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Quantized Conductance Without Reservoirs: Method of the Non-Equilibrium Statistical Operator

B. Sorée and W. Magnus
Interuniversitary Microelectronics Center (IMEC), Kapeldreef 75, B-3001 Leuven, Belgium
e-mail: bart.soree@imec.be or wim.magnus@imec.be

INTRODUCTION

We introduce a generalized time-dependent statistical operator to calculate nonequilibrium statistical averages of inhomogeneous current-carrying dissipative nanoscale conductors. We show that the method of the nonequilibrium statistical operator (NSO) [1] and the boosted statistical operator [2], [3] yield the same result for an appropriate choice of the thermodynamic parameters responsible for time-reversal breaking in homogeneous systems.

Next we demonstrate the method of the generalized statistical operator that also leads to a quantized conductance $G_{\rm LB} = 2e^2/h$ [6], [7] for a single-channel quantum point contact (QPC) and we infer that energy dissipation must be included to obtain a finite conductance.
Moreover a connection is made between our approach and the method of M.P. Das and F. Green [4] who have obtained the Landauer-Büttiker conductance without making the ”Landauer assumptions”.

THE GENERALIZED NON-EQUILIBRIUM STATISTICAL OPERATOR

Within the framework of the NSO method of Zubarev our generalized non-equilibrium statistical operator corresponds the following form of the quasi-equilibrium statistical operator :

$$\hat{\rho}_t^{\rm B} = \frac{1}{Z(t)} e^{-\beta_{\rm e}(t)(\hat{H}_{\rm e}^{\rm B} - \mu(t)\hat{N})} e^{-\beta(t)\hat{H}_{\rm P}} \qquad (1)$$

with

$$\hat{H}_{\rm e}^{\rm B} = \hat{H}_{\rm e} + \tau(t) \int_\Omega d\mathbf{r}\, \hat{\mathbf{J}} \cdot \mathbf{E} \qquad (2)$$

where $\hat{H}_{\rm e}$ and $\hat{\mathbf{J}}$ denote the Hamiltonian and current density operator of the unperturbed electron system and $\hat{H}_{\rm P}$ refers to the free phonon bath. Eq. (1) represents a current-carrying quasi-equilibrium statistical operator due to the presence of the time-reversal breaking term :

$$\hat{H}_{\rm B}(t) = \tau(t) \int_\Omega d\mathbf{r}\, \hat{\mathbf{J}} \cdot \mathbf{E}. \qquad (3)$$

It is possible to show that the generalized statistical operator can also be derived from the principle of maximum entropy under the constraint that it yields the correct total current $\langle \hat{I} \rangle$. In the steady-state regime where the quasi-equilibrium statistical operator becomes time-independent the integral containing the dot product of $\hat{\mathbf{J}}$ and $\mathbf{E}$ can be disentangled [5] and we obtain $\hat{H}_{\rm B} = \tau \hat{I} V_\epsilon$ where V_ϵ is the applied electromotive force. The time-reversal breaking term $\hat{H}_{\rm B}(t)$ is a measure of the average energy increase of the electron ensemble at time t due to the power supplied by the nonconservative electric field $\mathbf{E}$.

SELF-CONSISTENT SOLUTION OF POISSON AND BALANCE EQUATIONS IN THE STEADY-STATE

In the steady-state the parameters $\beta_{\rm e}$, μ and τ are obtained from a set of balance equations for energy and momentum [2] which are given by :

$$IV_\epsilon = \frac{i}{\hbar} \langle [\hat{H}_{\rm e}, \hat{H}_{\rm ep}] \rangle \qquad (4)$$

$$\int d\tau\; \rho_{\rm e} \mathbf{E} = \frac{i}{\hbar} \langle [\hat{\mathbf{P}}, \hat{H}_{\rm ep}] \rangle + \frac{i}{\hbar} \langle [\hat{H}_{\rm e}, \hat{H}_{\rm imp}] \rangle. \qquad (5)$$

Eqs. (4)-(5) are solved self-consistently together with Poisson's equation :

$$\nabla^2 \Phi = \frac{e}{\epsilon} \left[n(\mathbf{r}) - n_0 \right]. \qquad (6)$$

Due to the presence of the electron-phonon interaction Hamiltonian $\hat{H}_{\mathrm{ep}}$ in the balance equations (4)-(5) energy dissipation is explicitly included.

QUANTIZED CONDUCTANCE BEYOND THE RESERVOIR PICTURE

For the case of the QPC we show that the Poisson equation together with the requirement of charge neutrality in the asymptotic regions of the QPC yields $\tau = L/2v_{\mathrm{F}}$ where L is the operational length of the QPC, while v_{F} is the Fermi-velocity. Calculating the current I with this value for τ, we obtain for a one-channel QPC at low temperature in the linear-response regime :

$$I = -2e\sum_k F(\epsilon_k + \tau V_\epsilon I_k) I_k \approx \frac{2e^2}{h} V_\epsilon \quad (7)$$

where

$$I_k = -\frac{e\hbar k}{mL} \quad (8)$$

is the one-particle current.
As a result we have obtained the Landauer-Büttiker quantized conductance through a self-consistent calculation without referring to the reservoir picture. For the particular case of the QPC this value of the corresponding total relaxation time $\tau = L/2v_{\mathrm{F}}$ was also obtained by Das and Green [4] from the Kubo-Greenwood formula for the conductance. In their case the requirement that $\tau_{\mathrm{in}} = \tau_{\mathrm{el}} = L/v_{\mathrm{F}}$ was necessary to obtain the quantized conductance. The total relaxation time τ was then obtained through Matthiessen's rule :

$$\tau^{-1} = \tau_{\mathrm{in}}^{-1} + \tau_{\mathrm{el}}^{-1} = \frac{2v_{\mathrm{F}}}{L}. \quad (9)$$

The corresponding total scattering length $\lambda = v_{\mathrm{F}}\tau = L/2$ is thus half the length L of the QPC and is due to both inelastic (phonons) and elastic scattering.

Finally, we also mention the result obtained by Kamenev and Kohn [8] who have also obtained the Landauer-Büttiker conductance without using the reservoir picture. Their calculation is based upon a self-consistent solution of the Schrödinger, Poisson and continuity equations.

CONCLUSION

The use of a generalized NSO allows us to obtain a self-consistent solution of the energy and momentum balance equations and Poisson equation. The self-consistent solution involves the Lagrange multipliers $\tau(t)$, $\mu(t)$ and $T_{\mathrm{e}}(t)$ which are in general time-dependent. Applying the generalized NSO method to a one-channel QPC in the low-temperature linear-response regime yields the Landauer-Büttiker conductance G_{LB}. The corresponding value of the Lagrange multiplier τ is given by $L/2v_{\mathrm{F}}$ and is in agreement with the results obtained by [4]. Moreover we have corroborated the result of Green and Das, stating that inelastic scattering is essential for the Landauer-Büttiker conductance.

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