Boundary Green's function for spin-incoherent interacting electrons in one dimension

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The spin-incoherent regime of one-dimensional electrons has recently been explored using the Bethe ansatz and a bosonized path integral approach, revealing that the spin incoherence dramatically influences the correlations of charge excitations. We here introduce a bosonization scheme for strongly interacting electrons, allowing us to generalize the description to account for the presence of an open boundary. By calculating the single-electron Green's function we find that the charge sector power-law scaling is highly sensitive to the boundary. Our result allows for a detailed description of the crossover between boundary and bulk regimes. We predict that scanning tunneling microscopy on a spin-incoherent system will pick up oscillations in the differential tunneling conductance as a function of the applied voltage V at "intermediate" distances x from a real or a dynamically generated boundary. The wavelength of the oscillations, $\pi v_c/x$, probes the speed v_c of the charge excitations, and therefore the strength of the electron-electron interaction.

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I. INTRODUCTION

The spin-incoherent regime of one-dimensional strongly interacting, very low-density electrons has recently attracted a lot of interest. For zero temperature the kinetic energy of an electron can be estimated by the Fermi energy $E_F = (\pi \hbar n)^2 / 8m$. For low densities, $n \ll a_B^{-1}$, this energy is small compared to the Coulomb potential energy e^2n/ϵ (with ϵ being the dielectric constant and $a_B = \epsilon \hbar^2 / me^2$ the effective Bohr radius of the material). In the limit of low densities the system turns into a Wigner crystal, which—in a classical picture—can be viewed as a system of electrons placed equidistantly so as to minimize the potential energy. Quantum fluctuations induce an exponentially small antiferromagnetic spin exchange J > 0 between the electrons. In the case when J is the smallest energy scale, $J \ll T \ll E_F$, the spin exchange can no longer support collective spin excitations, and the system is driven to a spin-incoherent regime. The physics of the spin-incoherent regime has been addressed using the Bethe ansatz^{3,4} and a bosonized path integral approach.⁵ Surprisingly, it was found that the spin incoherence dramatically influences the correlations of charge excitations, leading to a power-law decay in the charge sector with an interactiondependent nonunitary exponent.

In this paper we generalize the description in Ref. 5 to account for the presence of an open boundary. For this purpose we introduce a bosonization scheme, valid for strongly interacting electrons, and presented in Sec. II. In Sec. III we then derive the single-electron Green's function in the presence of an open boundary condition. Scanning tunneling microscopy (STM) as a possible experimental probe of the spin-incoherent regime is discussed in Sec. IV. The last section contains a brief summary of our results.

II. BOSONIZATION IN THE STRONG COUPLING REGIME

We here introduce a bosonization scheme for strongly interacting electrons, for which the applicability of an ordinary PACS number(s): 71.10.Pm, 71.27.+a, 73.21.-b

bosonization⁶ becomes questionable. In the strong-coupling regime, the electrons are localized at the lattice sites of the Wigner crystal, and the usual procedure of linearizing the spectrum around the Fermi points $\pm k_F$ and then expanding the electron fields in left and right movers is no longer justified. In what follows we show that one can nonetheless perform an "effective" bosonization, valid for low energies and large distances.

To begin with, it can be shown that a bosonic Hamiltonian correctly describes the low-energy properties of a one-dimensional (1D) Wigner crystal. To justify this statement we turn to the classical picture and describe a 1D Wigner crystal as a system of electrons vibrating around their equilibrium positions. This is very similar to the classical description of phonons as lattice vibrations. For low energies (long-wavelength limit) the vibrations can be described by elasticity theory, with the energy of the system expressed by the Hamiltonian

$$H = \int dx \left[\frac{p^2}{2mn} + \frac{1}{2}mns^2(\partial_x u)^2 \right]. \tag{1}$$

Here u(x) is the displacement of the medium and p(x) is the momentum density. Density fluctuations are given by $\delta n = -n\partial_x u$, and s plays the role of the speed of density waves.

