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CHARGE–VOLTAGE RELATIONS IN QUANTUM DOT ARRAY FIELD-EFFECT TRANSISTORS

Yurii Sibirnovskii [1]
Khayratdin Kamalov[2]
Abdumukhamed Khudaybergenov[3]
National Research Nuclear University MEPhI
Department of Condensed Matter Physics, Moscow, Russia
Karakalpak State University, Department of Physics, khayratdinkamalov@gmail.com
Karakalpak State University, Department of Physics, abdumuxammed2198@gmail.com

ABSTRACT

This paper presents a numerical modeling approach to analyze the characteristics of a field-effect transistor (FET) with a quantum dot array channel. The study primarily considers the quantum size distribution, gamma distribution as a function of density, and the resulting energy distributions. Newton's method is employed to solve the system of nonlinear equations governing quantum transport phenomena. The Laplace equation is used to describe the electrostatic potential, and simulations are conducted in MATLAB and R. The results provide insight into the transistor's behavior under varying conditions, highlighting the influence of size-dependent energy levels and quantum confinement effects.

KEYWORDS

Introduction

Quantum dot array-based field-effect transistors (FETs) have emerged as promising candidates for next-generation nanoelectronic devices due to their discrete energy levels, tunable quantum confinement effects, and strong electrostatic control. The unique transport properties of these transistors are governed by several critical factors, including the quantum dot size distribution, energy broadening effects, and charge transport mechanisms.

The variation in quantum dot sizes leads to fluctuations in the density of states, which in turn influences the current-voltage (I-V) characteristics, energy level distributions, and overall device performance. Additionally, the current flowing through the quantum dot array is affected by the stochastic nature of

[1] National Research Nuclear University MEPhI Department of Condensed Matter Physics, Moscow, Russia
[2] Karakalpak State University, Department of Physics, khayratdinkamalov@gmail.com
[3] Karakalpak State University, Department of Physics, abdumuxammed2198@gmail.com

electron transport, making it essential to incorporate statistical distributions such as gamma functions to describe energy broadening effects.

This study presents a numerical approach to analyzing quantum transport in quantum dot array FETs by solving complex nonlinear equations using Newton's method. The proposed model accounts for the impact of quantum dot size variations, energy distribution effects, electrostatic potential variations, and their influence on charge transport. By integrating these factors, we aim to provide a more comprehensive understanding of the physical mechanisms governing such devices and to enhance predictive modeling for their future applications in nanoelectronics.

Literature Review

Initially, I decided to review several books and articles for my research. The most suitable book is . In this book , a more detailed and specific explanation relevant to my work is provided.

The research focuses on studying the source and drain of a field-effect transistor as a double-barrier structure. Between the source and drain, there is a quantum dot array, and the goal is to analyze and compare various characteristics such as the current-voltage (I-V) characteristics, charge transport, and energy distribution in quantum dot array field-effect transistors, among other aspects.

In the matrix model (Fig. 1), an additional third "contact," referred to as the s-contact, has been introduced to represent scattering processes. This inclusion is essential for establishing the transition to Ohm's law. The formulation presented in Fig. 1 a can be considered a special case of this general formalism, where all matrices are of size 1×1. If there exists a representation that diagonalizes all the matrices, then the matrix model without the s-contact can be directly obtained from Fig. 1.

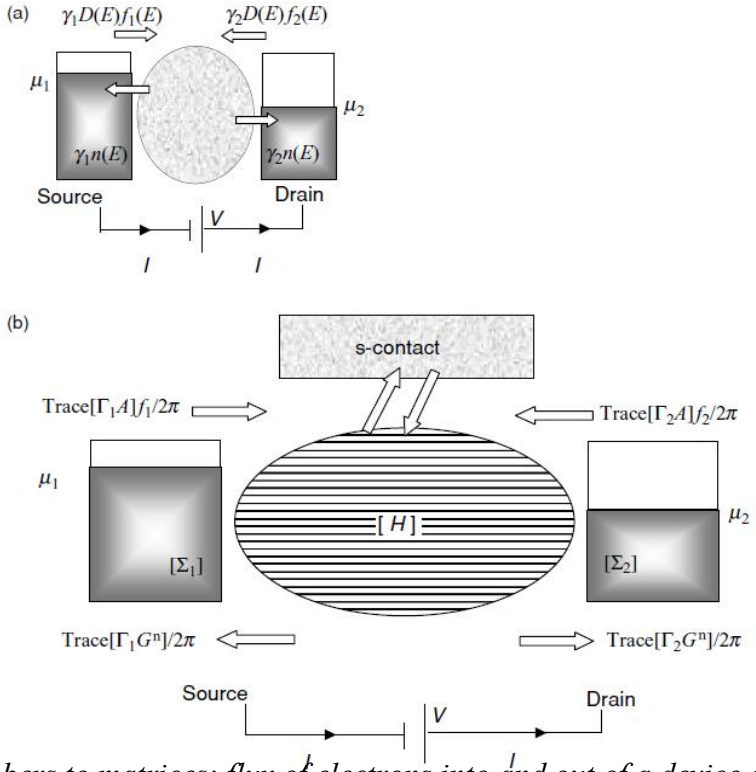

Figure 1:From numbers to matrices: flux of electrons into and out of a device at the source and drain ends. (a) Simple result for independent level model, (b) General matrix model, to be developed in this book. Without the "s-contact," this model is equivalent to that of Meir and Wingreen (1992). The "s-

contact" distributed throughout the channel describes incoherent scattering processes . In general, this "contact" cannot be described by a Fermi function, unlike the real contacts.

