Negative dynamic conductivity of ballistic quantum wires

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We develop a theory of the admittance of a quantum wire in the presence of an applied DC bias voltage, which under conditions of ballistic transport of electrons leads to a population inversion of the electronic states in the wire. We show that for a sufficiently strong inversion the real part of the admittance (the dynamic conductivity) becomes negative over a certain frequency interval. The admittance is determined both by electrons injected from the cathode and drifting through the wire to the anode and by electrons entering the wire from the anode and returning once again to that electrode. The negative dynamic conductivity is caused by the injected electrons. The electron flux from the anode creates a positive conductivity and has a marked effect on the shape of the frequency dependence of the admittance, the value of the negative conductivity, and its dependence on applied voltage. We establish that there are two basic regimes of negative dynamic conductivity: 1) in long wires, where the admittance oscillates with increasing frequency and the dynamic conductivity becomes negative at frequencies determined by the drift time of electrons in the wire, and 2) in short wires, where the dynamic conductivity becomes negative near a frequency equal to the lowest energy of the band of states occupied by the injected electrons above the bottom of the conduction band.
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1. INTRODUCTION

In recent years, interest in the high-frequency conductivity of semiconducting quantum structures in the ballistic regime has grown rapidly, driven both by attempts to identify overall regularities of the dynamic conductivity (similar to the Landauer formula),[1–3] and by the promise of applications related to the detection and generation of electromagnetic radiation in the terahertz range.[4–6] In particular, the quantum ballistic wire, which is a convenient system for implementing quantum interference phenomena, has attracted much attention. The admittance of a quantum wire has an oscillatory dependence on frequency, caused by spatial resonances of one-dimensional charge waves in the wire.[8] These resonances are the result of interference between electron waves at the fundamental frequency and "sideband" (quasienergy) waves. An interesting feature of these systems is that the real part of the admittance, which characterizes the energy loss, can vanish at certain frequencies, indicating that electrical instability could occur under nonequilibrium conditions. In Ref. 9, Fedichkin and V'yurkov studied the classical motion of electrons in a wire and showed that in the presence of a constant applied voltage it is possible for negative dynamic conductivity to appear, connected with the classical drift instability, which has been known in vacuum electronics for thirty years.[10,11]

The goal of this paper is to discuss quantum mechanically the admittance of a ballistic quantum wire in the presence of a DC bias voltage, and to clarify the conditions under which negative dynamic conductivity can appear. In Sec. 2 we describe our formulation of the problem. In Sec. 3 we study the admittance of a wire with a distribution of electron potential energy along its length that is smooth (on the scale of the electron Fermi wavelength), and analyze the conditions for the appearance of negative dynamic conductivity. In this analysis we take into account the fact that the admittance is determined by the sum of currents created by electrons injected from the cathode and electrons entering into the wire from the anode. Both of these currents give comparable contributions to the total current through the wire, but the negative dynamic conductivity is caused only by the first. The flux of electrons from the anode determines the form of the frequency dependence of the admittance to a significant degree, and strongly affects the frequency at which the largest negative conductivity is achieved. The mechanism of negative dynamic conductivity is analyzed in more detail in Sec. 4, based on a model in which we treat only one flux of electrons from the cathode to the anode in a certain band of energies above the bottom of the conduction band. Here we discuss the contributions to the total current from the upper and lower energy sidebands, which are connected with absorption and emission of a photon with energy $\hbar\Omega$, respectively (where Ω is the external field frequency). The dynamic conductivity arising from the upper sideband is always positive, while that arising from the lower sideband is negative. It is possible for the wire to exhibit negative dynamic conductivity, connected with the fact that the partial conductivities arising from the upper and lower sidebands are functions of frequency. We consider two basic cases: 1) the long-wire case (long compared to the electron wavelength), where both conductivities are oscillatory functions of frequency due to spatial charge-wave resonances, and 2) the short-wire case, where the negative dynamic conductivity arising from the lower sideband has a sharp maximum connected with an increase in the one-dimensional density of states of the wire as the energy approaches the bottom of the conduction band.

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2. STATEMENT OF THE PROBLEM

Let us consider a quantum wire of length L that joins two highly conducting regions (electrodes), to which we apply a DC bias voltage V_a and an AC voltage $V_1 \cos(\Omega t)$. The electrodes are reservoirs in which electrons are in a state of thermodynamic equilibrium. While in the wire, electrons cannot undergo collisions. We use a one-dimensional model of the wire, i.e., we will treat the motion of electrons along the wire by assuming that it is decoupled from the transverse motion. This model is easily justified in the case where the width of the wire varies smoothly as we approach the electrodes.[12] In this case the energy of transverse quantization enters in as potential energy in the equation of longitudinal motion. If the width of the wire varies rapidly, then although the one-dimensional model, strictly speaking, can no longer be used, it nevertheless leads to qualitatively correct results. We can convince ourselves of this by calculating the static conductivity of the wire in the one-dimensional model and comparing it with the results of calculations by Kirchenov[13] for a two-dimensional model.[1)]

Thus, we write the Schrödinger equation in the form

$$i\hbar \frac{\partial \psi}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}-U_0(x)\psi-H_1\psi=0. \tag{1}$$

Here $U_0(x)=U_{bi}(x)-eV_a(x)$, where $U_{bi}(x)$ is the "built-in" potential of the wire, which includes both the potential caused by the electrodes and the quantization energy for transverse motion; $V_a(x)$ is a DC potential connected with the applied DC voltage. H_1 is the Hamiltonian for the interaction of an electron with the AC electric field E_1, for which it is convenient to use the vector potential

$$H_1=\frac{e\hbar V_1}{2m(\Omega+i0)}\left[F(x)\frac{\partial}{\partial x}+\frac{1}{2}F'(x)\right]e^{-i\Omega t}-\text{c.c.}, \tag{2}$$

where $F(x)=E_1(x)/V_1$. The voltage V_1 is assumed to be small ($eV_1 \ll \hbar\Omega$), so that in solving Eq. (1) it is enough to take into account processes with emission or absorption of only one photon with energy $\hbar\Omega$.

