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Impurity induced current oscillations in one-dimensional conductors

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Abstract. We study theoretically electronic transport through an isolated local defect in a 1D conductor described in terms of the Luttinger liquid, and show that the well-known tunneling regime of electronic transport leading to power-law I-V curves takes place only in the limit of small voltage. At voltages exceeding a threshold value a new dynamic regime of transport starts in which the DC current $I$ induces AC oscillations of frequency $f = I/e$. In gated quantum wires where interaction between electrons is short-ranged, generation linewidth is small provided the inter-electronic repulsion is strong enough, otherwise a wide-band noise is generated. In case of long-range Coulomb interaction generation is coherent at any interaction strength. The effect is related to interaction of the current with Friedel oscillations of the electronic density around the impurity. Manifestations of the effect resemble the Coulomb blockade and the Josephson effect. Oscillations of the electric current are accompanied by spin current oscillations. The results are related to semiconducting quantum wires, metallic atomic chains, carbon nanotubes, graphene nanoribbons and others.

Basic electronic properties of three-dimensional (3D) solids are usually well described within Landau’s Fermi-liquid picture. This is not the case in 1D systems where interaction is always strong. In 1D systems of interacting electrons single-electron quasi-particles (electrons and holes) do not exist, the only low energy excitations are charge and spin collective modes with a sound-wave-like spectrum. These excitations form the Luttinger liquid (LL) that is an alternative to Fermi liquid in 1D (for a review see Ref. [1]). Inter-electronic interaction greatly affects electronic transport in conducting 1D systems. In particular, isolated impurities form effectively large barriers in 1D systems with repulsive inter-electronic interaction and strongly suppress conductivity which is reflected in power-law dependences of conductivity on voltage and/or temperature [1]. This was confirmed experimentally in various 1D systems, including carbon nanotubes [2] and semiconductor quantum wires [3]. This effect was described in terms of macroscopic tunneling between different minima of an inclined by external bias periodic potential of interaction of the electronic system with the impurity. The periodic potential is associated with Friedel oscillations induced by impurity. We have shown recently [4] that the power-law regime takes place only in the limit of small enough currents/voltages, while above a threshold voltage a new dynamical regime starts in which current increases rapidly and the DC current is accompanied by oscillations with the washboard frequency $f = I/e$. This regime takes place when applied voltage exceeds a threshold value corresponding to the slope at which the system can roll out from the minimum of the washboard potential renormalized by fluctuations. The effect is induced by the inter-electronic repulsion and cannot be found by means of an approach.
based on non-interacting electrons. Theoretical study of the effect is complicated by strong fluctuations that in many respects determine behavior of 1D systems. The approach of ref. [4] is strict in the limit of strong inter-electronic repulsion, when fluctuations at the impurity site are not large, while for the general case the Gaussian model has been used that is not justified strictly. Here we study the effect in the limit of large voltages/currents, where non-Gaussian part of fluctuations is small. This enabled us to calculate I-V curves and generation linewidth strictly.

For brevity we consider first the response of a spinless repulsive LL to an external DC voltage at zero temperature using the Tomonaga-Luttinger model [1] with short range interaction between electrons characterized by a constant $K_\rho < 1$. The short-range interaction describes gated quantum wires where the long-range part of the interaction is screened by 3D gate electrodes. At the end we will discuss essential modifications induced by spin, the long-range Coulomb interaction, and finite temperature.

We consider a 1D conductor with impurity at $x = 0$ and apply boundary conditions [5] derived for a wire adiabatically connected to ideal Fermi-liquid reservoirs at $x = \pm L/2$ with voltage difference $V$. We start with the Hamiltonian

$$\hat{\mathcal{H}} = \int dx \left\{ \frac{h \pi v_F}{2} \left[ \hat{\Pi}^2 + \frac{1}{\pi^2 K_\rho^2} (\partial_x \hat{\Phi}_\rho)^2 \right] - \frac{1}{\pi} W_i \delta(x) \cos 2\hat{\Phi}_\rho \right\}$$

(1)

that includes the standard bosonized Tomonaga-Luttinger (TL) Hamiltonian in written in terms of the bosonic (plasmon) displacement field $\Phi_\rho(t, x)$, and the impurity term with strength $W_i$ related to $2k_F$-matrix element of the impurity potential [1]. Time and coordinate derivatives of $\Phi_\rho(t, x)$ determine the operators of current, $\hat{I} = (e/\pi) \partial_t \hat{\Phi}_\rho$, and charge density, $\hat{\rho} = (e/\pi) \partial_x \hat{\Phi}_\rho$.

