A.C.-Transport Through a Two-Dimensional Quantum Point Contact

I.E. Aronov¹, G.P. Berman¹, D.K. Campbell⁴, and S.V. Dudiy²

¹ Theoretical Division, MS-B213, Los Alamos National Laboratory, Los Alamos, New Mexico, 87545, USA, ² Institute for Radiophysics and Electronics, National Academy of Sciences of Ukraine, 310083, Kharkov, Ukraine, ³ Kirensky Institute of Physics, 660036, Krasnoyarsk, Russia, ⁴ Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green St., Urbana, IL 61801-3080, U.S.A.

We calculate the admittance of a two-dimensional quantum point contact (QPC) using a Boltzmann-like kinetic equation derived for a partial Wigner distribution function in an effective potential. We show that this approach leads to the known stepwise behavior of the admittance as a function of the gate voltage. The admittance contains both a quantum inductance determined by the harmonic mean of the velocities for the propagating electron modes and a quantum capacitance determined by the reflected modes.

PACS numbers: 05.60; 72.10. Bgn; 72.30

Recent technological progress in manufacturing nanoscale solid state structures has made it possible to fabricate devices in two-dimensional electronic systems (2DES) which operate in the quantum ballistic regime. A particular system that has attracted much attention is the ballistic quantum point contact (QPC) [1,2].

In this letter we investigate a.c.-electron transport through a QPC. Despite detailed investigations, both experimental [3,4] and theoretical [3,5,6], of the d.c. transport, a.c. transport effects have so far not drawn comparable attention, but see recent important papers [3,7,4] (and [4,3,6] for the kinetic response of the resonant tunnel junction).

Several experiments [3,4] have exhibited such quantum coherent phenomena as quantization of the d.c.-conductance versus the gate voltage (or the number of propagating modes through the QPC). The theory of this phenomenon [3,4,5] explains the d.c.-conductance quantization as a consequence of the adiabaticity of the electrons’ motion through the QPC with smooth boundaries. In an adiabatic geometry (see Fig.1), which is smooth on the scale of the Fermi wavelength, the longitudinal and transverse motion of electrons can be separated in the Schrödinger equation [1]. In this case, the number of the transverse quantization modes is an adiabatic invariant, and the transverse energy plays the role of the potential energy for the one-dimensional longitudinal motion of each mode. Depending on whether the total energy of a given electron state is greater or less than the effective potential energy of each mode, the mode is propagating or non-propagating (see Fig. 2).

Frequency dependent transport phenomena in QPCs are clearly of interest, for the a.c. frequency introduces a time-scale that may reveal qualitatively new effects.

The a.c.-transport has been considered by M. Böttiker et al., [8-11], who showed that it is described at low frequency $\omega$, by an a.c.-admittance, $Y \equiv 1/Z = G - i\omega \mathcal{E}$ ($Z$ is the impedance). $G$ is the conductance and $\mathcal{E}$ is the emittance, a term first introduced in this context by M. Böttiker [10]. Christen and Böttiker [11] derived the general expression for the electrochemical capacitance and for the displacement current, and established the steplike behavior of the QPC emittance in synchronism with the conductance steps, and discussed the admittance for quantized Hall conductors. In paper [8-11], the emittance was expressed in terms of the geometric capacitance, transmission probability, and the densities of states of the “mesoscopic capacitor plates”.

Below we develop a simple method for calculating the transport characteristics for the QPC, which is based on the Wigner distribution function (WDF) formalism. (The effectiveness of the WDF approach to modeling of the mesoscopic devices was demonstrated in [13].) Our approach allows us to represent the emittance in terms of the capacitance and the inductance, which are expressed in the explicit form through the microscopic characteristics. Assuming adiabaticity, we derive a Boltzmann-like quantum kinetic equation for the partial WDF for the QPC. This equation allows us to treat the 2DES in a QPC in terms of classical trajectories for the effective 1D motion. We calculate the a.c.-admittance of the QPC, considering propagating and non-propagating (reflected) electron modes and show that the real part of the admittance (the conductance) is quantized versus of the gate voltage, consistent with earlier calculations [1] based on the Landauer formula [14]. We also show that the emittance $\mathcal{E}$ has a negative part (the quantum inductance), which arises from the propagating electron modes and whose value is determined by the harmonic mean of the electron velocities. The non-propagating electron modes give a positive contribution (the quantum capacitance) to $\mathcal{E}$. This contribution is determined by the which depends on a geometrical form of the QPC, which is controlled by the gate voltage.

