Interacting one-dimensional electron gas with open boundaries

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We discuss the properties of interacting electrons on a finite chain with open boundary conditions. We extend the Haldane-Luttinger-liquid description to these systems and study how the presence of the boundaries modifies various correlation functions. In view of possible experimental applications to quantum wires, we analyze how tunneling measurements can reveal the underlying Luttinger-liquid properties. The two-terminal conductance is calculated. We also point out possible applications to quasi-one-dimensional materials and study the effects of magnetic impurities.

I. INTRODUCTION

Physical properties of one-dimensional (1D) metals are well understood theoretically. Unlike higher dimensional metal, where interaction slightly modifies the free Fermi gas behavior (Landau-Fermi liquid picture), in 1D metals the electron-electron interaction plays a fundamental role and strongly affects their physical properties as compared to the ideal Fermi gas. The most interesting feature is the absence of well defined single-particle excitations. The only stable low-energy excitations turn out to be collective charge and spin density fluctuations (zero sound modes). Charge and spin sounds are dynamically independent, which, together with the absence of the continuum of electron-hole excitations, gives rise to the so-called spin-charge separation. The interaction also modifies the asymptotic behavior of all the correlation functions: at large distances (times) they are shown to decay as a power law with interaction dependent exponents (Luttinger-liquid behavior, for a review see Ref. 1).

Before the recent achievements of the submicrometer-size technology in the fabrication of 1D quantum wires, 1D electron gases have been studied either on their own rights (as interesting mathematical objects) or in view of applications to quasi-one-dimensional materials.[2] For these purposes, it was sufficient to investigate infinite systems (or to impose periodic boundary conditions, which are relatively easy to treat). Semiconductor devices with 1D confining potentials (quantum wires) represent a promising realization of 1D electron systems, which provide an alternative way to study experimentally the Luttinger-liquid properties. For instance, the collective nature of the low-energy excitations has been successfully probed by inelastic light scattering experiments.[3] Other experiments particularly suited for quantum wires are those measuring transport properties, and an interesting question is whether these measurements are able to reveal the Luttinger-liquid character of 1D systems. Regarding the measurements of bulk properties in a clean system (e.g., optical conductivity), the answer would be no. In fact, although many properties are anomalous, the (bulk) transport properties of a clean 1D metal are expected to be qualitatively similar to those of an ordinary 3D metal. Regarding the surface measurements or, more generally, the response to any local probe, it is claimed that the answer is positive. This result has been reached by extending the analysis of idealized 1D chains to physical quantum wires, which are finite systems with open boundaries or contacts of 1D electron gases with normal 3D metals.

The anomalous response of an interacting 1D Fermi gas to a local probe was first recognized by Kane and Fisher.[4] Subsequently, many different experimental situations have been proposed and analyzed in the framework of the Luttinger-liquid theory of 1D metals.[5] Several effects due to open boundary conditions have been studied by means of conformal field theory.[6] All these studies suggest that the interaction affects (in a nontrivial way) the behavior of the Fermi gas close to the boundaries. Consequently, transport measurements probing the edge properties should, in principle, reveal the Luttinger-liquid behavior.

In this paper, we study the properties of a 1D chain of interacting electrons with open boundary conditions from a more traditional point of view, not assuming conformal invariance. Some of the results will be new, some not; our intention is to provide a simple but powerful tool to tackle different problems that arise, while studying finite 1D systems.

The layout of the paper is as follows. In Sec. II, we develop the bosonization technique appropriate for open boundary conditions, generalizing Haldane's approach (which was originally deviced for periodic systems). The bosonization for noninteracting electrons is discussed first. Then, we study the interacting case. In Sec. III, several correlation functions are calculated and

the Friedel oscillation caused by the boundary is discussed. We also give an alternative derivation, based on Ward's identity method, of correlation functions and outline some applications of the open boundary analysis to slightly doped quasi-one-dimensional electron systems. Section IV is devoted to the analysis of transport phenomena in quantum wires. The two-terminal conductance is calculated and some other tunneling processes at the edge of the wire are discussed. In Sec. V we study a magnetic impurity coupled to a 1D electron gas in the presence of a potential scattering. There are four appendixes. In Appendix A, some formulas used in computation of correlation functions are given. The remaining appendixes are devoted to extensions of our approach: an x-ray edge type problem related to the scattering potential sign changing operator is investigated in Appendix B, effects of long-range electron-electron interaction are examined in Appendix C, and gaped phases of finite systems are studied in Appendix D.

II. OPEN BOUNDARY BOSONIZATION

This section is intended to give a general method of bosonizing an interacting Fermi system in the case of open boundaries (i.e., of a finite system of the length L).

The bosonization method has a long history. The equivalence between the excitation spectra of interacting fermions and free bosons in 1D was established by Mattis and Lieb[7] in their solution of the Luttinger model.[8] The bosons were identified as particle-hole excitations over the Fermi sea, and their dynamics turned out to be that one predicted by random-phase approximation. However, the full power of the bosonization method became clear later, when the representation for the electron creation (annihilation) operator in terms of free bosons was discovered.[9–11] This provided a powerful tool to calculate fermionic correlation functions in terms of free boson correlation functions. (Actually, this representation is very close in spirit to the famous Jordan and Wigner representation.) The finite size effects (assuming periodic boundary conditions) were studied by Haldane.[12]

We start with the Hamiltonian:

$$H = H_0 + H_{\rm int} ,$$

where the first term represents the kinetic energy,

$$H_0 = \sum_{s=\uparrow,\downarrow} \int_0^L dx \psi_s^\dagger(x) \varepsilon(-i\partial_x) \psi_s(x) , \tag{1}$$

and the second one describes the electron-electron interaction,

$$H_{\rm int} = \frac{1}{2} \sum_{ss'} \int dx dy \psi_s^\dagger(x) \psi_{s'}^\dagger(y) U_{ss'}(x-y) \psi_{s'}(y) \psi_s(x) , \tag{2}$$

$\varepsilon(k)$ is the dispersion law of the 1D band, and $\psi_s(x)$ is the spin s electron annihilation operator subject to the open boundary conditions:

$$\psi_s(0) = \psi_s(L) = 0 . \tag{3}$$

A. Noninteracting electrons

We consider the noninteracting case first. This situation has already been discussed in the literature (see, e.g., Ref. 13), but we still find it useful to give all of the details that we are going to use while studying the interacting case.

The Fourier mode expansion of the ψ operator, appropriate for the boundary conditions (3), takes the form

$$\psi_s(x) = \sqrt{\frac{2}{L}} \sum_k \sin(kx) c_{sk} , \tag{4}$$

with $k = \pi n/L$, n being a positive integer. The single electron spectrum is $\varepsilon(k)$ and the Fermi surface consists of the *single* point $k = k_F$ (see Fig. 1). Concentrating on the vicinity of this point, we define slow varying right and left moving fields:

$$\begin{aligned} \psi_{sR}(x) &= -\frac{i}{\sqrt{2L}} \textstyle\sum_p e^{ipx} c_{s,k_F+p} , \\ \psi_{sL}(x) &= \frac{i}{\sqrt{2L}} \textstyle\sum_p e^{-ipx} c_{s,k_F+p} , \end{aligned} \tag{5}$$

such that ($p = \pi n/L$)

$$\psi_s(x) = e^{ik_F x} \psi_{sR}(x) + e^{-ik_F x} \psi_{sL}(x) . \tag{6}$$

These fields, however, are *not* independent, as in the case of periodic boundary conditions,[12] but satisfy

$$\psi_{sL}(x) = -\psi_{sR}(-x) . \tag{7}$$

Therefore, one can actually work with the right moving field only, the left moving one is then defined by the above relation. The boundary condition

$$\psi_s(0) = 0$$

is automatically satisfied, whereas the condition

$$\psi_s(L) = 0$$

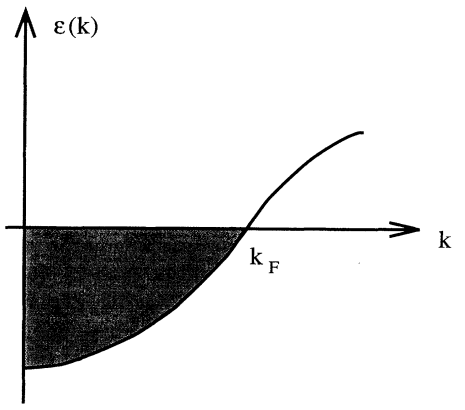

FIG. 1. Single-particle spectrum: for the case of open boundaries the Fermi surface consists of the single point k_F.

implies that the operator $\psi_{sR}(x)$ should obey

$$\psi_{sR}(-L) = \psi_{sR}(L) .$$

So we can regard the field $\psi_{sR}(x)$ as defined for all x, but obeying the periodicity condition with the period $2L$:

$$\psi_{sR}(x + 2L) = \psi_{sR}(x) . \tag{8}$$

In terms of the right moving field, the kinetic energy (1) takes the form

$$H_0 = v_F \sum_s \int_{-L}^{L} dx \psi_{sR}^{\dagger}(x)(-i\partial_x)\psi_{sR}(x) ,$$

where we have linearized the electron spectrum and the energy is accounted for from the Fermi energy of a reference system with N_{s0} number of spin s electrons.

