

## Low-temperature conductivity of quasi-one-dimensional conductors: Luttinger liquid stabilized by impurities

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(Received 6 May 2005; published 21 September 2005)

A new non-Fermi-liquid state of quasi-one-dimensional conductors is suggested in which electronic system exists in a form of collection of bounded Luttinger liquids stabilized by impurities. This state is shown to be stable towards interchain electron hopping at low temperatures. Electronic spectrum of the system contains zero modes and collective excitations of the bounded Luttinger liquids in the segments between impurities. Zero modes give rise to randomly distributed localized electronic levels, and long-range interaction generates the Coulomb gap in the density of states at the Fermi energy. Mechanism of conductivity at low temperatures is phonon-assisted hopping via zero-mode states. At higher voltages the excitations of Luttinger liquid are involved in electron transport, and conductivity obeys power-law dependence on voltage. The results provide a qualitative explanation for recent experimental data for NbSe<sub>3</sub> and TaS<sub>3</sub> crystals.

DOI: [10.1103/PhysRevB.72.125118](https://doi.org/10.1103/PhysRevB.72.125118)

PACS number(s): 71.10.Pm, 71.10.Hf, 71.27.+a, 71.45.Lr

### I. INTRODUCTION

The concept of single-electron quasiparticles is one of the central ideas of solid state physics. Indeed, systems of interacting electrons in metals and semiconductors are well described by Landau's Fermi-liquid picture in which interaction modifies free electrons making them quasiparticles that in many respects behave similar to noninteracting electrons. Basic electronic properties of many solids, including phase transitions into symmetry-breaking states such as superconducting or charge-density wave (CDW) states, are well described within this concept. Therefore, possibility to observe non-Fermi-liquid behavior in conducting materials attracts much interest. The concept of Luttinger liquid is an alternative to the Fermi liquid elaborated for one-dimensional (1D) electronic systems. It was found that in 1D electronic systems the Fermi-liquid picture breaks down even in case of arbitrarily weak interaction. Single-electron quasiparticles cannot exist in 1D metals, and electrons form the Luttinger liquid in which the only low energy excitations turn out to be charge and spin collective modes with the soundlike spectrum. Dynamical independence of these modes gives rise to a spin-charge separation in 1D systems. Furthermore, correlation functions at large distances and times decay as a power law with interaction dependent exponents (for a review see Refs. 1–3).

One may expect to observe formation of Luttinger liquid in quasi-1D conductors, i.e., highly anisotropic 3D conductors with chainlike structure. However, according to present theoretical point of view, the formation of Luttinger liquid in quasi-1D conductors at low enough temperatures is problematic because of the instability towards 3D behavior in the presence of arbitrarily small interchain hopping.<sup>4–9</sup> So interchain hopping induces a crossover to 3D behavior at low energies, while Luttinger-liquid behavior can survive only at high enough energy scale where it is not affected by 3D coupling. In contrast to interchain hopping, the Coulomb interaction between electrons on different chains does not destroy the Luttinger-liquid state, it merely modifies the electronic spectrum of the Luttinger liquid.<sup>10–13</sup>

Numerous experimental studies of both organic and inorganic quasi-1D conductors at low temperatures demonstrate, commonly, Fermi-liquid metallic behavior and/or transitions to broken-symmetry states, which are described in terms of Fermi-liquid ideas (for a review see Refs. 14 and 15). For instance, the most studied inorganic quasi-1D metals [e.g., blue bronze K<sub>0.3</sub>MoO<sub>3</sub>, TaS<sub>3</sub>, (TaSe<sub>4</sub>)<sub>2</sub>I, etc.] undergo the Peierls transition from metallic to a semiconducting CDW state, or to semimetallic CDW state such as NbSe<sub>3</sub>. Typically, this transitions occur in the temperature range 50–250 K. Some quasi-1D materials, e.g., TaSe<sub>3</sub> do not undergo the Peierls transition and remain in the normal metallic state at low temperatures as well.

However, a transition from room-temperature metallic behavior to nonmetallic one accompanied by disappearance of the CDW state at temperatures below 50–100 K was detected in recent experimental studies of temperature and field dependence of conductivity of TaS<sub>3</sub> and NbSe<sub>3</sub> nanoscale-sized crystals.<sup>16–18</sup> The low-temperature nonmetallic state was characterized by power-law dependencies of conductivity on voltage and temperature similar to that expected in Luttinger liquid, or by more strong temperature dependence corresponding to the variable-range hopping.<sup>18</sup> Resembling dependencies of conductivity were also reported in focused-ion beam processed or doped relatively thick NbSe<sub>3</sub> crystals.<sup>19</sup> Transition to nonmetallic conductivity at low temperatures was observed earlier in fragmented into small pieces and then sintered NbSe<sub>3</sub> crystals.<sup>14</sup> Hopping conductivity was also found out in heavily doped by iron bulk NbSe<sub>3</sub> crystals<sup>20</sup> in dirty quasi-1D conductors KCP and organic TCNQ-based metals,<sup>21</sup> while pure materials are known to undergo the Peierls transition to the CDW state.

In order to account for such behavior a possibility of stabilization of the Luttinger state by defects in quasi-1D metals was put forward recently in the letter of one of the authors.<sup>22</sup> Such a possibility is based upon finding made in Refs. 23–25 that a local impurity potential in Luttinger liquid acts, at low energies, as effectively infinite barrier. This leads to a discrete spectrum of collective charge and spin density fluctua-

tions, so that the electronic system can be considered as a collection of bounded Luttinger liquids. In this case, at temperatures below the minimum excitation energy of the collective modes, weak interchain hopping can be considered as small perturbation, and, therefore, hopping does not destroy the Luttinger-liquid state.

However, in order to make comparison with the experimental data and to find further evidences that the low-temperature nonmetallic state observed in quasi-1D conductors can, actually, be interpreted as a collection of impurity-induced bounded Luttinger liquids, calculation of conductivity in the latter state is needed. Such calculations are the main goal of this paper. We calculate conductivity in a collection of weakly coupled metallic chains with defects in the limit of low temperatures, considering both the case of the contact interaction used in the standard Tomonaga-Luttinger model<sup>1,3</sup> and the case of more physical long-ranged Coulomb potential.

Note that we consider the case of conductivity limited by impurities, i.e., we study the bulk effect, so we do not consider contribution due to contacts in this work. In the opposite limit of a wire without defects the contacts are known to strongly influence the transport properties (see, e.g., Refs. 26–28).

The paper is organized as follows. In Sec. II we present main equations and formulate the problem in terms of bosonization technique generalized to the case of long-range Coulomb interaction between electrons in a multichain problem in presence of impurities. In Sec. III we study electronic structure of quasi-1D conductors. We consider, first, interacting electrons neglecting interchain hopping and find the solution for the phase operators in the limit of strong impurity potential ignoring, at the first step, the Coulomb interaction of electrons at different chains. Modifications induced by the long-range nature of the Coulomb interaction are discussed in the next subsection. In the last subsection we show that at low temperatures the interchain hopping can be considered as small perturbation, provided the hopping matrix element is small enough. Section IV is devoted to transport properties of the system. We show that in the limit of low voltages conductivity is described in terms of variable-range hopping, while at large voltages it turns into conductivity described by a power-law dependence on voltage. And, finally, in Sec. V we discuss relation of the theoretical results to experimental data, and make conclusions. In this paper we use units with Planck and Boltzmann constants equal to unity,  $\hbar=1$ ,  $k_B=1$ .

## II. GENERAL EQUATIONS

First of all we start with the Tomonaga-Luttinger model ignoring interchain hopping integral  $t_{\perp}$  in order to formulate the problem in the zero approximation in  $t_{\perp}$ . Electronic operators for right ( $r=+1$ ) and left ( $r=-1$ ) moving electrons with spin  $s$  on chain number  $\mathbf{n}$  are given in terms of phase fields as (see Refs. 1, 3, and 11)

$$\psi_{\mathbf{n},s}(r,x) = \lim_{\alpha \rightarrow 0} \frac{e^{irk_F x}}{\sqrt{2\pi\alpha}} \eta_{\mathbf{n},r,s} e^{-iA_{\mathbf{n},r}(x,\mathbf{n})},$$

$$A_{\mathbf{n},r} = \frac{1}{\sqrt{2}} \{ \Theta_{\rho}(x,\mathbf{n}) - r\Phi_{\rho}(x,\mathbf{n}) + s[\Theta_{\sigma}(x,\mathbf{n}) - r\Phi_{\sigma}(x,\mathbf{n})] \}. \quad (1)$$

Phase fields  $\Phi_{\nu}(x,\mathbf{n})$  are related to charge ( $\nu=\rho$ ) and spin ( $\nu=\sigma$ ) densities, while fields  $\Theta_{\nu}(x)$  are related to the momentum operators  $\Pi_{\nu}=(1/\pi)\partial_x\Theta_{\nu}$  canonically conjugate to  $\Phi_{\nu}$ . Further,  $\eta_{r,s}$  are Majorana (“real”) Fermionic operators that assure proper anticommutation relations between electronic operators with different spin  $s$  and chirality  $r$ , and the cut off length  $\alpha \sim 1/k_F$  is assumed to be of the order of interatomic distance.

