Electroneutrality and the Friedel Sum Rule in a Luttinger Liquid

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Screening in one-dimensional metals is studied for arbitrary electron-electron interactions. It is shown that for finite-range interactions (Luttinger liquid) electroneutrality is violated. This apparent inconsistency can be traced to the presence of external screening gates responsible for the effectively short-ranged Coulomb interactions. We also draw attention to the breakdown of linear screening for wave vectors close to $2k_F$. [S0031-9007(97)04370-6]

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Screening is one of the most important and useful concepts in condensed-matter physics [1,2]. If some external charge is brought into a conductor, the internal charge carriers will reorganize with the new distribution of charge eliminating the electric field at large distances. The screened potential set up by the external charge together with its screening cloud is then rather short ranged. Typically, one ends up with only weakly correlated systems, despite originally long-range electrostatic forces.

Most theories employ linear screening as a working hypothesis, where the effects of (possibly time-dependent) external test charges onto the conduction electrons are determined by the linear response theory. Given the validity of linear screening, the wave vector- and frequency-dependent dielectric function $\epsilon(q,\omega)$ contains all relevant information about screening. An important result of the theory is the Friedel sum rule [3], which states that the total electronic screening charge exactly compensates any external (impurity) charge brought into the system. This charge neutrality requirement on large scales arises because in equilibrium there can be no net electric field at large distances. The validity of the Friedel sum rule is usually taken for granted, generally by referring to the analysis in Ref. [4] where this was proven explicitly for the Anderson model.

In this paper, we discuss screening and the Friedel sum rule for interacting electrons in one dimension (1D). At low energy scales, provided no lattice or spin instabilities are present, the properties of 1D fermions can be described by the Luttinger liquid model [5] (or slight generalizations thereof; see below). The Luttinger liquid is a strongly correlated 1D metal which does not support the existence of Landau quasiparticles. It is of importance for a number of applications of current interest, e.g., quantum wires in semiconductor heterostructures in the limit of one transport channel [6], transport in carbon nanotubes [7], or quasi-1D organic conductors [8], to mention a few. Here we show that in a Luttinger liquid the screening charge does not balance the impurity charge. Nevertheless, Friedel's phase shift sum rule [3] remains valid in terms of an adequately defined phase shift.

Our investigation of screening in 1D is based on the standard bosonization method [9]. From a comparison with alternative techniques, this method is known to give a proper description of 1D fermions at low energy scales (we consider zero temperature below). Since spin and charge are decoupled in a Luttinger liquid, it is sufficient to study only the spinless case in the following, with the same conclusions applying to spin-$\frac{1}{2}$ electrons. The low-lying excitations in a spinless Luttinger liquid are described by a bosonic phase field $\theta(x)$, in terms of which the electron density operator can be written in the form

$$\rho(x) = \frac{k_F}{\pi} + \frac{1}{\sqrt{\pi}}\partial_x\theta(x) + \frac{k_F}{\pi}\cos[2k_F x + \sqrt{4\pi}\,\theta(x)]. \quad (1)$$

The first term describes the mean charge density (which is supposedly neutralized by a positive background), the second term gives long-wavelength ($q \simeq 0$) fluctuations, and the last term yields rapidly oscillating ($|q| \simeq 2k_F$) contributions. Putting $\hbar = 1$, the Luttinger liquid Hamiltonian is then given by [5,9]

$$H_0 = \frac{v_F}{2}\int dx\,[\Pi^2(x) + (\partial_x\theta)^2] + \frac{1}{2\pi}\int dx\,dx'\,\partial_x\theta(x)U(x-x')\partial_{x'}\theta(x'), \quad (2)$$

where $\Pi(x)$ is the canonically conjugate momentum to $\theta(x)$ and v_F the Fermi velocity. The potential $U(x)$ can describe either an unscreened Coulomb interaction, $U(x) \sim 1/|x|$, or an externally screened finite-range potential which arises due to the presence of mobile charge carriers close to the 1D metal, e.g., on screening gates or other nearby chains. To simplify notation, we shall make the inessential assumption that $U(x)$ is sufficiently long ranged such that its Fourier transform $\tilde{U}(q)$ has a very small component at $q = 2k_F$. Then electron-electron backscattering can be neglected, as implied in Eq. (2). Even if this should not be the case, the bosonization technique can still be applied and yields qualitatively the same results. The Luttinger liquid model in the strict sense is obtained by effectively using a local interaction $U(x) = \tilde{U}(0)\delta(x)$. Here we shall employ the usual dimensionless Luttinger liquid interaction parameter g defined as

$$g = [1 + \tilde{U}(0)/\pi v_F]^{-1/2} \qquad (3)$$

for all finite-range interactions. Then $g = 1$ is the noninteracting limit, while for repulsive interactions we have $g < 1$. In the absence of screening gates, g approaches zero in an infinitely long system [5,9].