The right moving Fermi field (5) obeys *periodic* boundary condition (8), so it can straightforwardly be bosonized. We will conveniently employ the following version of the bosonization formula:

$$\psi_{sR}(x) = \frac{\eta_s}{\sqrt{2L}} e^{-i\theta_s} e^{i\pi \frac{x}{L} \Delta N_s} e^{i\phi_s(x)} , \tag{9}$$

where ΔN_s is the number of extra electrons with spin s,

$$\Delta N_s = N_s - N_{s0} ,$$

the variable θ_s, canonically conjugate to ΔN_s,

$$[\theta_s, \Delta N_s] = i ,$$

is defined modulo 2π. The operators η_s are real (Majorana) fermions,

$$\{\eta_\uparrow, \eta_\downarrow\} = 0 , \eta_s^2 = 1 ,$$

which stand to assure the correct anticommutation rules for electron operators with different spin s. The phase field $\phi_s(x)$ is given by the expression

$$\phi_s(x) = \sum_{q>0} \sqrt{\frac{\pi}{qL}} e^{iqx - \alpha q/2} b_q + \text{H.c.}$$

and satisfies periodic boundary condition:

$$\phi_s(x + 2L) = \phi_s(x) . \tag{10}$$

Here, b_q are canonical Bose operators; $q = \pi n/L$, n is an integer, and we have introduced a high-energy cutoff α. It is straightforward to check that the operators $\psi_{sR}(x)$, defined by Eq. (9), obey standard fermionic commutation relations (in the limit $\alpha \to 0$).

Alternatively one could write the Fermi operator (9) in a normal ordered form, noticing

$$\frac{1}{\sqrt{2L}} : e^{i\phi_s(x)} : \to \frac{1}{\sqrt{2\pi\alpha}} e^{i\phi_s(x)} ,$$

we shall use both normal ordered and not normal ordered forms of Fermi operators.

The presence of the momentum space cutoff α reflects the finite bandwidth of the original electron band (α is understood to be much larger than the lattice spacing; actually, $1/\alpha$ is the region around k_F where the electron band spectrum can be linearized).

The density of right moving electrons is given by

$$\rho_{sR}(x) = \frac{\Delta N_s}{2L} + \frac{\partial_x \phi_s(x)}{2\pi} .$$

We notice that

$$\rho_{sL}(-x) = \rho_{sR}(x) .$$

The bosonized form of the kinetic energy is

$$H_0 = \pi v_F \sum_s \int_{-L}^{L} dx : \rho_{sR}(x)\rho_{sR}(x) := v_F \sum_{sq>0} q b_{sq}^{\dagger} b_{sq} + \frac{\pi v_F}{2L} (\Delta N_s)^2 .$$

Before we turn to the interaction effects, we define the bosonic variables corresponding to charge and spin excitations:

$$b_{\rho(\sigma)q} = \frac{1}{\sqrt{2}} (b_{\uparrow q} \pm b_{\downarrow q}) ,$$

and

$$\Delta N_{\rho(\sigma)} = \Delta N_\uparrow \pm \Delta N_\downarrow .$$

B. Interaction effects

In order to make use of the above bosonization procedure also for the case of interacting electrons, we try the *same* trick; namely, we express the part of the Hamiltonian, which is responsible for the interaction, Eq. (2), in terms of the right moving Fermi field ψ_{sR} only. The cost is that the resulting expression is highly nonlocal in space as illustrated in Fig. 2. Nevertheless, as we show below, at least in the case of short-range electron-electron interaction $U(x-y)$, the problem can be quite simply treated in terms of bosonic fields.

Here, we focus on the case of $R \simeq \alpha$, where R is the characteristic radius of the region where the function $U(x-y)$ is essentially nonzero. Then the q dependence of corresponding Fourier transforms can conveniently be neglected. (This implies that all the distances considered should be much larger then R.)

The interaction part of the Hamiltonian contains several terms classified in what follows.

The terms, diagonal in the electron densities, can be written in conventional way:

$$\frac{g_{\rho(\sigma)}}{2} \int_0^L dx \left[\rho_{\rho(\sigma)R}(x)\rho_{\rho(\sigma)R}(x) + \rho_{\rho(\sigma)L}(x)\rho_{\rho(\sigma)L}(x)\right] = \frac{g_{\rho(\sigma)}}{2} \int_{-L}^{L} dx \rho_{\rho(\sigma)R}(x)\rho_{\rho(\sigma)R}(x) . \tag{11}$$

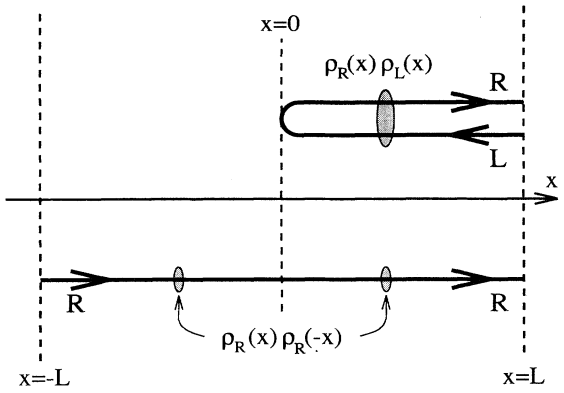

FIG. 2. The system with open boundaries can be described either in terms of right and left moving Fermi fields (the upper part of the figure) or in terms of the right moving field only (the lower part); in the latter case, the density-density interaction becomes nonlocal.

This renormalizes the sound velocity:

$$v^0_{\rho(\sigma)} = v_F + \frac{g_{\rho(\sigma)}}{2\pi} .$$

The term mixing right and left densities is of the form

$$\tilde{g}_{\rho(\sigma)} \int_0^L dx \rho_{\rho(\sigma)R}(x)\rho_{\rho(\sigma)L}(x) = \frac{1}{2}\tilde{g}_{\rho(\sigma)} \int_{-L}^{L} dx \rho_{\rho(\sigma)R}(x)\rho_{\rho(\sigma)R}(-x) , \quad (12)$$

i.e., it is nonlocal in space (see Fig. 2). Still, this term is quadratic in the electron densities and, therefore, takes a simple form in terms of bosonic operators (the remaining terms, which do not assume a form quadratic in densities are discussed in the last part of this section).

Consequently, the Hamiltonian becomes

$$H = \sum_{\nu=\rho(\sigma)} \left\{ \sum_{q>0} v^0_\nu q \left[b^\dagger_{\nu q} b_{\nu q} - \frac{\tilde{g}_\nu}{4\pi} \left(b_{\nu q} b_{\nu q} + b^\dagger_{\nu q} b^\dagger_{\nu q} \right) \right] + \frac{\pi v_{\nu N}}{4L} (\Delta N_\nu)^2 \right\} , \quad (13)$$

where

$$v_{\nu N} = v_F + \frac{g_\nu + \tilde{g}_\nu}{2\pi} .$$

This can be diagonalized in a standard way by the Bogolubov rotation,

$$b_{\nu q} \to \cosh(\varphi_\nu) b_{\nu q} - \sinh(\varphi_\nu) b^\dagger_{\nu q} , \quad (14)$$

where

$$\tanh(2\varphi_\nu) = -\frac{\tilde{g}_\nu}{2\pi v^0_\nu} . \quad (15)$$

[Notice that whereas the rotation angles φ_ν are defined in the same way as in the bulk case, Eq. (15), there is an important difference in sign in Eq. (14).] This rotation is achieved by the canonical transformation,

$$H \to UHU^\dagger = \sum_\nu \left\{ \sum_{q>0} v_\nu q b^\dagger_{\nu q} b_{\nu q} + \frac{\pi v_{\nu N}}{4L} (\Delta N_\nu)^2 \right\} , \quad (16)$$

where

$$v_\nu = \frac{v^0_\nu}{\cosh(2\varphi_\nu)} .$$

The previously defined $v_{\nu N}$ can be alternatively written as

$$v_{\nu N} = \frac{v_\nu}{K_\nu} , \quad (17)$$

being

$$K_\nu = \exp(2\varphi_\nu) .$$

The unitary operator U is defined by

$$U = \exp\left\{ \frac{1}{2} \sum_{\nu,\, q>0} \varphi_\nu \left(b^\dagger_{\nu q} b^\dagger_{\nu q} - b_{\nu q} b_{\nu q} \right) \right\} . \quad (18)$$

The next step is to find how the Fermi operators transform by applying U. Employing the method of Mattis and Lieb,[7] after lengthy but straightforward calculations, we arrive at the main result of this section, i.e., the expression for the electron annihilation operator in terms of free bosons for the case of the interacting Fermi system with open boundaries:

$$U\psi_{sR}(x,t)U^\dagger = \frac{\eta_s}{\sqrt{2\pi\alpha}} e^{-i\theta_s} e^{\frac{i\pi}{4L}\sum_\nu v_{\nu N} t} \times \exp\left\{ i \sum_\nu \varepsilon_{\nu s} \left[\pi \Delta N_\nu \frac{(x - v_\nu t)}{2L} + \frac{c_\nu}{\sqrt{2}} \phi_\nu(x - v_\nu t) - \frac{s_\nu}{\sqrt{2}} \phi_\nu(-x - v_\nu t) \right] \right\} \quad (19)$$

where $\varepsilon_{\nu s}$ is $+1$ unless $s = \downarrow$ and $\nu = \sigma$, when its value is -1. We have defined

$$c_\nu = \cosh(\varphi_\nu), \quad s_\nu = \sinh(\varphi_\nu).$$

It is important to notice that, if one would write the expression (19) in the normal ordered form, this results in x-dependent preexponential factors:

$$U\psi_{sR}(x,t)U^\dagger = A_\psi \frac{\eta_s}{\sqrt{2L}} e^{-i\theta_s} e^{\frac{i\pi}{4L}\sum_\nu v_{\nu N} t} [P(2x)]^{\sum_\nu s_\nu c_\nu/2} \times :\exp\left\{ i \sum_\nu \varepsilon_{\nu s} \left[\pi \Delta N_\nu \frac{(x - v_\nu t)}{2L} + \frac{c_\nu}{\sqrt{2}} \phi_\nu(x - v_\nu t) - \frac{s_\nu}{\sqrt{2}} \phi_\nu(-x - v_\nu t) \right] \right\} : , \quad (20)$$

where the constant A_ψ is given by

$$A_\psi = \left[\frac{\pi\alpha}{L}\right]^{\frac{1}{4}\sum_\nu (K_\nu^{-1}-1)} ,$$

and the function $P(z)$ is defined in the Appendix A. Although the preexponential factor in (20) is x dependent, it does not depend on t. This explicitates the asymmetry between space and time coordinates in the present problem (for the translation invariant system, the factors resulting from normal ordering are just constants[12]).