The Hamiltonian of the system includes three terms, the Hamiltonian of the interacting electrons, the impurity scattering term, and the interchain hopping Hamiltonian. The first term containing kinetic and potential energies of the electrons is described by the Tomonaga-Luttinger Hamiltonian generalized for the multichain case with long-range interaction that couples electrons on different chains.<sup>1,3,11</sup> This Hamiltonian ignores the backscattering terms in the electronic coupling, i.e., it neglects components of interaction potential with  $q_{\parallel} \approx 2k_F$ . In the bozonized form the Hamiltonian reads

$$H_0 = \frac{\pi v_F d^2}{2} \sum_{\nu=\rho,\sigma} \int \frac{d\mathbf{q}_{\perp} d q_{\parallel}}{(2\pi)^3} \left\{ \Pi_{\nu}^2 + \frac{1}{\pi^2 K_{\nu}^2} q_{\parallel}^2 \Phi_{\nu}^2 \right\}, \quad (2)$$

where  $d^2$  is the area per single chain, and integration over  $\mathbf{q}_{\perp}$  is taken within the first Brillouin zone

$$K_{\nu}(\mathbf{q}_{\perp}, q_{\parallel}) = \left( 1 + \frac{2g_{\nu}}{\pi v_F} \right)^{-1/2}, \quad (3)$$

$K_{\nu}$  is the standard Luttinger-liquid parameter describing the strength of the interaction.  $K_{\nu}$  determines velocities of the charge ( $\nu=\rho$ ) and spin ( $\nu=\sigma$ ) modes,  $v_{\nu}=v_F/K_{\nu}$ . We study the case of spin-independent interaction, therefore, in our case, the coupling constant for spin channel is equal to zero,  $g_{\sigma}=0$ , and  $K_{\sigma}=1$ . For charge channel  $g_{\rho}(\mathbf{q})$  coincides with the matrix element measuring the strength of the forward scattering due to interaction between electrons on the same or on different branches of the electronic spectrum. The exact form of  $g_{\rho}(\mathbf{q})$  depends on crystalline and electronic structure of a crystal, but in the long-wavelength limit  $qd \ll 1$ , one can describe interaction by the standard Fourier transform of the Coulomb interaction potential:

$$g_{\rho} = \frac{4\pi e^2}{d^2(q_{\perp}^2 + q_{\parallel}^2)}, \quad v_{\rho}^2 = v_F^2 + \frac{\omega_{pl}^2}{q_{\perp}^2 + q_{\parallel}^2}, \quad \omega_{\rho}^2 = q_{\parallel}^2 v_{\rho}^2, \quad (4)$$

where  $\omega_{pl}$  is the plasma frequency and  $\omega_{\rho}$  is the frequency of the charge mode.

In the coordinate representation

$$K_{\rho}^{-2}(x,\mathbf{n}) = \delta_{\mathbf{n}0} \delta(x) + \frac{2e^2}{\pi v_F \sqrt{x^2 + n^2 d^2}}, \quad (5)$$

where the last term is induced by the Coulomb interaction. Its contribution to the Hamiltonian (2) in the coordinate representation reads

$$\sum_{\nu=\rho,\sigma} \sum_{\mathbf{n},\mathbf{n}'} \int dx dx' \times \left\{ \partial_x \Phi_\nu(x, \mathbf{n}) \frac{e^2}{\pi^2 \sqrt{(x-x')^2 + (\mathbf{n}-\mathbf{n}')^2 d^2}} \times \partial_{x'} \Phi_\nu(x', \mathbf{n}') \right\}. \quad (6)$$

Since the operator of the particle density is given by expression  $\rho = -(\sqrt{2}/\pi) \partial_x \Phi(x)$ , this term has rather transparent physical meaning.

The second part of the total Hamiltonian is  $2k_F$  impurity backscattering term<sup>1-3</sup>

$$H_{\text{imp}} = - \sum_{\mathbf{n}} \int dx \sum_i \frac{V(x-x_i)}{\pi\alpha} \cos(\sqrt{2}\Phi_\rho + 2k_F x) \times \cos[\sqrt{2}\Phi_\sigma(x)], \quad (7)$$

where  $k_F$  is the Fermi wave number that is assumed to be the same for all conducting chain,  $V(x)$  is potential of impurity centered in position  $i$ . In calculations below we assume  $V(x) \approx V_0 \lambda \delta(x)$ , where  $V_0$  and  $\lambda \sim \alpha$  are amplitude and radius of the scattering potential, respectively.

When interchain electron hopping is ignored, equation of motion for Heisenberg phase operators  $\Phi_\rho$  and  $\Theta_\rho$  can be obtained in standard way from the Hamiltonian  $H_0 + H_{\text{imp}}$  given by Eqs. (2) and (7):

$$\partial_t \Theta_\rho(t, x, \mathbf{n}) = v_F \sum_{\mathbf{n}'} \int dx' K_\nu^{-2}(x-x', \mathbf{n}-\mathbf{n}') \partial_{x'} \Phi_\nu^{(0)}(t, x', \mathbf{n}'), \quad (8)$$

$$\begin{aligned} \partial_t^2 \Phi_\rho(t, x, \mathbf{n}) &= -v_F^2 \sum_{\mathbf{n}'} \int dx' \partial_x K_\rho^{-2}(x-x', \mathbf{n}-\mathbf{n}') \partial_{x'} \Phi_\rho(t, x', \mathbf{n}') \\ &= \frac{\sqrt{2} V_0 d v_F}{\alpha} \sum_i \delta(x-x_i) \sin(\sqrt{2}\Phi_\rho + 2k_F x) \cos(\sqrt{2}\Phi_\sigma). \end{aligned} \quad (9)$$

Kane and Fisher<sup>23</sup> found that the backscattering impurity potential for repulsive potential ( $K_\rho < 1$ ) flows to infinity under scaling. This conclusion was made for the case of single chain and a contact interaction potential.

The results of Refs. 23–25 were generalized by Fabrizio and Gogolin<sup>29</sup> to the case of many impurities. It was shown that the impurity potential can be considered as effectively infinite provided that the mean distance,  $\bar{l}$ , between impurities satisfies the condition

$$\bar{l} \gg \frac{1}{k_F} \left( \frac{D}{V_0} \right)^{2/(1-K_\rho)}, \quad (10)$$

where  $D$  is the bandwidth. We assume that the impurity potential is of the atomic scale,  $V_0 \leq D$ , and the interaction between electrons is not too weak (i.e.,  $K_\rho$  is not too close to 1). Then condition (10) is satisfied for  $\bar{l} \gg 1/k_F$ , so the limit

of strong impurity potential should be a good approximation in a wide range of impurity concentrations.

Similar conclusions can be derived for the multiple-chain system when interaction between electrons on different chains is taken into account. Indeed, calculations in Ref. 23 are based upon dominant contribution to Euclidian action expressed in terms of the value of the field  $\Phi_\rho$  at the impurity site by means of solution of equation of motion in imaginary time. One can act, similarly, in case of multiple-chain system. We express the solution of imaginary-time version of Eq. (9) for Fourier component of  $\Phi_\rho$  in terms of its value at the impurity site  $\Phi_0$  and find

$$\Phi(\omega_n, \mathbf{q}) = \frac{\Phi_0}{\omega_n^2 + q_\parallel^2 v_\rho^2} \left( \int \frac{d^2 \mathbf{q}_\perp d q_\parallel}{(2\pi)^3} \frac{1}{\omega_n^2 + q_\parallel^2 v_\rho^2} \right)^{-1}. \quad (11)$$

In the spirit of renormalization group approach the last factor in Eq. (11) must be calculated in the limit of small energies. Since at small  $\omega$  this integral diverges at small  $q_\parallel$ , we use  $v_\rho^2 = v_F^2 / K_\rho^2$  at  $q_\parallel = 0$ . Then we obtain

$$\int \frac{d^2 \mathbf{q}_\perp d q_\parallel}{(2\pi)^3} \frac{1}{\omega_n^2 + q_\parallel^2 v_\rho^2} = \frac{\bar{K}}{2v_F \omega},$$

where

$$\bar{K} \equiv \langle K_\rho(\mathbf{q}_\perp, q_\parallel = 0) \rangle_{\mathbf{q}_\perp} \equiv \frac{\int d\mathbf{q}_\perp K_\rho(\mathbf{q}_\perp, q_\parallel = 0)}{\int d\mathbf{q}_\perp}.$$

Then using Eq. (11) one finds the action

$$S = \sum_{i\omega_n} \frac{1}{v_F} \langle (\omega_n^2 + q_\parallel^2 v_\rho^2) \Phi^2(\omega_n, \mathbf{q}) \rangle_{\mathbf{q}} = \sum_{i\omega} 2 \frac{1}{\bar{K}} \omega \Phi_0^2(0). \quad (12)$$

This equation is similar to the action in Ref. 23 that was used to derive the renormalization equation for the interaction parameter, the only difference being that in case of long-range interaction action (12) contains the averaged value  $\bar{K}$  of the interaction parameter instead of parameter  $K_\rho$  itself. Thus impurity potential flows to infinity under scaling if  $\bar{K} < 1$ .