To study screening properties, we now consider some external time-dependent charge distribution $eQ(x,t)$ brought into the system. The interaction with the 1D metal reads

$$H_Q(t) = \int dx\, dx'\, Q(x,t) U(x - x') \rho(x'). \qquad (4)$$

In view of the representation (1) for the electronic density, there are two contributions. The first comes from the $q \simeq 0$ component, and the second from the $q \simeq 2k_F$ part. We note that the interaction potentials in Eqs. (2) and (4) are the same because we deal with the internally unscreened, microscopic interaction at this stage.

Let us first discuss the long-wavelength ($|q| \ll 2k_F$) response of the electrons. Ignoring the $2k_F$ part in Eq. (4), the now Gaussian Hamiltonian yields straightforwardly

$$\langle \rho(q,\omega) \rangle = \frac{v_F}{\pi} \frac{q^2 \tilde{U}(q)}{\omega^2 - \omega^2(q)} Q(q,\omega) \qquad (5)$$

with the plasmon dispersion relation

$$\omega(q) = v_F |q| \sqrt{1 + \tilde{U}(q)/\pi v_F}\,.$$

Apparently, in the long-wavelength limit, the Luttinger liquid model implies linear screening

$$\langle \rho(q,\omega) \rangle = \tilde{U}(q) \chi(q,\omega) Q(q,\omega)$$

with the polarizability $\chi(q,\omega)$. The response of the electrons to $Q(x,t)$ is thus fully described by a dielectric function. One finds from Eq. (5) and the definition [2]

$$\epsilon^{-1}(q,\omega) = 1 + \tilde{U}(q)\chi(q,\omega) \qquad (6)$$

the small-q result

$$\epsilon^{-1}(q,\omega) = 1 + \frac{v_F}{\pi} \frac{q^2 \tilde{U}(q)}{\omega^2 - \omega^2(q)}\,.$$

In the static case, $\omega = 0$, this yields

$$\epsilon(q) = 1 + \tilde{U}(q)/\pi v_F\,. \qquad (7)$$

We mention in passing that for large impurity charge eQ the bosonization approach breaks down [10]. For instance, Eq. (5) would incorrectly predict that the electron density becomes negative for sufficiently large Q.

One can now define the internally screened interaction potential $\tilde{U}_{\rm eff}(q) = \tilde{U}(q)/\epsilon(q)$ which determines the effective potential between two charges [2]. From Eq. (7), its long-wavelength part is $\tilde{U}_{\rm eff}(q) = \tilde{U}(q)/[1 + \tilde{U}(q)/\pi v_F]$, which gives for a finite-range interaction $\tilde{U}_{\rm eff}(q) = g^2 \tilde{U}(q)$ as $q \to 0$. For an externally unscreened $1/|x|$ interaction, one has $\tilde{U}(q) = 2e^2 |\ln(qd)|$, where d is the width of the 1D channel [5]. Apart from a hard core at small distances, this leads to the large-distance behavior valid at $|x| \gg d$

$$U_{\rm eff}(x) \sim \frac{1}{|x| \ln|x/d|}\,. \qquad (8)$$

Therefore the long-range character of the interaction is not significantly reduced. The only logarithmic suppression of the $1/|x|$ law explicitly demonstrates the very weak screening in 1D.

The condition for perfect screening

$$\epsilon^{-1}(q \to 0, \omega = 0) \to 0$$

is seen to be violated in any finite-range model. This follows directly from Eq. (7) since $\epsilon(q \to 0) = 1/g^2$. The implications are best discussed for a point charge sitting at $x = 0$, i.e., $Q(x,t) = Q\delta(x)$. The corresponding long-wavelength response is given in Eq. (5). For the total screening charge, $eQ_s = e \int dx \langle \rho(x) \rangle$, this leads to the strikingly simple result

$$Q_s = -(1 - g^2) Q\,, \qquad (9)$$

where g has been defined in Eq. (3). We stress that this relation holds for any finite-range Coulomb interaction. Asserting that the $2k_F$ Friedel oscillation in the charge density does not contribute to the total screening charge (see below), we observe that only a fraction $1 - g^2 < 1$ of the external charge Q is screened by the conduction electrons. Therefore the *electroneutrality condition* for impurity plus screening charge, $Q_s + Q = 0$, is apparently *violated* in models with a finite-range interaction. Of course, this reasoning carries over to lattice models with effectively short-ranged interactions, e.g., the 1D Hubbard model. For a long-range $1/|x|$ interaction, the parameter g effectively approaches zero, and electroneutrality is then seen to hold.

