Energy Dissipation in Mesoscopic Circuits

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***Abstract*— We will show that energy dissipation in mesoscopic circuits can be included in a consistent manner by the use of a quantum transport formalism developed by the authors. In particular we show how energy dissipation is induced by the presence of elastic scattering barriers. This will enable us to derive the Landauer formula for the conductance of a quantum wire and the Landauer-Büttiker formula for the conductance of a quantum point contact in a consistent way. The derivations of these conductances is realized without referring to so-called reservoirs where all the dissipation is assumed to take place. A study of the energy density for a quantum wire containing a localized elastic scattering barrier will clearly show that we are able to investigate the local dissipative properties of mesoscopic systems.**

I. Introduction

We developed a formalism for modeling quantum transport in closed electric circuits [2], [3], [4]. This transport formalism differs from the conventional approach towards mesoscopic transport in that we are considering the electric circuit as a whole, i.e. we are not explicitly chopping the circuit into different regions. The electric circuit thus constitutes a region Ω which is simply connected. As a consequence we are not following the conventional approach of attaching reservoirs to mesoscopic structures in which different chemical potentials are present. This transport formalism is based upon a consistent solution of energy and momentum balance equations in the steady-state regime together with Poisson's equation for the electrostatic potential :

$$IV_\epsilon = \frac{i}{\hbar} < [\hat{H}_e, \hat{H}'] > \tag{1}$$

$$\int_\Omega d\tau \rho_e E = -\frac{i}{\hbar} < [\hat{P}_x, \hat{H}'] > - \int_\Omega d\tau \rho_e \frac{dV(x)}{dx} \tag{2}$$

$$-\frac{d^2V(x)}{dx^2} = -\frac{e}{\epsilon}[n(x) - n_0(x)] \tag{3}$$

where $\rho_e = -e\rho$ is the electron charge density, I is the current, V_ϵ is the applied EMF, $\hat{H}$' is the electron-phonon interaction Hamiltonian, $\hat{H}_e$ is the electron Hamiltonian, $\hat{P}_x$ is the momentum operator, while V represents the internal potentials. In Eq. (3) $n(x)$ is given by

$$n(x) = 2\sum_{kn} F(\epsilon_{kn} + \gamma_0 I_k - eV(x))\rho_{kn}(x) \tag{4}$$

where $\rho_{kn}(x)$ is the electron probability density. $n_0(x)$ is the equilibrium electron density. The electric field E in Eq. (2) is in general not homogeneous and satisfies $\oint E(x)dx = V_\epsilon$. In order to solve the set of Eqs. (1)-(3) we will separate the homogeneous and local forces by splitting the electric field into a homogeneous and localized part, i.e. $E = E_H + E_\delta$. The homogeneous part of the electric field is then related to the homogeneous electron-phonon friction force, while the localized part is related to the presence of the localized internal potential $V(x)$ [2]. As a result the voltage drop over the circuit can be written as $V_\epsilon = V_H + V_\delta$. This allows us to derive the transport properties of a quantum circuit under various circumstances without referring to so-called reservoirs to which a mesoscopic region within the circuit would be attached. Furthermore we are able to look at the global and *local* properties of the system under investigation. Solving the balance equations results in a boosted Fermi-Dirac distribution for the electrons given by $F_e(\epsilon_k + \gamma_0 I_k - \mu)$ where $\beta_e = 1/kT_e$, while μ is the chemical potential. For a nonzero value of the parameter γ_0 we thus have a current-carrying electron ensemble. It is important to bear in mind that γ_0 is determined by the set of Eqs. (1)-(3). This means that γ_0 is determined by the dissipative properties of the mesoscopic system under consideration. In what follows we will first show in Sec. II how our quantum transport formalism enables us to derive the Landauer-Büttiker (LB) conductances of a quantum point contact (QPC) and a quantum wire and how energy dissipation is related to this quantized conductance. In Sec. III we will investigate the energy density for a quantum wire containing a localized elastic scattering barrier. This will show that our quantum transport formalism is able to probe the local dissipative properties of the system under investigation.