The classical Hamiltonian in Eq. (1) can be straightforwardly quantized by imposing a canonical commutation relation between u(x) and p(x),

$$[u(x), p(x')] = i\delta(x - x'). \tag{2}$$

The resulting quantum Hamiltonian describes the propagation of density fluctuation in the Wigner crystal, and can be written in terms of a bosonic field $\varphi_c(x)$ and its conjugate momentum $\Pi_c(x)$, connected to u(x) and p(x) by

$$u(x) = -\frac{\sqrt{2}}{\sqrt{\pi n}}\varphi_c(x), \quad p(x) = -\frac{\sqrt{\pi n}}{\sqrt{2}}\Pi_c(x). \tag{3}$$

It follows that

$$H = \frac{v_c}{2} \int dx \left[K_c \Pi_c^2 + \frac{1}{K_c} (\partial_x \varphi_c)^2 \right], \tag{4}$$

where

$$v_c = s, \quad K_c = \frac{v_F}{s},\tag{5}$$

with v_c the speed of the propagating charge density fluctuations, and with $v_F = \pi n/2m$ the Fermi velocity for noninteracting spinful electrons.

We have thus managed to write the Hamiltonian for a 1D Wigner crystal in bosonized form although we did not know the bosonization formula which connects electron and boson fields. We next derive such a formula, applying a kind of "reverse engineering" to the bosonic description of the Wigner crystal above. First we observe that in the $J \rightarrow 0$ limit, electrons behave like *spinless* fermionic particles, i.e., only charge degrees of freedom survive and spin degrees of freedom simply define the huge degeneracy of the ground state. We may thus omit the spin index and write

$$\Psi(x) = \psi_{-}(x) + \psi_{+}(x), \tag{6}$$

where $\psi_{-}(x)$ [$\psi_{+}(x)$] is the part of the electron operator which contains negative [positive] momenta. In analogy with ordinary bosonization of spinless fermions⁶ we introduce two chiral boson fields ϕ_{c-} and ϕ_{c+} , connected to φ_c by $\varphi_c = \phi_{c-} + \phi_{c+}$. We can then write an effective bosonization formula, valid for low energies,

$$\psi_{\ell}(x) \approx \frac{1}{\sqrt{2\pi\alpha}} e^{\ell i \tilde{k}_F x} e^{\ell i \sqrt{\lambda} \phi_{c\ell}(x)}, \quad \ell = \pm,$$
(7)

with α a short-distance cutoff, and where \tilde{k}_F and λ are to be determined. Using that the density operator is given by

$$\rho = \Psi^{\dagger}(x)\Psi(x) = n + \sqrt{\frac{2}{\pi}} \partial_x \varphi_c, \tag{8}$$

with the product of electron fields defined by point splitting,⁶ and where n is the average electron density and $(\sqrt{2/\pi})\partial_x \varphi_c$ is a fluctuation term [cf. Eqs. (1) and (3)], we find that

$$\tilde{k}_F = \pi n, \quad \lambda = 8\pi.$$
 (9)

We have here used that the fast oscillating nonchiral terms $\psi_{\pm}^{\dagger}\psi_{\mp}$ contained in $\Psi^{\dagger}\Psi$ effectively average out to zero over large distances, and hence can be neglected in the longwavelength limit. Also note that the doubling of the Fermi momentum in Eq. (9) is in agreement with our description of spinless fermions, since now only a single fermion can occupy a given momentum state. As can be easily verified, the case of noninteracting spinless fermions corresponds to $K_c = 1/2$. It follows that in this bosonization scheme interactions are absorbed in two steps: Local interactions among the spinful electrons are incorporated in a free Hamiltonian for spinless fermions (with $K_c = 1/2$), while long-range interactions renormalize the value of K_c (away from $K_c=1/2$). To see this explicitly, note that for a delta function interaction among the electrons—corresponding to the low-energy, long-wavelength limit of the infinite-U 1D Hubbard model²—the description as noninteracting spinless fermions becomes exact (with $K_c = 1/2$).