So at energies close to the Fermi energy the limit of strong impurity potential can be used. In the main approximation this limit corresponds to boundary conditions for the phase operators at the impurity site

$$\sqrt{2}\Phi_\rho + 2k_F x_i = n\pi, \quad \sqrt{2}\Phi_\sigma = m\pi, \quad (13)$$

where  $n$  and  $m$  are integers. Furthermore,  $n+m$  must be an even integer in order to ensure the minimum value of the impurity Hamiltonian (7). This connection violates independence of spin and charge modes similar to violation of spin-charge separation in bounded Luttinger liquid discussed by Eggert *et al.*<sup>30,31</sup>

The last term to be added to the total Hamiltonian describes next-neighbor interchain hopping in the standard way

$$\begin{aligned}
H_{\perp} &= t_{\perp} \sum_{m,n,r,s} \int dx \psi_{r,s,m}^{\dagger}(x) \psi_{r,s,n}(x) + \text{H.c.} \\
&= \sum_{m,n,r,s} \int dx \frac{it_{\perp} \eta_{r,s,n} \eta_{r,s,m}}{\pi \alpha} [\sin(A_{r,m} - A_{r,n}) \\
&\quad + \sin(A_{r,m} - A_{-r,n} + 2irk_F x)], \tag{14}
\end{aligned}$$

where indices  $n$  and  $m$  denote the chain numbers related to the nearest neighbors.

### III. ELECTRONIC STRUCTURE AT LOW TEMPERATURES

We consider first the case of interacting electrons neglecting interchain hopping and find the solution for the phase operators in the limit of strong impurity potential. According to discussion in the previous section this limit should be a good approximation in a wide range of impurity concentrations. In this approximation the system breaks up into a set of independent segments. At the beginning we ignore the long-range Coulomb interaction and consider the case of contact interaction as in the standard Tomonaga-Luttinger model, and then discuss modifications induced by long-range interaction. At the end of the section we will show that at low temperatures the interchain hopping does not produce qualitative modification of the electronic structure based on the concept of Luttinger liquid.

We begin with solutions for phase operators in case of contact interaction, taking into account that  $\Theta_{\nu}$  and  $\Phi_{\nu}$  must obey the commutation relations<sup>1-3</sup> ensuring anticommutation of electronic operators (1). Using then the analogy of  $H_0$  in Eq. (2) with the Hamiltonian of an elastic string strongly pinned at impurity sites, and taking into account commutation relations, we can write down solutions for the phase operators in the region between impurity positions at  $x=x_i$  and  $x_{i+1}$  as

$$\begin{aligned}
\Phi_{\nu} &= \frac{(\delta\phi_i \delta_{\nu\rho} - \pi \Delta N_{\nu i}) \tilde{x}}{l_i} - \pi \sum_{j < i} \Delta N_{\nu j} \\
&\quad + \sum_{n=1}^{\infty} \sqrt{\frac{K_{\nu}}{n}} (b_{n\nu i} e^{-i\omega_{n\nu} t} + b_{n\nu i}^{\dagger} e^{i\omega_{n\nu} t}) \sin \frac{\pi n \tilde{x}}{l_i}, \tag{15}
\end{aligned}$$

$$\begin{aligned}
\Theta_{\nu} &= \theta_{\nu} + \frac{(\delta\phi_i - \pi \Delta N_{\nu i}) v_{N\nu} t}{l_i} \\
&\quad + i \sum_{n=1}^{\infty} \sqrt{\frac{1}{K_{\nu} n}} (b_{n\nu i} e^{-i\omega_{n\nu} t} - b_{n\nu i}^{\dagger} e^{i\omega_{n\nu} t}) \cos \frac{\pi n \tilde{x}}{l_i}, \tag{16}
\end{aligned}$$

where  $\tilde{x} = x - x_i$ ,  $l_i = x_{i+1} - x_i$ .

Solutions (15) and (16) consist of two parts. The terms with summation present a general solution with zero boundary conditions, they describe excitations. Excitation spectra of the eigenmodes are  $\omega_{n\nu i} = n\pi v_{\nu} / l_i$ .

The first terms present the particular solution with boundary conditions (13), they describe zero modes. In the zero modes

$$\begin{aligned}
v_{N\nu} &\equiv \frac{v_F}{K_{\nu}^2} \equiv \frac{v_{\nu}}{K_{\nu}}, \quad \Delta N_{\rho i} = \frac{(\Delta N_{\uparrow i} + \Delta N_{\downarrow i})}{\sqrt{2}}, \\
\Delta N_{\sigma i} &= \frac{(\Delta N_{\uparrow i} - \Delta N_{\downarrow i})}{\sqrt{2}},
\end{aligned}$$

$\Delta N_{\uparrow i} (\Delta N_{\downarrow i})$  is the number of extra electrons with spin up (down) in the region between impurities number  $i$  and  $(i+1)$ ,  $\sqrt{2} \delta\phi_i$  is equal to the modulo  $2\pi$  residue of  $2k_F l_i$  and finally  $\theta_{\nu i}$  is the phase canonically conjugate to  $\Delta N_{\nu i}$  obeying commutation relations  $[\theta_{\nu i}, \Delta N_{\nu i}] = i$ .

Note that inside the segments between the impurities the expressions for the phase fields between the impurity sites turn out to be similar to those found for bounded 1D Luttinger liquid with open boundary conditions at the sample ends.<sup>29-31</sup> The main difference is that Majorana operators  $\eta_s$  in Eq. (1) are the same for electrons moving right and left, and that Eq. (15) contain the summation over  $j < i$  that insure proper commutation relations between the electron operators related to different segments. Thus we conclude that the system breaks up into a set of independent segments described as bounded Luttinger liquids with main properties similar to those discussed in Refs. 29-31. In particular, as long as eigenvalues of  $\Delta N_{\uparrow i}$  and  $\Delta N_{\downarrow i}$  are integers we find that  $\Delta N_{\rho i} = n_{\rho i} / \sqrt{2}$  and  $\Delta N_{\sigma i} = n_{\sigma i} / \sqrt{2}$  are not independent, because  $n_{\rho i} + n_{\sigma i}$  must be an even number. Such a limitation ensures the minimum value of the impurity Hamiltonian (7). This also means violation of spin-charge separation due to zero modes as discussed by Eggert *et al.*<sup>30,31</sup> for bounded Luttinger liquids.

Hamiltonian in the region between impurity positions at  $x=x_i$  and  $x_{i+1}$  can be presented as

$$H = \sum_{\nu} (\epsilon_{\nu} + \sum_n \omega_{n\nu} b_{n\nu}^{\dagger} b_{n\nu}) + \text{const}, \tag{17}$$

where contribution of zero modes has a form

$$\epsilon_{\rho} = \frac{v_{N\rho} (\delta\phi_i - \pi \Delta N_{\rho})^2}{2\pi l_i}, \quad \epsilon_{\sigma} = \frac{v_F (\pi \Delta N_{\sigma})^2}{2\pi l_i}. \tag{18}$$

One can see that energies of the zero-mode states depend on number of extra electrons at a segment confined by impurities.

From the constitutive relation (1) one can see immediately that temporal dependence (16) of zero-mode part of  $\Theta$  should result in local energy levels

$$\begin{aligned}
\psi_{\mathbf{n},r,s}(t) &\propto \exp \left[ \frac{1}{\sqrt{2}} (\Theta_{\mathbf{n},\rho} + s \Theta_{\mathbf{n},\sigma}) \right] \\
&\propto \exp \left[ i \frac{(\delta\phi_i - \pi \Delta N_{\rho i}) v_{N\rho} + \pi \Delta N_{\sigma i} v_{N\sigma} t}{\sqrt{2} l_i} \right].
\end{aligned}$$

Strictly speaking, the single-electron energy levels can be found from poles of single-particle Green's functions. Its calculation is similar to that in Ref. 31. As long as we study the low-temperature behavior of the system, we need explicit expressions for Green's function at  $T \ll \omega_{0,\nu}$ . It is presented in the Appendix.

