The Coulomb Luttinger liquid

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Accurate expressions, valid in experimentally relevant regimes, are presented for the effect of long-ranged Coulomb interaction on the low energy properties (momentum distribution function, density of states, electron spectral function, and 4k_F correlation function) of one-dimensional electron systems. The importance of plasmon dispersion (as opposed to exponent) effects in the spectral function is demonstrated.

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The low energy behavior of one-dimensional (1D) electron systems is known not to be consistent with Fermi liquid theory [1]. However, the theoretically well established [2] and extensively studied [3] Luttinger liquid model of one-dimensional physics is, strictly speaking, not applicable to electronically conducting one-dimensional systems such as quantum wires (QWR) [3], carbon nanotubes [4], organic conductors [5] and doped chain or ladder compounds [6], because the electrons in these compounds interact via the Coulomb force, which is long-ranged, whereas the standard Luttinger model assumes short-ranged interaction. The long range of the Coulomb interaction leads to a scale dependence of the Luttinger exponents and velocities [9], which have been discussed [2,3] on the assumption that it is well approximated by its leading (lnL) divergence. As we show, this approximation is not accurate in any physically relevant regime. One exception is a very interesting recent renormalization group treatment [11] which found an effective exponent very similar to ours but did not discuss the implications for physical quantities. Some numerical results have also appeared [12], but a general understanding of the experimental implications of the Coulomb interaction is lacking.

In the present paper we use direct analytical and numerical evaluation of the relevant bosonization expressions to determine the momentum distribution function, tunneling density of states, and spectral function for 1D electron systems interacting via the physically relevant Coulomb interaction at zero temperature. We define an important but previously overlooked energy scale, present an accurate expression for the scale dependent exponent, show how the scale dependent velocity affects the spectral function, and qualitatively discuss the 4k_F correlation function. Our results should apply directly to 1D QWRs [3] and nanotubes [4].

We consider a 1D electron system with a noninteracting dispersion ε_p which we linearize near the Fermi point, defining a bare velocity v_F. We here assume the only important interaction is the Coulomb interaction in the forward scattering channel, and neglect Umklapp scattering and other interactions. This is a good approximation for QWR and nanotube systems. (For the organic and doped spin chain materials a modification, discussed below Eq. (2), is needed.) The Hamiltonian is (here we do not write the spin index explicitly),

\[ H = \sum_{r,p} v_F (p-r_F) c_r^+ c_p + \frac{1}{L} \sum_{r,q} V_c(q) (\rho_r(q) \rho_r(-q) + \rho_r(q) \rho_{r-\epsilon}(q)), \]  

where c_r^+ is the electron creation operator and \( \rho_r(q) \) is the density operator describing density fluctuations at momentum q and branch \( r = \pm \) for the right(left) movers. For 1D systems \( V_c(q) \rightarrow \ln(1/q) \) as \( q \rightarrow 0 \), and becomes \( 1/q \) for q larger than some scale \( q_0 \) set by the geometry and the wave function size. A reasonable approximate form, which we will use in our subsequent analysis, is

\[ V_c(q) = \frac{\pi v_F V_0}{2} \ln \left[ \frac{q_0 + \sqrt{q}}{q} \right], \]  

where \( V_0 \) is a dimensionless measure of the interaction strength and \( q_0^{-1} \) is the length scale parameter. \( V_0 \) and \( q_0 \) are system dependent factors. For a cylindrical quantum wire of radius a, \( V_0 = 4e^2/\pi \varepsilon_0 v_F \) and \( q_0 \sim 2.5/a \), where e is the electron charge, and \( \varepsilon_0 \) is the background dielectric constant, about 10 for GaAs. These values give the correct long wavelength limit and are within 10% of the correct \( 1/q \) coefficient at large momentum. In carbon nanotubes \( V_0 \) is of the same form as in QWR but \( \varepsilon_0 \sim 1.4 \) and \( q_0 \sim 2.97/R \), where R is the radius of the tube. For organics or doped chains, additional short-ranged exchange interactions may be important. The usual arguments [2] show that these interactions lead, at low energies, to an additive constant term in \( V_c(q) \).