Commuting $\Phi_\rho$ with the Hamiltonian we derive the equation of motion for the Heisenberg operator

$$\left( v^2 \partial_x^2 - \partial_t^2 \right) \hat{\Phi}_\rho(t, x) = \frac{2v_F}{\hbar} W_i \sin 2\hat{\Phi}_\rho(t) \delta(x),$$

(2)

where $\Phi_\rho(0) \equiv \Phi_\rho(t, x = 0)$, and $v = v_F/K_\rho$ is the velocity of plasmons.

In ref. [4] we considered the limit of a long conducting channel with the length much larger than the damping length of plasmon excitations. Now we consider a short channel, so we cannot neglect reflections of current pulses generated at the impurity from the contacts.

Using Eq. (2) with boundary conditions at the contacts we express operator $\Phi_\rho(t, x)$ in terms of $\Phi_\rho(0)$ and find equation of motion for the expectation value $\Phi_\rho(t) = \langle \Phi_\rho(t) \rangle$:

$$\partial_t \Phi_\rho(t) + \int_0^\infty dt' Z(t - t_1) \langle \sin 2\Phi_\rho(t_1) \rangle = \frac{eV}{2\hbar}, \quad Z(t) = \int e^{-i\omega t} d\omega \frac{W_i K_\rho (1 - iK_\rho \tan \frac{\omega L}{2\hbar})}{h(K_\rho - i \tan \frac{\omega L}{2\hbar})}. \quad (3)$$

The non-linear term in Eq. (3) depends on fluctuations, $\langle \sin 2\Phi_\rho(t_1) \rangle = \langle \cos 2\hat{\Phi}_\rho \rangle \sin 2\hat{\Phi}_\rho$. Correlation function of fluctuations can be calculated from Keldysh Green’s function $D^K = -i\langle \{ \delta \hat{\Phi}_\rho(t), \delta \hat{\Phi}_\rho(t') \} \rangle$. This function can be expressed via retarded and advanced Green’s functions $D^{R(A)}(\omega, \omega') = \pm i\theta(\omega - \omega')D^{R(A)}(\omega, \omega')$ by relation of their Fourier transforms, $D^K(\omega, \omega') = D^R(\omega, \omega')f(\omega) - f(\omega)D^A(\omega, \omega')$, where $f$ is related to the distribution function of bosonic excitations $N(\omega)$, $f(\omega) = 1 + 2N(\omega)$. In the equilibrium state $N(\omega)$ is the Planck distribution function. At low temperatures, smaller than all characteristic energies of the system, one can neglect contribution of thermally excited excitations and $D^K$ can be expressed via the retarded and advanced functions.

Now we derive equations of motion for the retarded and advanced Greens functions of fluctuations. This can be done in a standard way multiplying Eq. 2 by $\Phi_\rho(t', x')$ from the
left and from the right, and combining them in order to obtain corresponding Green’s function after averaging. Then using the Fourier transformation we express Greens functions at the impurity site and get rid of the coordinate dependence of Green’s function. After that we subtract expectation values and obtain equations of motion for $D^{R(A)}$. The equation for $D^R$ reads
\[
\partial_t D^R(t,t') + \frac{1}{\hbar} W_l K_\rho D^R(t,t') = -\frac{\pi K_\rho}{2} \delta(t-t'),
\]
where $D^R_s(t,t') = i\theta(t-t') \left[ \sin 2\Phi_\rho(t), \delta\Phi_\rho(t') \right]$. Eq. (4) is not close since it contains $D^R_s$. The latter can be easily related to $D^R$ when fluctuations are Gaussian. In the Gaussian model the cosine term is substituted by self-consistent quadratic term $\cos 2\delta\Phi_\rho \rightarrow e^{-2(\delta\Phi_\rho^2)}/2(\delta\Phi_\rho^2)$). We calculate $D^R_s$ with full Hamiltonian (1), considering difference between cosine terms and its self-consistent harmonic approximation perturbatively, and find that non-Gaussian terms decay at large voltages, $V \gg V_T \sim (W_l/e) \left( \frac{K_\rho^2 W_l}{\Lambda} \right)^{\frac{1}{2-K_\rho}} \sqrt{1-K_\rho}$ (here $\Lambda \sim p_F v$ is a large cut-off energy of the TL model), and become a small correction to the Gaussian part of correlation functions. Here $V_T$ is the threshold voltage above which the dynamical regime of transport starts, it is smaller than impurity potential $W_l$ due to quantum fluctuations [4].