### A. Zero modes

Now we concentrate on zero modes. Consider the zero-mode state  $(n_\rho, n_\sigma)$  with extra charge  $n_\rho$  and extra spin  $n_\sigma$  in one of the segments. Such a state contains  $(n_\rho + n_\sigma)/2$  extra electrons with spin  $s$  and  $(n_\rho - n_\sigma)/2$  electrons with spin  $-s$ . Energy (18) for formation of the zero-mode state  $(n_\rho, n_\sigma)$  can be conveniently presented in a form (in this subsection, for brevity, we drop the index related to the number of a segment)

$$\epsilon = \epsilon_\rho + \epsilon_\sigma, \quad \epsilon_\rho = \frac{\omega_{0\rho}(\xi - n_\rho)^2}{4}, \quad \epsilon_\sigma = \frac{\omega_{0\sigma}n_\sigma^2}{4}, \quad \omega_{0\nu} = \frac{\pi v_F}{K_\nu^2 l}, \quad (19)$$

where we introduced a random factor  $\xi = \sqrt{2} \delta\phi / \pi$ ,  $|\xi| < 1$ . Since factor  $\xi$  is related to  $2k_F l$  and, hence, depends on positions of impurities confining the segment under consideration, it is different for different segments.

The low-lying frequencies of the single-particle Green's function  $G^{+-}$  and  $G^{-+}$  introduced by Keldysh (see Ref. 32 describe, respectively, energy levels of electron and hole states. So according to Eqs. (A2) and (A3) the energy levels induced by zero-mode states  $(n_\rho, n_\sigma)$  are

$$\epsilon_{n_\rho, n_\sigma} = \frac{1}{2} [\omega_{0\rho} n_\rho + \omega_{0\sigma} n_\sigma s - \omega_{0\rho} (\xi \pm \xi_0)], \quad (20)$$

where signs  $\pm$  are related to electron and hole states, respectively,  $\xi_0 = \frac{1}{2} [1 + (K_\rho/K_\sigma)^2]$ . (We remind that we consider spin-independent interaction, so in our case  $K_\sigma = 1$ .)

As long as typical values of  $\xi$  and  $\xi_0$  are of the order unity, a characteristic energy for formation of a zero-mode state (19) and characteristic energy scale for position of a zero-mode level (20) can be estimated as

$$\bar{\omega}_0 = \frac{\pi v_F}{K_\nu^2 \bar{l}},$$

with  $\bar{l} = 1/N_{\text{imp}}$ , where  $N_{\text{imp}}$  is the impurity density per single chain. If impurities are distributed randomly, then probability to find a segment of length  $l$  is given by the Poisson distribution,  $w(l) = N_{\text{imp}} \exp(-N_{\text{imp}} l)$ . Then, for a given segment, probability to find a value of frequency  $\omega_0$  that is much smaller, than  $\bar{\omega}_0$ , is exponentially small. Hence, at low temperatures  $T \ll v_F / \bar{l}$ , only energies of modes with  $(n_\rho, n_\sigma)$  equal to  $(0, 0)$ ,  $(1, \pm 1)$ , and to  $(-1, \pm 1)$  can be of the order of temperature. Other frequencies except mentioned above are at least by  $\omega_0$  larger. Furthermore, for a given value of  $\xi$  not more than two states can have energies near the Fermi level simultaneously.

So in the statistically averaged zero-mode part of the Green's function presented in the Appendix we can keep only terms related to the states mentioned above

$$\begin{aligned} & \langle e^{i(\delta\phi - \pi\Delta N_\nu)(x_a - v_{N\nu} t_a) / \sqrt{2}l} \rangle e^{\pm i\pi(x_a - v_{N\nu} t_a) / 4l} \\ & \simeq \frac{1}{2} (e^{i(q_{1,1} x_a - \varepsilon_{1,1} t_a)} + e^{i(q_{1,-1} x_a - \varepsilon_{1,-1} t_a)}) n_1 + \frac{1}{2} (e^{i(q_{-1,1} x_a - \varepsilon_{-1,1} t_a)} \\ & \quad + e^{i(q_{-1,-1} x_a - \varepsilon_{-1,-1} t_a)}) n_{-1} + e^{i(q_{0,0} x_a - \varepsilon_{0,0} t_a)} (1 - n_1 - n_{-1}), \end{aligned} \quad (21)$$

with  $q_{n_\rho, n_\sigma} = (\pi/2l)(n_\rho + s n_\sigma \mp 1 - \xi)$ . Distribution functions for electrons at zero-mode level are given by expressions

$$n_{\pm 1} = \frac{1}{1 + \frac{1}{2} \exp\left[\frac{\omega_{0\rho}(\xi_0 \mp \xi)}{2T}\right]}. \quad (22)$$

Note that the distribution functions must not coincide necessarily with Fermi-Dirac ones because electrons are correlated, and factor  $1/2$  in the denominator of Eq. (22) reflects the presence of two spin states.

Thus zero modes form the system of local electronic levels near the Fermi energy. The energies of these levels are determined by random factors  $|\xi| < 1$ , and density of these states at the Fermi energy is finite in case of short-range interaction.

### B. Modifications of zero modes by long-range interaction

Zero modes in case of long-range Coulomb interaction can be found from equations of motion (8) and (9) with time derivative equal to zero,

$$\partial_x \Theta_\nu^{(0)}(x, \mathbf{n}) = 0, \quad (23)$$

$$\begin{aligned} \Theta_\nu^{(0)}(x, \mathbf{n}) &= \theta_\nu + \sum_{\mathbf{n}'} \int dx' v_F K_\nu^{-2}(x - x', \mathbf{n} - \mathbf{n}') \partial_{x'} \Phi_\nu^{(0)} \\ &\quad \times (t, x', \mathbf{n}') t, \end{aligned} \quad (24)$$

with boundary conditions  $\sqrt{2} \Phi_\rho + 2k_F x = \pi k$ , where  $k$  is an integer.

The energy of zero modes in coordinate representation reads

$$\begin{aligned} E &= \frac{1}{2\pi} \sum_{\nu, \mathbf{n}, \mathbf{n}'} \int dx \int dx' v_F K_\nu^{-2}(x - x', \mathbf{n} - \mathbf{n}') \\ &\quad \times \partial_x \Phi_\nu^{(0)}(x, \mathbf{n}) \partial_{x'} \Phi_\nu^{(0)}(x', \mathbf{n}') \\ &= \frac{1}{4} \sum_{\nu, \mathbf{n}, \mathbf{n}'} \int dx \int dx' v_F K_\nu^{-2}(x - x', \mathbf{n} - \mathbf{n}') \\ &\quad \times \rho_\nu^{(0)}(x, \mathbf{n}) \rho_\nu^{(0)}(x', \mathbf{n}') \end{aligned} \quad (25)$$

with  $K_\nu$  determined by Eq. (5).

Analytical solution of Eqs. (23) and (24) is not a simple matter. Therefore, we consider a simplified model in which we neglect variations of the interaction when each coordinate varies inside a segment between the impurities. That is, we approximate interaction parameter  $K_\nu^{-2}(x - x', \mathbf{n} - \mathbf{n}')$  by its value  $K_\nu^{-2}(\mathbf{i} - \mathbf{j})$ , spatially averaged with respect to coordinates  $x, \mathbf{n}$  and  $x', \mathbf{n}'$  inside given segments labeled as  $\mathbf{i}$  and

**j**. This model does not violate effects of long-range interaction which determine conductivity at low temperatures calculated in the next section. It is not difficult to find solution of Eqs. (23) and (24) for such model interaction. The solution for the zero-mode part of the phase operators  $\Theta_\nu$  has a form

$$\Theta_{\nu i}^{(0)} = \theta_\nu + v_F \sum_{\mathbf{j}} K_\nu^{-2}(\mathbf{i} - \mathbf{j})(\delta\phi_{\mathbf{j}}\delta_{\nu p} - \pi\Delta N_{\nu j})t. \quad (26)$$

This expression for the phase operator enables us to calculate the energy levels of zero-mode states given by eigenfrequencies of Green's function. This is not difficult because contributions from zero modes are separated from excitation in the Green's function similar to the case of the short range interaction considered in the Appendix. So for the energy levels in segment  $\mathbf{i}$  we find

$$\varepsilon_{\mathbf{i}} = -\frac{v_F}{\sqrt{2}} \sum_{\nu j} K_\nu^{-2}(\mathbf{i} - \mathbf{j})(\delta\phi_{\mathbf{j}}\delta_{\nu p} - \pi\Delta N_{\nu j}) \pm \frac{\pi v_F}{4} \sum_{\nu} K_\nu^{-2}(0), \quad (27)$$

where signs  $\pm$  are, again, related to electron and hole states, respectively.

