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1993 J. Phys.: Condens. Matter 5 L633

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## LETTER TO THE EDITOR

# A new definition of the local chemical potential in a semiconductor nanostructure

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Received 14 September 1993

**Abstract.** A new definition is given for the local chemical potential  $\mu_L$  in a semiconductor nanostructure which is transmitting currents. It is determined by the equation  $n(\mathbf{r}, \mu_1, \mu_2, \dots) = n(\mathbf{r}, \mu_L, \mu_L, \dots)$  where  $n$  denotes the electron density,  $\mathbf{r}$  is the point at which  $\mu_L$  is required and  $\mu_t$  denotes the chemical potential in the reservoir feeding terminal  $t$ . This equation for  $\mu_L$  avoids any reference to non-invasive voltage probes which have been used in previous definitions. It is used to discriminate between previous formulae which use the ideas.

We have recently made calculations of the Hall resistance of a ballistic 2D electron gas which is confined in a quantum wire by hard walls [1,2]. The calculations made use of a particular expression given by Imry [3] for the local chemical potential in the wire. Büttiker [4] derives a similar expression for the self-consistent electrostatic potential and other authors [5,6,7] have sometimes used a different expression for the local chemical potential. All these results are restricted to the low-temperature, linear-transport regime. Moreover, their derivations involve severe approximations. In this letter we give a precise definition of the local chemical potential in a nanostructure described in the one-electron picture. The definition is valid in the non-linear transport regime at all temperatures. In the low-temperature, linear regime it immediately reduces to the formula given by Imry [3].

Imry's formula for the chemical potential at  $\mathbf{r}$  in the low-temperature, linear regime is

$$\mu(\mathbf{r}) = \frac{\sum_t p_t \mu_t}{\sum_t p_t} \quad (1a)$$

where

$$p_t = \sum_\alpha |\theta_{t\alpha}(\mathbf{r})|^2 / v_{t\alpha}. \quad (1b)$$

Here  $t$  labels the terminals feeding the nanostructure,  $v_{t\alpha}$  is the group velocity of mode  $\alpha$  in terminal  $t$  and  $\theta_{t\alpha}(\mathbf{r})$  is the scattered wave generated by an incident wave of unit amplitude in a mode  $\alpha$  in terminal  $t$ . All the quantities involved are evaluated at the equilibrium Fermi level.

The derivation of equation (1) rests on a particular view of the behaviour of non-invasive voltage probes [9,10]. Akera and Ando [7] also use equation (1) for  $\mu(\mathbf{r})$  in an electron waveguide. They justify the equation by envisaging a non-invasive probe which removes an infinitesimal current proportional to the local electron density in the mode considered. They [6,7] and Peeters [5] also calculate results for  $\mu(\mathbf{r})$  from equation (1) when the group

velocity factors are omitted from equation (1b). In this case the probe is envisaged as removing an infinitesimal current which is proportional to the local current density in the mode considered. Both these hypothetical probes fit well into the one-electron formalism but it is not clear how either of them could be fabricated so as to behave in the manner assumed.

Büttiker [4] calculates the self-consistent electrostatic potential  $U(\mathbf{r})$  in a nanostructure when currents are transmitted. He uses the Thomas–Fermi approximation and assumes strong screening. The physics behind the calculation is completely different from that used on the calculations of  $\mu(\mathbf{r})$  described above. Surprisingly, the result in equation (1) again *but* with  $\mu(\mathbf{r})$  replaced by  $U(\mathbf{r})$  in equation (1a). Neither of the approximations made in the calculation of  $U(\mathbf{r})$  are very appropriate to the one-electron formalism which is usually employed to describe the electronic behaviour of semiconductor nanostructures [4, 8]. Moreover in [1] and [2] we have calculated a Hall resistance from the numerically determined self-consistent electrostatic Hall potential which arises when current flows in the presence of a magnetic field. It behaves completely differently from the Hall resistance calculated from  $\mu(\mathbf{r})$  and, in particular, it does not exhibit the expected quantization.