To find the conductivity of a 2DES of a QPC (see Fig. 1) taking account of both frequency dependence and spatial dispersion, we shall use an approach based on the Wigner distribution function [15,20], $f^W_p(\vec{r})$ =
\[
\int d\mathbf{r} \rho \exp\left\{-\frac{i}{\hbar} (\mathbf{p} + \mathbf{A}(\mathbf{r})) \cdot \mathbf{r} / 2 - i(\mathbf{r} - \mathbf{r}' / 2) / 2\right\} \Psi^+ (\mathbf{r}) \Psi (\mathbf{r} + \mathbf{r}' / 2).
\]

Here \( \hat{\rho} \) is the density matrix operator of the system and obeys the quantum Liouville equation; \( \Psi^+ (\mathbf{r}) (\Psi (\mathbf{r})) \) is the Fermi operator creating (annihilating) a particle at \( \mathbf{r} \); and \( \mathbf{A} \) is the vector-potential of the electromagnetic field. When the characteristic scale of the spatial inhomogeneities exceeds both the radius of interaction among the particles and the electron de Broglie wavelength, the kinetic equation for the WDF takes the form equivalent to the classical kinetic equation [2]. From the WDF, we can find the charge density \( \rho \) and the current density \( j \) [19,20].

In the adiabatic model [12] of the QPC shown in Fig. 1, one assumes the conduction to be smoothly varying \( d'(x) \approx d(x)/L \ll 1 \), where \( 2L \) is a characteristic adiabatic length scale of the QPC. With this assumption, the variables in the Schrödinger equation can be separated, and the wave function can be written in the form: \( \psi_n(x,y) = \psi_n(y) \Phi_n(x,y,d(x)) \) , where the transverse wave function \( \psi_n(y) = (1/\sqrt{d(x)}) \sin (\pi n (y + d(x))/2d(x)) \theta (d(x) - y') \) , satisfies the boundary conditions \( \Phi_n(y)|_{y = \pm d(x)} = 0 \), and \( \theta (x) \) is the Heaviside-step function. The effective Hamiltonian for the longitudinal wave function \( \psi_n(x) \) is \( \tilde{H} = -(h^2/2m) \partial^2_x + \varepsilon_n(x) + e\phi(x) \), where \( \phi(x) \) is the electric potential averaged with respect to the transverse coordinate \( y \).

Adiabaticity and the quantization of the transverse motion imply that the energy \( \varepsilon_n(x) \) in the Hamiltonian \( \tilde{H} \) has the form \( \varepsilon_n(x) = \pi^2 n^2 \hbar^2 / 8 m d^2(x) \) , with the transverse quantum number \( n \) an adiabatic integral of motion. Thus the motion of electrons in the QPC can be viewed as a set of \( n \) effective one-dimensional electron systems. Each effective electron system is influenced by both the potential \( \varepsilon_n(x) \) and the self-consistent electric potential \( \phi(x) \). To describe these separate systems we introduce a partial WDF (PWDF) via

\[
f_n^W (x,p_x) = \int dx' \exp \left\{-i p_x x' / \hbar\right\} \text{Tr} \hat{\rho} \Psi^+_n (x' - x' / 2) \Psi_n (x + x' / 2).
\]

Then we can represent the WDF in the form

\[
f_n^W (\mathbf{r}) = \sum_{n=1}^{\infty} f_n^W (x,p_x) \int dy' \exp \left\{-i p_y y' / \hbar\right\}
\]

\[
\Phi_{n,x} (y - y' / 2) \Phi_{n,x} (y + y' / 2).
\]