C. Luttinger-liquid picture

We now pause to discuss how the open boundary conditions modify the standard Luttinger-liquid picture. According to the Haldane analysis,[12] a gapless 1D system with periodic boundary conditions is described by a low energy Hamiltonian of the general form,

$$H = \sum_{q>0} v_S q b_q^\dagger b_q + \frac{\pi v_N}{2L}(\Delta N)^2 + \frac{\pi v_J}{2L} J^2 , \qquad (21)$$

ΔN being related to the total number of particles, and J to the total current. The different velocities in (21) obey the relations:

$$v_J = K v_S , \quad v_N = \frac{v_S}{K},$$

where K is the parameter which governs the asymptotic power low decay of all the correlation functions. Two parameters, e.g., v_S and v_J, are therefore sufficient to determine all the low-energy properties of the system (concept of the Luttinger-liquid universality). For electrons with spin, due to the spin-charge separation, low-energy behavior of the system is also described by the Hamiltonian of the form (21) in each charge and spin sector.

As we learned from the above analysis, in an interacting Fermi gas with open boundary conditions (i) spin-charge separation still occurs; (ii) each (spin or charge) sector is described by the Hamiltonian (16), similar to (21). The important difference with Haldane's analysis is that the Fermi system with open boundaries is bosonized with the help of the right moving Bose fields only, and, therefore, there is only one (in each spin and charge sector) conserved "topological number," ΔN. The total current J is not any more conserved; its dynamics we discuss in Appendix B. The Luttinger-liquid concept still holds since the two parameters (v_S and $v_N = v_S/K$) are sufficient to describe the low-energy behavior of the system. In the spirit of Ref. 12, v_N and K should be treated as *phenomenological* parameters, though they are related to the interaction constants g and $\tilde{g}$, which are in turn determined by the interaction potential $U(x-y)$ in the starting Hamiltonian (2).

Notice that we started the above analysis with local (in real space) interactions: $g_\rho(x) = g_\rho \delta(x)$, etc. (The interaction becomes nonlocal only *after* formulating the problem in terms of right moving fields.) If we would have readily started with long-range interactions of radius $R \gg \alpha$ (but nevertheless $R \ll L$), the interaction term in (13) acquires off-diagonal corrections (in q space). In Appendix C, we show that these off-diagonal terms do not contribute to the asymptotic behavior of the correlation functions for $|x| \gg R$ and $v_F|t| \gg R$ and can, therefore, be neglected. The exponents are thus determined by the $q \to 0$ limit of the Fourier transform of the interaction constants g_ν.

As it is well known, for the case of electrons with spin, the above considered terms—quadratic in the electron densities—do not account all the possible interaction processes effective at low energy. The remaining process is the so-called spin backscattering process which is described by the following term in the Hamiltonian:

$$\frac{g_{\rm bs}}{2}\sum_s \int_0^L dx \left[\psi_{sR}^\dagger(x)\psi_{sL}(x)\psi_{\bar{s}L}^\dagger(x)\psi_{\bar{s}R}(x) + (R \to L)\right]$$

$$= \frac{g_{\rm bs}}{2}\sum_s \int_{-L}^L dx \psi_{sR}^\dagger(x)\psi_{sR}(-x)\psi_{\bar{s}R}^\dagger(-x)\psi_{\bar{s}R}(x) , \qquad (22)$$

where $\bar{s}$ denotes $-s$. Using Eq. (19) we find that, under the transformation (16), the spin backscattering term takes the form

$$\frac{g_{bs}}{(2\pi\alpha)^2}\int_{-L}^L dx e^{-i\sqrt{2K_\sigma}\phi_\sigma(x)} e^{i\sqrt{2K_\sigma}\phi_\sigma(-x)} e^{-2iK_\sigma f(2x)} . \qquad (23)$$

Equation (23) cannot be diagonalized, in general. Nevertheless, one can analyze the effects of the spin backscattering by applying the renormalization group (RG) method, as it has been done for the infinite system.[1]

For $K_\sigma > 1$ the operator (23) is irrelevant, and it flows to zero under RG process, meanwhile renormalizing K_σ to a smaller value $K_\sigma^* \geq 1$. For spin isotropic interaction, the fixed point value is

$$K_\sigma^* = 1 . \qquad (24)$$

In this case, therefore, the approach we have developed above correctly describes the low-energy properties of the system.[15]

On the contrary, if $K_\sigma < 1$, the spin backscattering interaction is relevant, i.e., it flows to strong coupling under RG process. This is interpreted as the opening of a gap in the spin excitation spectrum. It is known that,[1] under scaling procedure, K_σ decreases and eventually crosses the value $K_\sigma = 1/2$ at which the model has been exactly solved by Luther and Emery.[14] Therefore, the solution at this point is believed to give a qualitatively correct description of the gapped phase for any $K_\sigma < 1$. The influence of open boundary conditions on the *gapped* phase is analyzed in Appendix D.

Finally, we notice that although we have modeled the finite electron system by imposing vanishing boundary conditions (3), one could equivalently switch on a binding wall potential. For instance, a potential $V(x)$ such that $V(x \to \infty) \to 0$ but $V(x \to -\infty) \to V_0$ is equivalent (if V_0 is larger then the Fermi energy) to a left boundary. In this case, one should use as a basis the eigenfunctions of this potential $\varphi_k(x)$, while defining the electron field

operator:

$$\psi_s(x) = \sqrt{\frac{2}{L}} \sum_k \varphi_k(x) c_{sk}. \tag{25}$$

Since at large positive x the eigenfunctions $\varphi_k(x)$ are *standing waves*, the expression (25) asymptotically coincides with (4) and our above considerations are applicable also to the binding wall potential case.

III. CORRELATION FUNCTIONS

Given the bosonized form of the electron operators, Eqs. (19)–(20), one can compute various correlation functions. Here, we discuss some examples of physical interest.

A. The Friedel oscillation

Since the system under study is obviously not translation invariant, the mean electron density is not homogeneous, so that the Friedel oscillation is build in the ground state. Namely, we obtain

$$\begin{aligned}\delta\rho(x) &= -e^{2ik_F x} \sum_s \langle \psi^\dagger_{Rs}(-x)\psi_{Rs}(x)\rangle + (x \to -x) \\ &= -\frac{e^{2ik_F x}}{\pi\alpha}[P(2x)]^{\frac{1}{2}\sum_\nu K_\nu} e^{-if(2x)} + (x \to -x)\ .\end{aligned} \tag{26}$$

Consider distances $x \ll L$. The Friedel oscillation then takes the form

$$\delta\rho(x) = -\frac{1}{\pi\alpha}\left[\frac{\alpha}{\sqrt{\alpha^2+4x^2}}\right]^{\frac{1}{2}\sum_\nu K_\nu} \sin(2k_F x)\ .$$

This expression describes how the perturbation of the electron density, caused by the boundaries in a semi-infinite system, decays at large distances.

It is interesting to examine to which extend the open boundary consideration applies to doped systems. Kane and Fisher noticed that a local impurity potential

$$V(x)\sum_s \psi^\dagger_s(x)\psi_s(x),$$

is equivalent, at low energy, to an infinite barrier, i.e., to a boundary (for infinite system).[4] Indeed, they found that the backscattering part of the impurity potential flows to infinity under scaling according to

$$\frac{dV}{d\ln\omega} = -\frac{1}{2}(1-K_\rho)\,V\ , \tag{27}$$

where the energy ω is scaled to zero starting from the bandwidth $\omega = D$. Repulsive ($K_\rho < 1$), spin isotropic ($K_\sigma = K^*_\sigma = 1$) interaction is assumed. The proof is completed by studying the opposite limit of *strong potential*, which results in a *weak link* between two independent semi-infinite systems — the electron tunneling through a weak link is described by an irrelevant operator (which flows to zero under scaling).