For  $\mathbf{i}=\mathbf{j}$  the averaged interaction parameter can be estimated as

$$K_\rho^{-2}(0) \approx \frac{1}{\bar{l}} \left( 1 + \frac{8e^2}{\hbar v_F} \ln \frac{\bar{l}}{d} \right), \quad (28)$$

where we used dimensional units with  $\hbar$  for clarity.

The second term in Eq. (28) for typical values of Fermi velocity in quasi-1D conductors is quite large. For  $v_F \approx 2 \times 10^7$  cm/s, which is typical value for transition metal trihalogenides, its value is about 80. This corresponds to the case of strong interaction and leads to quite large values of coupling parameters. So we can estimate the typical energy of zero-mode levels as

$$\bar{\omega}_0 \sim \frac{e^2}{\bar{l}}.$$

Thus the zero modes describe quantization energy levels taking into account Coulomb interaction. And if the interaction is strong, the energy of the zero modes is determined by the charging energy of the segments.

Since interaction factor  $K_\rho$  has the long-range contribution, the energy of "single-electron local levels" in Eq. (27) are shifted due to interaction with charges in other segments. Further, because of the slow decay of interaction factor  $K_\rho^{-2}$  with distance described by the Coulomb law, the summation in Eqs. (26) and (27) may diverge. In particular,  $\langle \Theta_{\nu i}^2 \rangle$  and  $\langle \varepsilon_{\mathbf{i}}^2 \rangle$  diverge for random distribution of "number of particles"  $\sqrt{2}(\delta\phi_{\mathbf{j}}/\pi - \Delta N_{\nu j}) \equiv \xi_{\mathbf{j}} - n_{\nu j}$ , at segments  $\mathbf{j}$ . The problem can be resolved by correlated distribution of localized charges in different segments resulting in the Coulomb gap at the Fermi energy similar to the case of localized shallow impurity levels in semiconductors.<sup>33,34</sup> Indeed, Eq. (27) has some similarity to the energy of a local impurity level in the potential induced by all other impurities. Furthermore, energy of zero-

mode local levels has a form somewhat resembling the expression for the electrostatic energy of localized impurities

$$E = \frac{v_F}{2\pi} \sum_{\nu, \mathbf{i}, \mathbf{j}} (\delta\phi_{\mathbf{i}}\delta_{\nu p} - \pi\Delta N_{\nu i}) K_\nu^{-2}(\mathbf{i} - \mathbf{j})(\delta\phi_{\mathbf{j}}\delta_{\nu p} - \pi\Delta N_{\nu j}). \quad (29)$$

So we adopt to our case arguments by Efros and Shklovskii<sup>33</sup> for the Coulomb gap originally used for a system of shallow impurities in semiconductors, though there are considerable differences between equations used in Ref. 33 and Eqs. (26)–(29). First, the latter contain operators of number of extra electrons  $\Delta N_{\nu i}$ . But at low temperatures only a single eigenvalue of these operators plays a role, because the states with other eigenvalues  $n_{\sigma i}$  correspond to energies much larger than temperature. So we can consider the operators as  $c$  numbers. Another difference is the presence of the terms related to the spin channel. Below we will see that this does not change the result.

So following Ref. 33 we consider process of transfer of an electron with spin  $s$  from segment  $\mathbf{i}$  in the ground state to segment  $\mathbf{j}$ . An increase of the energy of the system induced by such transfer calculated from Eq. (29), with Eq. (27) taken into account, is equal to

$$\Delta E = \varepsilon_{\mathbf{j}} - \varepsilon_{\mathbf{i}} - \frac{e^2}{r_{\mathbf{i}, \mathbf{j}}} + \frac{\pi v_F n_{\sigma i}(s + \delta n_{\sigma i})}{2l_{\mathbf{i}}} - \frac{\pi v_F n_{\sigma j}(s - \delta n_{\sigma j})}{2l_{\mathbf{j}}} > 0, \quad (30)$$

where  $\delta n_{\sigma i}$  is the difference of  $n_{\sigma i}$  values in the state  $i$  after and before the transfer of the electron, and  $r_{\mathbf{i}, \mathbf{j}}$  is the distance between segments  $\mathbf{i}$  and  $\mathbf{j}$ . Since for the process of transfer considered here, variation of  $n_{\sigma i}$  in the initial state due to removal of an electron with spin  $s$  equals  $\delta n_{\sigma i} = -s$ , while addition of the electron to the final state is described by  $\delta n_{\sigma j} = s$ , two last terms in Eq. (30) vanish, and we obtain the relation similar to that derived for the case of impurity levels in semiconductors. One can see that small energy differences between the zero-mode levels can be found only for segments situated far from each other

$$r_{\mathbf{i}, \mathbf{j}} > \frac{e^2}{\varepsilon_{\mathbf{j}} - \varepsilon_{\mathbf{i}}}. \quad (31)$$

As it was shown in Ref. 33, this results in a minimum in the density of localized states,  $g(\varepsilon) \propto \varepsilon^2$  near Fermi energy, i.e., to the Coulomb gap. In particular, for electron transitions with energies  $\Delta E \ll v_F/\bar{l}$  important at low temperatures, the distance between the segments participating in electron transitions must be much larger, than the typical segment length. For such remote segments our simplified model, in which we neglected the spatial variation of the interaction within distance of the order of segment length, is asymptotically exact.

### C. Effect of long-range interaction on excitation spectrum

Solution of equation of motion (9) with long-range interaction (5) satisfying boundary conditions (13) is similar to

the problem of interacting segments of elastic strings of random length. Analytical solution of this problem is difficult. So, again, we consider a simplified model in which the impurities are nearly arranged in planes perpendicular to the conducting chains, so that positions of the impurities differ by the value much smaller, than the mean distance between the impurities. Solution of Eqs. (8) and (9) consists of two parts. The first part corresponding to particular solution with boundary conditions (13) describes zero modes, their spectrum having the form of the randomly distributed localized levels discussed above. Levels are situated randomly because the values of  $2k_F x_i$  which determine positions of zero-mode levels are random.

The part describing the excitations corresponds to general solution with zero boundary conditions. The latter can be found by means of Fourier transformation with respect to chain numbers. We take into account that according to Eq. (4) only excitations with long wavelengths along the chains correspond to low lying excitations (otherwise frequencies are of the order of plasma frequency). So we consider the limit  $q_\perp \gg q_\parallel$  and neglect  $q_\parallel$  in the denominator of the interaction parameter  $K_\rho$  (5). Then we easily find expressions similar to the last terms in Eqs. (15) and (16) describing the excitations, but with interaction factors and eigenfrequencies depending on  $q_\perp$ ,

$$\frac{1}{K_{\rho 0}^2} = 1 + \frac{8e^2}{v_F d^2 q_\perp^2}, \quad \omega = n \frac{\pi}{l_i} \sqrt{v_F^2 + \frac{\omega_{pl}^2}{q_\perp^2}}. \quad (32)$$

Thus the spectrum of the modes in this case consists of the bands, the minimum excitation energy being fixed by the maximum value of  $q_\perp$  determined by the transverse reciprocal lattice vector  $\sim \pi/d$ . Its characteristic value can be estimated as

$$\omega_{\min} = \frac{v_F}{l} \sqrt{\pi^2 + \kappa^2 d^2} = \frac{v_F}{l} \sqrt{\pi^2 + \frac{8e^2}{v_F}}, \quad (33)$$

where  $\kappa = \omega_{pl}/v_F$  is Thomas-Fermi screening length in the metallic state.