II. Dissipation and Conductance Quantization

In the low-temperature linear response regime we are able to derive the Landauer formula $G = (2e^2/h)T/R$ [5], [2] for the conductance associated with an elastic scattering barrier in the low-temperature linear-response regime for a quantum wire with only one subband. Not only does this allow us to proof that the resistance associated with an elastic scattering barrier is originating from the induced dissipation due to the presence of such a barrier [2], [3]. We are also able to reproduce one of the most important results from mesoscopic physics, i.e. the conductance associated with a scattering barrier described by the Landauer formula. Here we take a closer look at the conductance of a quantum point contact (QPC) [7] with our transport formalism and we will derive the LB conductance $G = (2e^2N/h)T$. The starting point of our calculation is the 2D constriction depicted in Fig. (1). Here L is the length of the circuit circumference, while Δx is the constriction length and L_c is the length of the wire in the constriction. We emphasize that we are considering a so-called WKB approximation in

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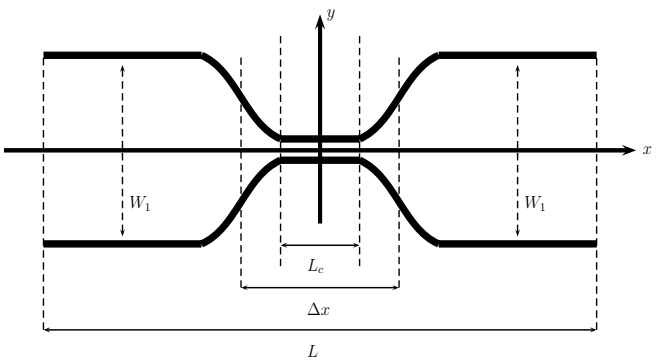

Fig. 1. Schematic representation of the WKB constriction in a 2DEG

which the constriction funnel is sufficiently smooth, i.e. the transition from the leads to the quantum wire happens slowly in order to avoid additional reflections. We also allow for the presence of an additional elastic scattering potential $U(x)$ with $U(x) = 0$ for $|x| > x_0$ where $x_0 \ll L_c$. This means that in a limited region within the constriction an elastic scattering potential is present which will be responsible for reflection and transmission. The Schrödinger equation for the electron wave functions in this 2DEG can be written as follows

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(x,y) + U(x)\Psi(x,y) = \epsilon\Psi(x,y), \qquad (5)$$

with the boundary condition $\Psi(x, y = \pm W(x)/2) = 0$. Using the ansatz $\Psi(x,y) = \xi_n(x)\phi_{nx}(y)$ we obtain an effective 1-dimensional Schrödinger equation in the WKB approximation :

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\xi_{nk}(x) + (V_n(x) + U(x))\,\xi_{nk}(x) = \epsilon_{nk}\xi_{nk}(x) \quad (6)$$

where $V_n(x) = \hbar^2\pi^2n^2/2mW(x)^2$ is the effective potential and

$$\phi_{nx}(y) = \sqrt{\frac{2}{W(x)}} \begin{cases} \sin(\frac{n\pi y}{W(x)}) & \text{n even} \\ \\ \cos(\frac{n\pi y}{W(x)}) & \text{n odd} \end{cases} \qquad (7)$$

The exact form of $W(x)$ and thus $V_n(x)$ is not of interest here as long as the variation of $W(x)$ is sufficiently smooth. In this sense $W(x)$ only determines the number of "channels" or current-carrying states denoted by N. In Fig. (2) we have depicted the effective potential $V_n(x)$ for $n = 1, 2, 3$ in the case of 2 channels, while in Fig. (3) we have depicted the width $W(x)$ as a function of x. For example, the width $W(x)$ may be modeled by

$$W(x) = \begin{cases} W_2 & |x| < L_c/2 \\ W_1 - (W_1 - W_2)e^{-(x-L_c/2)^2/\Delta x^2} & x > L_c/2 \\ W_1 - (W_1 - W_2)e^{-(x+L_c/2)^2/\Delta x^2} & x < L_c/2 \end{cases} \qquad (8)$$

where $W_1 = 10^{-3}$ m, $W_2 = 10^{-8}$ m, $L_c = 1$ μm and $\Delta x \approx 0.5$ mm. The minimum width at $x = 0$ is then given by $W(0) = 10^{-8}$ m, while the width of the contacts is given by $W(x) = 10^{-3}$ m for $|x| >> 0$. In Fig. (2) we also indicated the Fermi-level ϵ_F at $\epsilon_F \approx 0.04$ eV. For this Fermi-level only the states $n \leq 2$ are current-carrying, while for $n > 2$ we assume total reflection so that there is no contribution to the current from these states. The calculation of the conductance