Eq. (1) may be bosonized as usual [2,3]: the charge excitations are plasmons with dispersion \( \omega_q = qv_q \), and velocity \( v_q \equiv v_F \sqrt{1 + 2V_c(q)/\pi v_F} \) is

\[ v_q = v_F \sqrt{1 + V_0 \ln \left[ \frac{q_0 + q}{q} \right]}. \]  

1
(Note that we have \( \lim_{q \to \infty} \omega_q \sim qv_F + V_0q_0 / 2 \neq qv_F \) for Coulomb interaction). The electron Green function \( G_r(x, t) \equiv \langle \psi_r(x) \psi_1^*(0) \rangle \) is

\[
G_r(x, t) = \lim_{\epsilon \to 0} \frac{e^{i\kappa x}}{2\pi} \frac{\exp[-\Phi_r(x, t)]}{x - rv_F t + i\epsilon},
\]

where the phase function \( \Phi_r(x, t) \) is

\[
\Phi_r(x, t) = \frac{1}{2} \int_0^\infty \frac{dp}{p} e^{-rp} \left( e^{i(xrv_F t)} - e^{-i(xrv_F t)} \right)
+ 2\sinh^2(\theta_p) \left( 1 - \cos(px) e^{-irpv_F t} \right).
\]

The exponent parameter \( \theta_p \) is defined by

\[
e^{-2\theta_q} = \sqrt{1 + V_0 \ln \left( \frac{q_0 + q}{q} \right)} \sim \sqrt{V_0 \ln^{1/2} \left( \frac{q_s}{q} \right)},
\]

where \( q_s = q_0 e^{1/V_0} \) and the last approximation is good for large wavelengths, \( q \ll q_0 \).

We now use Eqs. (4)-(6) to study electronic quantities. We begin with the momentum distribution function

\[
n_r(\delta p) = \frac{-i}{2\pi} \int_0^\infty dx \frac{e^{-i\delta px}}{x^2 - i\epsilon} \exp[-\Phi_r(x, 0)],
\]

where \( \delta p \equiv p - rK_F \). In a noninteracting Fermi gas, \( n_r(\delta p) = \theta(-\delta p) \). For a short-ranged LL, the generally accepted result [12] is that in the vicinity of the Fermi momentum, \( 0.5 - n_r(\delta p) \sim \text{sgn}(r\delta p) \times \{C_1|\delta p| + C_2|\delta p|^\gamma \} \) with \( \gamma \) a LL exponent and \( C_1 \) and \( C_2 \) two constants. The first term is the non-critical background coming from high energies, while the second (critical) term comes from low energies where LL physics is important. For the long-ranged interacting model we now consider, attention to the singularity structure of the noninteracting electron Green function leads to

\[
n_r(\delta p) = \frac{1}{2} - \frac{1}{\pi} \int_0^\infty dx \frac{\sin(\delta px)}{x} \exp[-\Phi_r(x, 0)]
= \frac{1}{2} + C_1|\delta p| + C_2 \left( \frac{\delta p}{q_0} \right) \gamma_\delta(\delta p) + \text{higher orders},
\]

where again the non-singular \( C_1 |\delta p| \) term is from the integration over small \( x \), while the singular \( C_2 |\delta p| \) term comes from integration over large \( x \) and is a weak function of \( \ln^{1/2}(1/|\delta p|) \). The scale dependent exponent \( \gamma_\delta(\delta p) \) is found to be

\[
\gamma_\delta(q) \sim \frac{1}{2} \left( e^{-2\theta_q} + e^{2\theta_q} - 1 \right)
\sim \frac{\sqrt{V_0}}{6} \ln^{1/2} \left( \frac{q_s}{q} \right) + \frac{\ln^{-1/2}(q_s/q)}{2\sqrt{V_0}} - 1/2.
\]

Fig. 1 shows results obtained by numerically evaluating Eq (8) for typical QWR parameters. An enhanced curvature near the Fermi momentum is evident.

