Interaction-induced corrections to conductance and thermopower in quantum wires

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We study transport properties of weakly interacting spinless electrons in one-dimensional single channel quantum wires. The effects of interaction manifest as three-particle collisions due to the severe constraints imposed by the conservation laws on the two-body processes. We focus on short wires where the effects of equilibration on the distribution function can be neglected and collision integral can be treated in perturbation theory. We find that interaction-induced corrections to conductance and thermopower rely on the scattering processes that change number of right- and left-moving electrons. The latter requires transition at the bottom of the band which is exponentially suppressed at low temperatures. Our theory is based on the scattering approach that is beyond the Luttinger-liquid limit. We emphasize the crucial role of the exchange terms in the three-particle scattering amplitude that was not discussed in the previous studies.

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Introduction.— The quest for fundamental theory of interacting low-dimensional many-body quantum liquids and solids continues. Over the past several decades the traditional framework for discussing one-dimensional (1D) systems was provided by the Luttinger-liquid (LL) theory. It exploits an approximation of linearized fermionic dispersion relation which makes this model exactly solvable. While being extremely fruitful in many cases an ideal LL model, however, possesses certain deficiency. For example, elementary bosonic excitations (plasmons) of the LL have infinite lifetime so there is no relaxation toward the equilibrium within this description regardless of the strength of interaction. The effects of interaction show no sign in application to the dc transport coefficients of clean, single channel short quantum wires. Indeed, it has been shown that within LL model the interactions inside the wire do not affect conductance which is simply given by its noninteracting value. Clearly, a model with the linearized spectrum is an idealized one. It is really the delicate interplay between the dispersion nonlinearity and interactions in reduced dimensions that bring new insights. Thus, current interest in the properties of 1D systems is focused on the physics that lies beyond the Luttinger-liquid limit.

In support of this general interest a number of recent experiments in the low-density quantum wires revealed deviations from the perfect conductance quantization a lower value of the thermal conductance than predicted by the Wiedemann-Franz law and enhanced thermopower. Although there is no consensus on the theoretical interpretation of these observations it is widely accepted that interaction effects are crucial in understanding of these features. The goal of this paper is to elucidate the role of inelastic scattering processes (i.e., processes which change the number and energy of, say, right-moving electrons), not captured by the LL theory, for the description of transport properties of one-dimensional quantum wires. We evaluate the interaction-induced corrections to conductance and thermopower in a particularly interesting case of spinless (spin-polarized) electrons. Unlike the recent work, see Ref. 2 where the model of interacting electrons with sharp momentum cutoff was used, we consider more generic situation which requires to account for both the direct and exchange terms in the three-particle scattering rate.

Formalism.— We consider a clean single channel quantum wire connected adiabatically to the bulk noninteracting leads, and biased by a small voltage $V$ and temperature difference $\Delta T$, see Fig. 1. The distribution function of noninteracting electrons is purely determined by the leads and has the form

$$f_p = \frac{\theta(p)}{e^{\varepsilon_p/T_L} + 1} + \frac{\theta(-p)}{e^{\varepsilon_p/T_R} + 1}$$

where the chemical potentials and temperatures in the leads are $\mu_L = \mu + eV$, $T_L = T$ and $\mu_R = \mu$, $T_R = T + \Delta T$. The energy of an electron with momentum $p$ is $\varepsilon_p = p^2/2m$, and $\theta(p)$ is the unit step function.

In the general interacting case even weak processes of electron scattering will modify nonequilibrium distribution Eq. (1). Indeed, some right-moving electrons will

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1.png}
\caption{[Color online] Quantum wire of length $L$ in the regime of small voltage $\mu_L - \mu_R = eV$ and/or temperature $T_R - T_L = \Delta T$ bias. The interaction-induced backscattering changes the number of right-moving electrons, $N^R \neq 0$, thus affecting electrical conductance $G$ and thermopower $S$.}
\end{figure}
backscatter thus become left-movers. In that way electrons lose the memory of the lead the originated from and tend to equilibrate. To what extent the equilibration occurs depends on the strength of interaction and length of the wire.