Contribution of the excitations to the Green's functions can be calculated similarly to the case of the contact interaction presented in the Appendix. Factors in the square brackets in functions  $B$  in Eq. (A4) originate from summations over eigenfrequencies in products of phase fields  $\Phi_\nu$  and  $\Theta_\nu$ . If interaction parameter  $K_\rho$  depends on  $q_\perp$  these factors acquire a more complicated form, e.g., the first factor in square brackets in  $B$  must be substituted for

$$\exp \left\langle -\frac{1}{8} \left( \frac{1}{K_{\rho 0}} + K_{\rho 0} + 2 \right) \ln(1 - e^{-iz - \tilde{\alpha}}) \right\rangle_{\mathbf{q}_\perp}, \quad (34)$$

where  $z = \pi(x_a - v_\rho t_a)/l$ . Similar substitutions occur in other factors in square brackets in Eq. (A4)

In the next section we will need Green's functions for calculation of conductivity at large voltages, so we need to calculate Green's functions at energies  $\varepsilon \gg \bar{\omega}_0$ . Then in time and coordinate representation we need Green's functions for  $v_\rho t_a, x_a \ll l$ , where  $t_a$  and  $x_a$  are differences of time and coordinate arguments of the Green's functions (see the Appendix). In the same time we consider  $v_\rho t_a, x_a \gg \alpha$  since the energy is small compared to Fermi energy. In this limit, expression (34) reduces to factor  $\propto z^{-(1/2)(\delta+1)}$  with

$$\delta = \frac{1}{4} \left\langle \frac{1}{K_{\rho 0}} + K_{\rho 0} - 2 \right\rangle_{\mathbf{q}_\perp}. \quad (35)$$

Since density of states  $N(\varepsilon)$  is determined by Fourier transformation of Green's function in  $t_a$  at  $x_a = 0$ , and distribution function  $n(p)$  of electrons on momentum along the chains can be found by means of Fourier transformation with respect to  $x_a$  at  $t_a = 0$ , this means that at energies  $\varepsilon \gg \bar{\omega}_0 N(\varepsilon) \propto \varepsilon^\delta$  and  $n(p) \propto (p - k_F)^\delta$ , similarly to the case of Luttinger liquid without impurities (see Refs. 1, 3, and 11). Furthermore, if we neglect weak logarithmic dependence of  $v_\rho$  in Eq. (34) on  $\mathbf{q}_\perp$ , then we find that Green's function in the considered limit behave similar to that in the unbounded Luttinger liquid at any relation between  $v_\rho t_a$  and  $x_a$ . In other words, for such relatively large energies effect of impurities on Green's function and, hence, on energy spectrum can be neglected. So we conclude that in the electronic system with Coulomb interaction the electronic spectrum consists of discrete levels due to zero modes, and of quasicontinuum spectrum of excitations of the Luttinger liquid at energies more than  $\bar{\omega}_0$  apart from Fermi energy.

#### D. Effect of interchain hopping

Now we demonstrate that inter-chain hopping of electrons do not destroy the description of quasi-1D conductor with impurities at low temperatures based on the picture of collection of bounded Luttinger liquid. We take into account the hopping in a standard way, considering the perturbative series for Green's functions with respect to the hopping integral  $t_\perp$ . It is not difficult to calculate corrections to the Green's functions due to hopping for small energy  $\varepsilon \ll \bar{\omega}_0$ , because at such energies Fourier-transformed Green's functions presented in the Appendix acquire a simple form. For example, at such energies the zero-temperature causal Green's function reduces to a form

$$G^{--} = \frac{\tilde{\alpha}^{(1/4)(1/K_\rho + K_\rho + 2)} [(\tilde{\alpha}^2 + 4 \sin^2 q_0 x_1)(\tilde{\alpha}^2 + 4 \sin^2 q_0 x_2)]^{(1/16)(1/K_\rho - K_\rho)} e^{ik_F x_a + iq_\perp x_a}}{2\pi\alpha(\varepsilon - \varepsilon_i + i0 \operatorname{sgn} \varepsilon)}, \quad (36)$$

where  $\varepsilon_i$  and  $q_i$  are energy and wave vector of the zero-level state at segment number  $\mathbf{i}$  [see Eq. (21)].

So calculating in a standard way corrections to the mass operator in the second order in  $t_\perp$  we find that hopping results in a shift of the zero-mode level by

$$\delta\varepsilon_0 \sim \sum_j \frac{t_\perp^2}{\varepsilon_i - \varepsilon_j} \left(\frac{\alpha}{l}\right)^{2\delta}, \quad (37)$$

where  $\varepsilon_j$  are zero-level energies at neighboring segments.

Note that the probability to find similar values of zero-state energies at neighboring segments is negligible, so the energy difference in the denominator of Eq. (37) is of the order of typical energy of the zero level  $\bar{\omega}_0$ . So the shift of the energy due to hopping can be estimated as

$$\delta\varepsilon_0 \sim \frac{t_\perp^2}{\bar{\omega}_0} \left(\frac{\alpha}{l}\right)^{2\delta}. \quad (38)$$

The higher order terms give smaller corrections proportional to higher order powers of factor

$$\left(\frac{t_\perp}{\bar{\omega}_0}\right)^2 \left(\frac{\alpha}{l}\right)^{2\delta}. \quad (39)$$

So corrections are small provided this factor is small.

Note that our calculations are based on discrete nature of the electron spectrum near the Fermi energy, because we used an assumption that both characteristic energy and the hopping matrix element  $t_\perp$  are much smaller than typical energy of zero-mode levels  $\bar{\omega}_0$ . The characteristic energy is determined by temperature  $T$ . Thus interchain hopping does not destroy the Luttinger-liquid picture in the limit  $T \ll \bar{\omega}_0$ , which does not exist in pure infinite Luttinger liquid. In the opposite limit of larger temperatures there are many levels in the energy interval of the order of temperature, and, hence, the continuum limit is applicable, our approach is not valid. So at temperatures  $T \gg \bar{\omega}_0$ , the discreteness of the excitation spectrum cannot be neglected, hence, according to Refs. 4 and 6–9, interchain hopping is expected to give significant contributions and to destroy the Luttinger liquid.

#### IV. ELECTRON TRANSPORT

In this section we calculate current in the Luttinger-liquid state of quasi-1D conductors by means of Keldysh diagrammatic approach.<sup>32</sup>

##### A. Conductivity at low voltages

Consider, first, Ohmic conductivity due to hopping between the segments confined by impurities. Taking into account the similarity with the case of impurities in semiconductors, discussed above, it is natural to expect that the mechanism of conductivity is phonon assisted variable-range hopping.

There are two ways for electron transfer: via inter-chain transitions, and via transitions along conducting chains through potential barriers induced by impurities. In case of hopping conductivity there is no principal difference between both channels. So we concentrate on the case when

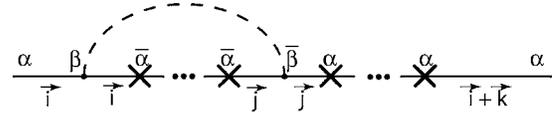


FIG. 1. A diagram for calculation of the current. The dashed line symbolizes the phonon propagator, Greek letters denote Keldysh time indices “+” and “-,” and  $\bar{\alpha}$  means the time index opposite to  $\alpha$ . Crosses denote hopping matrix elements  $t_\perp$ . Dots between the crosses stand for a way connecting segments  $\mathbf{i}$  and  $\mathbf{j}$  corresponding to sequential transitions via the neighboring segments. The lowest order contributions to current in  $t_\perp$  are given by diagrams with the least number of transitions.

probability of transitions between conducting chains dominates over probability of tunneling through impurities. Current flowing from segment  $\mathbf{i}$  to its neighbors can be calculated as

$$I \propto t_\perp \sum_k [F_{\mathbf{i},\mathbf{i}+\mathbf{k}}(1,1) - F_{\mathbf{i}+\mathbf{k},\mathbf{i}}(1,1)], \quad (40)$$

where  $F_{\mathbf{i},\mathbf{i}+\mathbf{k}} = G_{\mathbf{i},\mathbf{i}+\mathbf{k}}^{--} + G_{\mathbf{i},\mathbf{i}+\mathbf{k}}^{++}$ , and summation is performed over neighboring segments. Green’s functions  $G_{\mathbf{i},\mathbf{i}+\mathbf{k}}^{\alpha\alpha}$  can be calculated by means of diagrams presented in Fig. 1.

Having in mind that conductance is determined by the states with energies in vicinity of the Fermi energy we can use in the diagrams electron Green’s functions in the form given by Eq. (36). Performing calculations we find that the total current through segment  $\mathbf{i}$  consists of contributions describing currents flowing via numerous segments  $\mathbf{j}$ . Current from segment  $\mathbf{i}$  to segment  $\mathbf{j}$  is induced by a voltage difference  $V_{\mathbf{i},\mathbf{j}}$  defined as the difference of the electrochemical potentials at these segments. Expression for such current resembles corresponding expressions of the variable-range hopping theory<sup>33,34</sup> and has a form that has very transparent physical interpretation

$$I_{\mathbf{i},\mathbf{j}} \propto \int d\omega_{\text{ph}} \left[ \frac{t_\perp}{\bar{\omega}_0} \left(\frac{\alpha}{l}\right)^\delta \right]^{2m} \times \{ [n_i(1-n_j)N_{\text{ph}} - n_j(1-n_i)(1+N_{\text{ph}})] \times \delta(\varepsilon_i - \varepsilon_j + \omega_{\text{ph}} + V_{\mathbf{i},\mathbf{j}}) + [n_i(1-n_j)(1+N_{\text{ph}}) - n_j(1-n_i)N_{\text{ph}}] \delta(\varepsilon_i - \varepsilon_j - \omega_{\text{ph}} + V_{\mathbf{i},\mathbf{j}}) \}. \quad (41)$$

Here  $\varepsilon_i$ ,  $\varepsilon_j$  and  $n_i$ ,  $n_j$  are electron energies and distribution functions for zero-mode levels at the respective segments, and  $N_{\text{ph}}(\omega_{\text{ph}})$  is the distribution function of phonons. It is clear that different items in Eq. (41) describe processes of electron hopping between segments accompanied with phonon emission or absorption. The first factor under the integral originates from virtual transitions between the segments along the way between segments  $\mathbf{i}$  and  $\mathbf{j}$ , and power index  $m$  describes the number of virtual transitions

$$m \propto \sqrt{|\mathbf{n}_i - \mathbf{n}_j|^2 + \left(\frac{x_i - x_j}{l}\right)^2}. \quad (42)$$

Contribution of each virtual transition to the current is reflected by factor similar to that presented in Eq. (39).

