CALCULATIONS OF CONDUCTANCE OSCILLATIONS IN QUANTUM DOTS*

G. Hałdaś and A. Kolek

Department of Electronics Fundamentals, Rzeszów University of Technology
W. Pola 2, 35-959 Rzeszów, Poland

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When all 3 dimensions of electron device drop to a nanometer size, a 0-D device or a quantum dot appears. In this case the conductance shows oscillations with varying gate voltage. In this paper the results of numerical simulations, which clearly show the above behavior, are presented. The dot conductance is calculated with the help of Landauer formula after the Green's function corresponding to device Hamiltonian is evaluated. Coulomb interactions are included as the Hartree potential associated with the charge of all particles inside a dot. This forces us to use self-energies which describes interactions between device and leads not only to propagating states but also to non-propagating, localized states below the band.

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1. Introduction

The modern semiconductor technology makes now possible fabrication of devices that are only a few tens nanometers in size. The way to confine electrons in such small regions is to use material boundaries and/or electric fields. If the electrons are confined in all 3-dimensions: a zero dimensional (0-D) device or a quantum dot forms. Recent experiments at low temperatures revealed that conductance g of such quantum dot oscillates with varying gate voltage V_{g}. The commonly accepted explanation of this effect is that each oscillation corresponds to precisely one electron added to the device.

The aim of this paper is to present the results of numerical calculations in which the effect of conductance oscillations in quantum dot is reproduced. The method we have employed was the Green's function technique applied to

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discretized 2-D space. The problem was simplified in that way that electron-electron interactions were included only within Hartree approximation. Also the spin degeneracy has been omitted.

2. The model and computational technique

The model of rectangular quantum dot together with quasi 1-D leads is sketched in Fig. 1. We consider two strips connected to the opposite edges of the device. Within the Hartree approximation the tight-binding

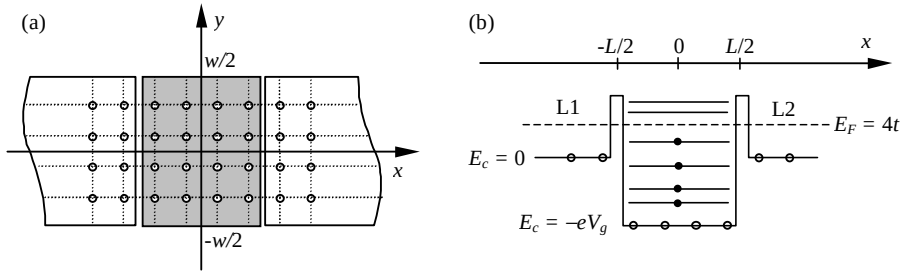


Fig. 1. (a) The model of 0-dimensional device weakly coupled to the leads: L1 (left) and L2 (right). The dimensions of the device are w (width) and L (length). The leads stretch to infinity. The uniform discretization mesh of lattice spacing a used in numerical simulations is marked. (b) Energetic structure of the model in (a). Sites in the leads have zero-energies, $[E_c]_i = 0$. Energies of the sites in the device depend on gate voltage, $[E_c]_i = -eV_g$. The height of the barriers describes the value of coupling parameter τ. Fermi level is assumed in the band center $E_F = 4t$.

Hamiltonian becomes a matrix $[H]$ with elements $[H]_{ij}$

$$\begin{aligned} [H]_{ii} &= 4t - e[V_H]_i + [E_c]_i\,, \\ [H]_{ij} &= -t\,, \qquad \text{for} \quad i,j \text{ being nearest neighbors (n.n.)} \\ [H]_{ij} &= 0 \qquad\quad \text{otherwise}\,. \end{aligned} \tag{1}$$

$[E_c]_i$ is the conduction band edge at site i, $t \equiv \hbar^2/2m^*a^2$, m^* is electron effective mass, a is the site separation and the elements of the vector of Hartree potential are [4]

$$[V_H]_i = -\frac{e}{4\pi\varepsilon a}\left(\sum_{j\neq i}\frac{[n]_j a^2}{|r_{ij}|/a} + 3.52[n]_i a^2\right), \tag{2}$$

where $|r_{ij}|$ is the distance between sites i and j, ε is dielectric constant and $[n]_i$ is the electron density at site i. It can be calculated as

$$[n]_i = \sum \mathrm{res}[G]_{i,i}\,(z = E_b) + \int\limits_{[E_c]_i}^{E_\mathrm{F}} -\frac{1}{\pi}\mathrm{Im}[G^\mathrm{R}]_{i,i}(E)dE\,, \tag{3}$$

