

Electrostatic and electrochemical potentials in quantum transport

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1989 J. Phys.: Condens. Matter 1 4931

(<http://iopscience.iop.org/0953-8984/1/30/006>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.93

The article was downloaded on 10/05/2010 at 18:30

Please note that [terms and conditions apply](#).

Electrostatic and electrochemical potentials in quantum transport

M C Payne

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

Received 23 January 1989, in final form 13 March 1989

Abstract. Self-consistent solutions for the electrostatic and electrochemical potentials are presented for idealised systems of perfect conductors connected to a perfect battery. A variety of phenomena are observed including electron transport against the gradient of the electrochemical potential.

1. Introduction

There has recently been a significant increase in interest in the subject of quantum transport following the successful fabrication of devices that show quantised conductances attributable to quantum transport (van Wees *et al* 1988, Wharam *et al* 1988b). The modelling of such devices is a complicated theoretical problem which involves the self-consistent solution of the Schrödinger equation of the device in the non-equilibrium current-carrying state. The devices studied experimentally contain narrow quasi-one-dimensional constrictions. It is straightforward to show that the conductance of such systems could be quantised. The electrons in a quasi-one-dimensional conductor occupy a set of sub-bands due to quantisation of the electronic states in the transverse directions but the electronic states are free-electron-like in the longitudinal direction. If there is no scattering of electrons between sub-bands the electrons in each sub-band can be considered as a one-dimensional electron gas. In a one-dimensional conductor the density of states at energy ϵ for electrons propagating in one direction is

$$\rho(\epsilon) = 2(L/2\pi) dk/d\epsilon \quad (1)$$

where L is the length of the conductor and k is the wavenumber of the electronic states. The group velocity of the electrons that have energy ϵ is

$$v(\epsilon) = (1/\hbar) d\epsilon/dk. \quad (2)$$

If all the electronic states propagating to the right in the energy range between ϵ and $\epsilon + \Delta\epsilon$ are occupied and all the states propagating to the left are unoccupied the current carried by the electrons in the energy range $\Delta\epsilon$ is

$$I = (e/L) \rho(\epsilon)v(\epsilon) \Delta\epsilon = (2e/h) \Delta\epsilon \quad (3)$$

which is independent of ϵ . If the range of energies over which all the right-propagating electronic states are occupied and the left-propagating states are unoccupied were equal

to eV , where V is the voltage across the conductor, the conductance of the system would be

$$G = I/V = 2e^2/h. \quad (4)$$

This result suggests that each occupied sub-band in a quasi-one-dimensional conductor should have a quantised conductance, in which case the conductance of the devices studied experimentally would be

$$G = (2e^2/h)n \quad (5)$$

where n is the number of occupied sub-bands in the narrow constrictions.

The conductances of the systems containing narrow constrictions that have been studied experimentally are found to be quantised in agreement with (5). This suggests that the simple model described above accurately describes these systems. However, there are a number of difficulties in relating (5) to the experimental results. In the devices studied experimentally electrons move from a wide region of the device into the quasi-one-dimensional constriction and then back into a second wide region of the device. The model presented above does not take account of the effect of this variation in the transverse width of the device. Furthermore, there is no obvious reason for which the range of energies of the current-carrying states in the constriction should be related to a voltage measured between probes positioned away from the constriction. The conductance measured between probes positioned away from the constriction could be calculated using the Landauer formula for the conductance. Application of the Landauer multi-channel conductance formula (Landauer 1985)

$$G = (2e^2/h) \text{Tr}(\mathbf{t}^\dagger \mathbf{t}) \quad (6)$$

where \mathbf{t} is the transmission matrix, predicts a quantised conductance for a quasi-one-dimensional constriction provided that the magnitude of the transmission coefficient for each channel is unity. Landauer has criticised the use of this formula because it does not take account of self-consistency (Landauer 1988) and he has shown that an approximately quantised conductance is predicted from the following conductance formula which does take self-consistency into account (Buttiker *et al* 1985):

$$G = \frac{2e^2}{\pi\hbar} \left(\sum_i T_i \right) \left(\sum_i v_i^{-1} \right) / \sum_i v_i^{-1} (1 + R_i - T_i) \quad (7)$$

where the sum is over all incident channels and v_i , R_i and T_i are the longitudinal velocity, reflection coefficient and transmission coefficient for channel i .

