Temperature Dependent Suppression of Conductance in Quantum Wires: Anomalous Activation Energy from Pinning of the Band Edge

Kenji Hirose and Ned S. Wingreen

1 Fundamental Research Laboratories, NEC Corporation, 34 Miyukigaoka, Tsukuba, Ibaraki 305-8501, Japan
2 NEC Research Institute, 4 Independence Way, Princeton, New Jersey 08540

Abstract

For unpolarized electrons in a clean quantum wire, density functional theory reveals a thermally activated suppression of conductance. The activation temperature $T_A$ grows slowly (roughly quadratically) with gate voltage due to pinning of the band edge at the chemical potential. Similar results were obtained experimentally by Kristensen et al. [Phys. Rev. B62, 10950 (2000)] for the temperature dependence of the anomalous conductance plateau near 0.7 $(2e^2/h)$ in a quantum point contact.
The discovery of the quantization of the conductance through a point contact in steps of $2e^2/h$ [1, 2] was a milestone in mesoscopic physics. Recent observations of additional plateau-like structures at $0.7(2e^2/h)$ in quantum point contacts [3, 4] and at $0.5(2e^2/h)$ in clean quantum wires [5] have been the center of much attention. These plateau-like structures become more pronounced as the temperature is raised. In the quantum point contacts, the conductance is suppressed by temperature between $0.7(2e^2/h)$ and the plateau value $2e^2/h$, while very little temperature dependence is observed below $0.7(2e^2/h)$. Kristensen and co-workers [4] found that the conductance suppression has an activated behavior, with the activation temperature growing roughly quadratically with gate voltage.

The present paper reports density-functional-theory (DFT) results for the thermally activated suppression of conductance for unpolarized electrons in a clean quantum wire. As in the experiment [4], we find an activation temperature $T_A$ that depends roughly quadratically on side-gate voltage, $T_A \propto V_s^2$, in the plateau region. We show that this anomalous behavior of the activation temperature derives from self-consistent pinning of the band edge at the absolute electrochemical potential.

The electronic states of a clean quantum wire are obtained using density-functional theory within the local-density approximation [6]. This method allows us to study both confinement and electron-electron interactions in a unified framework. A number of works have considered the possibility of spontaneous spin polarization of electrons in a quantum wire [4, 7, 8, 9, 10]. Here we consider unpolarized electrons to highlight effects that are electronic but not magnetic in origin. Exploiting translational invariance in the $x$ direction, we expand the wavefunctions as $\Psi_{n,k_n}(r) = e^{ik_nx} \sum_m c_{n,m} \psi_m(y)$, where $n$ is the subband number and $\psi_m(y)$ is the $m$th eigenvector of the bare parabolic potential. The following Kohn-Sham equations [11] are solved numerically,

$$\left[ -\frac{\hbar^2}{2m^*} \nabla^2 + \frac{1}{2}m^* \omega_y^2 y^2 - \frac{e^2}{\kappa} \int_{-\infty}^\infty \rho(y') \ln \left( \frac{(y - y')^2}{(y - y')^2 + a^2} \right) dy' + \frac{\delta E_{xc}[\rho]}{\delta \rho(r)} \right] \Psi_{n,k_n}(r)$$

$$= \left( \epsilon_n + \frac{\hbar^2 k_n^2}{2m^*} \right) \Psi_{n,k_n}(r)$$

$$\rho(r) = \frac{1}{\pi} \sum_n \int_{-\infty}^\infty f(\epsilon_n + \frac{\hbar^2 k_n^2}{2m^*}) |\Psi_{n,k_n}(r)|^2 \, dk_n,$$

$$f(\epsilon_n) = \int_{-\infty}^{\infty} \left[ \frac{(y - y')^2}{(y - y')^2 + a^2} \right] \rho(y') \ln \left( \frac{(y - y')^2}{(y - y')^2 + a^2} \right) \, dy'$$

$$\delta E_{xc}[\rho] = \int \rho(r) \left( \frac{\partial^2}{\partial \rho(r)} \right) \delta \rho \, dr.$$

(1)
for each electron density

\[
 n_{1D} = \frac{1}{\pi} \sum_n \int_{-\infty}^{\infty} f(\epsilon_n + \frac{\hbar^2 k_n^2}{2m^*}) dk_n.
\]  (2)

In the above equations, \( \rho(\mathbf{r}) \) is the local electron density, \( \epsilon_n \) is the band-edge energy of the \( n \)th subband, and the Fermi distribution function is \( f(\epsilon) = 1/\left[\exp\left(\frac{(\epsilon - \mu_{\text{wire}})}{k_B T}\right) + 1\right] \), where the electrochemical potential in the wire \( \mu_{\text{wire}} \) is determined self-consistently for each density \( n_{1D} \).  

In the experiments [3, 4, 5], the side-gate voltage \( V_s \) is used to change the density \( n_{1D} \). The absolute electrochemical potential \( \mu \) is the sum of the internal electrochemical potential of the wire \( \mu_{\text{wire}} \) and the external potential energy. The latter varies linearly with side-gate voltage as \(-\alpha e V_s\), where the capacitive lever-arm \( \alpha \) depends on the detailed gate geometry [12]. To model the fixed leads, we set the absolute electrochemical potential at \( \mu = 0 \), and take \( \alpha = 1 \) for simplicity, so that \( eV_s = \mu_{\text{wire}} \). This also implies that at \( T = 0 \) the lowest subband energy is set at \( \epsilon_0 = 0 \) when \( V_s = 0 \).