The result (9) can also be obtained by a phase shift consideration. Forward scattering due to a pointlike impurity charge $Q\delta(x)$ in Eq. (4) can be eliminated by the standard unitary transformation

$$U = \exp\left\{-i\sqrt{\pi} \int dx\, \alpha(x) \phi(x)\right\},$$

where $\phi(x)$ is the dual field to $\theta(x)$ [9], and the Fourier transform of $\alpha(x)$ is

$$\tilde{\alpha}(q) = -\frac{\tilde{U}(q)/\pi v_F}{1 + \tilde{U}(q)/\pi v_F}\, Q\,. \qquad (10)$$

Comparing with Eq. (5) for $\omega = 0$, the induced electronic density is simply $\langle \rho(x) \rangle = \alpha(x)$. The unitary transformation U now leads to a phase shift appearing, e.g., in the $2k_F$ part of Eq. (1), which takes the form

$$\eta(x) = \pi \int dx' \operatorname{sgn}(x - x')\alpha(x') .$$

Defining the asymptotic phase shift $\eta_F = \eta(x \to \infty)$, we find

$$Q_s = \int dx\, \alpha(x) = \eta_F/\pi . \tag{11}$$

Despite the apparent violation of electroneutrality, Friedel's phase shift sum rule [3] is seen to hold. Clearly, the phase shift η_F characterizes some screened impurity charge and not the bare charge Q brought into the system. Finally, using Eqs. (10) and (11), one may verify Eq. (9) again.

We mention that the conventional Fermi liquid case is not directly included in Eq. (9) as the simple limit $g \to 1$. For a Fermi liquid, one assumes that quasiparticles with good screening exist and then adds a local potential scatterer in order to derive the Friedel sum rule [3]. Its scattering strength is related to a phase shift η_F, and the screening charge is $Q_s = \eta_F/\pi$ as in Eq. (11). By interpreting η_F/π as the impurity charge, the Friedel sum rule is then in fact *imposed* as a consistency relation ensuring electroneutrality of the system. In contrast, putting $g = 1$ for the Luttinger liquid model would imply a noninteracting system (Fermi gas) rather than a Fermi liquid.

The physical reason for the apparent failure of electroneutrality in finite-range models is due to induced charges outside the 1D system, e.g., on external screening gates, which cause the finite range of the interaction. These other conductors also contribute to the total screening charge. To give a concrete example, consider the gated 1D quantum wire shown in Fig. 1. For a wire of width d, the presence of a two-dimensional gate at a distance D leads to a short-range interaction characterized by

$$g = \left\{1 + \frac{2e^2}{\pi v_F} \ln(2D/d)\right\}^{-1/2} .$$

The induced 1D charge density (integrated over the y direction) on the gate, $e\rho_G(x)$, is obtained as

$$\rho_G(x) = -\frac{D}{\pi} \int dx' \frac{q(x')}{D^2 + (x - x')^2} ,$$

where $q(x')$ is the total density in the wire (including the impurity). Integration over x gives straightforwardly the total induced charge on the gate

$$Q_G = \int dx\, \rho_G(x) = -(Q + Q_s) .$$

In effect, the electroneutrality condition in the form

$$Q_s + Q + Q_G = 0 \tag{12}$$

is then restored for the total system including the screening gates. Ignoring the screening gates implicitly used to derive the Luttinger liquid model is thus responsible for the modified condition (9) within the 1D system. Parenthetically, we note that if the charge Q is not put directly into the 1D system but some distance away, the screening charge Q_s is not given by Eq. (9) anymore, yet Eq. (12) will still hold.

The underscreening of an external charge brought into the 1D system should also be experimentally observable. If charge is injected into, e.g., a carbon nanotube constituting a perfect experimental realization of a 1D conductor [7], the resulting image charge on nearby external screening gates can be detected by capacitance spectroscopy [11] or by using highly sensitive single-electron transistor (SET) electrometers on top of a scanning probe tip [12].