The Landauer formulae describe the conductance measured between reservoirs positioned well away from the constriction and they should not be used to predict the conductances that will be measured between arbitrary points in the system. The current flow through a quantum transport device depends on the electrostatic and electrochemical potentials at all points in the system. Understanding the form of these potentials is essential for modelling quantum transport devices and for interpreting measurements of potential differences and conductances made on such devices. It is the purpose of this paper to consider the form of these potentials in a number of ideal systems. The examples studied have been chosen to be as simple as possible. All the complexities involved in theoretical treatments of quantum transport have been deliberately avoided although some of the complications that occur in real systems will be briefly described. In the following section the definitions of electrostatic and electrochemical potentials will be discussed and the concepts of perfect batteries and

ideal conductors will be introduced. The electrostatic and electrochemical potentials in systems containing these idealised circuit elements will be presented in § 3.

2. Electrochemical and electrostatic potentials, perfect batteries and ideal conductors

The difference between electrostatic and electrochemical potentials and the difficulties involved in the measurement of these potentials have been discussed by a number of authors (see Engquist and Anderson (1981), and Landauer (1988) and references therein). Only the briefest discussion of these potentials will be presented here to provide the working definitions for the potentials used in this paper. The measurement process will not be considered. The potentials in a real system are determined by current conservation and by self-consistency between the potentials and the charge density. Whether any instrument can accurately and non-destructively measure these potentials will not be addressed here.

The electrostatic potential in a system is most easily detected by measuring the absolute energy of the bottom of a particular band or of a particular atomic core state. The difference between the absolute energies of either of these quantities measured at two points in space is equal to the change in the electrostatic potential between the points. The electrochemical potential is more difficult to define since it can be precisely defined only for a system in equilibrium. If a material carries a current the electrons are not in equilibrium and so an electrochemical potential cannot be uniquely defined. One way around this problem is to assume that the carriers moving in a particular direction are in equilibrium in which case a different electrochemical potential could be assigned to the carriers moving in each direction. Experimentally a difference in the electrochemical potentials at two points is measured by connecting a voltmeter between the points. The magnitude of the measured electrochemical potential difference is then given by a weighted average of the occupancy of the electronic energy levels where the weighting factor depends on the details of the measuring instrument. In this paper the electrochemical potential at a point will be taken to be the absolute position of the Fermi level that would produce the electron number density at that point. This electrochemical potential would correspond to a measuring instrument for which the weighting factor is a constant. Different electrochemical potentials will be assigned to the electrons travelling in opposite directions as required for a circuit that carries a current.

It will be seen from the examples presented later in this paper that a perfect battery can only be defined in terms of electrochemical potentials. The definition of a perfect battery that will be adopted in this work is that it is a device that controls the filling of the outgoing electron states such that the outgoing states from one terminal of the battery are filled to a higher energy than the outgoing states from the other terminal. The electrochemical potentials of the outgoing states are different at the two terminals of the battery and the difference between the potentials is equal to the battery voltage.

In the examples that follow it will be assumed that a perfect battery is connected by perfect leads to another perfect conductor. The leads are an intrinsic part of the battery since it is the occupancy of the states in these leads propagating away from the battery that is controlled by the battery. It will be assumed that the leads and the conductor are made of the same material so that there are no contact potentials between them, but it is trivial to remove this constraint. Two-dimensional systems will be considered but the results could be extended to three-dimensional systems by using a three-dimensional density of states. Three cases will be studied: in the first the conductor is much narrower

than the leads; in the second the leads and the conductor are of the same width; and in the final example the conductor is much wider than the leads. The leads and the conductor will be assumed to be much longer than their screening lengths and the spatial dependence of the screening will not be investigated in detail. It will be assumed that the electrons evolve adiabatically so that they remain in the same transverse quantum state throughout the system. If this is the case electrons are either wholly reflected or wholly transmitted at the interfaces between the leads and the conductor. This model for the evolution of the electronic states explains the quantised conductance observed in systems containing several narrow constrictions (Wharam *et al* 1988a, Beenakker and van Houten 1989). Adiabatic evolution of the electronic states requires that the interfaces between the leads and the conductor are not abrupt. Whether electrons evolve adiabatically or not in quantum transport devices will be investigated in detail in the following paper (Payne 1989). Finally, it will be assumed that the widths of the leads and the conductor are large enough for the density of states per unit area to be constant. The complications introduced when the conductor becomes very narrow and the sub-band structure in the density of states becomes apparent will be discussed after the first example.