Assume now that many scatterers are present in the system. This is what happens in the case of doped quasi-one-dimensional electron systems. Does the above argument imply that, upon doping, the electron gas will break up, according to the concrete realization of the impurity potential, into a set of almost independent segments (to which open boundary description is applicable) connected by weak links? To answer this question, we notice that these segments are finite, so that there is a minimal excitation energy (dimensional quantization), $\omega_{\min}$. Consequently, the above scaling procedure should be stopped at energies $\omega \sim \omega_{\min}$. The relevant question, therefore, is whether $\omega_{\min}$ is so small that the impurity potential grows large enough to produce effectively infinite barriers *before* ω reaches $\omega_{\min}$. Obviously, this is just a condition on the scatterers concentration. The energy $\omega_{\min}$ should be compared with the cross over scale, ω_0, between the weak coupling regime of the impurity potential and the strong coupling one (the latter being equivalent to a regime of tunneling through a weak link). The latter scale can be estimated by imposing the solution of Eq. (27) to be of the order of the bandwidth. That gives

$$\omega_0 \sim D\left(\frac{V_0}{D}\right)^{2/(1-K_\rho)}\ .$$

Hence, setting $\omega_{\min} \sim v_F/x_0$, where x_0 is the mean distance between scatterers, we find the following condition on doping:

$$x_0 \gg \frac{1}{k_F}\left(\frac{D}{V_0}\right)^{2/(1-K_\rho)}\ . \tag{28}$$

Notice also that a *short-range* character of the impurity scattering was implied: $a_0 \sim 1/k_F$, where a_0 is the radius of an individual scattering potential. Otherwise, we should impose an additional condition:

$$x_0 \gg a_0\ . \tag{29}$$

Thus, if the conditions (28) — low doping — and (29) — short-range scattering — are satisfied, we arrive at physical picture for doped quasi-one-dimensional materials: the impurity potential renormalizes to large values thereby breaking up the electron system as shown in the Fig. 3; the electron tunneling across weak links and from chain to chain can then be treated by perturbation theory. This picture essentially differs from those previously discussed in the the literature, which deal with perturbation expansions in the disorder potential.[1,16]

Let us briefly outline some consequences.

(i) The Friedel oscillation (26) will be frozen in, depending upon the concrete realization of doping. Of course, this oscillation will be smeared out by impurity averaging. Still, an effect should remain in the density-density correlation function, which acquires an extra *doping dependent* $2k_F$ component steming from the impurity averaged Friedel oscillation. This should, in principle, be experimentally measurable (e.g., by neutron scattering).

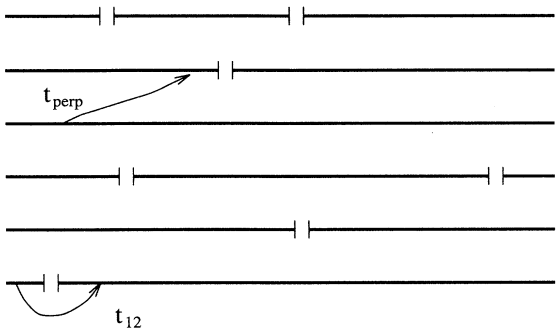

FIG. 3. Slightly doped quasi-one-dimensional conductor breaks up into independent segments of the electron gas (described by the open boundary analysis), these segments are coupled back by weak tunneling processes of two types: $t_{\rm perp}$ (tunneling between different chains) and t_{12} (tunneling between neighboring segments in the same chain).

(ii) The calculation of conductivity is, under these circumstances, an interesting but puzzling task dealing with a type of random resistance network.

(iii) At low temperatures the electron tunneling between chains becomes relevant, so that the 3D character of the problem takes over and a broken symmetry ground state forms (typically charge-density wave);[1,2,17] the effect of small doping (which increases a phase disorder but stabilizes the Friedel oscillation) on the formation of this state is unclear. These issues deserve, in our opinion, further investigations.

B. Green's function

The electron Green function is given by ($t > 0$):

$$G_{ss'}(x,y;t) = -i\langle\psi_s(x,t)\psi^\dagger_{s'}(y,0)\rangle = \sum_{a,b=\pm1} abe^{ik_F(ax-by)}G^R_{ss'}(ax,by;t)\ , \quad (30)$$

where we have substituted Eq. (6) and defined

$$G^R_{ss'}(x,y;t) = -i\langle\psi_{Rs}(x,t)\psi^\dagger_{Rs}(y,0)\rangle\ .$$

Making use of Eq. (19), we find

$$G^R_{ss'}(x,y;t) = -\frac{i\delta_{ss'}}{2\pi\alpha}\prod_\nu\Big\{[P(2x)P(2y)]^{s_\nu c_\nu/2}\Big[P(x^{(-)}-v_\nu t)\Big]^{c_\nu^2/2}\Big[P(x^{(-)}+v_\nu t)\Big]^{s_\nu^2/2} \times\Big[P(x^{(+)}-v_\nu t)P(x^{(+)}+v_\nu t)\Big]^{-s_\nu c_\nu/2}\Big\}e^{i\Phi(x,y,t)}\ , \quad (31)$$

where $x^{(\pm)} = x \pm y$, and the phase factor is given by

$$\Phi(x,y,t) = \frac{\pi}{L}x^{(-)} - \frac{\pi}{4L}\sum_\nu v_{\nu N}t + \frac{1}{2}\sum_\nu\Big[c_\nu^2 f(x^{(-)}-v_\nu t) - s_\nu^2 f(x^{(-)}+v_\nu t) + c_\nu s_\nu f(x^{(+)}+v_\nu t) - c_\nu s_\nu f(x^{(+)}-v_\nu t)\Big].$$

It is straightforward to calculate the finite temperature version of Eq. (31), that is, however, not of an immediate interest.

Let us now discuss some limiting cases of the expression (31).

(i) It is interesting to understand how the "bulk" behavior of Green's function is recovered. Clearly, one should impose the condition that the relative distance between points x and y is much less than all the distances to the boundaries:

$$x^{(-)} \ll \min\{x, y, L-x, L-y\}\ . \quad (32)$$

However, even if the above condition if fulfilled, the boundaries still influence the Green function behavior provided that the time interval t between the creation and the annihilation of the extra electron is large enough to allow the excitations to reach one of the boundaries and to be reflected from it. Hence the additional condition

$$(v_\rho t, v_\sigma t) \ll \min\{x, y, L-x, L-y\}\ . \quad (33)$$

Provided the conditions (32) and (33) are satisfied, Green's function (31) takes the following asymptotic form:

$$G^R_{ss'}(x,y;t) = -\frac{i\delta_{ss'}}{2\pi\alpha}\prod_\nu\Big\{\Big[\frac{\alpha}{x^{(-)}-v_\nu t+i\alpha}\Big]^{c_\nu^2/2} \times\Big[\frac{\alpha}{x^{(-)}+v_\nu t-i\alpha}\Big]^{s_\nu^2/2}\Big\}\ , \quad (34)$$

which is the electron Green function of the translation invariant system ($t > 0$). From the bulk behavior of Green's function (34) one can deduce, for instance, that

$$\langle\psi_s(x,t)\psi^\dagger_s(x,0)\rangle \sim \Big(\frac{1}{t}\Big)^{\frac{1}{2}\sum_\nu(K_\nu+K_\nu^{-1})}\ . \quad (35)$$

(ii) On the other hand, if our ψ operator is close to the boundary, the condition (32) can not be satisfied any more and one should use the general formula (31). Consider the case $x = y = 0$. Of course, strictly at the boundary, $x = 0$, the electron operator vanishes, Eq. (3). So, by writing $x = 0$, we mean that x is of the order of α. In this case, we find

$$G_{ss'}(0,0;t) \sim \delta_{ss'}\Big(\frac{1}{t}\Big)^{\sum_\nu K_\nu^{-1}/2}\ . \quad (36)$$

The latter formula holds actually for any x and y, satisfying

$$(x,y) \ll (v_\rho t, v_\sigma t) \ , \tag{37}$$

and means that the power law exponent of the Green function at the boundary differs from the bulk one. This result is implicit in the Kane and Fisher treatment[4,18] and also agrees with conformal field theory considerations.[6]

(iii) Different exponents come into play in the *static limit*: $G(x,y;t=0)$. For $t=0$ and $x=y$ the expression (31) coincides, of course, with (26). In the limit $x=0$, $y \gg \alpha$ (but $y \ll L$), however, one finds

$$G(0,y;0) \sim \left(\frac{1}{y}\right)^{(1/8)\sum_\nu (K_\nu + 3/K_\nu)} \ . \tag{38}$$

Notice the difference between (36) and (38).

C. Ward's identity

Because of the novelty of the bosonization approach to open boundary systems, the question arises whether any important physical processes have been missed in the above consideration. Put another way, is it possible to derive the Green function (31), and other correlation functions, by means of an alternative method not relying on specific tricks of the bosonization approach [like Eq. (9) to Eq. (19)]? An alternative method of deriving the correlation functions of 1D interacting Fermi systems, based on the classification of diagrams (Ward's identity), has been devised by Dzyaloshinskii and Larkin.[19] Everts and Schulz realized that Ward's identity can equivalently be derived using equations of motion for electron density operators.[20]

The starting point, as in Sec. II, is to formulate the problem entirely in terms of right moving fields. The full Hamiltonian then reads:

$$H = \int_{-L}^{L} dx \Big\{ v_F \psi_R^\dagger(x)(-i\partial_x)\psi_R(x) + \frac{g}{2}\rho_R(x)\rho_R(x) + \frac{\tilde{g}}{2}\rho_R(x)\rho_R(-x) \Big\} \ . \tag{39}$$

(For the sake of clarity, we consider the simplest case of spinless fermions.)

