Quantum simulation of an ultrathin body field-effect transistor with channel imperfections

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A B S T R A C T

An efficient program for the all-quantum simulation of nanometer field-effect transistors is elaborated. The model is based on the Landauer–Buttiker approach. Our calculation of transmission coefficients employs a transfer-matrix technique involving the arbitrary precision (multiprecision) arithmetic to cope with evanescent modes. Modified in such way, the transfer-matrix technique turns out to be much faster in practical simulations than that of scattering-matrix. Results of the simulation demonstrate the impact of realistic channel imperfections (random charged centers and wall roughness) on transistor characteristics. The Landauer–Buttiker approach is developed to incorporate calculation of the noise at an arbitrary temperature. We also validate the ballistic Landauer–Buttiker approach for the usual situation when heavily doped contacts are indispensably included into the simulation region.

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1. Introduction

The continuing progress in silicon VLSI technology motivates a transition to silicon-on-insulator (SOI) wafers. Just these structures definitely suppress short channel effects which substantially impair the bulk MOSFET performance. This is the ultrathin body (UTB) (1–5 nm) fully depleted (FD) silicon on insulator (SOI) structure (Fig. 1) that will take an ultimate advantage of SOI wafers and provide an advancement of the silicon technology to extreme channel lengths. As a result, such structures will exhibit higher frequencies and a lower power consumption.

As a carrier wavelength becomes commensurable with the channel size, the all-quantum simulation of such small devices becomes challenging. One of the most intriguing issues is an impact of realistic channel imperfections (random charged centers and wall roughness) on transistor characteristics. It is crucial for the evaluation of the statistical variability of transistors in large integrated circuits. The most vital is a variability of threshold voltages [1,2] which encumber lowering of the drive voltage necessary for lower power applications.

Methods of quantum simulation were in a rapid progress for more than two preceding decades. The leading ones are the non-equilibrium Green’s functions (NEGF) [3–12] and the Landauer–Büttiker (LB) approach [3,4,13–19]. In the ballistic regime they evidently coincide. To calculate the transmission coefficients one could exploit the transfer-matrix (T-matrix method) [20–23] or that of scattering-matrix (S-matrix) [3,4,24–29]. Previously, it was widely supposed that the conventional T-matrix method failed to cope with evanescent modes. However, recently an efficient method involving the arbitrary precision (multiprecision) arithmetic was put forward [30–32]. The advanced transfer-matrix technique is much faster in practical simulations than that of scattering-matrix. Moreover, the proposed means turned out to be powerful for simulations based on any wave equations, in particular, electromagnetic waves in non-uniform media, e.g., nanostructured solar cells [33,34].

Current noise is one of major transistor characteristics required for practical applications. We derive a general expression to calculate the current noise for an arbitrary temperature and voltage bias. This expression could be used in the same simulation of the field-effect transistor based on the Landauer–Buttiker approach.

We also address an issue of validity of the ballistic Landauer–Büttiker approach for the usual situation when heavily doped contacts with strong scattering are indispensably included into the simulation region. A question arises whether a transistor with a ballistic channel is really ballistic. Recently this ‘perpetual’ problem was also discussed in Ref. [35]. Here we argue that a fairly high and steep potential barrier at the contacts justifies the ballistic simulation.

2. Efficient T-matrix method for quantum simulation

We calculate transmission coefficients $T_\gamma$ from the Schrödinger equation and then evaluate dependence of the drain current $I$ on...
the source-drain voltage $V_D$ via the Landauer–Buttiker formula upgraded to the situation:

$$I = \frac{2e}{h} \sum_{i} \sum_{k} \int dE (f_k(E) - f_0(E))$$

(1)

where $f_k$ and $f_0$ are the Fermi–Dirac distribution functions in the source and drain contacts, respectively, shifted by a drain bias $eV_D$. $E$ is a total energy including the quantization energy and the longitudinal motion energy. Formula (1) implies the summation over all wave-guide modes $i$ involved into the simulation and all conduction band valleys $v$. The pre-summation factor originates in the conductance quantum for spin-unpolarized current $G_0 = 2e^2/h$, where $h$ is the Planck constant, namely,

$$T_i = \frac{\sum_{v} |c_{ij}|^2 k_i}{k_i} = 1 - R_i$$

is the total transmission coefficient of an incident wave belonging to the $i$-th mode with unity amplitude and the longitudinal wave vector $k_i$ at the channel entrance, $c_{ij}$ is an amplitude of the $j$-th outgoing mode at the channel exit with the wave vector $k_j$. The summation in the above formula for $T_i$ conserves the current.

