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## LETTER TO THE EDITOR

# Quantum transport in a three-dimensional wire

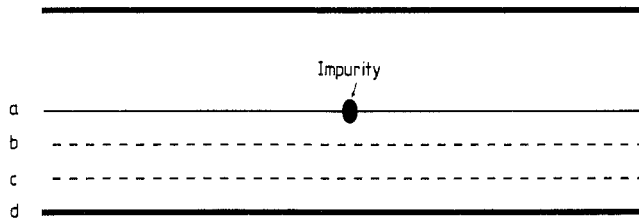
M C Payne and G E Engel

Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, UK

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**Abstract.** Electrostatic and electrochemical potentials are calculated for a current carrying cylindrical wire that contains a single impurity positioned on its axis. It is found that long-range electric fields are present in the region around the impurity despite the presence of metallic screening and that the direction of the electric field alternates along the axis of the wire.

Advances in semiconductor fabrication techniques have made it possible to fabricate devices in which the electronic mean free path exceeds the dimensions of the device so that transport through the device is ballistic. Experiments on systems that contain narrow one-dimensional channels have shown that the conductance of such devices is quantised in units of  $2e^2/h$  (van Wees *et al* 1988, Wharam *et al* 1988). In a previous publication (Payne 1989, hereafter referred to as I) the distribution of electrostatic and electrochemical potentials in a variety of one-dimensional devices was analysed (for a discussion of electrochemical and electrostatic potentials and their measurement see Landauer 1989). One-dimensional systems are particularly simple to study because different regions of the device are separated by well defined interfaces. The changes in the electrochemical potentials occur at the interfaces and the changes in the electrostatic potential occur within a screening length of the interfaces. In two- and three-dimensional devices there are no clearly defined interfaces between different regions of the device. In this letter we consider a three-dimensional wire that contains a single impurity and calculate the electrochemical and electrostatic potentials in the system. It is well known that the resistance of a wire at zero temperature results from the scattering of electrons from impurities. A simple model might assume that the voltage drops in such a device occur over regions of the size of the screening length around each impurity since the electric fields should be screened over this length-scale. However there is an obvious flaw in this model. One path through the device might pass through some of the impurities while another path may only pass through regions of perfect conductor. From the analysis presented in I it is easy to understand the presence of a voltage drop along a path that passes through impurities since it was shown that voltages are generated in regions of the device in which carriers are reflected. However, as it is expected that the electric fields around each of the impurities should be screened there should be no electric field in the regions of the device away from the impurities. If this were the case there would be no voltage drop along any path that avoided all the impurities in the wire. However, the voltage drop between the ends of the wire must be independent of the path taken through the wire so the previous argument must be incorrect. In this letter this



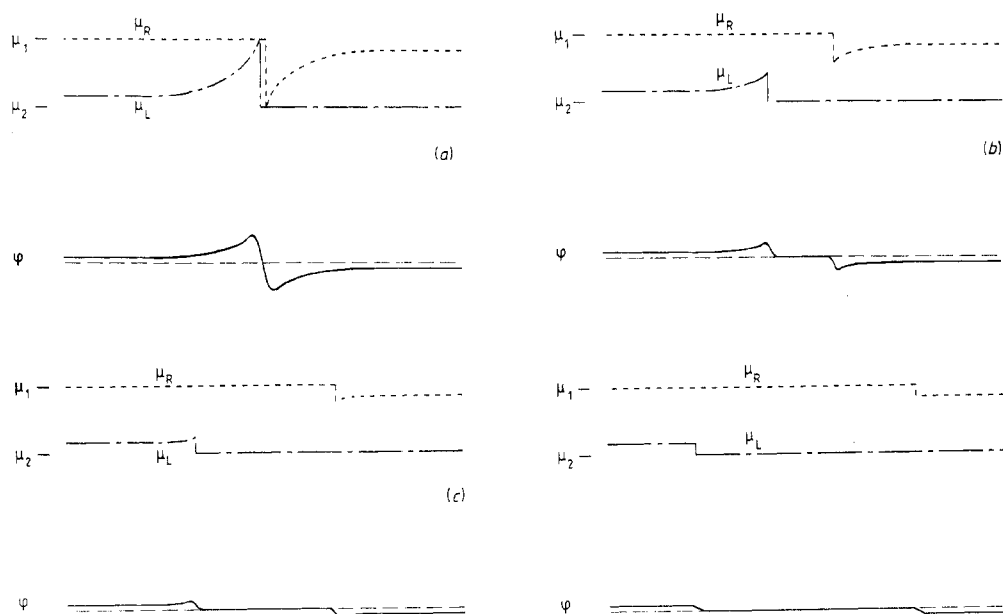
**Figure 1.** Schematic illustration of the cylindrical wire showing the position of the impurity on the axis of the wire and the four lines a, b, c and d along which the electrochemical potentials are plotted in figure 2.