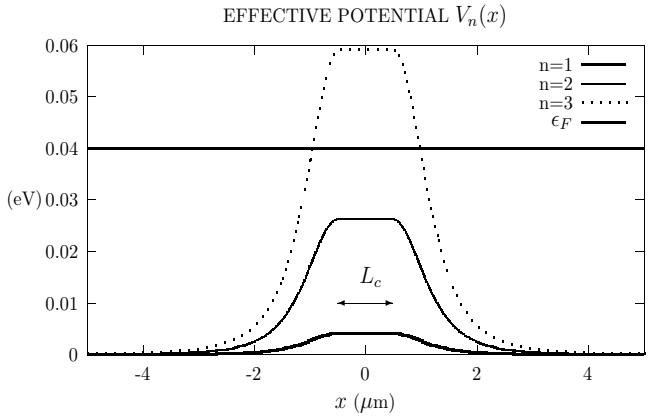

Fig. 2. Effective Potential $V_n(x)$ for $n = 1, 2, 3$ with 2 channels

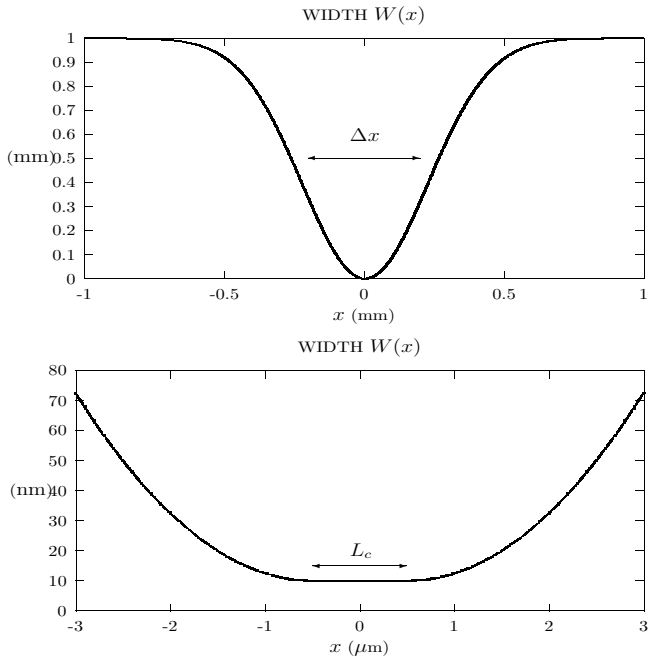

Fig. 3. Width $W(x)$ as a function of x

starts with the evaluation of the electrostatic potential $V(x)$ along the circuit satisfying Poisson's equation :

$$-\frac{d^2V(x)}{dx^2} = -\frac{e}{\epsilon}[n(x) - n_0] \qquad (9)$$

where the electron density is given by Eq. (4), while the electron probability density $\rho_{kn}(x)$ is derived from

$$\rho_{kn}(x) = \int dy\rho_{kn}(x,y) = \int dy\rho_{kn}(x)\rho_n(y). \qquad (10)$$

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with $\rho_{kn}(x,y) = |\xi_{nk}(x)\phi_{nx}(y)|^2$. Converting the sum over k into an integral, we obtain the following integro-differential equation :

$$\frac{d^2V(x)}{dx^2} = \frac{e}{\epsilon}\left[2\sum_n \int dk F(\epsilon_{kn} + \gamma_0 I_k - eV(x))\rho_{kn}(x) - 2\sum_n \int \frac{dk}{2\pi} F(\epsilon_{kn})\right]. \quad (11)$$

In the linear-response regime, i.e. for $eV(x) \ll \epsilon_F$ and $|\gamma_0| \ll |\epsilon_{kn}/I_k|$ and for asymptotic values of the coordinate x we can linearize Eq. (11) and we can set $V''(x) \approx 0$. This will lead to the following result for the asymptotic value of V_1 for $x \ll -\Delta x$ [1] :

$$\frac{2emV_1}{\hbar^2} = 2\gamma_0 k_F B(k_F). \quad (12)$$

A similar calculation for $x \gg \Delta x$ gives $V_2 = -V_1$. The potential difference V_δ is then given by

$$V_\delta = V_2 - V_1 = -4\gamma_0 \frac{\hbar^2 k_F B(k_F)}{2em} = -\gamma_0 \frac{2\hbar^2 k_F}{em} B(k_F). \quad (13)$$