To obtain a more conventional parametrization (where a unit value of an effective "charge parameter" K corresponds to the case of noninteracting spinless fermions) we define a bosonic field $\varphi \equiv \sqrt{2}\varphi_c$ with conjugate momentum $\Pi \equiv \Pi_c/\sqrt{2}$. Then the bosonization formula in Eq. (7) and the Hamiltonian in Eq. (4) take the forms

$$\psi_{\ell}(x) \approx \frac{1}{\sqrt{2\pi\alpha}} e^{\ell i \tilde{k}_F x} e^{\ell i \sqrt{4\pi}\phi_{\ell}(x)}, \quad \ell = \pm$$
 (10)

and

$$H = \frac{v_c}{2} \int dx \left[K\Pi^2 + \frac{1}{K} (\partial_x \varphi)^2 \right], \tag{11}$$

respectively, with $K \equiv 2K_c = 2v_F/s = \tilde{v}_F/s$ (in agreement with the doubling of the Fermi momentum \tilde{k}_F).

III. BOUNDARY GREEN'S FUNCTION

The bosonization procedure presented in the previous section can easily be adapted to the case when a boundary is present. Imposing an open boundary condition (OBC) at the end, x=0, of a semi-infinite system with $x \ge 0$, we have that

$$\Psi(0) = \psi_{-}(0) + \psi_{+}(0) = 0. \tag{12}$$

Analytically continuing the chiral fermion operators to negative coordinates,

$$\psi_{+}(x) = -\psi_{-}(-x), \tag{13}$$

and then following the standard procedure for an OBC⁸—using our Eq. (10)—we obtain a bosonization formula for strongly interacting spin-incoherent electrons with an OBC,

$$\psi_{-}(x) \approx \frac{1}{\sqrt{2\pi\alpha}} e^{-i\tilde{k}_F x} e^{-i\sqrt{4\pi}\left[\cosh(\vartheta)\tilde{\phi}_{-}(x) - \sinh(\vartheta)\tilde{\phi}_{-}(-x)\right]}. \tag{14}$$

Here $e^{2\vartheta} = K$, with $\widetilde{\phi}_- = \cosh(\vartheta)\phi_- - \sinh(\vartheta)\phi_+$ governed by the free chiral boson Hamiltonian

$$H = \frac{v_c}{2} \int dx [\partial_x \widetilde{\phi}_{-}(x)]^2.$$
 (15)

To calculate the zero-temperature single-electron Green's function in the presence of the OBC we follow the path integral approach introduced in Ref. 5. The averaging over spin introduces a factor $2^{-N(x,x',\tau)}$ in the expression for the Green's function, where $N(x,x',\tau)$ samples the number of electrons, or equivalently, the number of noncrossing world lines in the interval x-x'. In the spin-incoherent regime, here realized by first taking $J \rightarrow 0$ and then $T \rightarrow 0$, the spin configurations all carry the same weight, and the probability that the world lines in the interval x-x' all have the same spin (as required for a nonzero contribution to the low-energy Green's function) becomes equal to $2^{-N(x,x',\tau)}$. Given this, the calculation of the Green's function $G(x,x',\tau)$ translates into

the calculation of four correlators for spinless time-boosted fermions, with the spin averaging factor $2^{-N(x,x',\tau)}$ properly inserted.⁹

$$G(x,x',\tau) = \langle 2^{-N(x,x',\tau)} \Psi(x,\tau) \Psi^{\dagger}(x',0) \rangle$$

$$= \langle 2^{-N(x,x',\tau)} \psi_{-}(x,\tau) \psi_{-}^{\dagger}(x',0) \rangle$$

$$+ \langle 2^{-N(x,x',\tau)} \psi_{+}(x,\tau) \psi_{+}^{\dagger}(x',0) \rangle$$

$$+ \langle 2^{-N(x,x',\tau)} \psi_{-}(x,\tau) \psi_{+}^{\dagger}(x',0) \rangle$$

$$+ \langle 2^{-N(x,x',\tau)} \psi_{+}(x,\tau) \psi_{-}^{\dagger}(x',0) \rangle. \tag{16}$$

The operator $N(x, x', \tau)$ can be expressed as

$$N(x, x', \tau) = n|x - x'| + \frac{1}{\sqrt{\pi}} [\varphi(x, \tau) - \varphi(x', 0)], \quad (17)$$

where *n* is the average electron (or world line) density, and with $(1/\sqrt{\pi})[\varphi(x,\tau)-\varphi(x',0)]=[\cosh(\vartheta)+\sinh(\vartheta)][\tilde{\phi}_{-}(x,\tau)-\tilde{\phi}_{-}(-x,\tau)-\tilde{\phi}_{-}(x',0)+\tilde{\phi}_{-}(-x',0)/\sqrt{\pi}]$ the fluctuation term.