3. Applications

The first case to consider is when the width of the conductor is much smaller than the widths of the leads. This geometry resembles that of the systems containing narrow constrictions that have been studied experimentally. The model for the quantised conductance presented at the beginning of the paper requires that the range of energies of the current-carrying states in the constriction is equal to eV , where V is the voltage measured between probes positioned in the leads. The validity of this assumption will be examined later. The complications that occur when the width of the constriction becomes very narrow will be briefly discussed at the end of the example. The electrostatic and electrochemical potentials for the system are shown in figure 1. The electrostatic potential is represented by the absolute energy of the bottom of the band of electronic states shown by the full line in the figure. The electrochemical potential for the carriers moving to the right is shown by the broken line and the electrochemical potential for the carriers moving to the left is shown by the chain line. The figure shows an abrupt interface between the leads and the conductor whereas adiabatic evolution of the electronic states requires that the width of the channel varies continuously and in this case the electrochemical potentials would vary smoothly in the regions where the width of the channel changes. Only the electrons in the range of energies between the electrochemical potentials μ_1 and μ_2 imposed by the battery need to be considered to determine the magnitude of the current because below the lower of these energies all the electronic states are occupied so the currents due to electrons propagating to the right and to the left cancel and above the higher of these energies all the electronic states are empty. Since the leads are much wider than the conductor there is a higher density of states in the leads and so most of the electrons moving to the right in the left-hand lead are reflected at the interface between the lead and the conductor. If w is the width of the conductor and W is the width of the leads a fraction (w/W) of the states in the left-hand lead evolve adiabatically into states propagating to the right of the conductor filling all the right-propagating states in the conductor up to the electrochemical potential μ_1 . At the interface between the conductor and the right-hand lead all of these states are

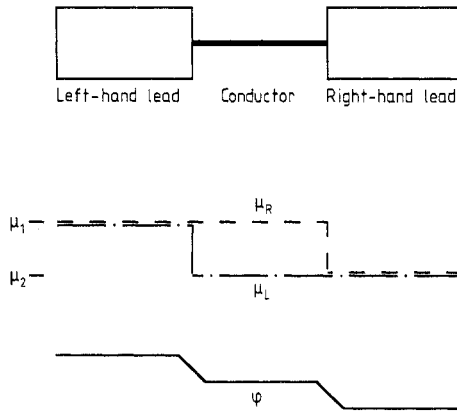


Figure 1. The electrostatic potential, ϕ , and the electrochemical potentials for carriers moving to the right, μ_R , and carriers moving to the left, μ_L , for a system consisting of a perfect battery connected by perfect leads to a perfect conductor. The width of the conductor is smaller than that of the leads. The negative terminal of the battery is connected to the left-hand edge of the left-hand lead and the positive terminal of the battery is connected to the right-hand edge of the right-hand lead. μ_1 is the electrochemical potential imposed by the battery on the carriers moving to the right in the left-hand lead and μ_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 $\mu_1 - \mu_2$. The variation of the electrostatic potential in the regions around the contacts is illustrated schematically.

perfectly transmitted into the lead. However, the density of states in the lead is larger than that in the conductor and so the electrochemical potential of the electrons propagating to the right in the right-hand lead is only $\mu_2 + (w/W)(\mu_1 - \mu_2)$. The arguments applied to electrons propagating to the right can be repeated for holes propagating to the left with the usual inversion of the energy scale which gives the electrochemical potential for electrons propagating to the left shown by the chain line in figure 1. The assumption of adiabatic evolution of the electronic states across the interfaces between the leads and the conductor makes it simple to determine the electrochemical potentials in the system and it only remains to determine the electrostatic potential. In general the electrostatic potential must be determined self-consistently so that the charge density in the system, which depends on the electrochemical and electrostatic potentials, generates the electrostatic potential. However, outside the regions where screening occurs the electrostatic potential is determined by the constraint that the system must be charge neutral. With the definition of the electrochemical potentials used in this paper charge neutrality occurs when the electrostatic potential is a constant energy below the average of the electrochemical potentials, so the number density of electrons is the same as that in the neutral material. The electrostatic potential varies smoothly between the regions of charge neutrality. Screening charges are generated because the electrostatic potential varies more slowly than the electrochemical potentials thus producing an excess of electrons to the left of each interface between the leads and the conductor and an excess of holes to the right of each interface.