The Dyson equation for the single-particle Green function,

$$G^R_{pp'}(t) = -i\langle T\{c_p(t)c^\dagger_{p'}(0)\}\rangle \ ,$$

where the operator c_p is defined by Eq. (5) with $k_F + p \to p$, takes the form

$$(i\partial_t - v_F p)\, G^R_{pp'}(t) = \delta_{pp'}\delta(t) - \frac{1}{2L}\sum_q \Big[g F^q_{p-q,p'}(t,t) + \tilde{g} F^{-q}_{p-q,p'}(t,t) \Big] \ , \tag{40}$$

F being the two-particle vertex function defined by

$$F^q_{p,p'}(t,t') = -i\langle T\{\rho_q(t)c_p(t')c^\dagger_{p'}(0)\}\rangle \ , \tag{41}$$

with

$$\rho_q = \sum_p c^\dagger_p c_{p+q} \ .$$

The crucial step in solving the 1D problem is to find a relation between the vertex function F and the Green function G, which enables one to express the former in terms of the latter thereby resulting in a closed equation for G. Since the nonlocal interaction in (39) does not conserve momentum, the diagrammatic approach of Ref. 19 is, in our case, less convenient then the equations of motion method of Ref. 20.

Standard commutation relations[7]

$$[\rho_q, \rho_{-q'}] = \frac{qL}{\pi}\delta_{qq'} \ ; \quad q,q' > 0$$

(the $1/2$ difference with Ref. 7 is due to q taking the values $\pi n/L$) lead to the following equation of motion for the density operator:

$$(i\partial_t - v_F q)\,\rho_q = \frac{g}{2\pi} q\rho_q + \frac{\tilde{g}}{2\pi} q\rho_{-q} \ . \tag{42}$$

Deriving Eq. (41) in t and substituting Eq. (42), we arrive at the version of Ward's identity applicable to the present problem:

$$\begin{aligned}(i\partial_t - v_F q)\, F^q_{p,p'}(t,t') &= \frac{g}{2\pi} q F^q_{p,p'}(t,t') + \frac{\tilde{g}}{2\pi} q F^{-q}_{p,p'}(t,t') \\ &\quad + i\delta(t-t')G^R_{p+q,p'}(t) - i\delta(t)G^R_{p,p'-q}(t'-t) \ .\end{aligned} \tag{43}$$

The Ward identity (43) can easily be solved with respect to the vertex function F (in ω space). Substituting this solution into Eq. (40) and transforming back to the (x,t) space, we find, after algebraic manipulations, the following closed equation for the Green function ($t>0$):

$$(\partial_t + v_F\partial_x)\ln G^R(x,y,t) = K(x,y,t) \ , \tag{44}$$

with

$$\begin{aligned}K(x,y,t) &= \frac{(v_F - v)sc}{x+y-vt} + \frac{(v_F+v)sc}{x+y+vt} \\ &\quad - \frac{v_F sc}{x} - \frac{(v_F - v)c^2}{x-y-vt} - \frac{(v_F+v)s^2}{x-y+vt} \ .\end{aligned} \tag{45}$$

The limit $L \to \infty$ (semi-infinite system) is taken. Here and below, we omit (imaginary) short-time cutoff terms (which can easily be restored). Analogously to the case of fermions with spin (see Sec. II), we have defined

$$c = \cosh(\varphi), \ s = \sinh(\varphi); \ \tanh(2\varphi) = -\frac{\tilde{g}}{2\pi v_F + g}$$

and the renormalized sound velocity v is given by

$$v = \sqrt{\Big[v_F + \Big(\frac{g}{2\pi}\Big)\Big]^2 - \Big(\frac{\tilde{g}}{2\pi}\Big)^2} \ .$$

Among many solutions of Eq. (44), the one which coincides with the free fermions Green function for the noninteracting case and is correctly symmetrized with respect to x and y, can be written in the form:

$$G^R(x,y,t) = -\frac{i}{2\pi\alpha}\left[\frac{(x+y-vt)(x+y+vt)}{4xy}\right]^{sc} \times \left[\frac{\alpha}{x-y-vt}\right]^{c^2}\left[\frac{\alpha}{x-y+vt}\right]^{s^2} . \quad (46)$$

The Green function (46) coincides with the appropriate asymptotic form of spinless version of Eq. (31), thus demonstrating the equivalence of "purely" bosonization methods of Sec. II and the approach based on Ward's identity for Fermi systems with open boundaries. [We remind you that the total Green function $G(x,y,t)$ is determined by $G^R(x,y,t)$ via the relation (30).]

The Ward's identity method can straightforwardly be extended to the case of finite L, finite temperatures, as well as to the case of fermions with spin. We are not presenting these calculations here since they anyway lead to the results identical to those of the bosonization technique.

IV. TUNNELING AT THE BOUNDARIES

In this section, we study several tunneling processes at the boundary of the wire, which might be relevant for experimental applications.

A. Two-terminal conductance

Consider a semi-infinite wire coupled to a normal (3D) metal through an insulating barrier, as shown in Fig. 4. A potential difference V is applied between the metal and the wire and we assume that the potential drop occurs just across the barrier, whereas both the metal and the wire have homogeneous chemical potentials. The Hamiltonian describing the system can be written in the form

$$\hat{H} = \hat{H}_M + \hat{H}_W + \hat{T} - V\hat{Q} , \quad (47)$$

where $\hat{H}_{M(W)}$ is the Hamiltonian of the isolated metal (wire), $\hat{T}$ describes the tunneling between them:

$$\hat{T} = \sum_s \int_W dx \int_M d\vec{r}\, T(x,\vec{r})\left[\psi^\dagger_{Ws}(x)\psi_{Ms}(\vec{r}) + \text{H.c.}\right] ,$$

where $T(x,\vec{r})$ the tunneling matrix element between the wire and the metal, which we take limited to the vicinity of the barrier. The last term in (47) is responsible for the potential difference between the wire and the metal, $\hat{Q}$ being their charge difference,

$$\hat{Q} = e(N_W - N_M),$$

where $N_{M(W)}$ is the total number of electrons in the metal (wire).

The potential drop induces a current $\hat{I}$, which is defined by

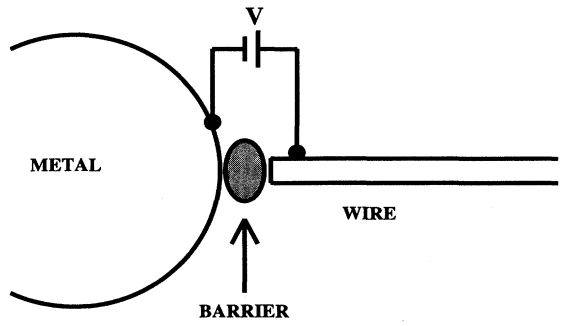

FIG. 4. Contact between a quantum wire and a 3D metal, with an applied potential difference V.

$$\hat{I}(t) = \frac{d\hat{Q}}{dt} = -2ie\sum_s \int_W dx \int_M d\vec{r}\, T(x,\vec{r}) \times \left[\psi^\dagger_{Ws}(x)\psi_{Ms}(\vec{r}) - \text{H.c.}\right] . \quad (48)$$

In linear response the average current at time t is given by

$$\langle\hat{I}(t)\rangle = i\int dt'\theta(t-t')\langle[\hat{I}(t),\hat{Q}(t')]\rangle V(t') .$$

Since $[\hat{I},\hat{Q}] = 4ie^2\hat{T}$, and $\hat{Q}$ is conserved in the absence of tunneling, the above correlation function vanishes if the thermal average is taken over the eigenstates of the Hamiltonian (47) with $\hat{T} = 0$. Therefore, one needs the next order correction in the tunneling, which leads to the following expression:

$$\langle\hat{I}(t)\rangle = i\int dt'\theta(t-t')\int dt''\theta(t'-t'')\langle[\hat{I}(t),\hat{I}(t'')]\rangle_0 V(t') , \quad (49)$$

where the thermal average $\langle\rangle_0$ is now taken at $\hat{T} = 0$.

Due to the relation (48), the current-current correlation function reduces to a product of the local single-particle Green functions for the metal and the wire. As we have shown previously, the local wire Green function behaves as

$$\langle\psi_{Ws}(0,t)\psi^\dagger_{Ws}(0,0)\rangle \sim \left(\frac{1}{t}\right)^{\sum_\nu K_\nu^{-1}/2} ,$$

while the metal Green function is

$$\langle\psi_{Ms}(0,t)\psi^\dagger_{Ms}(0,0)\rangle \sim \left(\frac{1}{t}\right) .$$

The latter result is true independently of the presence of electron-electron interaction in the 3D metal, as follows from the quasiparticle pole residue Z being finite in the Fermi liquid theory.

Plugging these results into (49), we find for low frequency conductance,

$$G(\omega) = \frac{I(\omega)}{V(\omega)} = G_0 \left(\frac{\omega}{D}\right)^{\sum_\nu K_\nu^{-1}/2-1} ,$$

where G_0 is a frequency independent constant that is determined by details of the barrier and D is a high-energy cutoff related to the metal and wire bandwidths. At zero frequency, the temperature dependence of the conductance is given by the same formula with the temperature replacing the frequency.

