Dissipative Transport in Quantum Wires

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Abstract

Starting from the quantum mechanical balance equations for a closed electric circuit represented by a closed region Ω and applying numerical solution methods we obtain information on the global and local transport properties. In particular we consider a quantum wire at low temperature containing a localized elastic scattering barrier. A new scheme is presented to calculate the localized electric field originating from the barrier. The resulting resistance associated with the localized barrier in the low-temperature linear response regime coincides with the Landauer formula.

1. Introduction

In ref. [1, 2, 3], it was argued that the reservoir concept is not suitable to set up a quantum transport formalism. An alternative approach was proposed based on the non-trivial topology of closed electric circuits. This formalism enables us to investigate various local and global quantum transport properties of electric circuits containing a mesoscopic region. The electric circuit is represented by a closed region Ω in which the electrons are confined. The region Ω also contains a battery that is responsible for the electromotive force (EMF) caused by an externally applied voltage. In general electromagnetic fields (E, B) will be present. The one-electron wave functions and the field operators \( \hat{\Psi} \) vanish at the circuit boundary \( \hat{\Psi}(r, t) = 0 \) at \( \partial \Omega \). The electromagnetic fields \( E \) and \( B \) are related to a scalar and vector potential \( (V, A) \). The total Hamiltonian can be written as
\[
\hat{H} = \hat{H}_c + \hat{H}_p + \hat{H}'
\]

where
\[
\hat{H}_c = \int_{\Omega} d\tau \left( \frac{1}{2} m \mathbf{v} \cdot \mathbf{v} + \mathbf{v} \cdot \hat{\mathbf{P}} + (U - eV) \hat{\mathbf{P}} \right).
\]

Eq. (1) represents the electron energy in the presence of internal potentials \( U \) and electromagnetic fields, where \( \mathbf{v} = (-i\hbar\nabla + e\mathbf{A})/m \) is the velocity operator. \( \hat{H}_p \) and \( \hat{H}' \) respectively represent the phonon bath energy and the electron-phonon interaction energy.

2. Balance equations

The following set of global balance equations in the steady-state regime were derived in [2, 3]:
\[
IV_e = \frac{i}{\hbar} \langle [\hat{H}_c, \hat{H}'] \rangle = P(\gamma_0, T_e)
\]
\[
\int_{\Omega} d\tau \langle \hat{\mathbf{P}}, \hat{H}' \rangle + \int_{\Omega} d\tau \langle \hat{\rho} \rangle \nabla U(r) = \mathbf{F}(\gamma_0, T_e),
\]

where \( IV_e \) is the power delivered by the battery, \( \gamma_0 \) a Lagrange multiplier conjugate to the current, \( T_e \) the electron temperature, while \( \mathbf{F}(\gamma_0, T_e) \) is the friction force arising from the phonons and the internal elastic scattering barriers. The product \( IV_e \) in Eq. (2) arises due to an integral theorem for closed electric circuits [4].

In order to solve the balance equations (2)-(3) in the steady-state regime we use first-order perturbation theory to calculate the ensemble average of an arbitrary Hermitian operator \( \hat{A}(t) \) in the Heisenberg picture
\[
\langle \hat{A}(t) \rangle = \langle \hat{A}^{(0)}(t) \rangle_0 - \frac{i}{\hbar} \int_0^t d\tau' \left[ \langle \hat{A}^{(0)}(t), \hat{H}_{int}(\tau') \rangle \right]_0
\]

where the superscript \( (0) \) denotes the interaction picture for operators. The total Hamiltonian is divided into an unperturbed part \( \hat{H}_0 \) and an interaction part \( \hat{H}_{int} \). The initial density operator \( \hat{\rho}_0 \) is not chosen to be the Gibbs-ensemble. Instead, it is taken to be a "boosted" initial density operator, i.e.
\[
\hat{\rho}^B_0 = \frac{1}{Z} \exp \left( -\beta_e (\hat{H}_c - eV) \right) \exp \left( -\beta H_p \right)
\]
\[
\hat{H}_c = \hat{H}_c - \sum_k c_k^+ c_k \gamma_0 I_k.
\]

The initial density operator \( \hat{\rho}^B_0 \) is parameterized by \( \beta_e = 1/k_B T_e \) and \( \gamma_0 \), where \( I_k \) is the current carried by the eigenstate \( |k\rangle \). Physically, it represents a moving and non-interacting electron system and a free phonon system in thermal equilibrium. The line integral of the electric field in the region \( \Omega \) must be equal to the EMF, i.e.
\[
V_e = \oint_C \mathbf{E} \cdot d\mathbf{l}.
\]
The independent variables $\gamma_0$, $T_e$ and $V_e$ are found by solving Eqs. (2), (3) and (7) in a self-consistent way. A similar approach was used in hot electron transport [5, 6].