The electron transport current $j(x,t)$, which is obtained by solving Eq. (1), depends on the coordinate x, because by virtue of the continuity equation $\operatorname{div} \mathbf{j}=-\partial|\psi|^2/\partial t \neq 0$. This also implies that a nonstationary charge density appears in the wire, which propagates in the latter in the form of traveling waves.[8] The total current, which remains constant along the wire, is also the current detected in the external circuit. It consists of a sum of transport current and displacement current; the latter in turn consists of two components. One is connected with the nonstationary charge in the wire; it is this current that provides continuity of the current. The other, which is connected with charges at the electrodes induced by the external source, consists of the usual capacitive current. The current detected in the external circuit is expressed in terms of the conduction current and the interelectrode capacitance C by using the Shockley theorem[14,11]:

$$j_{\text{ext}}(t)=\frac{1}{V_1}\int_0^L dx j(x,t)E_1(x)+C\frac{dV_1}{dt}. \tag{3}$$

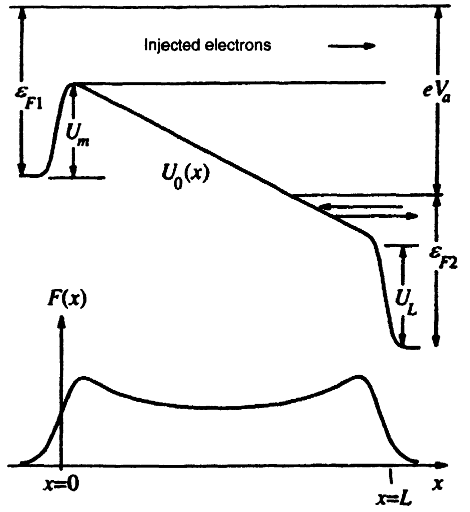

FIG. 1. Energy diagram of a quantum ballistic wire and plot of the distribution of AC electric field $F(x)$.

For the AC voltage $V_1 \exp(-i\Omega t)$, we write Eq. (3) in the form

$$j_{\text{ext}}(\Omega)=\left[\frac{e^2}{h}Y(\Omega)-i\Omega C\right]V_1,$$

where $Y(\Omega)$ is the dimensionless admittance of the quantum wire.

In calculating $Y(\Omega)$ we will assume that the built-in potential $U_{bi}(x)$ is a known function of x, determined by solving the steady-state problem. The potential $U_{bi}(x)$ depends on transverse quantization subband under discussion. In this paper we will discuss the conductivity arising from only a single lowest subband. The AC field $F(x)$ is determined, generally speaking, by charges both at the electrodes and in the wire itself. For simplicity we will assume, in this paper, that the charge on the electrodes is considerably larger than in the wire; therefore $F(x)$ is determined only by the geometry of the electrodes, and consequently can be considered a known function. For this it is necessary that the capacitance C be sufficiently large: $\Omega C \gg (e^2/h)|\operatorname{Im} Y(\Omega)|$.

3. ADMITTANCE OF A WIRE WITH A SMOOTH POTENTIAL

Let us consider a wire whose width varies so smoothly over an electron wavelength as we approach the electrodes that we may use the quasiclassical approximation to solve Eq. (1). The shapes of the potential curves $U_{bi}(x)$ and the AC field $F(x)$ are shown in Fig. 1. The electric current is created both by electrons injected from the cathode and drifting through the wire to the anode reservoir and by electrons that enter the wire from the anode. For a sufficiently large voltage ($eV_a > \varepsilon_{F1}-U_m$) all the electrons entering from the anode are reflected within the wire and pass back out into the anode reservoir.

Let us consider the contribution of these two electron fluxes to the total current. In the contact reservoirs, if they are sufficiently large, the thermodynamic equilibrium of the electrons is essentially undisturbed by the current passing through it. Under these conditions the wave functions of electrons entering the wire from the cathode and from the anode are not coherent, and consequently the currents connected with them can be treated separately.

3.1 Admittance of injected electrons

The wave function of electrons injected from the cathode has the form

$$\psi_0(x,t)\approx\sqrt{\frac{k_0}{k(x)}}\exp\left[iS(x)-\frac{i\varepsilon t}{\hbar}\right], \tag{4}$$

where $k(x)=\sqrt{2m[\varepsilon-U_0(x)]}/\hbar$, ε and m are the energy and effective mass of the electrons, $k_0=\lim k(x\to\infty)$, and

$$S(x)=\int_0^x dx'k(x').$$

When the electrons interact with the AC field in the wire, processes of absorption and emission of photons with energy $\hbar\Omega$ take place, as a result of which the wave function takes the form

$$\psi(x,t)=\psi_0(x,t)+[\psi_+(x)\exp(-i\Omega t)+\psi_-(x)\exp(+i\Omega t)]\exp(-i\varepsilon t/\hbar), \tag{5}$$

where $\psi_\pm(x)$ is determined from perturbation theory using the Hamiltonian (2):

$$\psi_+(x)=\frac{eV_1}{4\hbar\Omega}\sqrt{\frac{k_0}{k_+(x)}}\Bigg\{\exp[iS_+(x)]\times\int_{-\infty}^x dx'F(x')\frac{k_++k}{\sqrt{kk_+}}\exp[-i[S_+(x')-S(x')]]-\exp[-iS_-(x)]\int_x^\infty dx'F(x')\frac{k_+-k}{\sqrt{kk_+}}\times\exp[i[S_+(x')+S(x')]]\Bigg\}, \tag{6}$$