In spite of the fact that the Landauer–Buttiker approach is formulated explicitly, it is based on several suppositions which are not apparent. We discuss them in Appendix A.

The necessary transmission coefficients in Eq. (1) are determined via a self-consistent solution of the Schrödinger and Poisson equations (the Hartree mean field approach). To be more precise, the scattering problem for the three-dimensional stationary Schrödinger equation should be solved.

A brief description of the procedure is presented below. In fact, we follow a straightforward strategy which was widely used for a non-uniform electromagnetic wave-guide description long time ago. The stationary Schrödinger equation is:

$$\begin{align*}
- \frac{\hbar^2}{2m_x} \frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m_y} \frac{\partial^2}{\partial z^2} - \frac{\hbar^2}{2m_z} \frac{\partial^2}{\partial x^2} + U(x,y,z) & \psi(x,y,z) \\
= & E \psi(x,y,z),
\end{align*}$$

(2)

where $U(x,y,z) = -e \phi(x,y,z)$ is a potential energy inside the channel, $m_x, m_y, m_z$ are the electron effective masses along corresponding axes of the silicon conduction band structure (Fig. 2).

The exact wave function in any cross-section $x$ is expanded over all transversal modes $\phi_j(y,z)$ for the uniform wave-guide:

$$\psi(x,y,z) = \sum_{j=1}^{\infty} c_j(x) \cdot \phi_j(y,z).$$

(3)

The complete set of functions $\phi_j(y,z)$ obeys the two-dimensional Schrödinger equation.

Therefore, under such circumstances, transformation of the incident mode $i$ into upper modes $j$ is negligible. The necessary number of modes involved into consideration could be determined immediately during the simulation.

Eq. (8) is to be solved on a uniform mesh with nodes in $x = x_k$, $k = -1, 0, 1, \ldots, N, N + 1, N + 2$ and step $\Delta x$. The finite difference approximation of Eq. (8) is
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channel. However, it turns out that the number of modes necessary to stabilize the solution employ an approximation of the exact

exponential growth of evanescent modes, the finite-difference method

contacts may become evanescent in the channel. Due to the expo-

vantial is flattened (Fig. 3).

then we rewrite Eq.(12) as follows:

\[
\begin{bmatrix}
\mathbf{c}(x_{k,1}) \\
\mathbf{c}(x_0)
\end{bmatrix} = \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \mathbf{c}(x_{N,1}) \\
\mathbf{c}(x_{N,2}) \end{bmatrix} = \mathbf{T}_{\text{for}} \begin{bmatrix} \mathbf{c}(x_{N,1}) \\
\mathbf{c}(x_{N,2}) \end{bmatrix}.
\]

Eq. (14) relates the coefficients \( \mathbf{c} \) at the left boundary with that at the right one via the total transfer-matrix \( \mathbf{T}_{\text{tot}} \), which is a product of the individual transfer-matrices for particular nodes \( x_k \). To impose boundary conditions one should express the coefficients \( \mathbf{c} \) in terms of amplitudes of waves going to the right and going to the left in the extreme nodes placed fairly deep in contacts, where the potential is flattened (Fig. 3).

Aforesaid was a quite conventional description of the T-matrix method [20–23]. As soon as it is exploited, one immediately comes across a well-known encumbrance related to the evanescent modes in a non-uniform wave-guide [23]. The modes of this kind have a negative energy of longitudinal motion and, accordingly, an imaginary wave vector. The evanescent modes decay exponentially in one direction but they exponentially grow in the other. Those modes should be indispensably involved into consideration of the non-uniform waveguide. Moreover, propagating modes in contacts may become evanescent in the channel. Due to the exponential growth of evanescent modes, the finite-difference method on 3D-mesh becomes unstable and even diverges. Common means to stabilize the solution employ an approximation of the exact solution by an expansion over a finite number of transversal modes of the ideal rectangular wave-guide in any cross-section of the channel. However, it turns out that the number of modes necessary for the precise description of a quite complicated potential profile in the transistor channel with realistic imperfections (random charged impurities, charged defects on interfaces, or rough walls of the channel) is large, and, therefore, the instability still arises. The point is that the T-matrix technique implies a multiplication of T-matrices ascribed to different cross-sections of the channel. This method is quite straightforward and, therefore, ‘blindfolded’ with respect to exponentially increasing and exponentially decreasing modes. Consequently, very large and very small numbers appear during computation corresponding to those modes, respectively. In the case, to save accuracy one should employ the multi-precision arithmetic. This kind of arithmetic can be efficiently realized even on up-to-date desktop computers [38].