Thus considering the limit of large voltages we can use the Gaussian approximation for fluctuations and relating $D^R_s$ to $D^R$ we obtain close equation for $D^R$. Then this equation and similar equation for the advanced Green’s function can be solved analytically at $V \gg V_T$. The solutions are
\[
D^{R(A)} = -\frac{\pi K_\rho}{2} \theta[\pm(t-t')] e^{\mp 2W_l K_\rho \int_{t_1}^{t} C(t_1) dt_1}, \quad C(t) \equiv e^{-2(\delta\Phi_\rho^2(t))} \cos 2\Phi_\rho(t).
\]
This gives us
\[
\langle \delta\Phi(t) \delta\Phi(t') \rangle = \frac{K_\rho}{4} \left[ \int_{t-t'}^{\infty} dt_1 e^{-\frac{2}{\hbar} W_l K_\rho \int_{t_1}^{t_2} C(t_1) dt_1} + \int_{t'-t}^{\infty} dt_1 e^{-\frac{2}{\hbar} W_l K_\rho \int_{t_1}^{t_2} C(t_1) dt_1} \right].
\]
Eq. (6) must be solved self-consistently with (3) in order to find DC and AC currents and spectrum of fluctuations. For large voltages, $V \gg V_T$, it is not difficult to find analytical solutions perturbatively and to calculate current $I = (e/\pi) \langle \partial_t \Phi_\rho \rangle$ and its correlation function.
\[
I = I + I_{ac} \sin \omega_0 t, \quad I = V G_0 - I_{nl}, \quad \omega_0 = 2\pi f = \frac{2\pi I}{e} \approx \frac{eV}{\hbar},
\]
\[
I_{ac} \propto \frac{G_0 V_T \left( \frac{K_\rho^2 V_T}{V} \right)^{\frac{1}{2-K_\rho}}} {\sqrt{\sin^2 \frac{\omega_0 L}{2v_F} + K_\rho^2 \cos^2 \frac{\omega_0 L}{2v_F}}}, \quad I_{nl} \propto K_\rho V_T G_0 \left( \frac{K_\rho^2 V_T}{V} \right)^{\frac{1}{2-K_\rho}} \tan^2 \frac{\omega_0 L}{2v_F} + K_\rho^2
\]
\[
\langle \hat{I}(\omega) \hat{I}(-\omega) \rangle \propto \frac{e G_0 V_T K_\rho^2 (1-K_\rho)} {\sin^2 \frac{\omega_0 L}{2v_F} + K_\rho^2 \cos^2 \frac{\omega_0 L}{2v_F}} \left( \frac{eV}{\hbar |\omega - \omega_0|} \right)^{1-2K_\rho}
\]
where $G_0 = e^2/\hbar$ is the conductance quantum. These results are valid at $K_\rho < 1/2$, that is for strong enough inter-electronic repulsion. In the last expression we skipped a small term proportional to $\delta(\omega - \omega_0)$ that gives a negligible contribution to the fluctuation spectrum. At larger values of $K_\rho$ the Gaussian model yields that the pronounced maximum at $\omega = \omega_0$ in the fluctuation spectrum is absent and a wide-band noise is generated. For gated quantum wires the interaction parameter $K_\rho$ can be estimated roughly as
\[
K_\rho \sim \sqrt{\frac{\hbar v_F e}{e^2}} \approx 0.2 \sqrt{\frac{e v_F (cm/s)}{10^7}}.
\]
where $\epsilon$ is a background dielectric constant.