problem is investigated by calculating the electrochemical and electrostatic potentials in a cylindrically symmetric conductor that contains a single impurity positioned on its axis. It is shown that the scattering of the electrons by the impurity gives rise to long-range electric fields despite the metallic screening in the wire. These long-range electric fields explain the presence of a voltage drop along a path that avoids all the impurities in the wire. It is found that the electric field in the wire is not uniform; the magnitude of the electric field at the position of the impurity is significantly enhanced and the direction of the electric field alternates along the axis of the wire. These results are consistent with Landauer's model of residual resistivity dipoles (Landauer 1957).

The simplifications and approximations used in this letter are essentially those applied in the analysis of the one-dimensional system studied in I. Different electrochemical potentials will be assigned to left- and right-propagating electrons as must be the case for a current-carrying system; the magnitude of the electrochemical potential at a point will be taken to be the value of the Fermi energy that would produce the same electron density as actually exists at the point; screening will be described by a simple Thomas–Fermi model. Quantum interference effects which give rise to oscillations in the electronic density and consequent oscillations in the electrochemical potentials (Büttiker 1989) will be ignored: only the average of the electron density over distances of the order of the Fermi wavelength will be considered. It will be assumed that the impurity in the wire completely reflects the electronic wavefunctions over an area of  $\pi a^2$ . A number of these simplifications can be trivially removed. It is straightforward to consider an impurity that partially transmits the incident electrons and it is relatively straightforward to consider alternative positions of the impurity. It is simple to apply a similar analysis to two-dimensional systems. Quantum interference effects and a more detailed description of the electronic screening will be considered in future work.

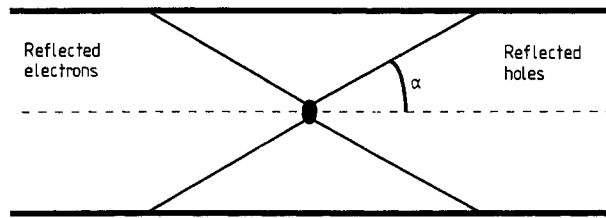
Figure 1 illustrates the system that will be studied. It will be assumed that a perfect battery as defined in I is attached to the system. The battery controls the occupancies of the outgoing electronic states so that the electrochemical potential for electrons propagating to the right far to the left of the impurity is  $\mu_1$  and the electrochemical potential for carriers propagating to the left far to the right of the impurity is  $\mu_2$ . The battery voltage is  $\mu_1 - \mu_2$ . All the electronic states that have energies less than  $\mu_2$  are occupied. Hence, carriers that have energies less than  $\mu_2$  give no contribution to the current.