The advanced T-matrix technique revealed a substantial speed-up in practical simulations compared to that of scattering-matrix (S-matrix) [3,4,24–29]. It is quite comprehensible because the S-matrix method implies solving the eigenvalue problem in all cross-sections of the channel with an arbitrary potential. This method is rather sophisticated. After an eigenvalue problem is solved in every channel cross-section one can distinguish the increasing and decreasing modes. The proper decomposition of S-matrix allows avoiding very small and very large numbers during computation. However, the S-matrix method is time consuming. Meanwhile, in the T-matrix method we do without that decomposition and employ the expansion over the eigenfunctions of the ideal wave-guide using the matrix elements of a potential to describe mode coupling.

As to the non-equilibrium Green’s functions [3,4,5–12], for non-interacting transport this method is equivalent to that of the S-matrix, and what one prefers is largely a matter of taste [3]. The Green’s functions method is a powerful tool to describe the effect of interactions (electron–electron or electron–phonon) which are negligible in the simulation of structures under consideration.

3. Results of simulation: imperfections in the channel

The results of simulation demonstrate the impact of realistic channel inhomogeneities on transistor characteristics. The elaborated simulation program can put into consideration a variety of realistic imperfections of the transistor channel, with these imperfections leading to a rather complicated potential profile. Imperfections may be random charged impurities, charged defects on interfaces, or rough walls of the channel.

The fully depleted extremely thin SOI field-effect transistor (FD ETSOI FET) under investigation (Fig. 1) is as follows: the gate length is 10 nm, the spacers are both equal to 5 nm, the channel thickness is 3 nm, the channel width is 10 nm, the equivalent gate oxide thickness is 1.5 nm, and the source/drain (S/D) contact doping is \( 10^{20} \text{ cm}^{-3} \). The gate voltage in presented figures is supposed to be equal to 0.0 V, provided the work-functions of the gate and the S/D contact are equal; otherwise, the gate voltage should be properly shifted. The conventional orientation of a silicon wafer with the Miller indices (100) is assumed. The present calculations involve the unstrained silicon body, however, if the stress exists, it may lead to a deformed band structure with split valleys and changed effective masses [39]. This results in a redistribution of the electrons among valleys and a drastic change of transistor characteristics [32].

We deal with continuous doping in the contacts. Previously, only a small mismatch in transistor characteristics was revealed for both continuous and discrete doping [32], because the interference on multiple discreet impurities is reasonably suppressed due to their random position.

The calculated potential profile in the perfect channel is presented in Fig. 3. The simulation region includes 5 nm of the source/drain contacts to make the potential flatten. This is important with the aim to impose exact boundary conditions for the Schrödinger and Poison equations. The steep potential walls near the source and drain could be a reason of interference peaks and dips of the transmission coefficients.
The calculated transmission coefficients for the electrons belonging to [100] valley of the silicon conduction band and the lowest propagating transversal mode are shown in Fig. 4. Just these electrons mostly contribute to the current due to an extremely thin silicon body and thus the high quantization energy for other valleys of the conduction band. Those valleys are almost empty. It should be emphasized that the pronounced oscillations of transmission coefficients also occur for a perfect channel (without any impurity) owing to the interference between the channel ends. The oscillations of transmission coefficients are also apparent for heavy holes in Fig. 5. Those holes mostly contribute to the current owing to the extremely thin silicon body and, therefore, the high quantization energy for light holes.

In spite of the oscillating behavior of transmission coefficients, the resultant I-V curves look quite smooth regardless of reasonable apprehensions and pioneering simulations of nanotransistors. Dependence of the drain current on the gate voltage drawn to logarithmic scale for the perfect nFET and pFET channels is presented in Fig. 6. The same dependence is depicted to linear scale in Fig. 7. A sub-threshold swing of 71 mV per decade of the current turns out to be quite close to the theoretical limit for a thermionic current at the room temperature $T = 300 \, \text{K}$: 60 mV/dec. This can be explained by a fairly small thickness of the channel compared to its length. Dependence of the drain current vs. the drain voltage (Fig. 8) demonstrates the channel resistance about $R = 10 \, \text{k} \Omega$.