$$k_+\equiv k_+(x)=\sqrt{2m[\varepsilon+\hbar\Omega-U_0(x)]}/\hbar,$$

$$S_+(x)=\int_0^x dx'k_+(x').$$

The expression for $\psi_-(x)$ when $\varepsilon>U_m+\hbar\Omega$ coincides with $\psi_+(x)$ if in the latter we replace Ω by $-\Omega$, and k_+ by k_- and S_+ by S_-, respectively. For $\varepsilon<U_m+\hbar\Omega$ the lower sideband possesses a classical turning point $x=x_-$, to the left of which the quantity k_- becomes imaginary; x_- is a positive root of the equation $\varepsilon+\hbar\Omega-U_0(x_-)=0$. In this case, neglecting the effects of tunneling, which is correct for sufficiently long wires, we have

$$\psi_-(x)=-\frac{eV_1}{4\hbar\Omega}\sqrt{\frac{k_0}{k_-(x)}}\Bigg\{\exp[i\tilde{S}_-(x)]\int_{x_-}^x dx'F(x')\times\left[\frac{k+k_-}{\sqrt{kk_-}}\exp[i(S(x')-\tilde{S}_-(x'))]+\frac{k-k_-}{\sqrt{kk_-}}\exp[i(S(x')+\tilde{S}_-(x'))]\right]+(\exp[i\tilde{S}_-(x)]+\exp[-i\tilde{S}_-(x)])\times\int_x^\infty dx'F(x')\frac{k-k_-}{\sqrt{kk_-}}\exp[i(S(x')+\tilde{S}_-(x'))]\Bigg\}, \tag{7}$$

where

$$\tilde{S}_-(x)=\int_{x_-}^x dx'k_-(x')-\frac{\pi}{4}.$$

The electron conduction current at frequency Ω is determined by the interference of electron waves at the fundamental and sideband energies, and is expressed in terms of the wave functions ψ_- and ψ_+ as follows:

$$j(x,t)=\frac{ie\hbar}{2m}\left(\psi_0^*\frac{d\psi_+}{dx}-\psi_+\frac{d\psi_0^*}{dx}-\psi_0\frac{d\psi_-^*}{dx}+\psi_-^*\frac{d\psi_0}{dx}-\frac{eV_1}{\hbar\Omega}\psi_0^*\psi_0F(x)\right)e^{-i\Omega t}+\text{c.c.} \tag{8}$$

The electric current in the external circuit, in accordance with (3), equals

$$j_{\text{ext}}=-\int_0^L dxF(x)\int_{U_m}^\infty d\varepsilon g(\varepsilon)f(\varepsilon)j(x,t), \tag{9}$$

where $g(\varepsilon)$ is the density of states in the cathode reservoir, and $f(\varepsilon)$ is the distribution function in the cathode.

Using Eqs. (6)–(9), we find the AC current connected with electrons injected from the cathode. The admittance Y_{c-a} corresponding to these electrons equals

$$Y_{c-a}=\frac{1}{4\hbar\Omega}\int_0^L dxF(x)\Bigg\{\int_{U_m}^\infty d\varepsilon\Bigg[[f(\varepsilon)-f(\varepsilon+\hbar\Omega)]\times\frac{k_++k}{\sqrt{kk_+}}\exp[i(S_+-S)]\times\int_{-\infty}^x dx'F(x')\frac{k_++k}{\sqrt{kk_+}}\exp[-i(S_+-S)]+\frac{k_+-k}{\sqrt{kk_+}}\Bigg[f(\varepsilon)\exp[-i(S_++S)]\times\int_x^\infty dx'F(x')\frac{k_+-k}{\sqrt{kk_+}}\exp[i(S_++S)]-f(\varepsilon+\hbar\Omega)\times\exp[i(S_++S)]\int_x^\infty dx'F(x')\frac{k_+-k}{\sqrt{kk_+}}\times\exp[-i(S_++S)]\Bigg]\Bigg]-\int_{U_m}^{U_m+\hbar\Omega}d\varepsilon f(\varepsilon)\times\int_{x_-}^L dxF(x)\Bigg[\frac{k+k_-}{\sqrt{kk_-}}\exp[i(S-\tilde{S}_-)]\int_{x_-}^x dx'F(x')$$

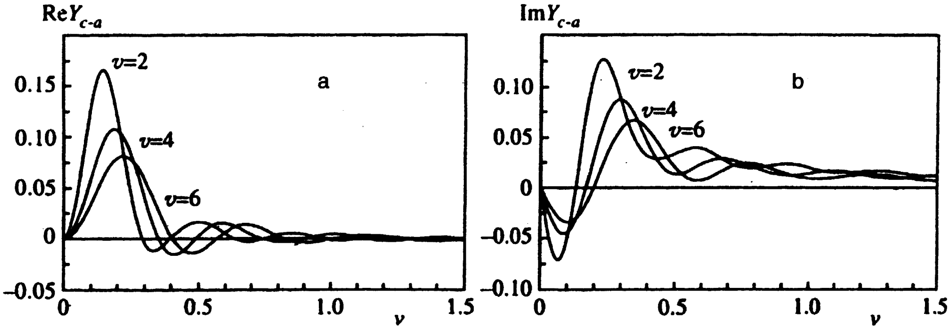

FIG. 2. Frequency dependences of the real (a) and imaginary (b) parts of the admittance associated with electrons injected from the cathode; $Lk_F=50$.

$$\times\left\{\frac{k+k_-}{\sqrt{kk_-}}\exp[-i(S-\tilde S_-)]+\frac{k-k_-}{\sqrt{kk_-}}\times\exp[-i(S+\tilde S_-)]\right\}+\frac{k-k_-}{\sqrt{kk_-}}\exp[i(S+\tilde S_-)]\times\int_{x_-}^{x}dx'F(x')\frac{k-k_-}{\sqrt{kk_-}}\exp[-i(S+\tilde S_-)]-4F(x)\times\left(\frac{\cos\tilde S_-}{k_-}+\frac{\sin\tilde S_-}{k}\right)\Bigg]\Bigg\}. \tag{10}$$