This result enables us to discuss the more realistic geometry of Fig. 5. In this case, the voltage drop V occurs at the two insulating barriers, i.e., $V = V_1 + V_2$ (the indices refer to each barrier), while the currents flowing across each barrier are the same $I = I_1 = I_2$. The latter condition holds since no accumulation of charge can occur in the wire. Therefore, the two-terminal conductance

$$G = \frac{G_1 G_2}{G_1 + G_2} \propto \left(\frac{\omega}{D}\right)^{\sum_\nu K_\nu^{-1}/2-1} .$$

Thus, in the physically relevant situation of spin isotropic repulsive interaction ($K_\rho < 1$ and $K_\sigma = 1$), the two-terminal conductance vanishes at low frequency (low temperature) with a power law. The conductance of a Luttinger liquid with an impurity has been predicted to vanish by Kane and Fisher.[4] Here, we have shown that such an effect should occur even in the case of a perfectly *clean* wire. This reflects the irrelevance of the tunneling $\hat{T}$ between the wire and the normal metal, as a consequence of the electron-electron interaction in the wire. Thus, a two-terminal experiment as the one we discussed above can provide a simple way of probing the Luttinger-liquid behavior in quantum wires. Notice, however, that those wires should be sufficiently long since the dimensional quantization introduces a low-energy cutoff v_F/L below which the conductance becomes temperature independent and moreover gives rise to a finite charging energy (causing Coulomb blockade type phenomena), which we have neglected.

B. Boundary operators

Similarly to what we have shown for a normal metal — quantum wire — normal metal contact, one can imagine other experimental setups in which different boundary processes are involved. In the case we just studied, the corresponding boundary operator was the single Fermi field operator. For example, at the contact between the quantum wire and a standard 3D superconductor, the tunneling of electron pairs should be considered.[21] In Table I, worked out by applying Eq. (19), we give a list of possible boundary operators $\hat{O}_b$ with their scaling dimensions x_b defined by

$$\langle \hat{O}_b(t) \hat{O}_b^\dagger(0) \rangle \propto \left(\frac{1}{t}\right)^{2x_b} .$$

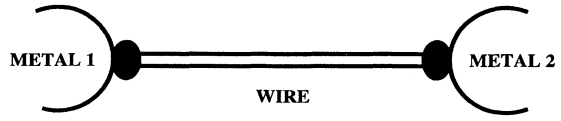

FIG. 5. Geometry for a two-terminal conductance measurement.

V. MAGNETIC IMPURITY

In this section, we consider the effects of a magnetic impurity in an interacting wire. The coupling to the conduction electrons is provided by an antiferromagnetic exchange J and a local potential V. On general grounds one expects $V \gg J$, but even in the unphysical case $V = 0$, a local potential will be generated by the exchange coupling.[22] The $V = 0$ problem has been previously studied by Lee and Toner[23] and by Furusaki and Nagaosa.[24] In Ref. 24 it was found that for repulsive electron-electron interaction the low temperature fixed point corresponds to the screened impurity spin, similarly to what happens in the conventional single-channel Kondo problem for noninteracting electrons.

Here, we study the opposite limit $V \gg J$. In this case, it is more appropriate to first diagonalize the Hamiltonian with only the local potential. For repulsive interaction that corresponds to cutting, the wire at the impurity site and treating the residual tunneling through the barrier as a (irrelevant) perturbation.[4] Taking into account also the spin exchange, one can, in general, write the following impurity Hamiltonian:

TABLE I. Boundary operators and their scaling dimensions.

Boundary operator $\hat{O}_b(t)$	Bosonized form	Exponent x_b
$\psi_{Rs}(t)$	$\exp\left\{i\frac{\phi_\rho(t)}{\sqrt{2K_\rho}} \pm i\frac{\phi_\sigma(t)}{\sqrt{2K_\sigma}}\right\}$	$\frac{1}{4}(K_\rho^{-1} + K_\sigma^{-1})$
$\psi_{Rs}^\dagger(t)\psi_{Rs}(t)$	$\partial\phi_\rho(t) + \partial\phi_\sigma(t)$	1
$\psi_{Rs}^\dagger(t)\psi_{R-s}(t)$	$\exp\left\{\mp i\sqrt{\frac{2}{K_\sigma}}\phi_\sigma(t)\right\}$	K_σ^{-1}
$\psi_{Rs}(t)\psi_{Rs}(t)$	$\exp\left\{i\sqrt{\frac{2}{K_\rho}}\phi_\rho(t) \pm i\sqrt{\frac{2}{K_\sigma}}\phi_\sigma(t)\right\}$	$K_\rho^{-1} + K_\sigma^{-1}$
$\psi_{R-s}(t)\psi_{Rs}(t)$	$\exp\left\{i\sqrt{\frac{2}{K_\rho}}\phi_\rho(t)\right\}$	K_ρ^{-1}

$$H_{\rm imp} = J\vec{S}\sum_{i=1,2}\sum_{\alpha\beta}\psi^{\dagger}_{i\alpha}\vec{\sigma}_{\alpha\beta}\psi_{i\beta} + \Gamma\vec{S}\sum_{\alpha\beta}\left(\psi^{\dagger}_{1\alpha}\vec{\sigma}_{\alpha\beta}\psi_{2\beta} + \text{H.c.}\right) + t\sum_{\alpha}\left(\psi^{\dagger}_{1\alpha}\psi_{2\alpha} + \text{H.c.}\right), \quad (50)$$

where 1(2) corresponds to the right (left) side of the impurity, $\vec{S}$ is the impurity spin-1/2 operator, and σ^a are the spin-1/2 matrices (see Fig. 6). The first term represents the exchange interaction of the electrons of each lead with the impurity spin. The second one corresponds to tunneling processes with spin flip, and the third one to the tunneling without spin flip.

For $\Gamma = t = 0$, the model is equivalent to the two channel Kondo model, which is known to exhibit anomalous behavior. Finite Γ and t will introduce anisotropy between the two channels. For noninteracting electrons, this anisotropy is known to be a relevant perturbation which brings the system back to the single-channel behavior at low temperature.[25] A repulsive interaction ($K_\rho < 1$, assuming $K_\sigma = 1$ to assure spin isotropy) changes the bare dimension of Γ getting it irrelevant, without affecting J (which remains marginal). The resulting renormalization group equations for weak interaction are

$$\frac{dJ}{d\ln L} = \frac{1}{2\pi v_F}(J^2 + \Gamma^2),$$

$$\frac{d\Gamma}{d\ln L} = \left(1 - \frac{1}{K_\rho}\right)\Gamma + \frac{1}{\pi v_F}\Gamma J.$$

Although a small Γ will firstly decrease under scaling due to $K_\rho < 1$, the contemporary increase of J will ultimately drive Γ to larger values. Therefore, the relevance of Γ should be more appropriately studied for large values of J. The best way to proceed is then to first assume $\Gamma = 0$, let J flow to the strong coupling fixed point, and analyze around it the relevance of a small Γ.

We bosonize the Fermi fields according to the procedure outlined in Sec. II. We introduce charge and spin bosonic variables for each lead $\phi_{1\nu}$ and $\phi_{2\nu}$ ($\nu = \rho, \sigma$), and their symmetric and antisymmetric combinations $\phi_{s\nu}$ and $\phi_{a\nu}$. In terms of these fields, the Hamiltonian (50) reads

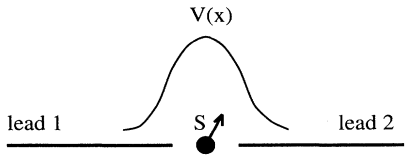

FIG. 6. Impurity spin S in a quantum wire in the presence of a strong potential scattering.

$$H_{\rm imp} = \frac{J_\perp}{2\pi\alpha}\left[S^+ e^{i\phi_{s\sigma}}\cos(\phi_{a\sigma}) + \text{H.c.}\right] + \frac{J_z}{2\pi}S^z\partial_x\phi_{s\sigma} + \frac{\Gamma_\perp}{2\pi\alpha}\left[S^+ e^{i\phi_{s\sigma}}\cos\left(\frac{\phi_{a\rho}}{\sqrt{K_\rho}}\right) + \text{H.c.}\right] + \frac{\Gamma_z}{\pi\alpha}S^z\sin(\phi_{a\sigma})\sin\left(\frac{\phi_{a\rho}}{\sqrt{K_\rho}}\right) + \frac{2t}{\pi\alpha}\cos(\phi_{a\sigma})\cos\left(\frac{\phi_{a\rho}}{\sqrt{K_\rho}}\right). \quad (51)$$

In the spirit of the Emery-Kivelson solution to the two-channel Kondo model,[26] we can get rid of the phase factors involving $\phi_{s\sigma}$ by performing the canonical transformation,

$$U = e^{-iS_z\phi_{s\sigma}}.$$

The transformed Hamiltonian is simply

$$H_{\rm imp} = \frac{1}{\pi\alpha}S^x\left[J_\perp\cos(\phi_{a\sigma}) + \Gamma_\perp\cos\left(\frac{\phi_{a\rho}}{\sqrt{K_\rho}}\right)\right] + \frac{\lambda}{2\pi}S^z\partial_x\phi_{s\sigma} + \frac{\Gamma_z}{\pi\alpha}S^z\sin(\phi_{a\sigma})\sin\left(\frac{\phi_{a\rho}}{\sqrt{K_\rho}}\right) + \frac{2t}{\pi\alpha}\cos(\phi_{a\sigma})\cos\left(\frac{\phi_{a\rho}}{\sqrt{K_\rho}}\right), \quad (52)$$

where $\lambda = J_z - 2\pi v_F$. If $\lambda = \Gamma_z = t = 0$ the Hamiltonian (52) can be easily studied since S^x commutes with the Hamiltonian and can be given a definite value $\pm 1/2$. For a fixed S^x, the Hamiltonian is equivalent to the one describing impurity scattering in a Luttinger liquid (for each field $\phi_{a\sigma}$ and $\phi_{a\rho}$). It is known that a local $\cos(\beta\phi)$ term is relevant if $\beta < \sqrt{2}$, marginal if $\beta = \sqrt{2}$, and irrelevant otherwise. Therefore, the $J_\perp$ operator is always relevant, whereas $\Gamma_\perp$ is relevant only if $1/2 < K_\rho < 1$.