The correlators in Eq. (16) are straightforwardly calculated by first using Eq. (13) to replace all occurrences of right-moving fermion fields by left movers, and then applying the bosonization formula (14). Introducing relative and center-of-mass coordinates, r=x-x' and R=(x+x')/2, respectively, we obtain for the G_{--} piece of the Green's function

$$G_{--}(x,x',\tau) \equiv \langle 2^{-N(x,x',\tau)} \psi_{-}(x,\tau) \psi_{-}^{\dagger}(x',0) \rangle$$

$$= \frac{1}{2\pi\alpha} e^{-(\ln 2/\pi)\tilde{k}_{F}|r|} e^{-i\tilde{k}_{F}r} e^{i\zeta_{-}} \frac{1}{(\alpha \operatorname{sgn} \tau + v_{c}\tau + ir)} \frac{1}{[(\alpha \operatorname{sgn} \tau + v_{c}\tau)^{2} + r^{2}]^{-2\Delta_{1} + 2\Delta_{2}}}$$

$$\times \left(\frac{\sqrt{[\alpha^{2} + (2R + r)^{2}][\alpha^{2} + (2R - r)^{2}]}}{(\alpha \operatorname{sgn} \tau + v_{c}\tau)^{2} + 4R^{2}} \right)^{2\Delta_{1} + 2\Delta_{3}}, \tag{18}$$

where

$$\zeta_{--} = \frac{\ln 2}{4\pi} K \left\{ \ln \frac{\left[\alpha^2 + (2R+r)^2\right] \left[\alpha^2 + (2R-r)^2\right]}{\left[(\alpha \operatorname{sgn} \tau + v_c \tau)^2 + 4R^2\right]^2} + 2 \ln \frac{(\alpha \operatorname{sgn} \tau + v_c \tau)^2 + r^2}{\alpha^2} \right\} + \frac{\ln 2}{4\pi} \left\{ \ln \frac{\left[\alpha - i(r+2R)\right] \left[\alpha - i(r-2R)\right]}{\left[\alpha + i(r+2R)\right] \left[\alpha + i(r-2R)\right]} + 2 \ln \frac{\alpha \operatorname{sgn} \tau + v_c \tau + ir}{\alpha \operatorname{sgn} \tau + v_c \tau - ir} \right\},$$
(19)

and with the exponents given by $\Delta_1 = \frac{K}{8}(\frac{\ln 2}{\pi})^2$, $\Delta_2 = \frac{1}{8}(\frac{1}{K} + K - 2)$, $\Delta_3 = \frac{1}{8}(\frac{1}{K} - K)$. The G_{-+} part of the Green's function reads

$$G_{-+}(x,x',\tau) \equiv \langle 2^{-N(x,x',\tau)} \psi_{-}(x,\tau) \psi_{+}^{\dagger}(x',0) \rangle$$

$$= \frac{1}{2\pi\alpha} e^{-(\ln 2/\pi)\tilde{k}_{F}|r|} e^{-i2\tilde{k}_{F}R} e^{i\zeta_{-+}} \frac{1}{(\alpha \operatorname{sgn} \tau + v_{c}\tau + 2iR)} \frac{1}{[(\alpha \operatorname{sgn} \tau + v_{c}\tau)^{2} + 4R^{2}]^{2\Delta_{1} + 2\Delta_{2}}}$$