For a long wire ($Lk(\varepsilon_F)\gg 1$) we can neglect the integrals of rapidly oscillating functions that contain $S+S_\pm$ in their exponents. They are associated with sideband electron waves that propagate counter to the incident fundamental wave. Then Eq. (10) simplifies

$$Y_{c-a}\approx\int_0^L dxF(x)\int_{U_m}^{\infty}\frac{d\varepsilon}{4\hbar\Omega}[f(\varepsilon)-f(\varepsilon+\hbar\Omega)]\times\frac{k_++k}{\sqrt{kk_+}}\exp\{i[S_+(x)-S(x)]\}\times\int_0^x dx'F(x')\frac{k_++k}{\sqrt{kk_+}}\exp\{-i[S_+(x')-S(x')]\}-\int_{U_m}^{U_m+\hbar\Omega}\frac{d\varepsilon}{4\hbar\Omega}f(\varepsilon)\int_{x_-(\varepsilon)}^{L}dxF(x)\frac{k+k_-}{\sqrt{kk_-}}\times\exp\{i[S(x')-\tilde S_-(x')]\}\times\int_{x_-(\varepsilon)}^{x}dx'F(x')\frac{k+k_-}{\sqrt{kk_-}}\exp\{-i[S(x')-\tilde S_-(x')]\}.$$

At low temperatures, where the function $f(\varepsilon)$ is close to a step function of $\varepsilon_F-\varepsilon$, the integration with respect to energy in this expression essentially reduces to selecting two energy bands of width $\hbar\Omega$ near ε_{F1} and U_m. Taking into account this fact, for relatively low frequencies ($\hbar\Omega\ll\varepsilon_{F1}-U_m$) we have

$$Y_{c-a}\approx\int_0^L dxF(x)\exp\{i[S_+(x)-S(x)]\}\times\int_0^x dx'F(x')\exp\{-i[S_+(x')-S(x')]\}-\frac{1}{\hbar\Omega}\times\int_{U_m}^{U_m+\hbar\Omega}d\varepsilon\int_{x_-(\varepsilon)}^{L}dxF(x)\exp\{i[S(x')-\tilde S_-(x')]\}\times\int_{x_-(\varepsilon)}^{x}dxF(x)\exp\{-i[S(x')-\tilde S_-(x')]\}. \tag{11}$$

Further simplification of the expression for Y_{c-a} is possible if we use a specific form for the potential U_0. Thus, for the case where U_0 varies linearly with x and for $\hbar\Omega\ll eV_a$, the integrals are calculable to the end, and we obtain the following expression for the admittance Y_{c-a}:

$$Y_{c-a}(\Omega)\approx\frac{4}{v^2w^2}\left\{1+i\frac{w}{3}[\sqrt{(1+v)^3}-\sqrt{v^3}-1]-\frac{(1+iw)(1-iw\sqrt{1+v})}{w^2}\exp[iw(\sqrt{1+v}-1)]+\frac{1-iw\sqrt{v}}{w^2}\exp(iw\sqrt{v})\right\}, \tag{12}$$

where we introduce the dimensionless applied voltage $v=eV_a/(\varepsilon_{F1}-U_m)$ and dimensionless frequency $w=\hbar\Omega Lk_F/eV_a$, $k_F=\sqrt{2m(\varepsilon_{F1}-U_m)}/\hbar$. It is clear that oscillations appear in the frequency dependence of the admittance with characteristic frequencies of order $(\sqrt{v})^{-1}$ and $(\sqrt{1+v}-1)^{-1}$ that are determined by the drift times of electrons with energies close to the lower and upper energy limits of the injected electron flux. For $v\gg 1$ these frequencies are both of order $(\sqrt{v})^{-1}$, which in dimensional units corresponds to

$$\Omega\sim L\sqrt{eV_a/m},$$

i.e., the characteristic frequency is determined by the drift time of electrons in a wire with energy eV_a.

Figure 2 shows the dependence of $\mathrm{Re}\,Y_{c-a}$ and $\mathrm{Im}\,Y_{c-a}$ on frequency for three values of the applied voltage. For simplicity, we normalize the frequency in a way that does not depend on applied voltage:

$$\nu=\frac{\hbar\Omega}{\varepsilon_{F1}-U_m}.$$

The frequency normalized in this way is connected with the drift time t_0 of electrons with energies equal to the upper energy boundary of the injected flux by the following relation:

$$\nu=\frac{\Omega t_0}{Lk_F}\frac{v}{\sqrt{1+v}-1}.$$

As is clear from Fig. 2, in the presence of an applied voltage the real part of the admittance is negative near certain frequencies determined by the drift times. The imaginary part of the admittance also oscillates, and can be either capacitive or inductive in character.

3.2 Admittance of backward-flux electrons

For a sufficiently large DC voltage the flux of electrons from the anode reservoir is cut off in the wire and does not create a through-current. Therefore, it does not contribute to the current at zero frequency. However, for an AC signal the contribution of electrons from the anode reservoir to the conductivity becomes significant. The current caused by electrons entering the wire from the anode is calculated in the same way as the current of electrons injected from the cathode, using Eqs. (3), (5), and (8). The wave function of the incident electrons has the form

$$\psi_0(x)\approx\begin{cases}0, & x<x_0,\\ 2\sqrt{k_\infty/k(x)}\cos\tilde{S}(x), & x>x_0,\end{cases} \tag{13}$$

where k_∞ is the wave vector in the anode reservoir ($x\rightarrow\infty$),

$$\tilde{S}(x_0)=\int_{x_0}^{x}dx'k(x')-\frac{\pi}{4},$$

and x_0 is the turning point for the energy ε.