3. Quantum wire

We study the local and global transport properties of a quantum wire containing a localized elastic scattering potential modeled by a Dirac delta potential. The parameters characterizing our quantum wire are given in Table 1. We further simplify the notation by remarking that only the lowest subband will be occupied.

Table 1. Physical parameters

<table>
<thead>
<tr>
<th>Number of electrons $N_e$</th>
<th>$5.0 \cdot 10^5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice temperatures $T$</td>
<td>$5.0, 10.0, 15.0 \text{ K}$</td>
</tr>
<tr>
<td>Effective mass $m$</td>
<td>$0.916 m_e$</td>
</tr>
<tr>
<td>Lateral dimensions $L_y, L_z$</td>
<td>$1.0 \text{ nm}$</td>
</tr>
<tr>
<td>Wire length $L_x$</td>
<td>$1 \text{ mm}$</td>
</tr>
<tr>
<td>Sound velocity $v_s$</td>
<td>$9.04 \cdot 10^3 \text{ m/s}$</td>
</tr>
<tr>
<td>Deformation potential $D$</td>
<td>$14.0 \text{ eV}$</td>
</tr>
<tr>
<td>Mass density $\rho_m$</td>
<td>$2.329 \cdot 10^3 \text{ kg/m}^3$</td>
</tr>
</tbody>
</table>

are distributed homogeneously over the wire, while the lattice temperature is taken to be sufficiently low. For strong enough confinement this allows us to restrict the calculations to the lowest subband only. The one-electron Schrödinger equation supplying the basis wavefunctions is given by $H_0 \phi_{k n y n_z}(x, y, z) = \epsilon_{k n y n_z}(x, y, z) \phi_{k n y n_z}(x, y, z)$, where $k$ is the longitudinal wavevector, while the one-electron Hamiltonian $H_0$ is given by

$$H_0 = -\frac{\hbar^2}{2m} \nabla^2 + U(x) + V_C(y, z)$$

$m$ is the electron band mass and the quantum numbers $n_y, n_z$ denote the lateral confinement quantum numbers. The confinement potential is given by

$$V_C(y, z) = \frac{1}{2} \sigma m \omega^2 (y^2 + z^2)$$

while the elastic scattering potential is taken to be:

$$U(x) = \Lambda \delta(x).$$

We emphasize that the elastic scattering potential (10) is explicitly included in the solutions of the Schrödinger equation which enables us to treat the barrier height $\Lambda$ non-perturbatively. We further simplify the notation by remarking that only the lowest subband will be occupied, i.e. we have that $n_y = n_z = 0$. The latter quantum numbers will not be written explicitly in the rest of our calculations. The electron wavefunctions thus have the following form for right- and left going states respectively:

$$\phi_k(x, y, z) = \varphi_k(x) \chi(y, z)$$

where $\varphi_k(x)$ are the well-known solutions of the Schrödinger equation containing a Dirac delta potential $\Lambda \delta(x)$, while

$$\chi(y, z) = N_0^2 e^{-\alpha^2(y^2+z^2)} \qquad \alpha = \left(\frac{\sigma m \omega_e}{\hbar}\right)^{1/2}$$

where $N_0$ is the normalization constant for the lateral wavefunction. The electron-phonon interaction is described by the Hamiltonian $\hat{H'}$ and is taken to be the standard bulk interaction [9], i.e.

$$\hat{H'} = \int d^3 x \hat{\rho}(r) \hat{V}(r)$$

where

$$\hat{V}(r) = \frac{1}{\Omega^{1/2}} \sum_{\mathbf{q}} e^{i\mathbf{r}\cdot \mathbf{q}} M(\mathbf{q}) \{ a_q + a^+_q \}$$

and $\hat{\rho}$ is the electron density operator. For acoustic phonons we have $|M(\mathbf{q})|^2 = \hbar \Omega D(\mathbf{q})^2 / 2 \rho_m \omega_q$ where $\omega_q = v_s |\mathbf{q}|$ is the phonon dispersion relation, $\rho_m$ is the mass density, $D$ is the deformation potential and $v_s$ is the sound velocity. The balance equations for energy and momentum in steady-state are given by