The potentials along the lines labelled a, b, c and d in figure 1 are shown in figures 2(a–d). Figure 2(a) shows the potentials along the axis of the wire. The effect of the impurity can be clearly seen by the step change in the electrochemical potentials at the position of the impurity. The step changes in the electrochemical potentials at this point result from the perfect reflection of the electrons in the energy range between  $\mu_1$  and  $\mu_2$



**Figure 2.** The electrostatic potential and the electrochemical potentials in the current-carrying wire illustrated schematically in figure 1. The electrostatic potential,  $\varphi$ , is shown by the full lines, the electrochemical potential for carriers moving to the right,  $\mu_R$ , is shown by the short-dashed lines and the electrochemical potential for carriers moving to the left,  $\mu_L$ , is shown by the chain lines. The long-dashed lines show the average electrostatic potential in the wire. The potentials are plotted along the lines a, b, c and d shown in figure 1. The wire is connected between the terminals of a perfect battery. The negative terminal of the battery is connected to the left edge of the left-hand lead and the positive terminal of the battery is connected to the right edge of the right-hand lead.  $\mu_1$  is the electrochemical potential imposed by the battery on the carriers moving to the right in the left-hand lead and  $\mu_2$  is the electrochemical potential imposed by the battery on the carriers moving to the left in the right-hand lead. The voltage of the battery,  $V$ , is equal to  $\mu_1 - \mu_2$ .

incident on the impurity from the left and the holes in this energy range incident on the impurity from the right. The step changes in the electrochemical potentials are reminiscent of the changes in the electrochemical potentials observed in the one-dimensional systems studied in I. However, in this three-dimensional system the electrochemical potentials are not constant away from the point where the reflection of the carriers takes place. The reflected electron and hole wavepackets are localised in a transverse area  $\pi a^2$  at the position of the impurity. The transverse wavefunctions at the position of the impurity contain a wide range of Fourier components which have different group velocities. Hence the reflected electron and hole wavepackets will spread in the lateral direction with time as they propagate away from the impurity. The actual form of the reflected wavepackets is quite complicated and to simplify the following analysis it will be assumed that the reflected electron and hole wavepackets spread over cones of half-angle  $\alpha$ . The curvature of the wavefronts of the reflected electron and hole wavepackets will be ignored and it will be assumed that there are no changes in the wavepackets once they have spread over the cross-section of the wire. It will also be assumed that the density of the reflected electrons and holes is uniform across each cross-section of the cone. The assumed form of the reflected electron and hole wavepackets is shown in figure 3.



**Figure 3.** Schematic illustration of the lateral spreading of the electron and hole wavepackets reflected from the impurity.

At the position of the impurity the reflected electrons and holes are spatially localised in the transverse direction. The wavepackets spread laterally as the reflected electrons and holes propagate away from the impurity and so the density of the reflected electrons and holes is not uniform away from the impurity. As the magnitudes of the electrochemical potentials depend on the local electron densities the electrochemical potentials are not constant away from the impurity. With the model for the reflected wavepackets introduced above the excess electron and hole densities along the axis of the wire are proportional to  $(1/d \tan(\alpha))^2$ , where  $d$  is the distance away from the impurity. The lateral spreading of the wavepackets will continue until the density of reflected electrons and holes is uniform across the wire. This occurs at distances  $W/\tan(\alpha)$  along the wire from the position of the impurity, where  $W$  is the width of the wire. Beyond these points the density of reflected electrons and holes is independent of the position in the wire.

The effect of the lateral spreading of the reflected electrons and holes on the electrochemical potentials can be seen in figures 2(b–d). These figures show the variation of the electrochemical and electrostatic potentials off the axis of the wire. There is no change in the magnitude of the electrochemical potentials at the points closest to the impurity along the lines b, c and d because these points are outside the cones formed by the reflected electron and hole wavepackets. The electron density off the axis of the wire only changes when the reflected electrons and holes have propagated some distance away from the impurity and their wavepackets have spread laterally. Along lines b and c there are step changes in the electrochemical potentials at the points where the cones formed by the reflected electron and hole wavepackets cut the lines. The step changes in the electrochemical potentials are followed by smooth changes in the potentials. The smooth variations in the electrochemical potentials occur because the densities of the reflected electrons and holes decrease as the wavepackets continue to spread laterally away from the impurity. The changes in the electrochemical potentials continue until the reflected electron and hole wavepackets have spread across the whole cross-section of the wire. In the case of the electrochemical potentials on the edge of the wire shown in figure 2(d) there are no smooth variations in the electrochemical potentials because the step changes in these potentials occur at the points where the lateral spreading of the reflected wavepackets is complete.