The sideband wave functions $\psi_\pm(x)$, taking (2) and (13) into account, have the form

$$\psi_\pm(x)=\pm\frac{eV_1}{\hbar\Omega}\sqrt{\frac{k_\infty}{k}\frac{1}{ik_\pm}}\Bigg\{\exp(i\tilde{S}_\pm)\int_{x_\pm}^{x}dx'F(x')$$
$$\times(k_\pm\cos\tilde{S}\sin\tilde{S}_\pm-k\sin\tilde{S}\cos\tilde{S}_\pm)$$
$$-\cos\tilde{S}_\pm\int_{x}^{\infty}dx'F(x')(k\sin\tilde{S}$$
$$+ik_\pm\cos\tilde{S})\exp(i\tilde{S}_\pm)\Bigg\}, \tag{14}$$

where

$$\tilde{S}_\pm(x)=\int_{x_\pm}^{x}dx'k_\pm(x')-\frac{\pi}{4},$$

and $x_\pm$ are turning points for energies $\varepsilon\pm\hbar\Omega$.

Using these wave functions, and also the fact that the currents arising from the upper and lower sidebands are expressed in terms of each other by simultaneously shifting the energy by $\hbar\Omega$ and the coordinates of the turning points by x_+-x_0, we obtain the following expression for the admittance Y_{c-a} of the backward-flux electrons:

$$Y_{a-c}=-\frac{2}{\hbar\Omega}\int_0^\infty d\varepsilon\int_{x_0(\varepsilon)}^{L}dxF(x)[f(\varepsilon)\tilde{A}(\varepsilon,x)$$
$$-f(\varepsilon+\hbar\Omega)\tilde{A}^*(\varepsilon,x)]+\frac{2i}{\hbar\Omega}$$
$$\times\int_0^\infty d\varepsilon\int_{x_0(\varepsilon)}^{x_-}dxF(x)\frac{\cos^2\tilde{S}}{k}. \tag{15}$$

Here $f(\varepsilon)$ is the distribution function in the anode reservoir, and

$$\tilde{A}(\varepsilon,x)=\frac{k\sin\tilde{S}+ik_+\cos\tilde{S}}{\sqrt{kk_+}}\exp(i\tilde{S}_+)\int_{x_0}^{x}dx'F(x')$$
$$\times\frac{k_+\cos\tilde{S}\sin\tilde{S}_+-k\sin\tilde{S}\cos\tilde{S}_+}{\sqrt{kk_+}}$$
$$+\frac{k_+\cos\tilde{S}\sin\tilde{S}_+-k\sin\tilde{S}\cos\tilde{S}_+}{\sqrt{kk_+}}$$
$$\times\int_x^L dx'F(x')\frac{k\sin\tilde{S}+ik_+\cos\tilde{S}}{\sqrt{kk_+}}\exp(i\tilde{S}_+).$$

We are most interested in the real part of Y_{a-c}, for which we have

$$\mathrm{Re}\,Y_{a-c}=\frac{2}{\hbar\Omega}\int_0^\infty d\varepsilon[f(\varepsilon)-f(\varepsilon+\hbar\Omega)]\Bigg[\int_{x_0(\varepsilon)}^{L}dxF(x)$$
$$\times\frac{k_+\cos\tilde{S}\sin\tilde{S}_+-k\sin\tilde{S}\cos\tilde{S}_+}{\sqrt{kk_+}}\Bigg]^2. \tag{16}$$

Thus, Re Y_{a-c} is always positive. If the frequency reduces to zero, then Re Y_{a-c} reduces to zero in accordance with the fact that the flux of electrons from the anode cannot cause a stationary current.

Under the same conditions used to obtain Eq. (12) for electrons injected from the cathode, Eq. (16) takes the form

$$\mathrm{Re}\,Y_{a-c}=8\left(\frac{w\cos w-\sin w}{vw^2}\right)^2. \tag{17}$$

The notation here is the same as in (12); for simplicity we set $\varepsilon_{F1}=\varepsilon_{F2}$ and $U_m=U_L$.

3.3 Total admittance

The admittance of the wire equals the sum of the partial admittances discussed above:

$$y=Y_{c-a}+Y_{a-c}.$$

Plots of the frequency dependence of the real part of the total admittance together with the partial components are shown in Figs. 3a, 3b for two values of the applied voltage. Both components of the admittance have frequency dependence of an oscillatory type with differing periods, which moreover depend on voltage. The partial admittances are the same or-

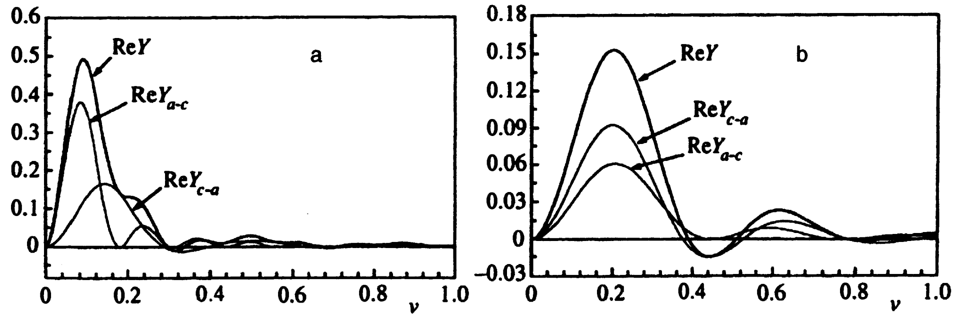

FIG. 3. Frequency dependence of the real part of the total admittance and its components connected with fluxes of electrons from the cathode and from the anode, for two values of the applied voltage: a—v=2, b—v=2; $Lk_F=50$

der of magnitude. For voltages $v \sim 1$ (Fig. 3a) the admittance Y_{a-c} is considerably larger than Y_{c-a}, but because Re Y_{a-c}, as an oscillatory function, reduces to zero when $w=w_n$ (where w_n is a root of the equation $w=\tan w$), the real part of the total admittance can become negative at those frequencies ω_n for which Re Y_{c-a} is negative. For large voltages ($v \gg 1$) the contribution of the admittance Y_{a-c} decreases rapidly (Fig. 3b) due to the repulsion of electrons from the wire into the anode reservoir under the action of the external electric field. In this case the region of frequencies in which Re $Y<0$ broadens. There also exist values of the voltage for which the oscillations of Re Y_{c-a} and Re Y_{a-c} are exactly out of phase: at the first extremum of the frequency dependence, the maximum of the negative conductivity (-Re Y_{c-a}) coincides with the maximum of the positive conductivity (Re Y_{a-c}). In this case a net negative conductivity appears at subsequent periods due to a gradually increasing phase shift between the oscillating partial conductivities.