The equation for the PWDF (1) can be derived using the Wigner transformation [19,20]:

\[
\frac{\partial f_n^W}{\partial t} + v_x \frac{\partial f_n^W}{\partial x} + \left[ - \frac{\partial \varepsilon_n(x)}{\partial x} + eE(x) \right] \frac{\partial f_n^W}{\partial p} = \hat{I}_n \left\{ f_n^W \right\},
\]

where \( p \equiv p_x \) and \( E(x) = -\partial \phi(x) / \partial x \). The equation (3) is derived in the semi-classical approximation, under the condition \( k_F L \gg 1 \). In terms of the PWDF the nonequilibrium charge density and current density can be defined as:

\[
\rho (x,y) = \sum_{n=1}^{\infty} \rho_n (x) \Phi_n^2 (y),
\]

\[
j (x,y) = \sum_{n=1}^{\infty} j_n (x, y) \Phi_n^2 (y),
\]

where \( \rho_n (x) \) and \( j_n (x, y) \) are the partial charge and current densities:

\[
\rho_n (x) = \int dp \left[ f_n^W (x,p) - f_n^W (0) (x,p) \right],
\]

\[
j_n (x, y) = \int dp \int dp' f_n^W (x,p) \delta (p - p').
\]

Here, \( f_n^W (0) (x,p) \) is the equilibrium PWDF. The kinetic equation (3) for the PWDF has the form as the classical kinetic equation in the effective potential \( \varepsilon_n(x) \). Thus we can solve this equation by the method of characteristics, i.e., by using the classical trajectories.

The collision integral in (3) includes quantum transitions [20] and intermixing of the different electron modes (the different PWDF). In this letter, we will approximate the collision integral by a single momentum relaxation frequency, \( \nu \), so that \( \hat{I}_n \left\{ f_n^W \right\} = -\nu \left[ f_n^W (x,p) - f_n^W (0) \right] \) , where \( f_n^W (0) \) is the equilibrium PWDF. The equilibrium distribution function \( f_n^W (0) \) within the adiabatic approximation is given by:

\[
f_n^W (0) (x,p) = n_F \left\{ [p^2 + 2m + \varepsilon_n (x) - \mu] / T \right\},
\]

where \( n_F \) is the Fermi function with the effective chemical potential \( \mu - \varepsilon_n (x) \), where \( \mu \) is the equilibrium chemical potential of the 2DEG. The characteristics of kinetic equation (3) are the phase trajectories of a one-dimensional motion in the potential \( \varepsilon_n (x) \), which is determined from the integral of motion, viz. the total energy:

\[
\varepsilon = p^2 / 2m + \varepsilon_n (x) = \text{const}
\]

We consider a symmetrical QPC, \( d(x) = d(-x) \) . In this case the phase portrait is shown in Fig. 2. The separatrix lines (the heavy lines) which pass through the hyperbolic point \( p = 0, x = 0 \), divide the phase space into four regions, within which four sets of phase trajectories exist.

The regions of propagating trajectories (\( \varepsilon > \varepsilon_n (0) \)) occupy the regions (see Fig. 2): 1) \( \varepsilon > \varepsilon_n (0), \ p > 0 \); 2) \( \varepsilon > \varepsilon_n (0), \ p < 0 \); 3) \( \varepsilon < \varepsilon_n (0) \); and 4) \( \varepsilon < \varepsilon_n (0), \ x < 0 \). Within each region, one can find the solution of the kinetic equation for the PWDF and derive the general formula for the partial charge \( \rho_n \) and the current densities \( j_n \) . Here we consider the most interesting case, when the temperature is very low (\( T \rightarrow 0, T < \mu \) ), so that we have a clear separation between open channels (\( \varepsilon_n (0) < \mu \)) and closed channels (\( \varepsilon_n (0) > \mu \)).

