary. However, for longer-range interactions, K_ℓ itself is expected to be dependent on ℓ even in the bulk, e.g., $K_\ell = 1/\sqrt{V_0 \ln(a/\ell)}$ for the case of a Coulomb potential [18]. There has been a controversy in the literature

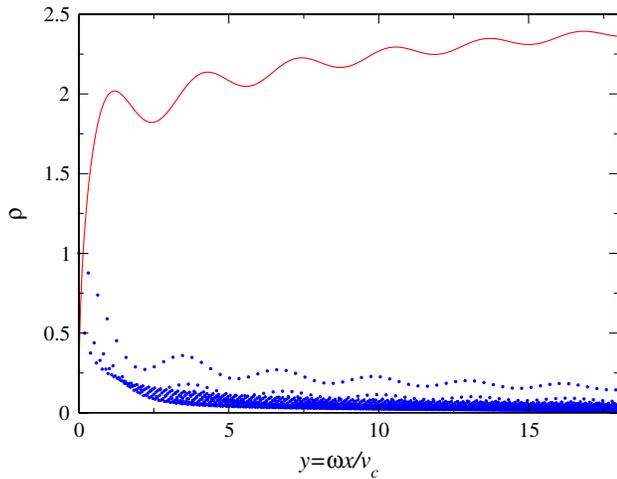


FIG. 3 (color online). The uniform spectral weights ρ_u in units of $|c_x|^2$ near a boundary as a function of $\omega x/v_c$ for $K_c = 0.531$, $K_s = 1$, and $v_c/v_s = 1.618$. The large number of spin and charge levels for $x = 0.1L$ (blue dots) follow Eq. (11) (red line) after averaging.

about the behavior of the corresponding DOS, for which an effective exponent $\rho \propto \omega^{\alpha(\omega)}$ was postulated in Ref. [19], which in turn lead to a debate [19,20]. Our analysis with $\gamma_\ell = \frac{1}{2}(\frac{1}{K_\ell} + K_\ell)$ using Eq. (5) now shows that over a limited range the true behavior can fit to the form postulated in Ref. [19] by some choice of parameters, but that there is an additional unknown scale dependence as the authors also mention [19]. Therefore, the description in terms of $\alpha(\omega)$ is not complete, but phenomenologically useful. An analysis with the help of Eq. (5) shows that corrections come from derivatives in γ_ℓ , which however cannot be summed exactly. Using the recursion formula it is possible to consider interactions K_ℓ of arbitrary form with relative ease. Also for harmonically trapped fermions a description of a mode dependent parameter K_ℓ has been predicted, albeit with a yet unknown dependence on ℓ [21].

This brings us to an important application of the recursion formula for systems which are *not* perfect Luttinger liquids. As outlined in the introduction, potentially all realistic models contain some scale dependence of the parameter K_ℓ , which is however not *a priori* known. Therefore, it will be very beneficial to use the recursion formulas (5) in reverse: Knowing the lowest m spectral weights ρ_ℓ , it is easily possible to uniquely determine the first $m - 1$ interaction parameters γ_ℓ . The analogous statement is also true for continuous spectra. This is especially promising considering the fast progress in numerical [12,13], exact [14], and experimental [8–10] techniques in determining the DOS.

In summary, we have obtained a straightforward tool for analyzing the local DOS in one-dimensional interacting systems. The crossover from individual levels to a continuous spectrum has been studied in detail for future comparison with possible STM experiments. A closed analytic expression was obtained for electrons in a system with

hard-wall boundaries. Long-range interactions can also be considered. The inversion of the recursion formula is useful to calculate the interaction parameters directly from the low energy spectral weights, which in turn can be obtained from numerical, exact, or experimental methods. In this way the theory can be generalized to systems which are not perfect Luttinger liquids, such as harmonically trapped ultracold fermions.

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