The maximum value of the negative conductivity max(-Re Y) depends on the applied voltage. Plots of this dependence are shown in Fig. 4a. Here the thick curves show the total conductivity, while the thin ones show the partial conductivity of electrons injected from the cathode. Negative conductivity occurs at all voltages for which the model can be used ($v>1$); however, for certain of its values (specifically, those for which the partial conductivities Y_{c-a} and Y_{a-c} oscillate with nearby frequencies and are out of phase) it is very small. As a result of the oscillations of the partial conductivities, the frequency at which the largest negative conductivity is reached changes discontinuously as the voltage varies (Fig. 4b).

The analytic expressions (12) and (16) presented here for the admittance were obtained in the case of a linear distribution of potential along the wire. For an arbitrary distribution of AC potential $V_a(x)$ and an arbitrary (but smooth) constant potential the admittance can be written using Eqs. (11) and (15). In this case, numerical calculations are required to find the admittance. These calculations show that the negative dynamic conductivity is more strongly manifested the more abrupt the change in potential is near the electrodes. The characteristic frequency of oscillation of the admittance, as is clear from (11), is determined by the drift time even for an arbitrary distribution of potential.

4. ON THE MECHANISM FOR NEGATIVE CONDUCTIVITY

In this section we will discuss a somewhat simplified model that allows us to understand the mechanism of negative dynamic conductivity and the basic conditions for its appearance. As we established above, negative dynamic conductivity is caused by a flux of electrons injected from the cathode and passing through the wire while in a certain band of energies above the bottom of the conduction band. The flux of electrons from the anode into the wire possesses a positive conductivity at all times; moreover, it is ejected from the wire by the external electric field. Therefore, we will consider a simple model of the system in which the nonequilibrium electron flux density moves over a flat-bottomed conduction band in the quantum wire between two ideally conducting electrodes, to which we apply an AC voltage $V_1 \cos(\Omega t)$ with an arbitrary distribution of AC electric field along the wire on the segment from $x=0$ to $x=L$.

Calculation of the AC current leads to the following expression for the wire admittance normalized by the conductivity e^2/h:

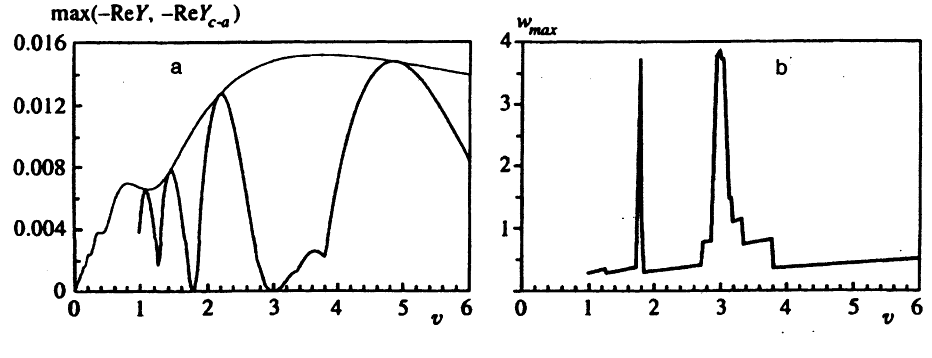

FIG. 4. a) Dependence of the maximum value of the negative dynamic conductivity (the thick curve corresponds to the total admittance, the thin curve to the admittance of injected electrons) on applied voltage. b) Dependence of the frequency at which the maximum negative conductivity is reached on voltage.

$$Y(\Omega)=\frac{1}{\hbar\Omega}\int_0^L dxF(x)\int_0^\infty d\varepsilon f(\varepsilon)[A_+(\varepsilon)+B_+(\varepsilon)-A_-^*(\varepsilon)-B_-^*(\varepsilon)], \tag{18}$$

where

$$A_\pm=\frac{(k_\pm+k)^2}{4kk_\pm}\exp[i(k_\pm-k)x]\int_0^x dx'F(x')\times\exp[-i(k_\pm-k)x'], \tag{19}$$

$$B_\pm=\frac{(k_\pm-k)^2}{4kk_\pm}\exp[-i(k_\pm+k)x]\times\int_x^L dx'F(x')\exp[i(k_\pm+k)x']. \tag{20}$$

Here $f(\varepsilon)$ is the distribution function with respect to the energy of the injected electrons; k, k_+, and k_- are wave vectors of electrons for the fundamental, upper, and lower sidebands respectively.

The real part of the admittance can be written in the form

$$\mathrm{Re}\,Y(\Omega)=\frac{1}{\hbar\Omega}\int_0^L dxF(x)\int_0^\infty d\varepsilon f(\varepsilon)\{[1-f(\varepsilon+\hbar\Omega)]\times\mathrm{Re}[A_+(\varepsilon)+B_+(\varepsilon)]-[1-f(\varepsilon-\hbar\Omega)]\times\mathrm{Re}[A_-^*(\varepsilon)+B_-^*(\varepsilon)]\}. \tag{21}$$

Equation (21) consists of a sum of the partial conductivities of the upper and lower sidebands:

$$\mathrm{Re}\,Y=\mathrm{Re}\,Y_+ +\mathrm{Re}\,Y_-.$$

Note that in Eqs. (19) and (20) the factor $1/kk_\pm$ is the product of one-dimensional densities of states in the wire for the ground-state energy ε and quasienergies $\varepsilon\pm\hbar\Omega$. The form of Eq. (21) coincides exactly with the Kubo–Greenwood formula.[15] Here the first term describes a current associated with absorption of a photon with energy $\hbar\Omega$. It is always positive. The second term describes current associated with emission of a photon; it is always negative.