The conductance is calculated from the Landauer formula,

\[
 G = \frac{2e^2}{\hbar} \sum_n \int_{-\infty}^{\infty} \left( -\frac{\partial f}{\partial \epsilon} \right) T_n(\epsilon) d\epsilon.
\]  (3)

To model a clean quantum wire, we assume that the transmission coefficients \( T_n(\epsilon) \) change abruptly from 0 to 1 at the band-edge energies \( \epsilon_n \). We fix the external confining potential as \( \hbar \omega_y = 2.0 \text{meV} \) and take an image-charge plane at \( a = 100 \text{nm} \). The material constants are those of GaAs, \( m^* = 0.067m \) and \( \kappa = 13.1 \).

Figure 1(a) shows the conductance \( G \) in the lowest subband as a function of side-gate voltage \( V_s \) at different temperatures \( T = 0.25K, 0.5K, 0.67K, 1.0K, \) and 2.0K, from top to bottom, respectively [13]. We see that the conductance is suppressed with increasing temperature. Guided by the experimental results of Kristensen et al. [4], we look for Arrhenius-type suppression of the conductance,

\[
 G(T) = G_0 (1 - e^{-T_A/T}),
\]  (4)

where \( G_0 = 2e^2/h \). In the inset of Figure 1(b), we plot the relative conductance suppression as \( \ln[1 - G(T)/G_0] \) versus the inverse of the temperature at different side-gate voltages.
(1) $V_s = 1.0\text{mV}$, (2) $V_s = 3.0\text{mV}$ and (3) $V_s = 5.0\text{mV}$. The linear behavior of Arrhenius plots of this type allows us to extract activation temperatures $T_A = -T\ln[1 - G(T)/G_0]$ for all side-gate voltages $V_s$. Figure 1(b) shows that the activation temperature has an approximately quadratic dependence on the side-gate voltage, close to that observed in the experiment of Kristensen et al. on quantum point contacts [4].

The roughly quadratic dependence of the activation temperature on side-gate voltage in our DFT results reflects “pinning” of the band edge at the absolute electrochemical potential. As electrons begin to enter the wire, their self-consistent potential buoys up the band-edge energy. The result is that the difference between the absolute electrochemical potential and the band edge grows slowly with side-gate voltage.

To explore the band-edge pinning effect, we use a simplified model consisting of a purely 1D wire with a classical capacitance [10]. We find that this model captures the essential features of the DFT results. The kinetic energy of the 1D electrons is $\epsilon_k = \hbar^2 k^2/2m^*$, and the band-edge energy $\epsilon_0 = -eV_s + (e^2/C)n_{1D}$ is the sum of the side-gate contribution and a classical capacitive energy, where $C$ is a fixed capacitance per unit length of the wire. The electron density, for two spins, is determined by

$$n_{1D} = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{dk}{\exp\{(\epsilon_k - \mu_0)/k_BT\} + 1}. \quad (5)$$

For each $V_s$, the chemical potential $\mu_0$ of the 1D electrons is determined self-consistently by the condition that the absolute electrochemical potential $\mu$ is fixed at zero, so that $\mu = \mu_0 + \epsilon_0 = \mu_0 - eV_s + (e^2/C)n_{1D} = 0$. To remove the explicit dependence on the parameters $m^*$ and $C$, this condition can be written in dimensionless form as

$$\bar{\mu}_0 - \bar{V}_s + \int_0^\infty \frac{d\bar{k}}{\exp\{(\bar{k}^2 - \bar{\mu}_0)/\bar{T}\} + 1} = 0. \quad (6)$$

Here all the energies $\mu, k_BT, \epsilon V_s$ are normalized by $U = (e^2/C)^2/(\pi^2\hbar^2/8m^*)$, and $\bar{k} = \pi\hbar^2k/[4m^*(e^2/C)]$.

In the inset to Figure 2(b), we show the chemical potential $\bar{\mu}_0$ as a function of $\bar{V}_s$, obtained by solving Eq. (6) for different temperatures. In the zero temperature case, $\bar{\mu}_0$ has a cusp where it crosses zero, i.e. where electrons first enter the wire. The relatively
slow increase of $\tilde{\mu}_0$ with gate voltage on the right side of the cusp reflects the pinning of the band edge at the absolute electrochemical potential. To elucidate this effect, we consider the zero-temperature limit of Eq. (6),

$$\tilde{\mu}_0 + \sqrt{\tilde{\mu}_0 - \tilde{V}_s} = 0, \quad (7)$$

which has the solution

$$\tilde{\mu}_0 = \frac{1}{2} \left[ 1 + 2\tilde{V}_s - \sqrt{1 + 4\tilde{V}_s} \right] \simeq \tilde{V}_s^2, \quad \tilde{V}_s \ll 1. \quad (8)$$

The quadratic growth of the chemical potential for side-gate voltage $\tilde{V}_s \ll 1$ can be traced to the square-root singularity $\rho_{1D}(\epsilon) \sim \epsilon^{-1/2}$ in the density of states of 1D electrons \[10\]: As electrons begin to enter the wire, because of this high density of states, a very small increase in the chemical potential $\mu_0$ causes a large increase in the density of electrons $n_{1D}$. This, in turn, produces a large increase in the band-edge energy $\epsilon_0$ through the self-capacitance of the wire $(e^2/C)n_{1D}$. The result is that a large increase of $V_s$ is required for a small increase of $\mu_0$. As seen in the inset to Figure 2(b), the pinning effect diminishes as temperature broadens the electron-energy distribution.