Relying only on the very general basis of particle number conservation, one may show that the electric current $I$ flowing through the wire is ultimately related to the electron backscattering

$$GV = I - e\mathcal{N}^R$$

where $\mathcal{N}^R$ is the rate of change in the number of right-moving electrons, see Fig. 1. The physical meaning of Eq. (2) is clear: without interaction $\mathcal{N}^R = 0$ and one then finds the Landauer conductance of noninteracting electrons, $G = I/V = (e^2/h)(1 + e^{-\mu/T})^{-1}$, which coincides with the conductance quantum, $e^2/h$, up to an exponentially small correction, $e^{-\mu/T}$, due to the states at the bottom of the band. In the presence of interaction some right-moving electrons are backscattered reducing the current. Therefore, the interaction-induced correction to conductance is $\delta G \propto \mathcal{N}^R$ and Eq. (2) can be considered as the generalization of Landauer formula.

Apart from the conductance we are interested also in the thermopower, $S$, which relates induced voltage across the wire to applied temperature difference. For the non-interacting electrons $S = V/\Delta T|_{T=0} \approx (\mu/eT)e^{-\mu/T}$, to the leading order at low temperatures $T/\mu \ll 1$. Within the LL model $S = 0$ due to particle-hole symmetry. The reason for such strong suppression of thermopower is the partial cancelation between heat currents carried by electron-like and hole-like excitations. Only the absence of electronic states below the bottom of the band prevents thermopower from vanishing exactly. Knowing $S$ one can also find the Peltier coefficient $\Pi$ via the Onsager relation $\Pi = ST$. As we discuss below the interaction-induced corrections to thermopower also result from the electron backscattering, so that $\delta S \propto \mathcal{N}^R$.

Within the Luttinger-liquid model we have $\mathcal{N}^R = 0$. It is because the constraints imposed by the energy and momentum conservations allow either zero-momentum exchange or an interchange of the momenta for two colliding particles. In either case $f_p$ given by Eq. (1) remains unchanged. Thus, the transport coefficients $G$ and $S$ remain intact by two-body interactions. Therefore, one can conclude then the leading backscattering mechanism is due to three-particle collisions.

Rather than working within the LL model with nonlinear dispersion, that would include the anharmonic interaction of plasmons and thus, in principle, contain equilibration and backscattering processes, we consider simpler situation of weakly interacting electrons, $e^2/\hbar v_F R \lesssim 1$, where $v_F$ is Fermi velocity while $\kappa$ dielectric constant. We account for the three-particle collisions within the Boltzmann equation (BE) formalism. The evolution of the distribution function of an interacting many-body system is governed by the BE, $\mathcal{I}_p = \mathcal{I}(f_p)$, where the collision integral is given by

$$\mathcal{I}(f_p) = - \sum_{p_2 p_3} W^{123}_{123} [f_{p_1} f_{p_2} f_{p_3} (1 - f_{p_1})(1 - f_{p_2}) (1 - f_{p_3})]$$

In general collision integral is a nonlinear functional of $f_p$ which we assumed here to be local in space. A particular combination of the distribution functions in Eq. (3) conventionally accounts for the probability to find filled $f_{p_3}$ and empty $1 - f_{p_2}$ states before and after the collision. The key element of the theory is the scattering rate $W^{123}_{123} = (2\pi/\hbar)|A^{123}_{123}|^2\delta(E - E')\delta_{P_3 P_3}$ from the set of initial states $\{p_1, p_2, p_3\}$ into the final states $\{p_1', p_2', p_3'\}$. The delta-functions in $W^{123}_{123}$ impose conservation of total energy $E(E') = \sum_i \varepsilon_i(p_i)$ and total momentum $P(P') = \sum_i P_i(p_i)$ in a collision, and $A^{123}_{123}$ is corresponding scattering amplitude. For the electrons with the bare pair-interaction potential three-particle amplitude can be found via generalized Fermi golden rule by iterating interaction to the second order. The result of such calculation gives

$$A^{123}_{123} = \sum_{\pi(123')} \text{sign}(123') A(11', 22', 33')$$

where $A(11', 22', 33')$ is an amplitude of a particular scattering process, see Fig. 2 which reads explicitly

$$A_{123}^{1'2'3'} = \frac{1}{\Delta \varepsilon_{12}} \left( \frac{1}{\Delta \varepsilon_{31}} - 1 \right)$$

$$a_{12}^{1'2'} \equiv a_{p_1 p_2}^{p_1' p_2'} = \frac{1}{T} V_{p_1 - p_2} V_{p_1' - p_2'} \left[ \frac{1}{E - \varepsilon_{p_1} - \varepsilon_{p_1'} - \varepsilon_{p_2} - \varepsilon_{p_2'}} + \frac{1}{E - \varepsilon_{p_1} - \varepsilon_{p_2} - \varepsilon_{p_1'} - \varepsilon_{p_2'}} \right]$$

Here $\pi(\ldots)$ and sign$(\ldots)$ denote permutations of the final momenta and parity of a particular permutation, finally $V_p$ is the Fourier component of the bare two-body interaction potential.