Transport through a QPC in principle involves non-local (integral) operators in that the charge and current densities at a given point \( x \) can be influenced by the electric field within the whole conductor. Nonetheless, it is well known that the static conductance is (to a good approximation) specified by the potential difference
(bias voltage) between the right and left reservoirs and that the detailed electric potential profile does not influence it significantly. This result was derived using the Landauer formula in which the conductance is determined by the matrix of the transmission coefficients of the electron waves corresponding to different propagating modes. We can readily show that this result follows from our PWDF approach. In the ballistic regime, when $L \ll l$, $(2L)$ is the distance between the reservoirs, $l$ is the mean free path and at $\omega, \nu \to 0$, we obtain for the open channels $j_n = (2e^2/h)V$, with $V = \int_{-L}^{L} \text{d}x E(x)$, and for the closed channels $j_n=0$. Hence for the static conductance we get the familiar result: $G = I/V = 2e^2N/e$, where $N$ is the number of the open channels: $N = ([2/k_Fd(0)]/\pi)$. Here the brackets $[\cdot]$ stand for an integer part. Clearly, the static conductance does not depend on the specific form of the smooth function, $d(x)$.

More generally, we can use the formalism of the PWDF to calculate the admittance at a finite frequency $\omega$. The partial current $j_n$ is a function of the longitudinal coordinate $x$ at $\omega \neq 0$.

The continuity equation, $\nabla \cdot j = \partial \rho / \partial t = 0$, in the QPC at $\omega \neq 0$ allows one to show that the total current, $I_{\text{tot}} = \sum_{n=1}^{\infty} \left( j_n - i(1/V) \int_{-L}^{L} \text{d}x' \rho_n(x') \right) \equiv 0$, which includes the electron current $\sum_{n=1}^{\infty} j_n(x)$ and displacement current $-i\omega \int_{-L}^{L} \text{d}x' \rho_n(x')$, is independent of the longitudinal coordinate $x$. Within the left reservoir the displacement current vanishes, so the total current is $I_{\text{tot}} = \sum_{n=1}^{\infty} j_n(-L)$, and the admittance can be determined as $Y = I_{\text{tot}}/V = (1/V) \sum_{n=1}^{\infty} j_n(-L)$. In the general case, we should determine the field $E(x)$ self-consistently within the QPC from Maxwell’s equations and afterwards calculate the admittance. For the present, we consider the long-wavelength approximation, where $v_n^* \gg \omega L_n$. Here $v_n^*$ is the typical velocity for electrons in the $n$th channel, and $L_n$ characterizes the length of a region for that channel. For the propagating modes, $L_n$ is the distance between the reservoirs ($L_n \sim 2L$) and $v_n^* = v_n(0)$.

For reflecting modes, $L_n$ is the doubled distance between the turning points ($\varepsilon_n(x_n) = \mu$) and the nearest reservoir ($L_n \sim 2(L - x_n)$). The typical velocity in this case is: $v_n^* = 2v_F \sqrt{x_n(x_n - L_n)}/L$, where $v_F = \sqrt{2\mu/m}$, $L$ is as above, the characteristic adiabatic length scale of the QPC. To calculate the current of the propagating modes, we can approximate the velocity $v_n$ as $v_n(x) \simeq v_n(0) = v_n^*$, while for the reflecting modes: $v_n(x) \simeq v_n^* \sqrt{1 - x_n(L - x_n)/L}$. Consistent with the symmetry of $d(x)$ we assume that $E(x) = E(-x)$ within the QPC and take $d(x) = d_0 \exp \left[ x/L \right]$. The contribution of the propagating modes to the total current is determined by the bias voltage $V$ and is independent of the detailed profile of the electric potential inside the QPC, while that of the reflecting modes depends on $d(x)$ and $E(x)$. We can write the admittance in the form $Y = G - i\omega \xi$, where as shown above the static conductance is given by $G = (2e^2/h)N$ and (after some calculation) one can show that the emittance $\xi$ can be expressed as

$$\xi = -G - \frac{L}{\tau^2} + C, \quad C = \frac{16e^2}{3h} \sum_{n=N+1}^{\infty} \xi_n^*(L - x_n). \quad (4)$$

Here $\tau^2$ is the harmonic mean of the velocities $v_n^*$ in the propagating modes: $1/\tau^2 = (1/N) \sum_{n=1}^{N} 1/v_n^*$. The integer $N$ determines the number of reflecting modes: $N = \left[ (2k_Fd_0/\pi) \exp[(L/L)^2] \right] - N_{\text{res}}$, $2L$ being the distance between the reservoirs. The dimensionless parameter value $\xi_n$ reflects the form of the electric field in the region $(x_n, L)$ filled with the electrons of the $n$th reflecting channel: $\xi_n = (3/2) \int_{x_n}^{L} \text{d}x' (E(xt)/V) \sqrt{x' - x_n}/(L - x_n)$.