Since the capacitance of interconnects corresponding to the technological node of 10 nm is approximately equal to $C_{\text{out}} = 1\, \text{aF} = 10^{-18} \, \text{F}$, the RC-delay in a circuit is about $10^{-11} \, \text{s}$. This opens prospects to a SOI FET application in THz logic (digital) circuits. It is worth noting that, unlike the SOI FET, the single-electron transistor (SET) has a fundamental restriction on the minimal channel resistance originating from a requirement of the Coulomb blockade. Indeed, the typical resistance of a SET channel is about $100 \, \text{k} \Omega$. Lower frequency is subsequent upon that value.

A positively charged center in the channel augments the ON-state current (Fig. 9). Merely, it means a shifted threshold voltage. This is confirmed by the inset in Fig. 9 where a fragment of gate voltage characteristic is depicted. This conclusion seems quite general and valid for any types of channels, for example, for that of nanotubes [40,41]. A charged center may originate from a random impurity inside the channel, or an interface defect, or a defect inside the gate dielectric. In our opinion, the most probable is a charged defect at the silicon/gate dielectric interface.

Surface scattering may dominate bulk scattering in thin silicon layers [42–45]. The calculations based on quantum description [45] give rise to an extremely high power of the dependence of the conductance $\sigma$ vs. the layer thickness $d$: $\sigma \sim d^m$, $m = 2 \div 6$, compared to $\sigma \sim d^2$ in the case of bulk scattering. However, for short channels one should take into account a definite wall shape. A step-like corrugation of the channel wall diminishes the ON-state current (Fig. 10). The step height of 0.5 nm corresponds to the one monolayer terrace edge which is a plausible geometrical imperfection inside the channel.

All kinds of inhomogeneities have much stronger effect on the current when they are located nearby the source contact compared to that located nearby the drain contact, where the carriers have larger kinetic energy. A preliminary estimation of dispersion caused by a realistic imperfection of transistors in a circuit gives rise to 10–20% variations of the current corresponding to variations of the threshold voltage 10–20 mV. In spite of the former intuitive suspicions, it is not dramatic. However, some improvements of the technology and the materials used for ultra-large integrated
circuits may become necessary, especially for low-power applications. It is well-known that the main reason of the high drive voltage and low frequency in up-to-date VLSI based on bulk silicon is the variability of threshold voltages.

In Fig. 11 we present a two-dimensional self-consistent potential energy relief in the channel cross-section, where a single impurity lies. The potential strongly varies in the vicinity of the impurity; therefore, a fairly big number of waveguide modes and a fairly dense mesh should be involved into simulation to attain the necessary accuracy of back-scattering. The distribution of electron density at zero bias (for better clarity) is shown in Fig. 12. The density is enhanced at the impurity site. Here the impurity is supposed to be unoccupied. However, any impurity (or other charged defects) in the channel could be a feasible source of the 1/f noise (the flicker noise) caused by charging and discharging.

In practical calculations the accuracy was estimated by doubling the number of modes enumerated in order of rising energy. The sufficient number of modes turns out to be 10–20 for different valleys of the conduction band to hit 1% accuracy. The required length of decimal numbers is equal to 80–90 digits to cope with evanescent modes [32]. The mesh contains 300 × 200 × 200 nodes.

4. Current noise

Current noise is one of the major characteristics of the transistor required for its practical application. Along with the shot noise and the Johnson–Nyquist noise well-known far before, an especial quantum excess noise was revealed in nanotransistors [46,47]. In this section, we undertake an attempt to derive a general expression to calculate the current noise for an arbitrary temperature.
and voltage bias. This expression could be used in the same simulation of the field-effect transistor based on the Landauer–Buttiker approach.

To begin with, let us consider the current and noise produced by the electrons in a fairly small energy interval $dE$, where the transmission coefficient $T(E)$ and the distribution function $f(E)$ are almost constant. Beforehand, we introduce the probability $T_S$ to find an electron coming from the source contact to the drain contact and the analogous probability $T_D$ for the drain electrons:

$$T_S = T(E)f_S(1 - f_D),$$

$$T_D = T(E)f_D(1 - f_S),$$

where the Pauli exclusion principle establishes the statistical correlations between the source and drain contacts.