If both $J_\perp$ and $\Gamma_\perp$ are relevant, the low temperature fixed point behavior is that of the single-channel Kondo model, as we previously discussed. Just this case has been analyzed in detail by Furusaki and Nagaosa.[24] Thus, we have shown that the presence of a strong potential scattering does not modify their conclusions, provided that $K_\rho \geq 1/2$.

The feature that arises from our analysis is that for $K_\rho < 1/2$ the two-channel Kondo behavior is stable, with respect to a channel asymmetry. The behavior of the model around the two-channel fixed point can be performed in a way similar to that of Ref. 26. Without repeating the calculation, we just remind that the low temperature impurity susceptibility $\chi \sim \ln(1/T)$ and the specific heat $C_V \sim T\ln(1/T)$. This situation could be realized in quantum wires with long-range Coulomb interaction, which may result in a very small K_ρ, see Ref. 27.

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APPENDIX A

The computation of average values of exponentials containing phase fields requires the knowledge of the sum:

$$S(z)=\sum_{q>0}\frac{\pi}{qL}e^{iqz-\alpha q}=\ln\left(\frac{L}{\pi\alpha}\right)+\ln P(z)+if(z)\ , \tag{A1}$$

where

$$P(z)=\frac{\pi\alpha}{2L\sqrt{\sinh^2\left(\frac{\pi\alpha}{2L}\right)+\sin^2\left(\frac{\pi z}{2L}\right)}};$$

$$f(z)=\tan^{-1}\left[\frac{\sin\left(\frac{\pi z}{L}\right)}{e^{\pi\alpha/L}-\cos\left(\frac{\pi z}{L}\right)}\right].$$

Let us consider the limit of these functions for z close to one of the boundaries. For $|z|\ll L$ (but $|z|\gg\alpha$), we have

$$P(z)=\frac{\alpha}{|z|};$$

$$f(z)=\tan^{-1}\left(\frac{z}{\alpha}\right)\to\frac{\pi}{2}\mathrm{sgn}(z).$$

The same expression holds at the other boundary ($z\to 2L$) with the replacement $z\to z-2L$.

APPENDIX B

As an interesting application of the open boundary bosonization, we consider the following problem: let us imagine that in a spinless Luttinger liquid on a ring of length L, we insert an impurity at the origin. This impurity has two possible states, which can be thought of as two spin states $|\uparrow(\downarrow)\rangle$. We model the impurity as a local backscattering potential,[4] and we assume that the sign of this potential depends on the impurity spin. This amounts to add to the electron Hamiltonian a term of the form,

$$V\sigma_z\cos(\phi_R+\phi_L), \tag{B1}$$

where the Pauli matrix acts on the impurity states, and $\phi_{R(L)}$ is the phase field corresponding to the right (left) moving electrons. Since there is no term in the Hamiltonian which flips the impurity spin, σ_z can be given a fixed value, which does not evolve with time. If the interaction is repulsive (parametrized by the exponent $K<1$), we know from Ref. 4 that the impurity at low energy effectively acts as an infinite barrier, thus cutting the chain into two disconnected leads of length L. Consider now the following x-ray edge type of problem: at time $\tau<0$, the impurity is in the state $|\downarrow\rangle$. Suddenly at $\tau=0$ the spin is reversed, thus changing sign of the scattering potential, and finally at time $\tau=t$ the spin is reversed back. This process is described by the correlation function:

$$\chi(t)=\langle\downarrow|\,\sigma^-(t)\sigma^+(0)\,|\downarrow\rangle\ . \tag{B2}$$

Can we calculate the long time behavior of (B2)? We recently encountered a similar problem analyzing the four-channel Kondo model,[28] and we think it may be relevant also for other impurity models. The way to evaluate (B2) is similar to the standard bosonization approach to the x-ray edge singularity. Notice that the unitary operator

$$U=\exp\left[i\frac{\pi}{2}J\right],$$

where $J=N_R-N_L$ is the total current, has the following property:

$$U\left[H_0+V\cos(\phi_R+\phi_L)\right]U^\dagger=H_0-V\cos(\phi_R+\phi_L),$$

i.e., it changes the sign of the potential term without modifying the bulk part of the Hamiltonian H_0. Thus, U is equivalent to the spin flip operator. This implies that the correlation function (B2) can also be written as

$$\chi(t)=\langle\downarrow|\,U(t)U^\dagger(0)\,|\downarrow\rangle\ ,$$

and in this representation its evaluation is straightforward. Since the low-energy fixed point corresponds to cutting the ring at the origin, we use the open boundary bosonization to rewrite the current operator,

$$\begin{aligned}J=N_R-N_L&=\int_0^L dx\rho_R(x)-\rho_L(x)\\&=\int_0^L dx\rho_R(x)-\rho_R(-x).\end{aligned}$$

By performing the Bogolubov rotation to get rid of the bulk interaction, we get

$$J=\frac{1}{\pi\sqrt{K}}[\phi(L)-\phi(0)]\ ,$$

and, therefore,

$$U=\exp\left[\frac{i}{2\sqrt{K}}[\phi(L)-\phi(0)]\right]\ .$$

Since the fields ϕ are now free Bose fields with logarithmic correlation, we immediately see that the dynamics of the total current is characterized by the following correlation function ($t\ll L/v_F$):

$$\langle J(t)J(0)\rangle=\frac{2}{\pi^2K}\ln t\ .$$

This result agrees with the analysis of Ref. 29. Hence,

the correlation function (B2) takes the form

$$\chi(t) \propto \left(\frac{1}{t}\right)^{\frac{1}{2K}} . \tag{B3}$$

$\chi(t)$ has the power law behavior typical of the x-ray edge singularity, but the exponent is determined by the interaction only and is not bounded from above.

APPENDIX C

This Appendix is intended to show that a long-range electron-electron interaction (i.e., interaction of finite radius R) does not modify the conclusions of Sec. II; namely, that the exponents of correlation functions are determined by zero-momentum Fourier components of interaction constants. In the case of long-range interaction, the bosonic Hamiltonian (13) is no more diagonal in q space. We proceed in two steps: first, we demonstrate how the diagonal part of the interaction can be separated from the off-diagonal one and, second, we observe that the latter is irrelevant (does not contribute to the exponents).

The interaction term (11) is now of the form

$$\frac{1}{2}\int_0^L dx \int_0^L dy g(x-y)\Big[\rho_{\rho(\sigma)R}(x)\rho_{\rho(\sigma)R}(y) + \rho_{\rho(\sigma)L}(x)\rho_{\rho(\sigma)L}(y)\Big] \tag{C1}$$

and the $\tilde{g}$ term (12) changes analogously. (The index $\nu = \rho, \sigma$ is suppressed, but the results are valid for both charge and spin sectors.)

Simplifying the problem (but not affecting qualitative results), we work in the limit of semi-infinite system ($L \to \infty$). Then, in q space, the Hamiltonian takes the form

$$H = H_0 + H_{\text{int}} , \tag{C2}$$

with the continuum version of the free part,

$$H_0 = \int_0^\infty dq v_F q b_q^\dagger b_q ,$$

and the interaction term,

$$H_{\text{int}} = -\frac{1}{4\pi}\int_0^\infty dq_1 \int_0^\infty dq_2 \sqrt{q_1 q_2}[I(q_1,q_2)(b_{q_1} b_{q_2} + \text{H.c.}) + I(q_1,-q_2)(b_{q_1}^\dagger b_{q_2} + \text{H.c.})] , \tag{C3}$$

where

$$I(q_1,q_2) = g(q_1,q_2) + \tilde{g}(q_1,-q_2) ,$$

and $g(q_1,q_2)$ is defined by

$$g(q_1,q_2) = \text{Re}\frac{1}{\pi}\int_{-\infty}^\infty \frac{dp}{2\pi}\frac{g(p)}{(p+q_1+i\delta)(p-q_2-i\delta)} . \tag{C4}$$

Here, $g(p)$ is the Fourier integral transform of $g(x)$ and δ a positive infinitesimal. The formula (C4) with $\tilde{g}(p)$ instead of $g(p)$ defines $\tilde{g}(q_1,q_2)$.