For the classical capacitance model, the conductance can be obtained analytically from the Landauer formula \[3\] with a single subband,

$$G = G_0 f(0) = \frac{G_0}{\exp(-\tilde{\mu}_0/\tilde{T}) + 1}, \quad (9)$$

where we have again assumed that the transmission coefficient jumps abruptly from 0 to 1 at the band-edge energy $\epsilon_0$. In Figure 2(a), the conductance is plotted as a function of side-gate voltage $\tilde{V}_s$ at different temperatures. At $\tilde{T} = 0$, the conductance $G$ abruptly jumps from 0 to $2e^2/h$ at $\tilde{V}_s = 0$, where the band edge drops below the absolute electrochemical potential. Increasing the temperature suppresses the conductance with an approximately activated form, $G(T) \simeq G_0[1 - \exp(-\tilde{T}_A/\tilde{T})]$.

The activation temperature $\tilde{T}_A$ for the suppression of conductance can be obtained exactly and analytically as a function of $\tilde{V}_s$ by considering the low temperature limit of the conductance,

$$\tilde{T}_A \equiv -\lim_{F/\tilde{\mu}_0 \to 0} \{ \tilde{T} \ln[1 - G(\tilde{T})/G_0] \} = \tilde{\mu}_0. \quad (10)$$
The activation temperature is just equal to the zero-temperature chemical potential. Hence, the initial quadratic behavior of the activation temperature \( \tilde{T}_A \) with gate voltage simply reflects the initial quadratic behavior of \( \tilde{\mu}_0 \) with gate voltage due to the pinning of the band edge. The activation temperature \( \tilde{T}_A \) is plotted in Figure 2(b) using the full expression for \( \tilde{\mu}_0 \) from Eq. (8).

These results may shed light on the observation by Kristensen et al. [4] of thermally activated suppression of conductance near the anomalous \( 0.7(2e^2/h) \) conductance plateau in a quantum point contact (QPC). In a phenomenological model, Bruus et al. [14] have attributed \( T_A \), and its gate-voltage dependence, to proximity of the absolute electrochemical potential to a subband edge. Our observation of band-edge pinning provides a microscopic justification for this model, insofar as a QPC can be regarded as a segment of clean quantum wire. However, various aspects of transport through QPCs remain unaccounted for microscopically, including the magnetic field dependence [3].

In conclusion, we have explored the thermally activated suppression of conductance in a clean quantum wire, using both density functional theory and a classical capacitance model for unpolarized electrons. The quadratic dependence of the activation temperature on the gate voltage in the plateau region reflects self-consistent pinning of the band edge by the absolute electrochemical potential. We hope that this work contributes to the understanding of the thermally suppressed conductance in quantum point contacts and clean quantum wires. The authors acknowledge valuable conversations with Yigal Meir.
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Figure Captions

Figure 1: (a) Conductance $G$ as a function of side-gate voltage $V_s$ at different temperatures $T = 0.25K$, 0.5K, 0.67K, 1.0K, and 2.0K (from top to bottom) within the DFT calculations with parameters appropriate to GaAs, $\kappa = 13.1$ and $\hbar \omega_y = 2.0\text{meV}$. (b) Activation temperature $T_A$ as a function of $V_s$ obtained from Arrhenius plots of conductance suppression. Inset – Arrhenius plots of conductance at fixed side-gate voltages of $V_s = (1) 1.0\text{mV}$, (2) 3.0mV, and (3) 5.0mV, respectively.

Figure 2: (a) Conductances $G$ as a function of side-gate voltage $\tilde{V}_s$ at different temperatures from $\tilde{T} = 0$ (above) to $\tilde{T} = 0.1$ (below) in steps of $\Delta \tilde{T} = 0.01$ within the classical-capacitance model. (b) The activation temperature $\tilde{T}_A$ as a function of $\tilde{V}_s$. Inset – Chemical potential $\tilde{\mu}_0$ as a function of $\tilde{V}_s$ at different temperatures from $\tilde{T} = 0$ to $\tilde{T} = 0.1$ (from top to bottom at $\tilde{V}_s = 0$) in steps of $\Delta \tilde{T} = 0.02$. Here $\tilde{V}_s$, $\tilde{T}$, $\tilde{T}_A$ and $\tilde{\mu}_0$ are all measured in units of $U = (e^2/C)^2/(\pi^2\hbar^2/8m^*)$. 