$$\times \{ \sqrt{[\alpha^{2} + (2R+r)^{2}][\alpha^{2} + (2R-r)^{2}]} [(\alpha \operatorname{sgn} \tau + v_{c}\tau)^{2} + r^{2}] \}^{2\Delta_{1}} \left\{ \frac{\sqrt{[\alpha^{2} + (2R+r)^{2}][\alpha^{2} + (2R-r)^{2}]}}{(\alpha \operatorname{sgn} \tau + v_{c}\tau)^{2} + r^{2}} \right\}^{2\Delta_{3}},$$
(20)

where

$$\zeta_{-+} = \frac{\ln 2}{4\pi} K \ln \frac{\alpha^2 + (2R+r)^2}{\alpha^2 + (2R-r)^2}$$

$$+ \frac{\ln 2}{4\pi} \left\{ \ln \frac{\left[\alpha - i(r+2R)\right] \left[\alpha - i(r-2R)\right]}{\left[\alpha + i(r+2R)\right] \left[\alpha + i(r-2R)\right]} \right\}$$

$$+ 2 \ln \frac{\alpha \operatorname{sgn} \tau + v_c \tau + ir}{\alpha \operatorname{sgn} \tau + v_c \tau - ir} \right\}.$$
(21)

The expressions for the G_{++} and G_{+-} pieces of the Green's

function are immediately obtained from Eqs. (18)–(20) by using that

$$G_{++}(x,x',\tau) = G_{--}^*(x,x',\tau),$$

$$G_{+-}(x,x',\tau) = G_{-+}^*(x,x',\tau).$$
(22)

Having derived the full expression for the boundary Green's function we can study boundary and bulk regimes by taking the proper limits. The bulk regime is defined by $R \gg v_c \tau, r$. For the chiral G_{--} piece we obtain

$$G_{--}(x,x',\tau) = \langle 2^{-N(x,x',\tau)} \psi_{-}(x,\tau) \psi_{-}^{\dagger}(x',0) \rangle$$

$$= \frac{1}{2\pi\alpha} e^{-(\ln 2/\pi)\tilde{k}_F|r|} e^{-i\tilde{k}_F r} e^{i\zeta_{--}} \frac{1}{(\alpha \operatorname{sgn} \tau + v_c \tau + ir)}$$

$$\times \frac{1}{[(\alpha \operatorname{sgn} \tau + v_c \tau)^2 + r^2]^{-2\Delta_1 + 2\Delta_2}},$$
(23)

in agreement with the result for the bulk Green's function derived in Refs. 3 and 5. In contrast to the chiral part G_{-} (G_{++}) of the Green's function, G_{-+} (G_{+-}) decays with a power law and vanishes in the bulk limit, as it must

$$G_{-+}(x, x', \tau) \sim \frac{1}{R^K}.$$
 (24)

For the boundary case, defined by $v_c \tau \gg r, R$, the chiral and nonchiral parts of the Green's function show the same behavior, with the asymptotic scaling

$$G_{--}(x,x',\tau) \sim G_{-+}(x,x',\tau) \sim \frac{1}{\tau^{1/K}}.$$
 (25)

This agrees with the result in Ref. 10 (see also Ref. 11). Importantly, our general result allows for a study of the crossover between boundary and bulk regimes.

IV. STM RESPONSE IN THE SPIN-INCOHERENT REGIME

In this section we discuss a possible experimental probe of the spin-incoherent regime, using scanning tunneling microscopy (STM). Assuming that the STM tip couples only to the conduction electrons, the differential tunneling conductance dI(V,x)/dV is directly proportional to the local electron tunneling density of states (LDOS) $\rho(V,x)$, where V is the applied voltage, and x is the position of the tip as measured from the boundary. The boundary may here be one of the end points of a quantum wire or a metallic nanotube, or generated dynamically by an impurity in the system (an antidot, or a deep "core level" hole created by an x-ray photon 10). The LDOS is related to the boundary Green's function in Eq. (16) by

$$\rho(x,\omega) \approx -\frac{1}{\pi} \operatorname{Im} G_R(x,\omega),$$
(26)