Oscillations of currents in Eqs. (7-9) as function of voltage are induced by reflections of current pulses from the contacts. The oscillatory dependence of conductivity versus voltage was, presumably, observed in [6]. Note that the shape of the oscillations will be different if the impurity is not situated at the middle of the wire. Note also that we assumed the regime of the fixed voltage bias at the contacts. Such a regime takes place if a small impedance $ZG_0 \ll 1$ is connected to the wire either in parallel or in series. In general case the results (7-9) would be modified.

For the case of long-range Coulomb interaction the results are qualitatively similar, the most important difference is that the maximum maximum at $\omega = \omega_0$ in the fluctuation spectrum is always present, that is at any values of parameter $\epsilon^2/(\hbar v_F e)$ measuring the strength of the Coulomb interaction.

In case of finite temperatures, modifications of the results (7-9) are negligible at temperatures $T \ll T_c$. The main modification is that thermal fluctuations change shape of the line at $|\omega - \omega_0| \ll T$, singularity of the peak being washed out and becoming approximately of Lorentzian form $\sim (G_0 W_i)^2 K^3 \omega_T^2/[(\pi K^2 \rho_T)^2 + (\omega - \omega_0)^2]$, where $\omega_T = k_B T/h$. At temperatures $T > T_c$ the effect of generation disappears because of thermal destruction of the impurity pinning.

Now we discuss what happens in the system of electrons with spin. In the spinful LL the impurity Hamiltonian contains contribution due to the spin phase field, $\Phi_\sigma$, and $\cos 2\Phi_\rho$ in (1) must be substituted for $\cos \sqrt{2}\Phi_\rho \cos \sqrt{2}\Phi_\sigma$ [1]. This leads to partial violation of the spin-charge separation and modifies the results. The threshold voltage becomes smaller than in the spinless case due to spin fluctuations. For a spin-independent interaction $L_{\sigma} = 1$ it reads

$$V_T \sim W_i \left( \frac{W_i}{h} \right)^{1/(1-2K_\rho)} K_{\rho}^{1+K_\rho} K_{\rho}^{1+K_\rho} K_{\rho}^{1+K_\rho}$$

Non-linear term in equation (2) for the charge phase is also changed, $\sin 2\Phi_\rho \rightarrow \sin \sqrt{2}\Phi_\rho \cos \sqrt{2}\Phi_\sigma$. Further, we have to solve equation of motion for the spin phase that can be obtained from (2) and (3) by exchanging subscripts $\sigma$ and $\rho$ and putting $K_{\sigma} = 1$. In the limit of small $K_{\rho}$ the characteristic time of variations of the spin phase is much smaller than that for the charge phase. Using this fact we can study phase evolution in the limit $V_T \ll V \ll V_T/K_\rho$. Then the phase $\Phi_\rho$ increases almost linearly, $\Phi_\rho \approx \frac{V_V}{\sqrt{2e}} t$, while $\Phi_\sigma$ stays, firstly, practically constant and equal to $2\pi n/\sqrt{2}$, and then, when $\cos \sqrt{2}\Phi_\rho$ changes its sign, $\Phi_\sigma$ rapidly changes by $\pm \pi/\sqrt{2}$ since the previous state of $\Phi_\sigma$ becomes unstable. This variations of the spin phase means generation of pulses of spin current corresponding to transport of one spin through the impurity, the time average of the spin current being equal to zero. However, if the wire is placed in a gradient of the magnetic field then a preferential direction for the spin current would appear resulting in a DC component of the spin current.

In conclusion, we predict the new regime of electronic transport through an impurity or a local defect in 1D conducting channel. The effect is induced by the inter-electronic repulsion. Manifestations of the effect resemble the AC Josephson effect and Coulomb blockade. The results are applicable to semiconducting quantum wires, metallic atomic chains, carbon nanotubes, graphene nanoribbons and other 1D conducting systems.

References