If we substitute this result in the expression for the current I, i.e. $I = -(4e\hbar k_F \gamma_0/2\pi m) NT(k_F) B(k_F)$, we obtain $I = (2e^2/h) NT(k_F) V_\delta$. As a result the conductance associated with the barrier $U(x)$ and the effective potential $V_n(x)$ is given by

$$G_{LB} = \frac{2e^2}{h} NT(k_F). \quad (14)$$

This is the LB conductance [5], [9], [10], [6]. The potential V_δ can then be set to V_{LB}, i.e. the voltage drop associated with the LB conductance. We emphasize that the derivation above is done in a consistent way because dissipation is included through the parameter γ_0. We stress again that the calculation of γ_0 is done by solving the energy and momentum balance equations [2]. It is clear that dissipation shows up in two different ways. First of all, we have the dissipation due to the presence of phonons. This is reflected in the homogeneous voltage drop V_H. On the other hand we also have *induced* dissipation due to the presence of elastic scattering barriers. In the case of the LB resistance we have two barriers : the effective potential $V_n(x)$ and the localized scattering barrier in the constriction $U(x)$. In the linear-response and low-temperature case, the homogeneous voltage drop of the phonons is very small, but it is still present. In other words the total conductance can be written as $G_{tot}^{-1} = G_P^{-1} + G_{LB}^{-1}$, where G_{LB} is the conductance associated with the presence of the barrier and the constriction given by (14), while G_P is the conductance associated with the presence of the phonons :

$$G_P = \frac{I}{V_H} = -\alpha \frac{4e\hbar k_F}{2\pi m} NT(k_F) B(k_F) \quad (15)$$

In (15) we have made use of the fact that γ_0 is obtained via the balance equation approach [2] in the linear-response regime. This means that we are allowed to write $\gamma_0 = \alpha V_H$ where α is determined by the properties of the electron-phonon system. We stress again that (15) is the conductance associated with the presence of the phonons.

III. Calculation of the Energy Density

In order to further support the statement that dissipation is induced by the presence of an elastic scattering barrier, we will now take a closer look at the energy density profile of a quantum wire containing a localized elastic scattering barrier modeled by a Dirac-delta function $U(x) = \Lambda\delta(x)$. Numerical simulations show that an energy jump occurs in the region where the scattering barrier is localized. In the low-temperature linear response regime we will calculate this energy jump Δw which will turn out to be given by $\Delta w = eV_\delta/\pi k_F$ where V_δ is the voltage drop associated with the scattering barrier. This shows that the energy jump is equal to the voltage drop associated with the scattering barrier and occurs over a Fermi-wavelength $2\pi/k_F$. Another way for obtaining a clear picture of the different dissipative mechanisms at work is to consider the different voltage drops as we have done at the end of Sec. II for the QPC. In the case of a quantum wire containing phonons and an elastic scattering barrier, we have two different voltage drops namely V_H and V_δ [2]. V_H is the so-called homogeneous voltage drop associated with the presence of the phonon bath. V_δ however is an induced voltage drop due to the presence of an elastic scattering barrier. This barrier changes the electron-phonon coupling *locally* and this results in a localized voltage drop V_δ. The energy density operator is given by

$$\hat{w}(\vec{r}) = \hat{\Psi}^+(\vec{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + U(x)\right] \hat{\Psi}(\vec{r}) \quad (16)$$

where the electron field operators are given by

$$\hat{\Psi}(\vec{r}) = \sum_{k\alpha} \hat{c}_{k\alpha} \phi_k(x) \Phi_\alpha(y,z). \quad (17)$$

As a result we may write for the expectation value of (16)

$$\langle \hat{w}(\vec{r})\rangle_0 = \sum_{k\alpha}\sum_{k'\alpha'} \langle \hat{c}^+_{k\alpha}\hat{c}_{k'\alpha'}\rangle_0 \epsilon_k \phi^*_k(x)\phi_{k'}(x) \Phi^*_\alpha(y,z)\Phi_{\alpha'}(y,z) \quad (18)$$

where $\langle \hat{c}^+_{k\alpha}\hat{c}_{k'\alpha'}\rangle_0 = F(\epsilon_{k\alpha} + \gamma_0 I_k)\delta_{kk'}\delta_{\alpha\alpha'}$ and we obtain for Eq. (18) :

$$\langle \hat{w}(\vec{r})\rangle_0 = \sum_{k\alpha} F(\epsilon_{k\alpha} + \gamma_0 I_k)\epsilon_k \rho_k(x) \Phi^*_\alpha(y,z)\Phi_\alpha(y,z). \quad (19)$$

Next we assume low-temperature and strong confinement, such that only the lowest sub-band is occupied. Eq. (19) then becomes

$$\langle \hat{w}(\vec{r})\rangle_0 = \sum_{k} F(\epsilon_k + \gamma_0 I_k)\epsilon_k \rho_k(x) \Phi^*_0(y,z)\Phi_0(y,z). \quad (20)$$

After integration over the (y,z)-coordinates we obtain

$$\langle \hat{w}(x)\rangle_0 = \sum_{k} F(\epsilon_k + \gamma_0 I_k)\epsilon_k \rho_k(x). \quad (21)$$