where the summation is over all discrete eigenenergies E_b of the Hamiltonian $[H]$ (or poles of $[G]_{ii}$) that lie below the Fermi level E_F, and the integral is over continuous spectrum of $[H]$: starting from the band edge $[E_c]_i$ up to E_F. The Green's functions that appear on the r.h.s. of Eq. (3) can be calculated as [2]

$$[G](z = E + i\eta) = (z[I] - [H] - [\Sigma_\mathrm{DL1}] - [\Sigma_\mathrm{DL2}])^{-1}, G^\mathrm{R}(E) = \lim_{\eta\to 0} G(z)\,. \tag{4}$$

In this equations the coupling between device and leads is taken into account in the form of self-energies $\Sigma_{\mathrm{DL}p}$, $p = 1, 2$. The matrix elements of self-energy due to the interaction between the device and the lead p are [2,4]

$$[\Sigma_{\mathrm{DL}p}]_{ij}(E) = -t\tau^2 \sum_m \chi_m(l_i)\chi_m(l_j) f_m(E)\,, \tag{5}$$

where τ is the coupling parameter and l_i is the point (site) in the lead p adjacent to the point i in the device. The meaning of the coupling parameter τ is that for $\tau = 0$ there is no coupling to the lead: $[\Sigma_{\mathrm{DL}p}]_{ij} = 0$. In this case we have closed device with only bounded states inside the dot and no transport takes place. On the contrary for $\tau = 1$ the system is entirely open. Tuning τ in the range [0, 1] continuously changes the coupling between the device and the lead. It is like controlling the height of the tunnel barrier separating device from the lead (see Fig. 1(b)). In Eq. (5) χ_m is the transverse component of the envelope function of mode (subband) m in lead p. The form of the function f_m in Eq. (5) depends on the difference between E and eigenenergy E_m of mode m [2,4]

$$f_m(E) = \left\{ \begin{array}{lll} q - \sqrt{q^2-1} & \text{for} & E \geq E_m + 2t \\ \exp(ik_m a) & \text{for} & E_m - 2t \leq E \leq E_m + 2t \\ q + \sqrt{q^2-1} & \text{for} & E \leq E_m - 2t \end{array} \right\}, \tag{6}$$

where $\cos k_m a = q \equiv -(E - E_m)/2t$. The meaning of the above cases is that while the first and third rows refer to localized (non-propagating) states, the row in the middle describes the propagation of extended states and for this reason is especially important when calculating conductance. For this reason the other two terms are usually ignored. When Coulomb interactions are considered the charge being captured in localized states must be taken into account. Thus, for a proper treatment the self-energy terms that describe interaction for localized states must not be omitted. One more reason for

this is that omitting self-energies that describes device-lead interaction for localized states gives incorrect density of extended states [5]. So, in our calculations we use the self-energies as in Eqs. (5) and (6). In this point this paper differs from others [3].

3. Results of calculations: 10×5 rectangular quantum dot

We have performed calculations for rectangular-shaped quantum dot. The discretization mesh was of 10 sites width and 5 sites length. The leads were of 10 sites width. The strength of Coulomb interaction $U = e^2/4\pi\varepsilon a$ was assumed as $U = 0.5t$. For GaAs material parameters m^* and e this corresponds to the lattice spacing $a \simeq 2.5$ nm, and the size of the device of approximately 25×12.5 nm^2. As a reference level we have assumed the conduction band edge in the leads $[E_c]_i = 0$. The influence of external voltage V_g was then simulated by the site energies in the device $[E_c]_i = -eV_g$. The Fermi level was fixed in the middle of the band, $E_F = 4t$ (see Fig. 1(b)). The calculations were performed for the value of the coupling parameter $\tau = 0.2$. The self-consistent solutions was achieved in the iterative procedure: calculate device Hamiltonian, Eqs. (1); calculate the self-energies due to the leads, Eqs. (5) and (6); calculate the Green's functions, Eq. (4); calculate electron density, Eq. (3); calculate the Hartree potential, Eq. (2); calculate the Hamiltonian, Eqs. (1) ..., go on unless electron density stops changing. Result are shown in Fig. 2. In Fig. 2(a) the density of states (DOS)

$$\Omega(E) = a^2 \sum_i [\rho]_i(E) = -\frac{a^2}{\pi} \sum_i \mathrm{Im}[G^{\mathrm{R}}]_{ii}(E)$$

calculated for gate voltage $V_g = -t/e$ is presented. Lorentzian peaks at the positions of dot energy levels are clearly visible. The width of these peaks depend on the value of coupling parameter τ, the greater τ the wider the peak.