$$IV_c = \frac{i}{\hbar} \langle \hat{H}_e, \hat{H}' \rangle_{t \to \infty}$$

$$e \int_{\Omega} d\tau \langle \hat{p}(\mathbf{r}) \rangle E(x) = \frac{i}{\hbar} \langle \hat{P}_e, \hat{H}' \rangle_{t \to \infty} - e \int_{\Omega} d\tau \langle \hat{p}(\mathbf{r}) \rangle \frac{dV(x)}{dx}$$

where the average $\langle \hat{A} \rangle_t = \text{Tr} \{ \rho_0^t \hat{A}(t) \}$ is taken with the boosted initial density operator. Bearing in mind that the elastic scattering is modeled by a delta-function, we assume that the total electric field can be written as the sum of a homogeneous and localized part, i.e.

$$E(x) = E_H + V_\delta \delta(x)$$

which leads to

$$\int_{-C}^C E(x) dx = E_H L_x + V_\delta = V_H + V_\delta = V_e$$

in order to comply with (7). However, the set of Eqs. (15)-(16) and (18) are insufficient to solve the set of independent unknowns $(\gamma_0, T_e, V_H)$ because the localized electric field $E_\delta(x)$ is still unknown. In other words, we tacitly assume that the homogeneous electric field $E_H$ results solely from the homogeneous electron-phonon frictional force, while the localized electric field $V_\delta \delta(x)$ relates to the presence of the localized delta potential scatterer $U(x) = \Lambda \delta(x)$ through an induced potential $V(x)$. The induced potential $V(x)$ is obtained using a self-consistent solution of the Poisson equation as we will show below. Finally, we remark that the influence of the localized elastic scatterer $U(x)$ is already included in the basis wavefunctions. This means that the homogeneous friction force $F_H(\gamma_0, T_e) = i \hbar \langle \hat{P}_e, \hat{H}' \rangle$ and the power dissipation $P(\gamma_0, T_e)$ originating from the phonons is also affected by the presence of $U(x)$. 
4. Localized electric field

The localized electric field originating from the presence of the Dirac-delta potential is obtained through a self-consistent solution of the Poisson equation. The total (screened) potential is derived from
\[ \frac{d^2 V(x)}{dx^2} = -\frac{e}{\varepsilon} [n(x) - n_0] \]  
where the total average electron charge density is given by
\[ -e n(x) = -2e \int dk F(\epsilon_k + \gamma_0 J_k - eV(x)) \rho_k(x) \]  
where \[ \rho_k(x) = |\varphi_k(x)|^2 \] is the electron probability density. The positive background charge density is
\[ e n_0 = 2e \int \frac{dk}{2\pi} F(\epsilon_k). \]
The asymptotic solutions of Eq. (19), i.e. the values of \( V(x) \) at \( x \ll 0 \) and \( x \gg 0 \), are given by
\[ V_1 = \frac{\hbar^2 k_F^2 \gamma_0}{em} B(k_F) R(k_F) \quad x \ll 0 \]  
\[ V_2 = -\frac{\hbar^2 k_F^2 \gamma_0}{em} B(k_F) R(k_F) \quad x \gg 0, \]
where \( R(k_F) \) is the reflection coefficient at Fermi level, while \( B(k_F) \) is a function of \( k \) given by
\[ B(k) = \left( \frac{d}{dk} \left( \frac{\epsilon_k}{I_k} \right) \right)^{-1}. \]
The resulting localized electric field is then given by
\[ E_\delta(x) = V_\delta \delta(x) \]
where
\[ V_\delta = V_2 - V_1 = -\gamma_0 \frac{2\hbar^2 k_F}{em} B(k_F) R(k_F). \]

5. The Landauer resistance revisited

The localized resistance \( R_\delta = V_\delta / I \), defined as the resistance of the barrier region, can be calculated from the current \( I \) given by
\[ I = -\frac{4e\hbar k_F \gamma_0}{2\pi m} T(k_F) B(k_F). \]
Combining (27) and (26) then results in
\[ I = \frac{2e^2}{\hbar} T(k_F) V_\delta. \]
As a result the localized resistance reads
\[ R_\delta = \frac{\hbar}{2e^2} \frac{R(k_F)}{T(k_F)}. \]
Our method for obtaining the localized electric field thus results in the Landauer resistance \([7, 8]\) for the localized barrier. It is important to point out that this resistance is not calculated by assuming different chemical potentials to be assigned to different reservoirs. Instead our calculation is a result of a consistent transport formalism.