The electrochemical potentials beyond the points where the reflected carriers have completely spread across the wire are  $\mu_1 - \{[1 - (a/w)^2](\mu_1 - \mu_2)\}$  for left-propagating electrons to the left of the impurity and  $\mu_2 + \{[1 - (a/w)^2](\mu_1 - \mu_2)\}$  for the right-propagating electrons to the right of the impurity. These potentials become  $\mu_2$  and  $\mu_1$  respectively as the cross-section of the wire becomes much larger than the cross-section of the impurity. These are the values of the electrochemical potentials that are expected for a perfect conductor where the left- and right-propagating carriers are not scattered

as they propagate through the system. Even though the wire contains a scatterer the system behaves as a perfect conductor in this limit because a negligible fraction of the current-carrying electrons are scattered as they propagate through the wire.

The electrostatic potential in the wire will now be considered. It is simple to calculate the value of the electrostatic potential in any region in which there is no change in the electrochemical potentials and so these regions will be considered first. In any region in which the electrochemical potentials are constant the value of the electrostatic potential beyond a few screening lengths from the edge of the region is determined by the condition of local charge neutrality. The electrostatic potential must be constant within any such region because this is the only self-consistent steady-state solution of the electrostatic and current transport equations. From the definitions of the electrochemical potentials adopted in this paper this implies that in regions in which the electrochemical potentials do not vary with position the electrostatic potential is a constant energy below the average of the electrochemical potentials for the left- and right-propagating carriers. If this fixed energy is  $\zeta$  the electrostatic potential in the region far to the left of the impurity lies at  $\mu_1 - \{[1 - (a/w)^2](\mu_1 - \mu_2)/2\} - \zeta$  and the electrostatic potential far to the right of the impurity lies at  $\mu_2 + \{[1 - (a/w)^2](\mu_1 - \mu_2)/2\} - \zeta$ . The difference in the electrostatic potential between the ends of the wire is  $(\mu_1 - \mu_2)(a/w)^2$ , which is the same as the differences in the electrochemical potentials between the ends of the wire. As the cross-section of the wire becomes much larger than the cross-section of the impurity the scattering from the impurity becomes negligible, the voltage drop along the wire goes to zero and the wire behaves as a perfect conductor.

The electrochemical potentials are constant in the region around the impurity outside the cones formed by the reflected electron and hole wavepackets. In this region the electrostatic potential lies at  $(\mu_1 + \mu_2)/2 - \zeta$ , which is half-way between the electrostatic potentials at the ends of the wire.

Finally, the electrostatic potential in the conical regions where the reflected electron and hole wavepackets spread laterally must be calculated. The reflected carriers generate non-uniform charge densities in these regions and the electric fields generated by these charge densities will be screened. A full analysis of the screening will be presented in a future publication and only a qualitative description of the screening will be presented here.