where the retarded Green's function $G_R(x,\omega)$ is obtained from the Fourier transform $G(x,\omega_n)$ of $G(x,x,\tau)$ in Eq. (16) by analytically continuing $i\omega_n \to \omega + i\eta_+$. The \approx sign in Eq. (26) is a reminder that the expression for the Green's function in Eq. (16) as derived above becomes exact only in the long-wavelength limit [cf. the text after Eq. (9)]. The LDOS has a uniform rapidly oscillating part originating from the chiral (nonchiral) Friedel-type terms $G_{--/++}(x,x,\tau)$ $[G_{-+/+-}(x,x,\tau)]$ in $G(x,x,\tau)$,

$$\rho(x,\omega) = \rho_{\text{uni}}(x,\omega) + \cos(2\tilde{k}_{F}x)\rho_{\text{osc}}(x,\omega). \tag{27}$$

Figure 1 shows ρ_{uni} for three choices of distance from the boundary, obtained from Eq. (16) by numerically computing the integrals which define the analytically continued Fourier

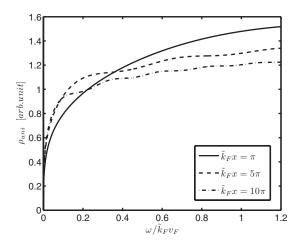


FIG. 1. Uniform part of the LDOS, $\rho_{\rm uni}$, as a function of energy ω for different boundary-to-tip distances x. Oscillations for intermediate distances are a result of interference of incoming and reflected charge modes at the boundary.

transforms. The most interesting feature is the oscillation pattern seen for "intermediate" distances where $\omega x \sim v_c$ (i.e., the crossover regime between boundary and bulk behavior). This pattern is due to the interference of incoming and reflected charge modes at the boundary. The oscillations, of wavelength $\pi v_c/x$, give immediate information about the speed v_c of the charge modes, and therefore about the strength of the electron-electron interaction. This unique signal of the spin-incoherent phase should be readily obtained in STM experiments as an oscillation pattern in the differential tunneling conductance as a function of the applied voltage V (which fixes the frequency for which the LDOS is probed). Let us here point out that the oscillations are present at any distance from the boundary, but that in the boundary [bulk] regime, defined by $\omega x \ll v_c [\omega x \gg v_c]$, the wavelength may become too long [short] to be possible to resolve experimentally. (Cf. Fig. 1 where the wavelength for the oscillation for the case $k_F x = \pi$ is roughly twice larger than the displayed frequency interval.) It is important to stress that the Friedel terms the last two terms in Eq. (16) do not change the result qualitatively. This is in contrast to an ordinary Luttinger liquid where the interference of charge and spin modes with different speeds produce an oscillation pattern with very different properties.¹⁴ In the case of a spinincoherent system there is only one propagating charge mode with a single speed v_c , and the oscillation pattern of $\rho_{\rm osc}$ will be the same as that of $\rho_{\rm uni}$.

Let us conclude this section by mentioning that other experimental probes of spin incoherence have been suggested in the literature, including momentum resolved tunneling experiments on cleaved-edge overgrowth quantum wires, ^{15,16} and quantum interference experiments on specially designed devices. ¹¹ It would be very interesting to explore how the characteristic crossover behavior of the single-electron Green's function identified above may influence these proposed experiments.

V. CONCLUSIONS

We have calculated the exact single-electron boundary Green's function for one-dimensional spin-incoherent electrons in the low-energy, long-wavelength limit, using a bosonization scheme valid in the strong-coupling regime. The Green's function thus obtained correctly reproduces known results in the bulk and extreme boundary regimes. As revealed by the expressions in Eqs. (18) and (21), the charge sector power-law scaling of the Green's function is highly sensitive to the presence of the boundary also at intermediate distances away from it, where the center-of-mass coordinate $R \sim \mathcal{O}(v_c \tau)$. This feature will strongly influence the local tunneling density of states, and may be probed experimentally

by scanning tunneling microscopy of one-dimensional conductors of spin-incoherent electrons.

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tomatically taken into account in our spinless fermion formulation. In Ref. 5, averages are carried out for spinless bosons, requiring the permutation factor to be explicitly inserted [cf. the discussion after Eq. 41 in Ref. 15].

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