In the linear response regime we have $|\gamma_0| \ll |\epsilon_k/I_k|$ which results in (after approximating the discrete sums into integrals) :

$$\langle \hat{w}(x) \rangle_0 = \int dk F(\epsilon_k)\epsilon_k \rho_k(x) + \gamma_0 \int dk \frac{dF(\epsilon_k)}{d\left(\frac{\epsilon_k}{I_k}\right)} \epsilon_k \rho_k(x) \tag{22}$$

where now $\rho_k(x)$ is renormalized. We start with the asymptotic value $x \ll 0$. We obtain for Eq. (22) (neglecting the oscillatory part of $\rho_k(x)$) in the low-temperature regime

$$\langle \hat{w}(x) \rangle \quad = \quad \int_0^{+\infty} \frac{dk}{\pi} F(\epsilon_k)\epsilon_k + \frac{\gamma_0}{\pi} R(k_F)B(k_F)\epsilon_F \tag{23}$$

where $B(k) = \left(d/dk\left(\epsilon_k/I_k\right)\right)^{-1}$. The same calculation for $x \gg 0$ gives

$$\langle \hat{w}(x) \rangle \quad = \quad \int_0^{+\infty} \frac{dk}{\pi} F(\epsilon_k)\epsilon_k - \frac{\gamma_0}{\pi} R(k_F)B(k_F)\epsilon_F \tag{24}$$

These two asymptotic values for $w(x)$ enable us to calculate the asymptotic energy density difference $\Delta w(x)$

$$\begin{aligned} \Delta w(x) \quad &= \quad w(x)|_{x\gg 0} - w(x)|_{x\ll 0} \\ &= \quad -\frac{2\gamma_0}{\pi} R(k_F)B(k_F)\epsilon_F. \end{aligned} \tag{25}$$

The value of γ_0 for a quantum wire is given by [2] :

$$\gamma_0 = -V_\delta \frac{em}{2\hbar^2 k_F R(k_F)B(k_F)}. \tag{26}$$

Combining Eqs. (25) and (26) then gives the following result for the energy density jump :

$$\Delta w = \frac{eV_\delta}{2\pi} k_F. \tag{27}$$

This means that the electron energy drop is given by eV_δ and occurs over a distance $2\pi/k_F$. It is important to point out that the electron energy density is calculated using the diagonal elements of the expectation value only, i.e. $\langle ... \rangle = \langle ... \rangle_0$. As a consequence, the energy drop due to the phonon distribution, is not contributing to the relation (27). The presence of the phonons is incorporated in the result (27) through the parameter γ_0. Although we have only calculated $w(x)$ asymptotically, i.e. for $|x| \gg 0$, we have numerically solved $w(x)$ for all x. The result is shown in Fig. (4) for different barrier heights Λ at a total voltage drop $V_\epsilon = 10\,\mathrm{mV}$. We also indicated the energy jump Δw for the largest barrier height Λ.

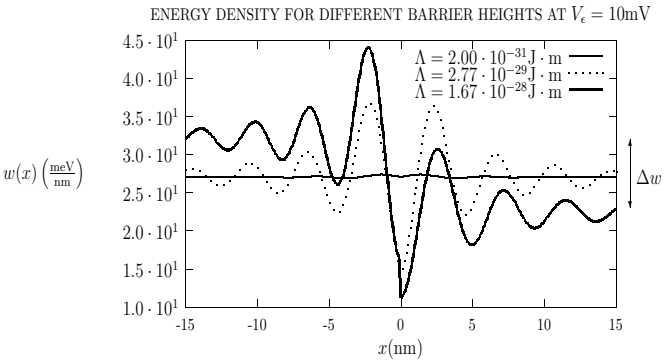

Fig. 4. Local energy density profile $w(x)$ for different values of the barrier height Λ

IV. Conclusion

We showed that energy dissipation is localized in the regions where elastic scattering barriers are present. This clearly demonstrates that our transport formalism which includes dissipation is not only able to reproduce the well-known results from mesoscopic physics, we also show that dissipation must be included in order to obtain a proper physical picture. Another important difference between our method and the "textbook" approach [8] towards mesoscopic quantum transport is that we do not assume that dissipation is taking place solely in the so-called reservoirs; dissipation is present everywhere. Experiments involving QPC's show the presence of a background resistance of the order of $100\,\Omega$ [7]. This background resistance is clear experimental proof that dissipation is always present. Furthermore we are able to account for this residual resistance because there is always a homogeneous voltage drop V_H associated with the presence of phonons. We have shown that dissipation is also present in the constriction of the QPC. As a result the very notion of ballistic transport is rejected by our formalism because dissipation is present in the constriction.

Acknowledgment

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