It is commonly assumed that static electric fields in metals are screened within a screening length  $\lambda$ . This is true in the case of electric fields generated by a point charge and the electric fields generated by a uniform charge density in some region of a metal. In the former case the electric field generated by the point charge is screened within a few screening lengths. In the latter case a dipole layer whose width is of the order of the screening length surrounds the region of constant charge density. The electric field is non-zero within the dipole layer and gives a uniform shift between the electrostatic potentials inside and outside the dipole layer. The shift in the electrostatic potential inside the region produces a constant screening charge density that effectively cancels the original charge density. The region becomes charge neutral so the electric field inside the region is zero. For the system studied in this letter it is easier to understand the behaviour of the electrostatic potential by writing the potential in terms of the unscreened charge density generated by the reflected electrons and holes. In the Thomas–Fermi screening model the screened charge density at wavevector  $\mathbf{q}$ ,  $\rho_{\text{scr}}(\mathbf{q})$ , is given by

$$\rho_{\text{scr}}(\mathbf{q}) = q^2 \rho_{\text{unscr}}(\mathbf{q}) / (\lambda^2 + q^2) \quad (1)$$

where  $\rho_{\text{unscr}}(\mathbf{q})$  is the unscreened charge density at wavevector  $\mathbf{q}$  and  $\lambda$  is the Thomas–

Fermi screening wavevector. Hence the electrostatic potential at wavevector  $\mathbf{q}$ ,  $\varphi(\mathbf{q})$ , is

$$\varphi(\mathbf{q}) = \rho_{\text{unscr}}(\mathbf{q})/\varepsilon_0(\lambda^2 + q^2). \quad (2)$$

Equation (1) shows that only at  $\mathbf{q} = \mathbf{0}$  is the screened charge density strictly zero. From equation (2) it can be seen that when the unscreened charge density only contains Fourier components that have wavevectors much smaller than the Thomas–Fermi wavevector the screened potential is approximately  $1/\varepsilon_0\lambda^2$  times the unscreened charge density.

Equation (2) shows that the electrostatic potential must vary continuously in any region in which the unscreened charge density is non-uniform. Hence in the case of the system studied in this letter the electric field surrounding the impurity must extend over the whole of the conical regions defined by the reflected electron and hole wavepackets. As the electric field extends over the whole of these regions there are no paths through the wire along which the electric field is zero everywhere, and hence there are no paths through the wire along which the voltage drop is zero.

The magnitude of the electrostatic potential in the wire is shown by the full lines in figures 2(a–d). These figures show a number of surprising features. The electric field reverses direction two times along the axis of the wire. An electron propagating to the right along the axis of the wire initially experiences an electric field directed against the direction of the current. Then it experiences an electric field in the direction of the current and finally it experiences an electric field directed against the current. This behaviour can be understood as follows. As the electron approaches the impurity it experiences a Coulomb repulsion from the electrons that have been reflected from the impurity. In the region immediately around the impurity the electric field points in the direction of the current but the magnitude of the electric field is considerably enhanced over the value that would be calculated if it was assumed that the voltage applied to the wire were dropped uniformly along the length of the wire. Finally an electron on the axis of the wire to the right of the impurity experiences an electric field directed in the opposite direction to the current due to the attraction between the electron and the excess holes that have been reflected from the impurity. The variations in the electrostatic potential that give rise to the curious behaviour of the electric field are simply the response of the electronic system which attempts to screen the electric fields generated by the reflected electrons and holes. The reflected electrons generate a negative charge density to the left of the impurity and the reflected holes generate a positive charge density to the right of the impurity. The screening acts to reduce the total charge density but in the Thomas–Fermi model the screened charge density must be of the same sign as the unscreened charge density. This implies that even after screening there is excess negative charge to the left of the impurity and excess positive charge to the right of the impurity which produces the electrostatic potential shown in figure 2.

The behaviour of a wire that contains a number of impurities will depend on the ratio of the separation between the impurities to the width of the wire. If the separation of the impurities is much larger than the width of the wire a distribution of electric fields similar to those described in this letter will exist around each impurity, the exact field distribution around each impurity depending on its position on the cross-section of the wire, and there will be regions of constant potential between the impurities. When the separation of the impurities becomes much less than the width of the wire there will be no field-free regions in the wire since the electric fields surrounding each impurity will overlap. However, even in this case the magnitude of the electric field in the wire will be non-uniform along the length of the wire.

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