The inset to Fig. 1 shows the logarithmic derivative \( \alpha_{\delta}(p) \equiv d\log |n(p)|/d\log(p) \), which shows that for small \( \delta p \) the behavior may be described in terms of a slowly changing effective exponent. We note \( \alpha_{\delta}(p) \) is always less than 1, because when the scale dependent exponent \( \gamma_\delta(p) \) of Eq. (9) is greater than 1, the background term dominates.

We now turn to the tunneling density of states,

\[
N(\omega) = \frac{1}{2\pi} \sum_r \int_{-\infty}^\infty dt e^{i\omega t} \left[ G_r(0, t) + G_r(0, -t) \right],
\]

for \( \omega \) measured from the chemical potential. We first show that \( N(\omega) \) vanishes faster than any power of \( \omega \) as \( \omega \to 0 \). We observe that if \( V_c(p) \neq 0 \), \( G \) vanishes faster than any power of \( t \) as \( t \to \infty \). Therefore the integral obtained by taking any number of \( \omega \)-derivatives of \( N(\omega) \) is absolutely convergent at long times, and may be evaluated straightforwardly by contour methods even at \( \omega = 0 \).

We further note that \( G_r(0, t) \) has no singularities in the lower (upper) half plane for \( r = +1(-1) \); thus by deforming the contours appropriately we find that \( d^nN(\omega)/d\omega^n |_{\omega=0} = 0 \) for any \( n \). This argument does not apply to \( n(p) \) because of the different analytic structure of the \( x \)-dependence. Thus the non-critical contributions which obscured the behavior of \( n(p) \) do not occur in \( N(\omega) \). By evaluating Eq. (10) we obtain

\[
N(\omega) \propto \left( \frac{\omega}{\omega_s} \right)^{\gamma_\omega(\omega)},
\]

where the scale dependent density of states exponent \( \gamma_\omega(\omega) \) is

FIG. 1. Calculated momentum distribution function, \( n(p) \), with respect to momentum \( p - K_F \) for a realistic QWR system of \( a = 70 \) nm. Solid, dashed and dotted lines are results for three different interaction strengths \( V_0 = 1.21, 2.42, 4.84 \) respectively, where \( V_0 = 1.21 \) is for electron density \( 0.65 \times 10^6 \) cm\(^{-1}\) and \( \epsilon_0 = 12.7 \) [5]. Inset: the effective exponent (around \( K_F \)) obtained by taking the logarithmic derivative of the numerical \( n(p) \) for \( |p - K_F| < 0.2K_F \).
FIG. 2. Calculated density of states, $N(\omega)$, with respect to energy $\omega$ for the same system as Fig. 1. Different line styles represent different interaction strengths as indicated. Inset is the effective exponent, $\alpha_\omega$ obtained by taking the logarithmic derivative of $N(\omega)$. The numerically calculated curves are well fitted by the analytical expression (dash-dot lines) of the exponent from Eq. (13) at the corresponding $V_0$’s and $\omega_* = 20q_s v_F \sqrt{V_0}$. The stars are the first order term of Eq. (13) only, for $V_0 = 1.21$, showing that the widely used leading logarithm approximation leads to factor of two errors.

$$\gamma_\omega(\omega) = \frac{V_0}{6} \ln^{1/2} \left( \frac{\omega_s}{\omega} \right) + \frac{\ln^{1/2} (\omega_s/\omega)}{2v_F} - \frac{1}{2} \frac{v_F}{V_0} \ln \left( \frac{\omega_s}{\omega} \right)$$