6. Numerical results

In Fig. 1 we show the homogeneous and localized voltage drop as a function of the barrier height \( \Lambda \) at lattice temperature \( T = 5K \). This figure shows that for low barrier heights the localized voltage drop is almost zero. As the barrier height of the delta-scatterer is increased, the homogeneous voltage drop \( V_H \) goes down, while the localized voltage drop \( V_L \) increases. As expected, the total voltage drop \( V_T \) is seen to satisfy Eq. (18).

In Fig. 2 we plotted the total resistance \( R \) as a function of the barrier height \( \Lambda \) at lattice temperatures \( T = 5K, 10K \) and \( 15K \) respectively. At first sight the resistance \( R \) in Fig. 2 at

Figure 1. Localized and uniform voltage drop of a quantum wire as a function of barrier height \( \Lambda \) at \( T = 5K \)

Figure 2. Resistance \( R \) as a function of barrier height \( \Lambda \) at temperatures \( T = 10K \) and \( T = 15K \) seems to behave in a paradoxical way. Classically one expects that for increasing barrier height the resistance would increase. Fig. 2 shows that initially, when the barrier height \( \Lambda \) increases, the resistance first decreases before increasing. This paradox is resolved by taking a closer look at the localized resistance and the homogeneous resistance. The local resistance \( R_\delta \) arises from the presence of an elastic scattering potential and the dissipative medium (phonons), while the homogeneous resistance \( R_H \) is solely due to the phonons. Fig. 3 clearly indicates where this resistance "anomaly" for sufficiently high lattice temperatures comes from. For increasing barrier height the homogeneous resistance \( R_H \)
First starts to decrease for a lattice temperature $T = 15\text{K}$, while $R_6$ increases at the same time. Initially the decrease of $R_H$ is not compensated by the increase of $R_6$ resulting in a decreasing total resistance $R$. At certain barrier height $\Lambda_3$ we get $R_6 = R_H$ as indicated on Fig. 3. The points $\Lambda_2$ and $\Lambda_3$ indicated on Fig. 2 are the corresponding points for lattice temperatures $T = 5\text{K}$ and $T = 10\text{K}$ respectively. Further increase of the barrier height beyond the points $\Lambda_2$ and $\Lambda_3$ results in an increase of the total resistance. Beyond this threshold the increasing localized resistance is larger than the decreasing homogeneous resistance resulting in an increasing total resistance. At very low temperature $T = 5\text{K}$ this initial decrease of the total resistance can not be noticed because until $\Lambda = \Lambda_1$ when $R_6 = R_H$, there is no decrease in homogeneous resistance $R_H$. Therefore, the total resistance at $T = 5\text{K}$ is seen to increase uniformly.

In order to study the spatial dependence of energy dissipation, we have calculated the local energy density profile $w(x)$ of the quantum wire containing a localized elastic scatterer. The result is presented in Fig. 4 for different values of the barrier height $\Lambda$ at $V_L = 10\text{mV}$ where the lattice temperature is taken to be $T = 15\text{K}$. For $\Lambda$ sufficiently small one observes that the energy density shows no fluctuations. One can readily see that an energy drop occurs at $x = 0\text{nm}$ for larger values of $\Lambda$. In the region $x < 0$ the electrons have on the average a larger energy density than for $x > 0$. The difference $\Delta w$ in energy density is indicated on Fig. 4 for $\Lambda = 1.67 \cdot 10^{-29}\text{J} \cdot \text{m}$. The energy density drop increases for increasing values of the barrier height $\Lambda$. This energy drop at is a clear indication that the electron energy drop is strongly localized in space. Besides the presence of this energy drop we can also see the presence of Friedel-like oscillations. These oscillations decay away for larger $x$.

7. Conclusion

The balance equation transport formalism for closed electric circuits clearly constitutes a valid new approach towards dissipative quantum transport. In particular we have shown that it is especially suited for investigating not only the global transport properties, but also local energy dissipation characteristics. We have shown how a single localized elastic scatterer influences the properties of energy dissipation. Moreover we have obtained the well established Landauer formula for the localized resistance associated with the elastic scattering barrier $U(x)$. We have also clearly shown how dissipation becomes highly localized when the barrier height increases. This is deduced from the resulting localized electric field $E_x = V_L \delta(x)$ and the resulting energy density profile $w(x)$.

It is clear that this new approach enables us to investigate the transport properties of various mesoscopic systems where quantum mechanical effects are inherently important.