We now turn to the new definition of the local chemical potential. To do so we consider an arbitrary nanostructure in two different situations. Firstly, a non-equilibrium situation in which the chemical potential in the reservoir feeding terminal  $t$  takes an arbitrary value  $\mu_t$ . We write  $n(\mathbf{r}, \mu_1, \mu_2, \dots)$  for the electron density at  $\mathbf{r}$  in this case. Secondly, we consider an *equilibrium* situation in which  $\mu_t = \mu_0$  for all  $t$ . The electron density at  $\mathbf{r}$  in this case is simply  $n(\mathbf{r}, \mu_0, \mu_0, \dots)$  which we abbreviate to  $n_e[\mathbf{r}, \mu_0]$ .

We may now define the local chemical potential at the point  $\mathbf{r}$  by the equation

$$n_e[\mathbf{r}, \mu(\mathbf{r})] = n(\mathbf{r}, \mu_1, \mu_2, \dots) \quad (2)$$

i.e.  $\mu(\mathbf{r})$  is the chemical potential in the equilibrium system which creates the same electron density at  $\mathbf{r}$  as that which is actually found there in the non-equilibrium system.

Equation (2) applies at all temperatures and all values of  $\mu_t$ . It is easily solved for  $\mu(\mathbf{r})$  in the linear, low-temperature regime assumed in equation (1). Since the reservoirs are phase randomizing, we have

$$n(\mathbf{r}, \mu_1, \mu_2, \dots) = \sum_t \sum_\alpha \int d\epsilon f_t(\epsilon) N_{t\alpha} |\theta_{t\alpha}(\mathbf{r})|^2 \quad (3)$$

where  $f(\epsilon)$  is a Fermi–Dirac function with chemical potential  $\mu_t$  and  $N_{t\alpha} = 2/hv_{t\alpha}$  is the density of states for mode  $\alpha$  in terminal  $t$ . To obtain  $n_e[\mathbf{r}, \mu(\mathbf{r})]$ , we have only to replace every  $f_t(\epsilon)$  in equation (3) by the Fermi–Dirac function  $f_\mu(\epsilon)$  which involves the local chemical potential  $\mu(\mathbf{r})$ . According to equation (2), the difference between these two quantities must vanish. The integrals in the difference involve

$$f_t(\epsilon) - f_\mu(\epsilon) \simeq -[\mu_t - \mu(\mathbf{r})] \frac{df_0(\epsilon_F)}{d\epsilon} \simeq [\mu_t - \mu(\mathbf{r})] \delta(\epsilon - \epsilon_F). \quad (4)$$

Here  $f_0(\epsilon)$  is the Fermi–Dirac function involving the equilibrium chemical potential  $\epsilon_F$  of the nanostructure before it was perturbed. The first approximation in equation (4) is valid in the linear regime because both  $\mu_t$  and  $\mu(\mathbf{r})$  remain close to  $\epsilon_F$ . The second approximation is standard at low temperatures. With the aid of equation (4) we find immediately that equation (2) reduces to equations (1).

The advantage of the new definition of  $\mu(\mathbf{r})$  is that it involves no assumptions or approximations which are not already involved in the Landauer–Büttiker formalism. No appeal is made to self-consistent fields, screening, or non-invasive probes of any sort. Moreover, the general formula (2) for  $\mu(\mathbf{r})$  is valid at high temperatures and in the non-linear regime. In the low-temperature, linear regime, the new definition reduces to Imry's formula (1) for the chemical potential. The Hall resistance calculated from  $\mu(\mathbf{r})$  in this regime exhibits the expected quantization [1, 2, 7]. The weighting factors  $p_i$  involve  $v_{\alpha}^{-1}$  and, as a consequence of this, the Hall resistance is *quenched* as the Fermi level approaches the bottom of an excited subband [2]. The alternative formula for  $\mu(\mathbf{r})$  in which  $v_{\alpha}^{-1}$  is omitted from  $p_i$  also yields a quantized Hall resistance but it does not quench [5, 6, 7].

Quenching is found in crossed ballistic quantum wire structures both theoretically [11] and experimentally [12–15]. However, the behaviour of the quench is strongly dependent on the geometry of the cross and it does not correlate well with the simple picture predicted by equation (1). Experimental studies of the effect of subband depopulation on the Hall resistance would be very interesting in this regard.

This work was supported by the United Kingdom Science and Engineering Research Council.

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