Shifting the integration contour in (C4) up in the complex p plane, we can write

$$I(q_1,q_2) = g(q_2)\delta(q_2+q_1) + \tilde{g}(q_2)\delta(q_2-q_1) + \delta I(q_1,q_2) . \tag{C5}$$

The first two terms in (C5) stem from the residual of the pole $p = q_2 + i\delta$. They are responsible for the diagonal part of the interaction. The off-diagonal part, $\delta I(q_1,q_2)$, is due to singularities of the functions $g(p)$ and $\tilde{g}(p)$ in the complex plane (see Fig. 7). Since the only regular complex function is a constant, the only case when $\delta I = 0$ corresponds to local (in real space) interactions.

In order to illustrate the properties of the off-diagonal part of the interaction, we consider now a specific example:

$$g(p) = \tilde{g}(p) = \frac{g_0}{2}\ln\left(\frac{p^2+\lambda_a^2}{p^2+\lambda_s^2}\right) . \tag{C6}$$

The interaction (C6) may model a screened Coulomb interaction in quantum wires (the cutoffs λ_s and λ_a are then related to the inverse screening length and inverse lattice spacing, respectively). Evaluating the branch cut integral (Fig. 7), we find

$$\delta g(q_1,q_2) = \frac{g_0}{\pi(q_1+q_2)}\sum_{i=1,2}\left[\tan^{-1}\left(\frac{q_i}{\lambda_s}\right) - \tan^{-1}\left(\frac{q_i}{\lambda_a}\right)\right] .$$

It is important to notice that δI tends to a constant in the limit of small q:

$$\delta I(0,0) = \frac{2g_0}{\pi}\left(\frac{1}{\lambda_s}+\frac{1}{\lambda_a}\right) .$$

Obviously we can, in general, write

$$\delta I(q_1,q_2) = g_0 R, \quad \text{for } (q_1,q_2) \ll 1/R . \tag{C7}$$

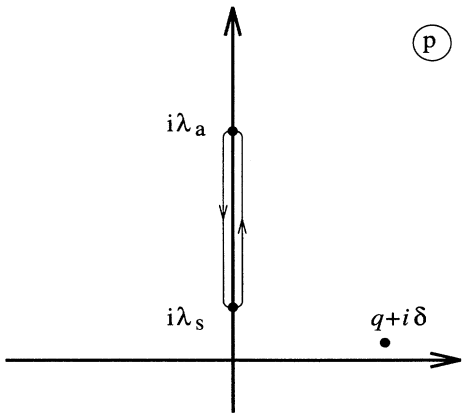

FIG. 7. Integration contour in Eq. (C4).

Here, g_0 is the interaction strength and R is related to the inverse distance to the first singularity of $g(p)$ from the real axis (i.e., to the radius of the interaction).

We can thus rearrange the total Hamiltonian (C2) writing it in the form

$$H = \tilde{H} + \delta H \ .$$

Here, $\tilde{H}$ is the continuum version of the Hamiltonian (13), it contains H_0 and the diagonal in q part of (C3). $\tilde{H}$ can immediately be diagonalized [the exponents are determined by $g(q=0)$ and $\tilde{g}(q=0)$]. The remaining part, in small-q limit, takes the form

$$\delta H = -\frac{g_0 R}{2\pi}\int_0^\infty dq_1 \int_0^\infty dq_2 \sqrt{q_1 q_2}\left(b_{q_1} - b^\dagger_{q_1}\right)\left(b_{q_2} - b^\dagger_{q_2}\right)$$

The irrelevance of δH is already clear from its scaling dimension (with is equal to 2). One can also demonstrate this more straightforwardly: since δH is quadratic in Bose fields, H can be diagonalized. Doing so, we find that the leading corrections (due to δH) to the correlation function $\langle\phi(x)\phi(y)\rangle$ [which behaves as $\ln(x-y)$ in the absence of δH] drop as $(R/x)^2$, $(R/y)^2$ at large distances thus do not modifying the asymptotic behavior of fermionic correlators.

APPENDIX D

Here, we study how the Luther-Emery solution is modified by open boundary conditions. If we define new Fermi operators

$$\Psi_\sigma(x) = \frac{1}{\sqrt{2\pi\alpha}} e^{-i\theta_\sigma} e^{i\frac{\pi}{L}x\Delta N_\sigma} e^{i\phi_\sigma(x)} \ ,$$

where θ_σ is conjugate to ΔN_σ, then exactly at $K_\sigma = 1/2$ the spin backscattering term (23) assumes a quadratic form in these operators. The Hamiltonian describing the spin excitations becomes

$$H_\sigma = v_\sigma \int_{-L}^{L} dx \Psi^\dagger_\sigma(x)(-i\partial_x)\Psi_\sigma(x)$$

$$-i\Delta\int_{-L}^{L} dx\, \mathrm{sgn}(x)\Psi^\dagger_\sigma(x)\Psi_\sigma(-x) \ , \qquad \text{(D1)}$$

where

$$\Delta = \frac{g_{bs}}{2\pi\alpha} \ . \qquad \text{(D2)}$$

The $\mathrm{sgn}(x)$ factor in (D1) stems from the phase factor $f(2x)$ in the $\alpha \to 0$ limit, which is necessary to preserve the particle-hole symmetry of the model,

$$\Psi_{sR}(x) \to \Psi^\dagger_{\bar{s}R}(-x) \ ,$$

or equivalently

$$\phi_\sigma(x) \to -\phi_\sigma(-x) \ .$$

This symmetry implies that the spectrum should be symmetric around zero energy.

Being quadratic in the fermion fields, the Hamiltonian (D1) can be brought into diagonal form

$$H_\sigma = \sum_\epsilon \epsilon C^\dagger_\epsilon C_\epsilon \ ,$$

where the new Fermi operators C_ϵ are related to the old ones by the canonical transformation,

$$C^\dagger_\epsilon = \int dx \chi_\epsilon(x)\Psi^\dagger_\sigma(x) \ .$$

The wave functions $\chi_\epsilon(x)$ satisfy the following nonlocal Schrödinger equation:

$$\epsilon\chi_\epsilon(x) = -iv_\sigma\partial_x\chi_\epsilon(x) - i\Delta\,\mathrm{sgn}(x)\chi_\epsilon(-x) \ . \qquad \text{(D3)}$$

Defining the functions $\chi^{(+)}_\epsilon(x) = \chi_\epsilon(x)$ and $\chi^{(-)}_\epsilon(x) = \chi_\epsilon(-x)$ (for $x > 0$), we can conveniently rewrite (D3) as the system of differential equations:

$$\begin{aligned} \epsilon\chi^{(+)}_\epsilon(x) &= -iv_\sigma\partial_x\chi^{(+)}_\epsilon(x) - i\Delta\chi^{(-)}_\epsilon(x) \ , \\ \epsilon\chi^{(-)}_\epsilon(x) &= +iv_\sigma\partial_x\chi^{(-)}_\epsilon(x) + i\Delta\chi^{(+)}_\epsilon(x) \ . \end{aligned} \qquad \text{(D4)}$$

Those functions obey the following boundary conditions:

$$\chi^{(+)}_\epsilon(0) = \chi^{(-)}_\epsilon(0) \ , \qquad \text{(D5)}$$

$$\chi^{(+)}_\epsilon(L) = \chi^{(-)}_\epsilon(L) \ , \qquad \text{(D6)}$$

where the latter derives from (10).

Each particular solution of (D4) has the form $\exp(\pm ipx)$. The dispersion relation turns out to be

$$\epsilon^2 = (v_\sigma p)^2 + \Delta^2 \ , \qquad \text{(D7)}$$

and the allowed values of p derive from imposing the boundary conditions (D5,D6), which lead to

$$\sin(pL)(i\Delta - \epsilon - v_\sigma p)(i\Delta - \epsilon + v_\sigma p) = 0 \ . \qquad \text{(D8)}$$

The solutions are $p = \pi n/L$ with n a positive integer, which correspond to energies $|\epsilon| > \Delta$, and $p = \pm i\Delta/v_\sigma$, with energy $\epsilon = 0$. Therefore, similarly to what happens in the case of an infinite system, the spin backscattering term opens a gap Δ in the continuum spectrum. The unusual feature is the existence of the zero energy states, which are bound states localized at the boundaries. So, in the $L \to \infty$ limit (semi–infinite system), the wave function of the bound state localized at $x = 0$ takes the form

$$\chi_0(x) = \sqrt{\frac{\Delta}{v_\sigma}} e^{-\Delta|x|/v_\sigma} \ .$$

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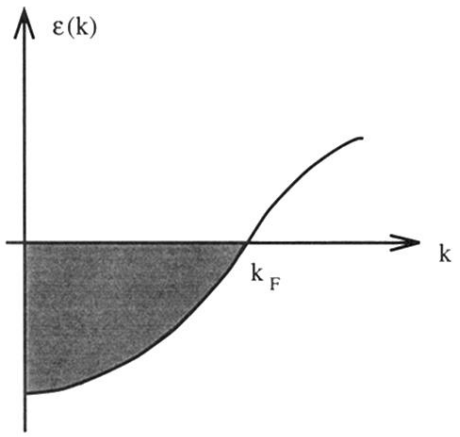

FIG. 1. Single-particle spectrum: for the case of open boundaries the Fermi surface consists of the single point k_F.