(12)

the same form as that of Eq. (9) with $q_s$ replaced by a characteristic energy scale $\omega_*$. From Eqs. (3) and (6) we expect $\omega_* = A q_s v_F \sqrt{V_0}$, with the numerical constant $A$ determined by subleading corrections to the asymptotic analysis of Eq. (5). $A$ may in principle have a weak scale and system-parameter dependence, but our numerical results show that for $\omega < \omega_*/\rho c < 0.1$ and interactions $1 < V_0 < 5$ it is very well approximated by the constant value $A = 20$. Fig. 2 shows the results of a numerical calculation of $N(\omega)$ from Eq. (10) for three different interaction strengths; the inset compares the numerically calculated effective exponent, $\alpha_\omega(\omega) = d\log(N(\omega))/d\log(\omega)$, with the analytical result obtained from Eqs. (11) and (12):

$$\alpha_\omega(\omega) = \frac{V_0}{4} \ln^{1/2} \left( \frac{\omega_s}{\omega} \right) + \frac{\ln^{1/2} (\omega_s/\omega)}{4V_0} - \frac{1}{2} \frac{v_F}{V_0} \ln \left( \frac{\omega_s}{\omega} \right)$$

(13)

One sees that the fit is very good (the small differences appearing at $\omega_*/\rho c \sim 0.01$ arise from noise in the numerical calculation).

The two crucial energy scales defined by $N(\omega)$ are $\omega_s$ and $\omega_*$ at which $\alpha_\omega(\omega_s) = 1$, corresponding to $\omega_* \sim \omega_s e^{-34/V_0} \ll \omega_*$. In the high energy region, $\omega > \omega_s$, one has essentially non-interacting behavior. For $\omega < \omega_s$ there is a LL with a scale dependent exponent. For $\omega < \omega_s$, $\alpha_\omega > 1$ and $N(\omega)$ is concave upwards at small $\omega$, suggesting a "pseudo-gap" in the electronic density of states. For most real QWR systems, $V_0$ is about 1-5 depending on $\varepsilon_0$ and $v_F$, and thus $\omega_s$ is typically many orders of magnitude smaller than $\omega_*$. In our calculation, using QWR parameters from Ref. [8], we have $\omega_s \sim 100$ meV and $\omega_* \sim 10^{-4}$ meV. For extremely small $\omega \ll \omega_*$, Eq. (13) gives $\gamma_\omega \sim \frac{V_0}{4} \ln^{1/2} (\omega_*/\omega)$, an approximate form used earlier in the literature [8][10]. However, as seen from the inset of Fig. 2, the leading logarithmic divergence is so weak that in all physically relevant regimes the other two terms in Eq. (12) are needed for quantitative accuracy. On the other hand, the constant (scale independent) exponent used in Ref. [8] for nanotubes is also not an adequate approximation for small energy region ($\omega < 0.05E_F$) either. We therefore propose Eqs. (9) and (12) as widely applicable fitting formulae for the effective exponents in the Coulomb Luttinger liquid.

The scale dependent exponent also appears in the single particle spectral function, $\rho(q, \omega) = (1/2\pi)[G(q, \omega) + G(\omega - q, -\omega)]$, however the scale dependent velocity in Eq. (5) is more important. To introduce our results, we briefly summarize known results for a short-ranged repulsive interaction in the spinless LL model [13]. At fixed $q$, one defines three $\omega$-ranges: (i) $\rho(q, \omega) = 0$ for $|\omega| < |q|$, (ii) $\omega$-conservation, and (ii) power-law singularities as $|\omega| \rightarrow \omega^+$, and (iii) an exponential decay at scales larger than the Luttinger cut-off. For the long-ranged Coulomb interaction, $\rho(q, \omega) = 0$ for $|\omega| < q|\omega|$ due to the energy-momentum conservation, but the behavior in both regions (ii) and (iii) are strongly modified. For $|\omega| > \omega_*$ (region (iii)), $\rho(q, \omega) \sim \exp[-|\omega|/E_c(\omega)]$ with a scale dependent cut-off

$$E_c(\omega) = \frac{q_0 v_F}{4} \ln \left( \frac{\omega}{q} \frac{v_F}{V_0} \right),$$

(14)

because of the slow $(1/q)$ decay of the Coulomb interaction in the large momentum region (Eq. (5)).