Taking into account both contributions to the current from the source and drain electrons, we obtain an expression for the resultant current $dI$

$$dI = \frac{2e}{h}(T_S - T_D)dE = \frac{2e}{h}T(E)(f_S - f_D)dE,$$

where the Pauli exclusion principle formally disappears. In the same way one can calculate the mean square current fluctuation

$$dI_n^2 = \langle dI^2 \rangle - \langle dI \rangle^2 = \frac{2e^2}{h} \Delta v[T_S(1 - T_D) + T_D(1 - T_S)],$$

where $\Delta v$ is a frequency interval. The Pauli exclusion principle is crucial in Eq. (18). Evidently, for zero bias ($f_S = f_D$) the current (17) vanishes at any temperature. Meanwhile, the noise (18) turns to zero only if both the temperature and the bias are equal to zero.

Formula (18) for zero temperature $T = 0$ and small bias ($V \ll dE/e$) could be easily reduced to that of Lesovik for the quantum excess noise [46,47].

$$dI_n^2 = \frac{2e^2}{h} \Delta v|eV|T(E)(1 - T(E)).$$

For small values of the transmission coefficient $T(E)$ the above expression turns to that for the shot noise, i.e. proportional to the current [46]. However, it is worth noting that for classical ballistics – when the transmission coefficient can acquire only two values: 1 or 0 – the quantum excess noise equals zero.

On integrating the expression (17) over energy, one arrives at the Landauer–Buttiker formula for the current (1). If there are no correlations between the electrons with different energies (e.g., if the states are disentangled) the expression for the noise (18) can be integrated to obtain the total noise:

$$P_n^2 = \frac{2e^2}{h} \Delta v \sum_i \sum_v \int dE[T_S(1 - T_S) + T_D(1 - T_D)].$$

For zero drain voltage this relation gives rise to the Johnson–Nyquist noise in quantum limit. This noise is also roughly proportional to the temperature. For a non-zero drain voltage there is a blend of the Johnson–Nyquist noise and the shot noise (including the excess quantum noise). Formula (20) is valid for fairly low frequencies $v \ll v_0$, namely, the ultimate frequency $v_0$ obeys the inequality

$$v_0 \ll \frac{\Delta E}{kT},$$

where $\Delta E$ is the energy interval where the transmission coefficient $T(E)$ substantially varies [46], $kT$ is the energy interval where the distribution function substantially varies, $\tau$ is a transit time limiting the validity of static current description on the whole. The typical energy of transmission coefficient variation could be estimated as the energy of longitudinal quantization in the channel of length $L$: $\Delta E = \frac{h^2}{8mL^2}$. (22)

where $m$ is a mass of longitudinal motion. The calculated transmission coefficients (Figs. 4 and 5) confirm that the inequality (21) is valid up to THz frequencies.

In Fig. 13 we depict the current calculated for the classical ballistic longitudinal motion [32] in a perfect channel, the current calculated for a quantum ballistic longitudinal motion, and the renormalized noise $I_n^2/e\Delta v$. Comparison of curves results in the estimation of the mean quantum transmission coefficient for conducting electrons which turns out to be about 0.7. The noise in Fig. 11 is primarily the shot noise (quantum excess noise), the thermal (Johnson–Nyquist) noise is clearly visible at zero drain voltage. The investigation of the noise just at low voltage and low current is challenging for low-power electronics.

5. Conclusions

The efficient program based on the Landauer–Buttiker approach for simulation of nanometer field-effect transistors is elaborated. The transmission coefficients are calculated via the advanced transfer-matrix technique. The multiprecision arithmetic is employed to cope with the evanescent modes. The simulations make it possible to estimate an impact of the realistic channel imperfections (random charged centers and wall roughness) on the transistor characteristics. All kinds of imperfections have a much stronger effect on the current when they are located nearby the source contact.

The Landauer–Buttiker approach is developed to incorporate calculation of the noise at an arbitrary temperature.

We also validate an applicability of the ballistic Landauer–Buttiker approach for the simulation of heavily doped contacts with rather strong scattering. An analytical solution of the kinetic equation with a collision integral in the modified $\tau$-approximation representation for a fairly high and steep potential barrier at the contacts justifies a purely ballistic simulation. Due to a strong scattering in the contacts, entangled and mixed states are supplied by the contacts rather than pure disentangled states adopted in the Landauer–Buttiker model. However, we show that those states have no effect on a steady current of the transistor.

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Appendix A

A.1. Validation of the Landauer–Buttiker approach

The Landauer–Buttiker approach has a hidden shortcoming inherent in the classical kinetic simulation though. The point is that any simulation of an open system (quantum as well as classical one) must start from the boundary where the distribution function of incoming particles (or waves) is known. In the case, the only region where this function is definitely known is a quasi-equilibrium heavily doped source/drain contact. However, the simulation becomes very much complicated and time-consuming when contacts are involved. The reason is a strong scattering and a big number of occupied modes inside the contact.