Let us assume that $f(\varepsilon)=1$ in a band of energies from ε_1 to ε_2, and $f=0$ outside this interval. For concreteness we will assume that the AC field $F(x)$ does not depend on x; then the expression for $\mathrm{Re}\,Y_\pm$ takes the form

$$\mathrm{Re}\,Y_+=\frac{\nu}{2b^2}[J(r_1,s_1)+J(r_2,s_2)],$$

$$\mathrm{Re}\,Y_-=\frac{\nu}{2b^2}[J(r_3,s_3)+J(r_4,s_4)]\theta(1-\nu), \tag{22}$$

where

$$J(r,s)=\int_r^s dx\,\frac{1-\cos(bx)}{x^5}.$$

Here we have introduced the normalized frequency, wire length, and value of the lowest energy of the occupied states:

$$\nu=\hbar\Omega/\varepsilon_2,\quad b=L\sqrt{2m\varepsilon_2}/\hbar,\quad \delta=\varepsilon_1/\varepsilon_2.$$

The quantities r and s are expressed in terms of ν and δ as follows:

$$r_1=\sqrt{1+\nu}-1,$$

$$s_1=\min[(1-\sqrt{1-\nu});(\sqrt{\nu+\delta}-\sqrt{\delta})],$$

$$r_2=\max[(1+\sqrt{1-\nu});(\sqrt{\nu+\delta}+\sqrt{\delta})],$$

$$s_2=1+\sqrt{1+\nu},$$

$$r_3=\max[(\sqrt{\delta+\nu}-\sqrt{\delta});(1-\sqrt{1-\nu})],$$

$$s_3=\min[(\sqrt{\delta}-\sqrt{\delta-\nu});\sqrt{\nu}],$$

$$r_4=\max[(\sqrt{\delta}+\sqrt{\delta-\nu});\sqrt{\nu}],$$

$$s_4=\min[(\sqrt{\delta}+\sqrt{\delta+\nu});(1+\sqrt{1-\nu})].$$

The limits of integration determined in this way reflect the fact that in Eq. (21) we have included only transitions from filled states to empty ones: $\varepsilon_2\geqslant\varepsilon\geqslant\max[(\varepsilon_2-\hbar\Omega),\varepsilon_1]$ in the first term and $\varepsilon_1\leqslant\varepsilon\leqslant\max[(\varepsilon_1+\hbar\Omega),\varepsilon_2,2\varepsilon_1]$ in the second.

Let us consider the frequency dependence of the quantities $\mathrm{Re}\,Y_+$ and $\mathrm{Re}\,Y_-$. For $\mathrm{Re}\,Y_+$ the presence of two characteristic frequencies is important: $\nu=1$ and $\nu=\nu_2\equiv4\pi/b$. The first is the frequency of electron waves with energy ε_2, while the second corresponds to the drift time of an electron with this energy through the wire. The shape of the frequency dependence of $\mathrm{Re}\,Y_+$ is determined by the value of ν_2. If $\nu_2\ll1$ (i.e., the length of the wire significantly exceeds the wavelength of the electrons), then $\mathrm{Re}\,Y_+$ oscillates and attenuates at a rate ν. The physical nature of the oscillations is connected with the spatial resonances of charge waves over the length of a wire.[8] For $\nu_2\sim1$ the oscillations disappear, while for $\nu_2\gg1$ there is a maximum at a frequency $\nu\approx1-\delta$ determined by the width of the band of occupied states.

The frequency dependence of $\mathrm{Re}\,Y_-$ has an analogous form; however, the characteristic frequencies in this case equal $\nu=\delta$ and $\nu=\nu_1\equiv\nu_2/\sqrt{\delta}$. They have the same meaning as for $\mathrm{Re}\,Y_+$, the only difference being that they are measured from the lowest value of the energy of occupied states ε_1. For $\nu_1\ll1$ the value of $\mathrm{Re}\,Y_-$ oscillates with increasing ν and decays. For $\nu_1\gg1$ a maximum appears at a frequency $\nu\approx\delta$. The appearance of this maximum, which is considerably more abrupt than it is for $\mathrm{Re}\,Y_+$, is connected with an increase in the one-dimensional density of states as the energy approaches the bottom of the conduction band in the wire.

The total conductivity of the wire is determined by adding the conductivities arising from the upper and lower sidebands. Characteristic plots of the frequency dependence of $\mathrm{Re}\,Y$ are shown in Figs. 5a, 5b for two of the most interesting relations between the characteristic frequencies: $\nu_2<\nu_1<1$: $1<\nu_2<\nu_1$.

From the figures we have shown it is clear that a negative dynamic conductivity appears in both cases: $\mathrm{Re}\,Y<0$. If the wire is long ($\nu_2\ll1$), then the characteristic instability frequency is determined by the drift time for the upper sideband: $\Omega\sim4\pi\sqrt{\varepsilon_2/2m}/L$. In particular, when $\nu_1\ll1$ we have