Near threshold ($|\omega| < |q| < \omega_*$) there are two effects: the scale dependence of the effective Luttinger exponent and the curvature of the plasmon dispersion, which prevents the different boson modes from adding coherently. Thus as one decreases $\omega$ towards $\omega_*$ (consider $\omega > 0$ part only) one obtains first a divergence $\delta \omega^{\alpha_\omega(\omega_*)}$ (here $\delta \omega \equiv \omega - \omega_*$). This divergence is cut off by curvature effects at a scale $\omega_c(q) = \max_{p<q}(\omega_p - p|\omega_*/q) \approx (1/4q v_F \sqrt{V_0} \ln^{1/2} (q_*/q))$, the difference between the exact dispersion and a linear approximation. We find that for $q > q_*$ (at which $\gamma_\omega(q_*) = 1$) the curvature effect is more important in cutting off the divergence, whereas for $q < q_*$ the effective exponent is more important. As $\delta \omega \rightarrow 0^+$ the spectral function decreases rapidly, ultimately vanishing faster than any power of $\delta \omega$ due to the increase of the effective exponent. Thus the generic behavior is a spectral function which increases rapidly as $\omega$ is increased above threshold $\omega_*$, goes through a maximum at $\omega_{peak} = \omega_0 + \Delta \omega$ with $\Delta \omega$ set by the larger of $\omega_*$ and $\omega_c(q_*)$, and then decreases exponent-
density-density correlation to decay more slowly than length scales the logarithm arising from the long-ranged relation. Schultz [9] observed that at long enough techniques used in [15] to simplify the evaluation for the \( \omega = 0 \) equal to the effective exponent of the Coulomb case at Luttinger liquid with exponent \( \alpha \).

The suppressed spectral weight in the near threshold region is compensated by the slower decay at high energies, which is sensitive to the electron density and experimental geometry, but is in general far too small to be experimentally relevant, and is also much less than the scale \( \omega_s \) at which \( N(\omega) \) develops a pseudo-gap.

In conclusion, we have presented a systematic theoretical analysis of the low energy properties of electron systems subject to long-ranged Coulomb interactions, including a reliable estimate of the scale dependent Luttinger parameter and apparently the first calculation of Coulomb effects on the spectral function, and values for the (unfortunately extremely low) scales at which the divergent behavior associated with the Coulomb interaction becomes manifest.

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\[ S_{4k_F}(\delta p) \sim \left( \frac{q_s}{\delta p} \right)^{1 - 8V_0^{-1/2} \ln^{-1/2}(q_s/\delta p)} \]  

where \( \delta p \equiv |p - 4k_F| \). Therefore we expect to see the \( 4k_F \) divergence when \( \sqrt{V_0} \ln^{1/2}(q_s/\delta p) > 8 \) or \( \delta p < q_s e^{-64/V_0} \), or in term of temperature at \( T < T_{w,x} = \omega_s e^{-64/V_0} \), which is sensitive to the electron density and experimental geometry, but in general far too small to be experimentally relevant, and is also much less than the scale \( \omega_s \).

Finally, we briefly discuss the ”Wigner crystal” correlation. Schultz [4] observed that at long enough length scales the logarithm arising from the long-ranged Coulomb interaction causes the \( 4k_F \) component of the density-density correlation to decay more slowly than \( x^{-4k_F} \) and also more slowly than the \( 2k_F \) component, leaving a state best interpreted as Wigner crystal. Using the notations of this paper, we obtain for the \( 4k_F \) term in the structure factor,

\[ \rho(q, \omega) = \begin{cases} \rho_{\text{regular}}(q, \omega) + \rho_{\text{Wigner}}(q, \omega), & \text{for } q < q_s \, \text{and } \omega > \omega_s, \\ \rho_{\text{regular}}(q, \omega), & \text{for } q < q_s \, \text{and } \omega < \omega_s, \\ \rho_{\text{Wigner}}(q, \omega), & \text{for } q > q_s \, \text{and } \omega > \omega_s. \end{cases} \]
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