The positions of the peaks in DOS in Fig. 2(a) depend on the gate voltage V_g. This is shown in Fig. 2(b) where the maxima in DOS are plotted versus eV_g. The origin of this step-like behavior is clear. As V_g increases every time the peak in DOS crosses E_F a new electron tunnels into the dot. This prevents moving DOS towards level energies because the (Coulomb) electrostatic energy of the system increases. The peak in DOS is pinned to E_F until the whole electron enters the dot. This effect is known as the Coulomb blockade.

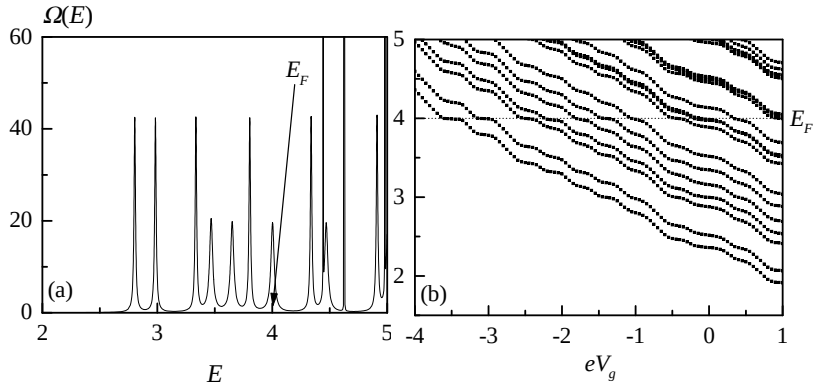


Fig. 2. (a) Density of states $\Omega(E)$ calculated for the device weakly coupled to the leads ($\tau = 0.2$). The gate voltage was $V_{\rm g} = -t/e$. The position of the Fermi energy, fixed at $E = E_{\rm F} = 4t$, is marked. The unit on horizontal/vertical axis is t/t^{-1}. (b) The positions of the maxima in the density of states $\Omega(E)$ versus $eV_{\rm g}$. The unit on both axes is t.

Another effect are the oscillations of the conductance. When the peak in DOS crosses $E_{\rm F}$ high DOS is probed. This correspond to large conductance. On the contrary for $E_{\rm F}$ in between the peaks, low DOS is probed and small conductance should be observed. Indeed, such oscillations are shown in Fig. 3. We were able to calculate conductance g since it can be expressed in terms of the retarded Green's function [2]

$$g = \frac{2e^2}{h} \mathrm{Tr} \left\{ [\Gamma_{\rm L1}][G^{\rm R}][\Gamma_{\rm L2}][G^{\rm R}]^{+} \right\} , \tag{7}$$

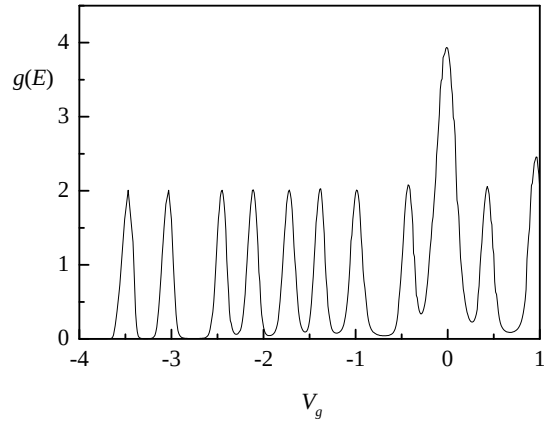


Fig. 3. Conductance g in units of e^2/h versus the gate voltage $V_{\rm g}$ in units of t/e.

where Tr{} stands for the trace of the matrix, $^+$ is Hermitian conjugate and the elements of the matrix $[\Gamma_{\mathrm{Lp}}]$ are [2]

$$[\Gamma_{\mathrm{Lp}}]_{ii'} = \sum_m \chi_m(i) \frac{\hbar v_m}{a} \chi_m(i') \,, \tag{8}$$

where $v_m = 2ta \sin k_m a$ is the longitudinal component of the velocity in mode m and the summation is over all modes in lead p.

4. Conclusions

The Green's function technique was used to calculate the conductance of 0-D device. The electron-electron interactions were treated within the Hartree approximation. The interactions between device and leads took into account both extended and localized sites. The oscillations of conductance have been observed in agreement with recent experiments.

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