So far we have discussed the long-wavelength part of the electronic response only. Turning now to the $2k_F$ part [13] and assuming linear screening, we have to compute the polarizability χ, which is essentially the double-Fourier transformed density-density correlation function of the unperturbed conductor

$$\chi(q, i\omega) = -\int dx\, d\tau\, e^{-i\omega\tau - iqx} \langle T_\tau \rho(x,\tau)\rho(0,0)\rangle . \tag{13}$$

Here T_τ is the time-ordering operator in Euclidean time, and one has to analytically continue Eq. (13) to real frequencies, $i\omega \to \omega + i0^+$, in order to obtain $\chi(q,\omega)$ needed in Eq. (6). The $2k_F$ part of χ for a Luttinger liquid is found to read

$$\chi(q, i\omega) = -\frac{C_g}{\pi v_F} \sum_{p,s=\pm} \left(\frac{is\omega}{v_F k_F} + \left| \frac{q}{k_F} - 2p \right| \right)^{2g-2} \times F\left(2 - 2g, 1 - g; 2 - g; \frac{is\omega - v_F|q - 2pk_F|}{is\omega + v_F|q - 2pk_F|}\right),$$

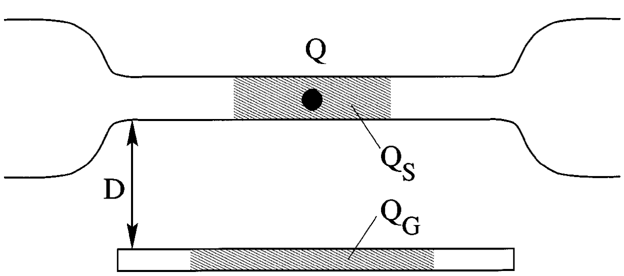

FIG. 1. Schematic view of a 1D quantum wire with short-range Coulomb interaction due to the presence of a 2D screening gate located a distance D away from the wire. The bare impurity charge is Q, the direct screening charge within the 1D system is $Q_s = -(1 - g^2)Q$ [see Eq. (9)], and the induced charge on the screening gate is Q_G.

where F denotes the hypergeometric function and $C_g = 4^{-g}\Gamma(2-2g)/\Gamma(g)\Gamma(2-g)$. In the static case, this gives algebraic singularities

$$\chi(q) = -\frac{\bar{C}_g}{\pi v_F} \sum_{p=\pm} \left| \frac{q}{k_F} - 2p \right|^{2g-2}, \qquad (14)$$

with the numerical constant

$$\bar{C}_g = \frac{\sqrt{\pi}\Gamma(2-2g)}{2\Gamma(g)\Gamma(3/2-g)}.$$

From these algebraic singularities one would infer a Friedel oscillation decaying as $\langle\rho(x)\rangle \sim \cos(2k_F x)x^{1-2g}$ and a similar contribution to the screened interaction potential $U_{\rm eff}(x)$. However, this represents only the first order in the perturbation expansion for the Friedel oscillation and determines merely the short-distance behavior, while the long-distance behavior of the Friedel oscillation necessitates a calculation in all orders of the impurity strength [14,15]. An important implication is the *breakdown of linear screening* for the $2k_F$ electronic response. This breakdown occurs for arbitrarily small impurity charge eQ at wave vectors close enough to $2k_F$. Following the results of Ref. [14], the singularity exponent $2g-2$ for $q \to 2k_F$ in Eq. (14) is turned into $g-1$. As a consequence, the effective screened potential as well as the Friedel oscillation asymptotically decay as $\sim\cos(2k_F x)x^{-g}$. Because of the intrinsically nonlinear screening, the dielectric function is of rather limited use for wave vectors close to $2k_F$.

The bosonization approach naturally separates the density operator (1), and therefore also the electronic screening response, into a slow and a fast $2k_F$ part. The total screening charge is determined by the $q=0$ component of the induced charge density, which in turn is exclusively given by the slow part (5). Therefore the Friedel oscillation obtained from the bosonized $2k_F$ part of Eq. (1) does not contribute to the total screening charge. In a microscopic calculation, one will in general not be able to separate the slow and the fast components so nicely, but within the bosonization approach, a quite simple derivation of the total screening charge (9) is possible.

To conclude, we have investigated screening in one dimension. We have shown that electroneutrality is not obeyed in models with a finite-range (screened) Coulomb interaction. In a 1D metal, the total induced screening charge is given by $Q_s = -(1-g^2)Q$, where Q is the impurity charge and g the Luttinger liquid interaction parameter. To resolve this apparent inconsistency, one needs to take into account induced charges on screening gates.

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