Fortunately, a fairly high and steep potential barrier originates at the junction of a heavily doped S/D contact and the undoped channel (Fig. 3). Most of particles (or waves) are reflected back at the junction of a heavily doped contact reservoirs supply only pure states (plane waves) into the channel and they sustain their coherence during transmission through the channel. However, the quite plausible assumptions are:

1. Mixed states are injected from the contacts instead of pure ones.
2. Entangled states are injected from the contacts because of a strong interaction inside them.
3. Electron–electron scattering inside the channel can smear interference.

The density matrix method is a powerful tool to describe the mixed states. For the simulation of the transistor one could use a representation of the density matrix in the basis of pure states. After averaging over the ensemble, the current coincides with that given by the Landauer–Buttiker formula.

The problem of entanglement is more subtle. It is well-known that the entanglement is a fundamental of quantum computing. At the same time, the influence of entanglement on a macroscopic behavior of a quantum many-particle system has not been so far recovered. Here we put forward only a cursory discussion of the problem regarding the interference in quantum simulations. The content

\[ f(x) = n_{0} \left[ 1 - \exp \left( \frac{x}{\tau} \right) \right] \]  \hspace{1cm} (A4)

for reverse particles above the barrier \((\nu < 0)\).

Indeed, it turns out that for fairly steep potential barrier the distribution function of injected particles is equilibrium. This makes the Landauer–Buttiker approach valid although it does not incorporate strong scattering in the contacts. At the same time, this imposes restrictions on steepness of doping profile in the contacts to ensure ballistic transport in the transistor. The required steepness is determined by a relaxation length in contacts.

There are other vague issues in the Landauer–Buttiker approach arising from quantum mechanics. This approach supposes that the contact reservoirs supply only pure states (plane waves) into the channel and they sustain their coherence during transmission through the channel. However, the quite plausible assumptions are:

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\[ I = I_1 + I_2 = \frac{i\hbar e}{2m} \left[ \int dx_1 (\psi \nabla x_1 \psi - \psi^* \nabla x_1 \psi)|_{x_1=x} + \int dx_2 (\psi \nabla x_2 \psi - \psi^* \nabla x_2 \psi)|_{x_2=x} \right]. \]  \hspace{1cm} (A5)

The pure disentangled state is

\[ \psi_0(x_1, x_2) = \psi_1(x_1) \psi_2(x_2). \]  \hspace{1cm} (A6)

At the channel exit the wave functions are \(\psi_1(x) = t_1 \exp(ik_1x)\) and \(\psi_2(x) = t_2 \exp(ik_2x)\), where \(t_1\) and \(t_2\) are the amplitude transmission coefficients.

The entangled state is

\[ \psi_{\text{ent}}(x_1, x_2) = \frac{1}{\sqrt{1 + |x|^2}} [\psi_1(x_1) \psi_2(x_2) + \alpha \psi_1(x_1) \psi_2(x_1)] \]  \hspace{1cm} (A7)

where \(x\) is an arbitrary complex number. If \(|x| \to 0\) or \(|x| \to \infty\), then the state becomes disentangled. Calculation of the current in accordance with Eq. (A5) for the entangled wave function \(\psi_{\text{ent}}(x_1, x_2)\) gives the same value as for the disentangled one \(\psi_0(x_1, x_2)\), which results in the Landauer–Buttiker formula. The point is that the off-diagonal terms of the form \(\psi_1(x) \psi_2^*(x)dx\) are equal to zero owing to orthogonality of wave functions.

As to the electron–electron scattering, it is commonly omitted in classical Monte Carlo simulations. This is substantiated by the fact that this kind of scattering, at least, does not influence the mobility due to the momentum conservation law. Such is not the case if we regard interference in quantum simulations. The content

Fig. 14. Idealized potential barrier near the source.
of the matter is that the interference requires coherence in the channel. On the other hand, the electron–electron scattering breaks the coherence. The decoherence time is reciprocal to the electron–electron scattering rate which is equal to $10^{12}$ s$^{-1}$ for the typical bulk density $n \sim 10^{18}$ cm$^{-3}$. It leads to the decoherence length about 100 nm for the thermal velocity $10^7$ cm/s. These estimates readily show that the electron–electron scattering can be neglected for fairly short channels. However, the problem needs more thorough consideration, possibly, based upon the Green's function method.

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