In the following we calculate $\mathcal{N}^R$ from the BE, having in mind that the distribution function at the ends of the wire are Fermi functions determined by the leads, Eq. (1). The rate of change in the number of right-moving electrons is defined as $\dot{\mathcal{N}}^R = \sum_{p > 0} \dot{f}_p = \sum_{p > 0} \mathcal{I}_p.$ Since we restrict our analysis to very short wires in which three-particle collisions are rare and thus effect of relaxation on the distribution function can be neglected, we can treat collision integral [Eq. (3)] in perturbation theory. Expanding the distribution function in Eq. (4) to the linear order in $V$ and $\Delta T$ as $f_p \approx f_p^0 + f_p^0 (1 - f_p^0) \left[ \frac{\alpha}{T} \theta(p) + \sigma \Delta T (\varepsilon_{p - p')^2} \theta(-p') \right]$, where $f_p^0 = [e^{\varepsilon_r - \mu/T} + 1]^{-1}$ is equilibrium Fermi function, we get with the help of Eq. (3)

$$\dot{\mathcal{N}}^R = 3 \sum_{\pi(123)} W^{123}_{123} \left[ \frac{\Delta T}{T^2} \left( \varepsilon_{p_1'} - \varepsilon_{p_3} + \varepsilon_{p_2'} - \mu - \frac{eV}{T} \right) \right]$$
where $W_{123}^{1'2'3'} = W_{123}^{1'2'} p_1^0 p_2^0 f_{p_3}^0 (1-f_{p_3}^0) (1-f_{p_{2'}}^0) (1-f_{p_{1'}}^0)$.

The notation $\sum^{++-}$ means $\sum_{p_1>0, p_2>0, p_3<0}$, etc. In deriving Eq. [7] we have used the symmetry of the scattering rate under: (i) the interchange of all primed and unprimed indices; (ii) a pairwise exchange and (iii) the inversion of all momenta $p_i \rightarrow -p_i$. In the course of the derivation one can see that in order to have $N^R \neq 0$ the number of right-moving electrons must change after the collision. In Eq. [7] we have kept only the leading contribution to $N^R$, namely an electron backscattered by one right mover and one left mover which preserve their direction of motion after the collision. This particular scattering process is compatible with the conservation laws, it involves only a single state at the bottom of the band, and it has all final scattering states in the vicinity of the initial ones. At low temperatures we expect $N^R \propto e^{-\mu/T}$ which stems from the Fermi occupation factors for the particle at the bottom of the band.

Scattering amplitudes. Let us look closer at the kinematics of backscattering processes. In general three-particle scattering amplitude [Eq. [4]] depends on all $p_i$ and $p_{i'}$. However, for the momentum configuration under consideration [see Fig. 2] $p_{2(2')}$ lies near the bottom of the band, while $p_{1(1')}$ and $p_{3(3')}$ lie near the right and left Fermi points, all within a small range $|p_i - p_{i'}| \sim T/v_F$ set by temperature $T \ll \mu$. We thus argue that, up to small corrections in $\delta p \sim T/v_F \ll p_F$, one can replace $p_1 \approx +p_F$, $p_2 \approx 0$ and $p_3 \approx -p_F$ in the expressions of Eqs. [1]–[6], which then becomes a function of $q_i = p_i - p_F$ only $A_{123}^{1'2'3'} \rightarrow A(q_1, q_2, q_3)$, with $q_i$ being momenta transferred in a collision. Furthermore, using the approximate forms of dispersion relation near Fermi points $\varepsilon_{p_i} - \varepsilon_{p_{i'}} \approx v_F q_i$ and $\varepsilon_{p_{i'}} - \varepsilon_{p_{i''}} \approx -v_F q_3$ the conservation laws allow one to express $q_1$ and $q_3$ in terms of $p_2$ and $p_{2'}$ as $q_{1,3} = p_2 - p_{2'} \mp q_{2,2'}$. One readily sees that $q_1 \approx q_3 \approx -q_2/2$ up to small contributions of order $p_2/p_F \ll 1$, such that amplitude effectively depends on a single momentum, $A(q_2) \equiv A(-q_2/2, q_2, -q_2/2)$. Applying these observations to Eq. [4] we can expand amplitude for $|q_2| \sim T/v_F \ll p_F$ to the leading order and obtain

$$A(q_2) = \frac{1}{2\mu L^2} \{V_{2F}^2 V_{q_2/2}^2 - V_{2F}^2 V_{q_2}^2 - V_{2F}^2 V_{q_2}^2 - 2p_F V_{2F}^2 (V_{q_2}^2 - V_{2F}^2) \}$$