From their respective expressions one sees immediately that the contribution to $\xi$ of the reflecting modes is positive while that of the propagating modes is negative. In this situation we can interpret our results in terms of an equivalent circuit in which a capacitance and resistance are in parallel followed by an inductance in series. The admittance of this circuit is

$$Y = G - i\omega(C - \frac{\Lambda^2}{\tau^2}), \quad \omega C \ll G, \quad \omega \Lambda \ll \frac{G^2}{\Lambda}. \quad (5)$$

The effective inductance in (5) is given by $\Lambda = e^2L/G\tau^2$, and the effective capacitance $C$ is given in (4). Note, that the formula (5) coincides with the general expression for the emittance derived in [11] (see formula (7) in [11]), where the emittance was expressed in terms of the geometric capacitance, transmission probability, and the densities of states of the “mesoscopic capacitor plates”. Our approach allowed us to represent the emittance in terms of the capacitance and the inductance, which are represented in the explicit form through the microscopic characteristics.

The dependence of the emittance on the number of open channels shows immediately that it is a stepwise function of the gate voltage. When the gate voltage approaches a point for which $2k_Fd/\pi$ is an integer, so that an additional channel opens (or closes), our expressions for the inductance and the capacitance diverge. In this case, our assumption that $v_n^* \gg \omega L_n$ is violated, and the contribution of these points into the admittance should be calculated separately, using the full self-consistent Maxwell equation approach $\gamma_n = (\mu - \varepsilon_n(0))/\varepsilon_n(0)$.

In conclusion, we have developed a new approach, based on a partial Wigner distribution function, to analyze the a.c. electron transport properties of a quantum
point contact. Treating the ballistic QPC in the adiabatic approximation, we derived a Boltzmann-like equation for the partial Wigner distribution function in an effective potential brought about by the quantized transverse modes. We analyzed this equation in terms of propagating and reflecting trajectories in the semi-classical approximation.

Our results establish that the a.c. electron transport depends directly on the number of propagating and reflecting modes and that certain features are sensitive to the form of the distribution of the electric field in the QPC. In particular, the real part of the admittance (the conductance) is determined by the harmonic mean of the velocities for the propagating electron modes and does not depend on the spatial distribution of the electric field inside the QPC. We are presently investigating this problem.

We stress that the effective quantum inductance and capacitance, and the equivalent circuit, are concepts valid within the linear response, low-frequency approximation. For the high-frequency case, and when new propagating and non-propagating modes can appear or disappear, the frequency dispersion of the admittance is more complicated than the linear one given by the equivalent circuit of Eq. (5). This case must be considered using the self-consistent Maxwell equations for the electric field in the QPC. We are presently investigating this problem.

We are grateful to L.I. Glazman, D.K. Ferry, R. Akis and G.D. Doolen for fruitful discussions. This work was partially supported by the Linkage Grant 93-1602 from the NATO Special Programme Panel on Nanotechnology and by the INTAS Grant No. 94-3862.