Energies in arguments of the distribution functions in Eq. (41) are shifted by values of electrochemical potential at given segment. Linearizing expression (41) with respect to potentials and performing the integration over phonon frequencies we find expression for the current between segments  $\mathbf{i}$  and  $\mathbf{j}$  similar to that describing current between localized impurity states in semiconductors<sup>33,34</sup>

$$I_{\mathbf{i},\mathbf{j}} = \frac{V_{\mathbf{i},\mathbf{j}}}{R_{\mathbf{i},\mathbf{j}}}, \quad R_{\mathbf{i},\mathbf{j}} \propto \exp \left[ 2m \ln \left[ \frac{\bar{\omega}_0}{t_{\perp}} \left( \frac{\bar{l}}{\alpha} \right)^{\delta} \right] + \frac{|\varepsilon_{\mathbf{i}} - \varepsilon_{\mathbf{j}}|}{T} \right]. \quad (43)$$

This expression leads to different results for the case of short-range interaction of the Tomonaga-Luttinger model, and for the case of long-range Coulomb interaction of electrons at different segments. In the former case, following standard arguments of theory of variable-range hopping<sup>33,34</sup> we arrive at Mott's law describing three-dimensional variable-range hopping conductivity

$$\sigma(T) \propto \exp \left[ - \left( \frac{T_M}{T} \right)^{1/4} \right], \quad T_M \sim \bar{\omega}_0 \ln^3 \left[ \frac{\bar{\omega}_0}{t_{\perp}} \left( \frac{\bar{l}}{\alpha} \right)^{\delta} \right]. \quad (44)$$

The result is different in case of long-range interaction. Then there is the Coulomb gap in the density of states at the Fermi energy, and hopping of electrons occurs effectively only between the segments situated far from each other, at distances given by condition (31). Since distances between impurities  $\bar{l}$  is much larger than the interchain distance  $d$  a given distance  $r_{\mathbf{i},\mathbf{j}} = \sqrt{|\mathbf{n}_{\mathbf{i}} - \mathbf{n}_{\mathbf{j}}|^2 d^2 + (x_{\mathbf{i}} - x_{\mathbf{j}})^2}$  can be found for much smaller values of  $m$ , Eq. (42), if the segments are situated at the same or at adjacent chains, than for segments situated at remote chains. As current (43) between the segments exponentially decreases with  $m$  increasing, the strong dependence of distance between the segments on direction results in effectively one-dimensional hopping. Using, again, the arguments of theory of variable-range hopping we find that conductivity obeys Efros-Shklovskii law

$$\sigma(T) \propto \exp \left[ - \left( \frac{T_{\text{ES}}}{T} \right)^{1/2} \right], \quad T_{\text{ES}} \sim \bar{\omega}_0 \ln \left[ \frac{\bar{\omega}_0}{t_{\perp}} \left( \frac{\bar{l}}{\alpha} \right)^{\delta} \right], \quad \bar{\omega}_0 \sim \frac{e^2}{\bar{l}}. \quad (45)$$

Nearly 1D character of hopping results in enhancement of anisotropy of conductivity. The anisotropy can be estimated as the ratio of the characteristic hopping lengths in directions parallel and perpendicular to the chains. It was argued above that hopping in the perpendicular direction occurs effectively over distances of the order of interchain distance  $d$ . The hopping length along the chains can be found as that corresponding to the minimum value of the exponent in Eq. (43). So for anisotropy of the conductivity we find

$$\frac{\sigma_{\parallel}}{\sigma_{\perp}} \sim \frac{e^2}{d\sqrt{T_{\text{ES}}T}}. \quad (46)$$

Note that the conduction mechanism in the considered system is similar not only to that in a system of shallow impurities in semiconductors. In disordered granular metals conduction is also controlled by the interplay of hopping of an electron to large distance and long-range Coulomb interaction, and conductivity is described by the Efros-Shklovskii law.<sup>34</sup> So our results on conductivity bear resemblance to recent studies of transport in disordered metals in Refs. 35–37.

## B. Nonlinear conductivity

Now we discuss electron transfer at high voltages and make rough estimates of nonlinear current-voltage dependencies. We assume that the typical voltage drop per single segment can reach the value of the order of or even larger than the typical energy of the local levels  $\sim \bar{\omega}_0$  but it is still small compared to the effective strength of the impurity potential  $V_0$  which is assumed to be of the atomic scale, see Eq. (10). As long as the average length between impurities  $\bar{l}$  is large compared to the interatomic distance, this condition is fulfilled easily.

Let the voltage between  $m$  segments is equal to  $mV$ . If the voltage drop over the hopping length becomes larger than the energy of the local levels  $\sim \bar{\omega}_0$  then electron transitions between the quasicontinuum spectrum of excitations in segments become possible without phonon absorption. This happens at electric field  $E \gtrsim \sqrt{TT_{\text{ES}}}/e\bar{l}$ . Current between such segments can be calculated by means of diagrams similar to that presented in Fig. 1, but without phonon line. The diagrams contain virtual transitions via intermediate segments that contribute to the expression for current small factors similar to the first factor in Eq. (41). Further, at large voltages current is roughly proportional to factor  $(mV)^{2\delta+1}$  because of the power-law energy dependence of the density of states in Luttinger liquid [see discussion below Eq. (35)]:

$$I \propto \left[ \frac{t_{\perp}}{\bar{\omega}_0} \left( \frac{\alpha}{\bar{l}} \right)^{\delta} \right]^{2m} (mV)^{2\delta+1}. \quad (47)$$

Consider, first, the case when the voltage is not too large so that electron transitions between the regions of quasicontinuum spectrum of excitations are possible at  $m \gg 1$  only. Then index  $m$  is related to the average electric field along the chains by relation  $meV \approx meE\bar{l} \gtrsim \bar{\omega}_0$ . So the most rapid, exponential, dependence of current on electric field originates from increase of  $m$  in the first factor in Eq. (47), in other words, from switching on new channels for nonlinear current flow between more and more closely situated segments. The second factor in Eq. (47) gives slowly varying function of field  $E$  of the order of  $\bar{\omega}_0^{2\delta+1}$ , its field dependence can be neglected in comparison to the exponential growth due to the first factor. So for this regime we find

$$I \propto \exp \left( - \frac{E_{0\parallel}}{E} \right), \quad E_{0\parallel} \sim \frac{T_{\text{ES}}}{e\bar{l}}. \quad (48)$$

Note that condition  $m > 1$  means  $E < E_{0\parallel}$ .

For current in direction perpendicular to conducting chains index  $m$  is related to the average electric field by the

relation  $meEd \geq \bar{\omega}_0$ . Then for this direction the characteristic field can be estimated as  $E_{0\perp} \sim T_{ES}/ed$ . This is much larger value than  $E_{0\parallel}$  which demonstrates strong anisotropy of the non-linear conductivity.

At larger voltages, when  $E \geq E_0$ , the voltage drop is large enough to induce electron transitions between the neighboring segments. In this case the  $I$ - $V$  curves can be estimated as

$$I \propto V^{2\delta+1}. \quad (49)$$

The power index here is different if tunneling along the chains via impurities is more effective than interchain tunneling. In the latter case the density of states at the ends of a segment is described by different power index, similarly to bounded Luttinger liquids,<sup>29-31</sup> so index  $2\delta$  in Eq. (49) must be substituted for  $\langle 1/K_{\rho 0} - 1 \rangle_{\mathbf{q}\perp}$ .