There are several useful checks we can make at this point. It is known from the context of *integrable* quantum many-body problem that for some two-body potentials, scattering of the particles of $N$-body system factorizes into a sequence of two-body collisions. In the context of this work, it means that three-particle scattering for the integrable potentials may result only in permutations within the group of three momenta of the colliding particles; all other three-particle scattering amplitudes must be exactly zero for such potentials. We have checked explicitly that the three-particle scattering amplitude in Eq. [4] vanishes for the several special potentials; for the contact interaction, $V_p \propto |p|$, for the Calogero-Sutherland model, $V_p \propto |p|^2$, and for the fermionic equivalent of the Lieb-Liniger model, $V_p \propto 1 - p^2/p_0^2$. Of course, the simplified version of the amplitude [Eq. [8]] obtained for a specific scattering process that we need [Fig. 2] also vanishes for these potentials. For generic non-integrable models the three-particle amplitude is not expected to be zero. In the following we take regularized Coulomb potential $1/|x| \rightarrow 1/\sqrt{x^2 + 4\Lambda^2}$ where cutoff $\Lambda = d$ is the distance to the screening gate at large $x$, while $\Lambda = w$ is the wire width at small $x$. Thus, the Fourier transformed component of the interaction reads $V_p = (2e^2/\kappa) [K_0(2|p|w/h) - K_0(2|p|d/h)]$, where $K_0(z)$ is Bessel function. In particular, for the case of screened Coulomb interaction, when $p \ll h/d \ll h/w$, we find from Eq. [6]

$$A(q_2) = -3(\ln 4 - 1)(2e^2/\kappa)^2 \lambda_a(k_Fd)/\mu L^2$$

where $\lambda_a(x) = x^4 \ln(1/x)$, while for the unscreened case, when $h/d \ll p \ll h/w$, we obtain

$$A(q_2) = (3/4)(2e^2/\kappa)^2 \lambda_a(k_Fw) \ln(p_F/|q_2|)/\mu L^2$$

where $\lambda_a(x) = x^2 \ln(1/x)$. Note, these forms of the amplitude require to keep all the exchange terms in Eq. [4].
Unlike in the previous studies\textsuperscript{23}, which assumed interaction with sharp momentum cut-off, keeping only direct term in the amplitude would give sub-leading contribution, namely $\mathcal{A}_{\text{dir}}(q_2) \propto q_2^2 \ln |q_2|$. Indeed, comparing this to the exchange contribution in Eq. (10) and using $q_2 \sim T/v_F$ one estimates $|\mathcal{A}_{\text{dir}}|/|\mathcal{A}_{\text{exc}}| \sim (T/\mu)^2 \ll 1$.

Results and discussions. Having determined scattering amplitude we are prepared to compute the rate of change of number of right-movers due to electron backscattering. In accordance with our earlier kinematic observations we approximate conservation laws implicit in the scattering rate $W_{123}^{\varepsilon \varepsilon \varepsilon}$ of Eq. (7) as $\delta(E-E')\delta_{p,p'} \approx \frac{1}{v_F} \delta(q_1 - q_3)\delta_{2q_1+q_2=0}$, which removes $q_2$ integrals. We can also complete $p_1,3$ integrals exactly

\begin{equation}
\sum_p f_p^0 (1 - f_{p+q}^0) = \frac{L}{2\hbar} \sinh \frac{\pi q}{2T} e^{\pm v_F q/2T}
\end{equation}

for $p$ near $\pm p_F$. This gives all together

\begin{equation}
\delta N^R = -\frac{3L^3}{16\pi^2 \hbar v_F} \left[ \frac{\mu \Delta T}{T^2} + \frac{eV}{T} \right] \sum_{p_2 > 0, q_1} \frac{q_1^2 |\mathcal{A}|^2 M(p_2, q_1)}{\sin^2 \frac{q_2}{2T}} \tag{12}
\end{equation}