The change in the electrostatic potential between the battery terminals in this system is equal to $(1 - w/W)(\mu_1 - \mu_2)$ which is the same as the changes in the electrochemical potentials for the electrons propagating to the right and to the left. The range of energies of the current-carrying states in the constriction is equal to $e(\mu_1 - \mu_2)$ which is not equal

to eV' , where V' is the potential difference measured between voltage probes in the two leads. Hence, the assumption used in the simple model for the quantisation of the conductance presented at the beginning of this paper is incorrect. The measured conductance will be larger than the quantised value by a factor of $(1 - w/W)^{-1}$. The changes in the electrochemical and electrostatic potentials across the system become equal to the voltage of the battery as the ratio of the widths of the battery leads to the width of the conductor tends to infinity, and so an approximately quantised conductance will be measured if the widths of the leads are much greater than the width of the constriction. The changes in the potentials do not occur continuously across the system but are restricted to the regions around the contacts between the leads and the conductor, so the approximately quantised conductance will only be measured between points in the electrodes that are far enough from the constriction for the potentials to have reached their asymptotic values. In the case of a measurement of the electrostatic potential difference this requires that the probes are outside the screening regions. Although the Landauer formulae should only be used to calculate the conductance measured between reservoirs it can be seen that different versions of the Landauer formula can give the correct values for the conductances measured between different points in the system. Measuring the change in any potential between points well inside the conductor or inside a single lead gives the infinite conductance predicted by (7) while either (6) or (7) would give the conductance measured between points in the two leads. A conductance equal to twice the quantised value would be measured between the conductor and either lead if the voltage probes measured the average electrochemical potential of electrons propagating in both directions.

The above analysis would be more difficult if the width of the constriction became very small. The electrochemical potentials will be as shown in figure 1 providing the electronic states evolve adiabatically through the system. However, the density of states per unit area is not constant if the constriction is very narrow and the minimum transverse kinetic energy of the electrons in the channel is no longer negligible. The total charge density in the channel must be calculated by summing the contributions of all the electrons propagating in the channel. If the channel is very narrow there can only be a small screening charge within the channel which may be insufficient to screen the electric field and in this case there would be an electric field along the entire length of the channel.

The changes in the electrostatic and electrochemical potentials across the system in the previous example are related to the battery voltage by a factor of $1 - w/W$. This suggests that when the leads and the conductor have the same width, so that the terminals of the battery are connected by a single perfect conductor, the differences in these potentials should be zero. The electrostatic and electrochemical potentials in such a system are shown in figure 2. It can be seen that this suggestion is correct: the electrochemical and electrostatic potentials are constant throughout the system. It should be noted that the battery voltage is still V according to the definition adopted in this paper. The conductance of the system is infinite because there is no change in the electrostatic potential or the electrochemical potentials across the system which is in accordance with (7). Even though the conductance of the system is infinite the current flowing through the system is finite because there is no change in the electrostatic or electrochemical potentials across the system. A system containing a battery is very different from a system in which the loop integral of the electric field is non-zero such as particle accelerator. The current in a circuit connected to a battery can never be infinite because only the states in a finite energy range between the electrochemical potentials of the battery, μ_1 and μ_2 , can contribute to the current. The electrons are not continuously

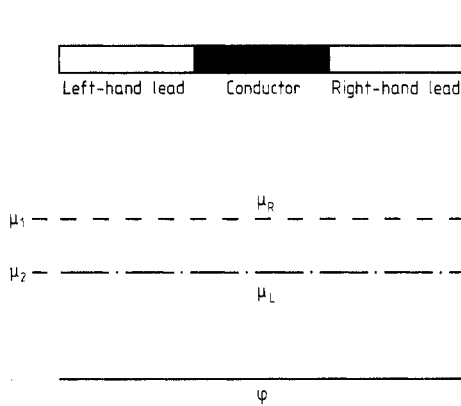


Figure 2. As figure 1 but for a system in which the leads and the conductor have the same width.