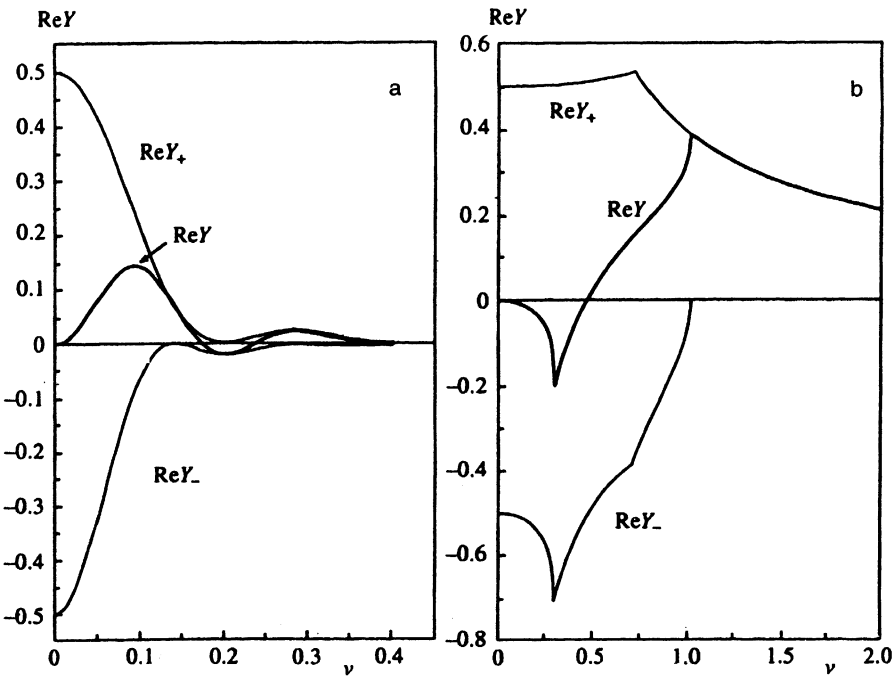

FIG. 5. Frequency dependence of the real part of the total admittance (Re Y) and the admittances connected with the upper (Re Y_+) and lower (Re Y_-) sidebands: a—$\nu_2=0.2$, $\nu_1=0.28$, $\delta=0.5$; b—$\nu_2=20$, $\nu_1=36.5$, $\delta=0.3$.

$$\mathrm{Re}\, Y=\frac{1}{2}\left[\left(\frac{\sin(b\nu/4)}{b\nu/4}\right)^2-\left(\frac{\sin(b\nu/4\sqrt{\delta})}{b\nu/4\sqrt{\delta}}\right)^2\right].$$

In this limiting case the instability under discussion is analogous to the classical drift-time instability.

If the length of the wire is small ($\nu_1\gg 1$), then an instability appears with a characteristic frequency determined by the lower edge of the energy of occupied states: $\Omega\approx\varepsilon_1/\hbar$. In this case the instability is connected with the fact that the density of states for electrons making transitions with emission of a photon with energy $\hbar\Omega$ turns out to be larger than the density of states for those making transitions with absorbtion of a photon. Thus, for $\nu_2\ll 1\ll\nu_1$ the admittance has the following form:

$$\mathrm{Re}\, Y\approx\frac{1}{2}\left(\frac{\sin(b\nu/4)}{b\nu/4}\right)^2-\frac{2\sqrt{\delta}}{\nu}\left[\sqrt{\delta+\nu}-\sqrt{\delta-\nu}\,\theta(\delta-\nu)\right].$$

It is interesting to note that in the steady-state limit ($\nu\to 0$) the conductivities arising from the upper and lower sidebands are the same in magnitude and completely compensate each other, which corresponds to zero differential conductivity. This is a consequence of saturation of the injection current with respect to the DC bias voltage. As ε reduces to zero, the contribution of the lower band disappears. As a result, there remains only the partial current of the upper sideband. It is this current that gives the usual expression for the conductance e^2/h.

5. CONCLUSIONS

In this paper, based on a first-principles quantum mechanical discussion, we have investigated the admittance Y of a quantum ballistic wire. We have shown that in the presence of an applied external voltage a negative dynamic conductivity appears (Re $Y<0$), which is associated with an inversion of the population of electronic states in the wire that occurs under conditions of ballistic transport of electrons.

The wire admittance, and in particular the value of the negative dynamic conductivity, are determined by adding the currents caused by electrons injected from the cathode reservoir and electrons entering the wire from the anode, being reflected within the wire and returning to the anode reservoir. The negative dynamic conductivity is connected with the injected electrons. The current of electrons entering the wire from the anode creates a positive contribution to the conductivity, which strongly affects the value of the negative dynamic conductivity and the frequency at which it is a maximum.

For the case of long wires ($Lk_F\gg 1$), the admittance oscillates as a function of frequency, with the characteristic frequency of the oscillations determined by the drift time of electrons in the wire. Due to the superposition of the currents created by electron fluxes from the cathode and from the anode, the dependence of the maximum value of the negative conductivity on the applied voltage becomes strongly nonmonotonic, and the frequency at which the negative conductivity reaches a maximum undergoes a sharp jump.

The mechanism for negative dynamic conductivity is connected with inversion of the populations of stationary electron states in the wire. A consequence of this is that downward transitions of electrons to unoccupied states with the emission of a photon with energy $\hbar\Omega$ become possible. These transitions give rise to a negative conductivity, while positive conductivity is associated with transitions that are energetically upward. The downward transitions turn out to be dominant in two cases: 1) the case of long wires, where due to spatial resonances of the charge waves over the length of the wire the conductivities arising from the lower and upper sidebands oscillate in frequency with different periods; 2) the case of short wires, when the conductivity arising from the lower sideband has a sharp maximum in frequency, connected with the increased density of states in the wire as the energy approaches the bottom of the conduction band, which causes the rate of transitions with emission of photons to become larger than that of transitions with absorption.

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[1)]One of the results of these calculations, which we have not published, is that the oscillations in the conductance as a function of the position of the Fermi level in the wire predicted by Kirchenov in Ref. 13 are also predicted by the one-dimensional model. These oscillations are connected with resonances in the above-barrier transport of electrons from one contact reservoir to the other, where the height of the barrier is determined by the quantization energy for transverse motion in the wire. The quantitative discrepancy between the calculated results for the one- and two-dimensional models does not exceed 15%.

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