## V. DISCUSSION

Now we discuss relation of our theoretical results to real materials and to experimental data. Our calculations are based on the Luttinger model which does not take into account backscattering terms, i.e.,  $2k_F$  Fourier component of the interelectronic interaction. These terms are known to lead to two qualitatively different consequences (for a review see Ref. 1). In case of attractive spin-independent interaction it results in the spin gap, while the backscattering terms are irrelevant if the interaction is repulsive. So, strictly speaking, our results can be applied for the case of Coulomb repulsion of the electrons at all wave vectors. On the other hand, the effective interelectronic interaction can be considered as containing both repulsive Coulomb interaction and attraction due to electron-phonon coupling. It can happen that the Coulomb repulsion dominates at small values of wave vectors, while attraction induced by electron-phonon coupling dominates at wave vectors close to  $2k_F$ . Though such picture ignores retardation effects in the electron-phonon coupling it is quite fruitful in description of quasi-1D CDW conductors,<sup>15</sup> electron-phonon interaction being described by means of attractive electron-electron coupling constant at  $2k_F$  wave vector. Note that the mean-field expression for the CDW gap<sup>15</sup> is similar to the expression for the spin gap obtained within the renormalization group approach with the cutoff length  $\alpha$  in equation for spin gap estimated as  $\alpha \sim 1/k_F$ . Therefore, we can conclude that a possible value of spin gap in such materials as NbSe<sub>3</sub> and TaS<sub>3</sub> can be of the order of few hundreds K. Since the spin gap implies long-range order in  $\Phi_\sigma$  field and expected values of spin gap are quite large, the fluctuations of this field at low temperatures must be small. The energy in the spin channel is minimized by  $\sqrt{2}\Phi_\sigma = 2\pi n$ , which satisfies boundary conditions (13) for even values of integer  $m$ . So we can expect that in the presence of large spin gap the electron system at low temperatures can be considered as spinless electrons in the Luttinger state, the spin degrees of freedom being frozen. In this case the results of the preceding sections are still valid, and only minor rather simplifications than modifications in the course of derivation of results are needed.

Thus we conclude that our results can be applied to quasi-1D conductors NbSe<sub>3</sub> and TaS<sub>3</sub> where transition from

metallic to nonmetallic behavior was observed. However, detailed quantitative comparison with experimental data is difficult. The first reason for this is some contradictory data on temperature dependence of Ohmic conductivity at low temperatures. In Ref. 18 the temperature dependence corresponding to the variable-range hopping described by the Efros-Shklovskii law was observed, while in Refs. 16 and 17 a power-law dependence of conductivity on temperature was observed down to liquid helium temperature. Another difficulty for making detailed comparison is that the impurity density in the samples is not known. However, our results agree with general tendencies observed in these materials. Namely, more impure samples demonstrate transition from metallic to nonmetallic behavior at higher temperatures, characteristic temperature in Eq. (48) increasing from few tens K in more perfect samples to few hundreds K in the most dirty samples. In a sample with characteristic temperature  $E_{ES} \approx 80$  K temperature dependence of Ohmic conductivity transforms from metallic to nonmetallic behavior in the temperature range 100–200 K. Then we conclude that  $\bar{\omega}_0 \sim 100$  K, and since  $\bar{\omega}_0 \sim e^2/\bar{l}$ , according to our approach we can estimate the mean segment length as  $\bar{l} \sim 10^{-5} - 10^{-4}$  cm. According to Eq. (48) this length corresponds to electric field of the order of  $10^2 - 10^3$  V/cm for transition from Ohm's law to power law dependence. This is in order of magnitude agreement with the experimental data of Ref. 18. But to make convincing conclusions more theoretical and experimental work is needed.

It is important to note that low temperature behavior of both NbSe<sub>3</sub> and TaS<sub>3</sub> in Refs. 16–19 is very similar, in spite of the fact that relatively pure samples of these materials behave quite differently: NbSe<sub>3</sub> remains metallic in the CDW state, while TaS<sub>3</sub> below the Peierls transition becomes an insulator with quasiparticle density obeying the Arrhenius law. Whereas the main properties of quasi-1D conductors at higher temperatures are well understood,<sup>14,15</sup> they demonstrate many intriguing properties at low temperatures which are still not explained convincingly. In particular, in TaS<sub>3</sub> at temperatures below 20 K a behavior typical for hopping conductivity was observed<sup>38,39</sup> instead of Arrhenius law, and anomalous behavior of the dielectric function interpreted as a new glassy phase<sup>40</sup> was detected at frequencies 1–10<sup>7</sup> Hz. One can speculate that this unusual behavior can be related to the formation of the Luttinger phase at very low temperatures because characteristic energy  $\bar{\omega}_0 \sim e^2/\bar{l}$  is small due to small impurity density  $N_{\text{imp}} = 1/\bar{l}$ .

## ACKNOWLEDGMENTS

We are grateful to S. V. Zaitsev-Zotov for useful discussions and to P. Monceau for helpful comments. In part the work was supported by the Russian Foundation for Basic Research (RFBR), by INTAS, and by CRDF. A part of this research was performed in the frame of the CNRS-RAS-RFBR Associated European Laboratory "Physical properties of coherent electronic states in condensed matter" between CRTBT and IRE RAS.

**APPENDIX: SINGLE-ELECTRON GREEN'S FUNCTION**

Here we present Green's functions introduced by Keldysh  $G^{+-}$  and  $G^{-+}$ :

$$iG_{\mathbf{n},s}^{+-}(1,2) = \langle \psi_{\mathbf{n},s}(1) \psi_{\mathbf{n},s}^{\dagger}(2) \rangle,$$

$$-iG^{-+}(1,2) = \langle \psi_{\mathbf{n},s}^{\dagger}(2) \psi_{\mathbf{n},s}(1) \rangle, \quad (\text{A1})$$

with notations  $1=(r_1, x_1, t_1)$ ,  $2=(r_2, x_2, t_2)$ . These functions are proportional to distribution function of holes and electrons, respectively. Other Green's functions can be easily derived by applying time ordering to expressions for  $G^{+-}$  and  $G^{-+}$ . In particular, the causal Green's function can be found as  $G^{--}=G^{+-}$  at  $t_1 > t_2$  and  $G^{--}=G^{-+}$  at  $t_1 < t_2$ .

Performing the calculations in the standard way<sup>1,3</sup> we find

$$G^{+-}(1,2) = -iB(1,2) \left\langle \exp \left( \frac{i(\delta\phi_i - \pi\Delta N_{vi})(x_a - v_{Nv}t_a)}{\sqrt{2}l_i} \right) \right\rangle$$

$$\times \exp \left( \frac{i\pi(x_a - v_{Nv}t_a)}{4l_i} \right). \quad (\text{A2})$$

The function related to distribution function of electrons has a form

$$G^{-+}(1,2) = iB(2,1) \left\langle \exp \left( \frac{i(\delta\phi_i - \pi\Delta N_{vi})(x_a - v_{Nv}t_a)}{\sqrt{2}l_i} \right) \right\rangle$$

$$\times \exp \left( -\frac{i\pi(x_a - v_{Nv}t_a)}{4l_i} \right), \quad (\text{A3})$$

where  $B(1,2)$  originates from bosonic excitations of the Luttinger liquid, and the last factors are related to zero modes. For  $r_1=+1$  and  $r_2=-1$  this function has a form

$$B(1,2) = \frac{e^{ik_F x_a}}{2\pi\alpha} \prod_v \tilde{\alpha}^{(1/4)(1/K+K)} \{ [\tilde{\alpha}^2 + 4 \sin^2 q_0 x_1]$$

$$\times [\tilde{\alpha}^2 + 4 \sin^2 q_0 x_2] \}^{(1/16)(1/K-K)}$$

$$\times [1 - e^{i(\omega_v t_a - q_0 x_a) - \tilde{\alpha}}]^{-(1/8)(1/K+K+2)}$$

$$\times [1 - e^{i(\omega_v t_a - q_0 x_s) - \tilde{\alpha}}]^{-1/8(1/K-K)}$$

$$\times [1 - e^{i(\omega_v t_a + q_0 x_s) - \tilde{\alpha}}]^{-(1/8)(1/K+K-2)}$$

$$\times [1 - e^{i(\omega_v t_a + q_0 x_s) - \tilde{\alpha}}]^{-(1/8)(1/K-K)}, \quad (\text{A4})$$

where  $x_a = x_1 - x_2$ ,  $x_s = x_1 + x_2$ ,  $t_a = t_1 - t_2$ ,  $q_0 = \pi/l_i$ ,  $\tilde{\alpha} = \pi\alpha/l_i$ .

Green's functions with other values of indices  $r$  describing branches of left(right) moving electrons can be found from relations

$$G(r_1 = +1, x_1; r_1 = -1, x_2) = G(r_1 = +1, x_1; r_1 = +1, -x_2),$$

$$G(r_1 = -1, x_1; r_1 = +1, x_2) = G(r_1 = +1, -x_1; r_1 = +1, x_2),$$

$$G(r_1 = -1, x_1; r_1 = -1, x_2) = G(r_1 = +1, -x_1; r_1 = +1, -x_2).$$

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