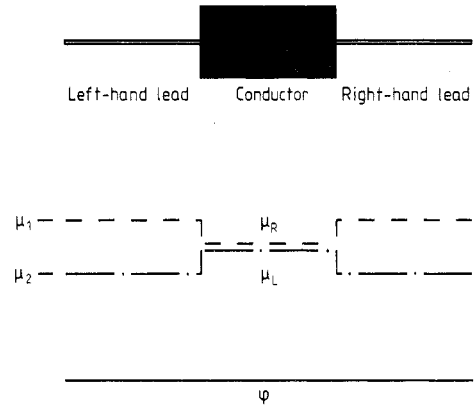


Figure 3. As figure 1 but for a system in which the conductor is wider than the leads.

accelerated as they are if the integral of the electric field round the circuit is non-zero, in which case the current would increase with time until the rate of gain of energy from the electric field was equal to the rate of loss of energy due to radiation.

The final example to be considered is a system in which the width of the conductor, w , is much greater than the widths of the leads to the battery, W . The electrochemical and electrostatic potentials in this system are shown in figure 3. All the electrons propagating to the right in the left-hand lead are transmitted into the conductor. However, the density of states in the conductor is larger than the density of states in the lead because the conductor is wider than the lead, so the electrochemical potential for the electrons propagating to the right in the conductor is only $(W/w)(\mu_1 - \mu_2)$ greater than that of the neutral conductor. The surprising feature in figure 3 is the increase of the electrochemical potential from the conductor to the right-hand lead for electrons moving to the right and similarly the increase in the electrochemical potential from the conductor to the left-hand lead for holes propagating to the left. In both cases the carriers are moving in the direction opposite to the gradients of their electrochemical potentials. This behaviour can be attributed to the adiabaticity of the evolution of the electronic states through the system. An electron propagating to the right in the left-hand lead is perfectly transmitted into the conductor into a state which is itself perfectly transmitted into the right-hand lead. This example provides a striking illustration of the limitations of the electrochemical potential for describing quantum transport. The distribution function for the electrons in the conductor would show that all the excess electrons propagating to the right in the conductor will be perfectly transmitted into the right-hand lead but the electrochemical potential does not contain this information.

There is no change in the electrostatic potential across this system and so the conductance of the system is infinite when defined with respect to changes in the electrostatic potential. If the conductance of the system is defined in terms of changes in the electrochemical potentials of the carriers moving in a particular direction then a variety of conductances including a *negative* conductance can be measured between different points in the system. If the probe used to measure the difference between electrochemical potential differences does not distinguish between electrons propagating in different directions and simply measures the average of the two electrochemical potentials the conductance of the system will be measured to be infinite.

The examples presented in this paper have been deliberately chosen to be as simple as possible and all the complex features associated with screening and with the precise details of the coupling between the leads and the conductor have been ignored. Nevertheless the examples give some insight into the electrochemical and electrostatic potentials that exist in systems used to investigate quantum transport phenomena and they illustrate under what conditions different forms of the Landauer formula describe the conductance of the systems.

Acknowledgments

The author thanks the Royal Society for financial support.

References

- Beenakker C W J and van Houten H 1989 *Phys. Rev. B* **39** at press
Buttiker M, Imry Y, Landauer R and Pinhas S 1985 *Phys. Rev. B* **31** 6207
Engquist H L and Anderson P W 1981 *Phys. Rev. B* **24** 1151
Landauer R 1985 *Localisation, Interaction and Transport Phenomena in Impure Metals* ed. G Bergmann, Y Bruynserade and B. Kramer (Heidelberg: Springer) p 38
——— 1988 *Which Version of the Formula for the Conductance as a Function of Transmission Probabilities is Correct?* (a technical comment available from the author)
Payne M C 1989 *J. Phys.: Condens. Matter* **1** 4939–46
van Wees B J, van Houten H, Beenakker C W J, Williamson J G, Kouwenhoven L P, van der Marel D and Foxon C T 1988 *Phys. Rev. Lett.* **60** 848
Wharam D A, Pepper M, Ahmed H, Frost J E F, Hasko D G, Peacock D C, Ritchie D A and Jones G A C 1988a *J. Phys. C: Solid State Phys.* **21** L887
Wharam D A, Thornton T J, Newbury R, Pepper M, Ahmed H, Frost J E F, Hasko D G, Peacock D C, Ritchie D A and Jones G A C 1988b *J. Phys. C: Solid State Phys.* **21** L209