where characteristic $p_2$ lies at the bottom of the band we can also approximate $f_{p_2}^0 (1 - f_{p_2-2q_1}^0) \approx e^{-\mu |T|} \left[ 1 + \frac{2q_2}{2m(q_2)T} \right]$ to the leading order at small temperatures, since $\frac{(T/v_F)^2}{\mu |T|} \sim (T/\mu) \ll 1$. Then, $p_2$ summation gives factor of $(2Lq_1/\hbar) e^{-\mu |T|}$ and remaining $q_1$ integration in Eq. (12) is straightforward. As a result, we find from $\delta G = e\delta N^R / V$ for the case of screened Coulomb interaction with the amplitude taken from Eq. (3), the interaction-induced correction to conductance

\begin{equation}
\delta G = -c(\ell_e^2/h)(k_F L)r_s^2 \lambda_s^2(k_F d)(T/\mu)^3 e^{-\mu |T|}
\end{equation}

where $r_s = e^2/\hbar v_F \kappa$ and $c = \frac{32\pi^2}{3\pi^2}$, while from $\delta S = -h\delta N^R / \Delta T$ correction to thermopower (restoring Boltzmann constant $k_B$)

\begin{equation}
\delta S = c(k_B/e)(k_F L)r_s^2 \lambda_s^2(k_F d)(T/\mu)^2 e^{-\mu |T|}
\end{equation}

Equally complete calculation for the unscreened case, with the amplitude taken from Eq. (10), gives additional logarithmic factor for conductance correction $\delta G \simeq (k_F L)^2 \lambda_s^2(k_F d)(T/\mu)^2 \ln^2 (\mu/T) e^{-\mu |T|}$ as compared to Eq. (13), and similar for the thermopower.

So far we have considered short wires when electrons propagate ballistically and experience rare backscattering. For longer wires three-particle collisions become more frequent and simplistic treatment of the collision integral in perturbation theory is not appropriate. For such longer wires electrons reach the state of partial equilibration where backscattering is achieved by means of multiple collisions at the bottom of the band\textsuperscript{31,30} While traversing form the right to left Fermi points electrons perform a random walk in momentum space with small momentum step $\delta p \sim T/v_F < p_F$ at every collision. For such diffusive type motion collision integral of the BE can be reduced to much simpler differential Fokker-Planck form. Corresponding calculation\textsuperscript{31} in this regime shows that interaction corrections to conductance and thermopower remain exponentially suppressed, namely $\delta G = -(c^2/h)(L/\ell_1) e^{-\mu |T|}$, where $\ell_1 = \sqrt{8\pi m T^3}/B$ and $B \propto r_s^2 \lambda_s^2(T/\mu)^5 k_{\text{FFPP}}^2$ is diffusion coefficient in momentum space. For even longer wires, $L > \ell_{eq} \propto e^{\mu |T|}$, small probability of scattering at the bottom of the band is compensated by the large phase space and effects of electronic equilibration in a wire are nonperturbative. When electrons are fully equilibrated then wire conductance saturates to the length and interaction strength independent universal value $\delta G = -(c^2/h)(\pi^2 T^2/12\mu^2)$, while thermopower grows from being exponentially small $\propto e^{-\mu |T|}$ to a power law $S = \pi^2 k_B T/6e\mu$, see Refs. [18][10] for details\textsuperscript{31}

Summary. We have calculated the leading order interaction corrections to the transport coefficients of a clean single-particle short 1D quantum wire. Our main results are Eqs. (13–14) for conductance and thermopower. The dominant scattering mechanism is three-particle collisions which are not captured by the ideal LL model. Note however that in the multi-mode case already two-particle inter-channel scattering gives correction to conductance.\textsuperscript{23} We have also emphasized crucial role of exchange terms in the three-particle amplitude Eq. (3) which was not discussed in the previous studies.\textsuperscript{23} Finally, our work also points on the open questions. First, it is interesting to explore the consequences of the exchange contributions in the spinfull case. Second, it is of great interest to understand the fate of interaction corrections in the limit of strong interactions which must simultaneously cope with the nonequilibrium effects.

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18 For the numerical estimates one can use $v_F \sim 10^5$ m/s, $k_F \sim 10^8$ m$^{-1}$, $\kappa \sim 10$ and $w \sim 10$ nm. This corresponds to $\mu = \hbar k_F v_F / 2 \sim 3$ meV, $k_F w \sim 1$ and $e^2/\hbar v_F \kappa \sim 1$. For temperatures $T \sim 1 \div 5$K the interaction-induced correction to conductance of fully equilibrated wire is $\delta G / G \sim 10^{-3} \div 10^{-2}$. The effect of interaction on the thermopower is much more pronounced $S \sim (k_B / e) \times (0.03 \div 0.15)$. 