[1] L. I. Glazman, G. B. Lesovik, D. E. Khmelnitskii, R. Shekhter, JETP Lett. 48, 238 (1988).
[2] C. W. J. Beenakker, H. van Hasen, p. 1 in Solid State Physics, Vol. 44, Eds: H. Ehrenreich, D. Turnbull, (Academic, San Diego, 1991); B. J. van Wees, H. van Houten, C. W. J. Beenakker, J. G. Williamson, L. P. Kouwenhoven, D. van der Mare, C. T. Foxon, Phys. Rev. Lett. 60, 848 (1988).
[3] D. A. Wharam, T. J. Thornton, R. Newbury, M. Pepper, H. Ahmed, J. E. F. Frost, G. G. Hasko, D. C. Peacock, D. A. Ritchie, G. A. C. Jones, J. Phys. C 21, L209 (1988).
[4] N. K. Patel, J. T. Nicholls, L. Martin - Moreno, M. Pepper, J. E. F. Frost, D. A. Ritchie, and G. A. C. Jones, Phys. Rev. B 44, 13549 (1991); R. Taboryski, A. K. Geim, M. Persson, and P. E. Lindelof, Phys. Rev. B 49, 7813 (1994).
[5] T. M. Eiles, A. Simons, M. E. Sherwin, and J. F. Klem, Phys. Rev. B 52, 10756 (1995).
[6] I. E. Aronov, M. Jonson, and A. M. Zagoskin, Phys. Rev. B 50, 4590 (1994).
[7] L. Gorelik, A. Grincwaig, V. Kleiner, R. Shekhter, M. Jonson, Phys. Rev. Lett. 73, 2260 (1994); A. Grincwaig, L. Gorelik, V. Kleiner, and R. I. Shekhter, Phys. Rev. B 52, 12168 (1995); F. Hekking and Y. V. Nazarov, Phys. Rev. B 44, 11506 (1991); Phys. Rev. B 44, 9110 (1991).
[8] M. Büttiker, H. Thomas, and Prêtre, Phys. Lett. A 180, 364 (1993); M. Büttiker, J. Phys.: Condens. Matter 5, 9361 (1993).
[9] M. Büttiker, Il Nuovo Cimento 110B, 509 (1995).
[10] M. Büttiker, In: Quantum Dynamics of Submicron Structures, Eds: H. A. Cerdeira et al., p.p. 657-672 (1995, Kluwer Academic Publishers, Netherlands).
[11] T. Christen, M. Büttiker, Phys. Rev. Lett. 77, 143 (1996); T. Christen, M. Büttiker, Phys. Rev. B 53, 2064 (1996).
[12] A. Yacoby and Y. Imry, Europhys. Lett. 11, 663 (1990).
[13] C.L. Fernando and W.R. Frensley, Phys. Rev. B 52, 5092 (1995).
[14] L.Y. Chen and C.S. Ting, Phys. Rev. Lett. 64, 3159 (1990).
[15] C. Jacoboni and P.Price, Solid State Commun. 75, 193 (1990).
[16] Y. Fu and S.C. Dudley, Phys. Rev. Lett. 70, 3159 (1990); C. Jacoboni and P.J. Price, Phys. Rev. Lett. 71, 464 (1993); Y. Fu and S.C. Dudley, Phys. Rev. Lett. 71, 466 (1993).
[17] D.K. Ferry and H.L. Grubin, Modelling of Quantum Transport in Semiconductor Devices, p. 283, In: Solid State Physics 49 (1995); N.C. Kluksdahl, A.M. Kriman, D.K. Ferry, C. Ringhofer, Phys. Rev. B 39, 7720 (1989).
[18] R. Landauer, IBM J. Res. Dev. 1, 233 (1957); Phil. Mag. 21, 863 (1970); Z. Phys. B 68, 217 (1987).
[19] E. Wigner, Phys. Rev. 40, 749 (1932).
[20] A. I. Akhiezer and S. V. Peletminskii, Methods of Statistical Physics, (Oxford, New York, Pergamon Press, 1981).
FIGURE CAPTIONS

Fig. 1: The geometry of the microconstriction. The width is denoted by $2d(x)$, the narrowest width is $2d_0$, and the effective length is $2\tilde{L}$.

Fig. 2: The plane of phase trajectories for one-dimensional motion determined by conservation of integrals of motion. The heavy lines are separatrices that separate the propagating modes (sections 1 and 2) and non-propagating (reflecting) modes (sections 3 and 4).
This figure "doc1.gif" is available in "gif" format from:

<http://arxiv.org/ps/cond-mat/9609239v3>
This figure "doc2.gif" is available in "gif" format from:

http://arxiv.org/ps/cond-mat/9609239v3