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

$$\rho(\omega, x) = \sum_m |\langle \omega_m | \Psi^\dagger(x)|0 \rangle|^2 \delta(\omega - \omega_m)$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t}(\Psi(x, t)\Psi^\dagger(x, 0))dt$$

(1)
describes the probability of inserting an electron at a given energy $\omega$ 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

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

(2)

where $A_{\ell}$ are linear combinations of bosonic annihilation operators, e.g., of the form $A_{\ell}(x) = \alpha_{\ell} e^{ik_{\ell}\ell} b_{\ell}^L + \beta_{\ell} e^{-ik_{\ell}\ell} b_{\ell}^R$ for a periodic system with length $L$, energy spacing $\Delta \omega = 2\pi \nu$, and $k_{\ell} = \ell \frac{2\pi}{L}$ [15]. Such operators $O^\dagger$ are used to represent left- or right-moving fermion operators $\psi^\dagger_{L,R}$. 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 \( \varepsilon_F \), 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 lattice model. The reason why bosonization remains useful is that the central information about the electron-electron lattice model. The reason why bosonization remains useful is that the central information about the electron-electron lattice model. The reason why bosonization remains useful is that the central information about the electron-electron lattice model. The reason why bosonization remains useful is that the central information about the electron-electron lattice model.
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 $x = L$. In this case, Eq. (5) becomes an integral equation

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

(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., $\gamma(\omega, x) = \frac{1}{4K_c} + \frac{K_c}{2} + (\frac{1}{4K_c} - \frac{K_c}{2}) \cos(\omega x/v_c)$ 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 $\gamma'' = 4(\frac{1}{4K_c} + \frac{1}{2} - \gamma)$, it is possible to obtain a third order differential equation, which in turn can be solved by the following hypergeometric function

$$\rho^{\text{uni}}(y) = y^{(1/2K_c)-1} F_2\left(\frac{1}{8K_c} - \frac{K_c}{8}, \frac{1}{4K_c}, \frac{1}{2}, -y^2\right),$$

(10)

where $F_2(a; b_1, b_2, z) = \frac{\Gamma(b_1)\Gamma(b_2)}{\Gamma(a)} \sum_{n=0}^\infty \frac{\Gamma(a+n)}{(b_1+n)(b_2+n)} \frac{z^n}{n!}$.

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

$$\rho_u = f(x) \frac{v_c}{v_s} \int_0^y \rho^{\text{uni}}(y') \rho^{\text{uni}}(v_c y'/v_s) dy'

\sim \frac{\left|c_{\text{ee}}\right|^2}{v_s} \frac{1}{\Gamma(1/2 + 1/2K_c)} \left(\frac{\omega}{\Delta \omega_c}\right)^{1/2K_c - 1/2}

\times F_2\left(\frac{1}{8K_c} - \frac{K_c}{8}, \frac{1}{4K_c}, \frac{1}{2}, -\left(\frac{\omega x}{v_c}\right)^2\right),$$

(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 $m_t$ quantum numbers from the discrete recursion formula (5). Clearly, the individual weights drop with increasing $\omega$, 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 $\alpha \sim \sum_y \gamma^{\text{uni/osc}} - 1$ 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, $K_\ell$ itself is expected to be dependent on $\ell$ 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. 1 (color online). $\rho_s(\omega, x)$ in units of $|c_{\text{ee}}-L/2|^2$ 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 $\Delta \omega_c$.

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.
about the behavior of the corresponding DOS, for which an effective exponent $\rho \approx \omega^{\alpha(\omega)}$ was postulated in Ref. [19], which in turn lead to a debate [19,20]. Our analysis with $\gamma_\ell = \frac{1}{2} ( 1 + K_\ell)$ 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 $\gamma_\ell$, which however cannot be summed exactly. Using the recursion formula it is possible to consider interactions $K_\ell$ of arbitrary form with relative ease. Also for harmonically trapped fermions a description of a mode dependent parameter $K_\ell$ has been predicted, albeit with a yet unknown dependence on $\ell$ [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 $K_\ell$, 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 $\rho_\ell$, it is easily possible to uniquely determine the first $m - 1$ interaction parameters $\gamma_\ell$. 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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