Theoretical Background

The model presented in Fig. 1 b, without the s-contact, is frequently used to analyze small devices. In this form, it is identical to the result obtained by Meir and Wingreen (1992), following the method of Caroli et al. (1972), which is based on the Non-Equilibrium Green's Function (NEGF) formalism. To make this approach accessible to readers unfamiliar with advanced many-body physics, I will derive these results using elementary arguments.

Previous studies have explored numerical methods for solving semiconductor equations . The application of Newton's method in quantum transport simulations has shown significant accuracy and computational efficiency . Recent advancements in MATLAB and R have facilitated the implementation of such methods .

Methodology

To obtain a high-quality dependence $\gamma(E)$, let us consider a model of a double-barrier structure .Resonant tunneling occurs in such a system.

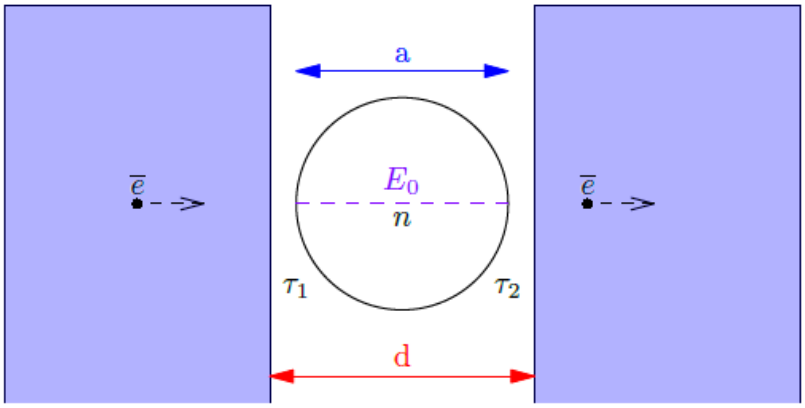

Figure 2:Positioning of the quantum dot between two electrodes.

Let us consider electron transmission through a double barrier described by the following potential:

$$U(x) = \alpha_1\delta(x) + \alpha_2\delta(x-a)$$

Compared to a rectangular barrier, we can set:

$$\alpha = Hw$$

where H is the barrier height (potential energy in eV) and w is the barrier width (in nm). For the delta-barrier model to work, H must be large and w small.

For a quantum dot between two metallic electrodes, H is approximately equal to the metal work function or the electron affinity in the semiconductor χ (around 4–5 eV), while $w = (d-a)/2$ is the distance between the metal and the quantum dot.

The probability current everywhere is given by:

$$j = \frac{\hbar k}{m}|T(E)|^2$$

Velocity:

$$v = \frac{j}{\rho}$$

For a double delta-barrier with spacing a and parameters α_1, α_2:

$$T = \frac{1}{(1+iq_1)(1+iq_2)+q_1q_2e^{2ika}}$$

where:

$$k = \sqrt{\frac{2m(E-E_c)}{\hbar^2}}$$

$$q_{1,2} = \frac{m\alpha_{1,2}}{\hbar^2 k}$$

To find the tunneling time τ and broadening γ, we need the following quantities:

$$A = (1+iq_2)T$$

$$B = -iq_2e^{2ika}T$$

$$|A|^2 = (1+q_2^2)|T|^2$$

$$|B|^2 = q_2^2|T|^2$$

Velocity:

$$v = \frac{\hbar k}{m}\frac{|T|^2}{|A|^2+|B|^2+2|A||B|\cos(2kx+\phi)}$$

$$v = \frac{\hbar k}{m}\frac{1}{1+2q_2^2+2q_2\sqrt{1+q_2^2}\cos(2kx+\phi)}$$

$$\frac{dx}{dt} = v$$

$$\tau = \frac{m}{\hbar k^2}\left[(1+2q_2^2)ka + 2q_2\sqrt{1+q_2^2}\cos(ka+\phi)\sin(ka)\right]$$

$$\gamma = \frac{\hbar^2k^2}{2m}\frac{k^2}{(k^2+2p_2^2)ka + 2p_2\sqrt{k^2+p_2^2}\cos(ka+\phi)\sin(ka)}$$

Define:

$$P = 1+q_1q_2[\cos(2ka)-1]$$

$$Q = q_1+q_2+q_1q_2\sin(2ka)$$

$$A = |T|^2(1+iq_2)(P-iQ)$$

$$B = |T|^2q_2(\sin 2ka - i\cos 2ka)(P-iQ)$$

Simplified expression:

For $\alpha_1 = \alpha_2 = \alpha$ (the quantum dot is located symmetrically between two electrodes):

$$\gamma = \frac{\hbar^2k^2}{2m^*}\frac{k^2}{(k^2+2p^2)ka}$$

$$k = \sqrt{\frac{2m(E-E_c)}{\hbar^2}}$$

$$p = \frac{m^*\alpha}{\hbar^2}$$

For GaAs:

$$\frac{m^*}{m_0} = 0.067$$

We consider a series of quantum dots positioned between the electrodes and not interacting with each other.

The primary influence on the I–V characteristics will be the size variation of these dots (parameter a). The distance between the electrodes remains constant, so when a changes, the parameter $w = (d - a)/2$ also changes, which in turn affects the parameter α in the delta-barrier model between the metal and the quantum dot.

Numerical Methods and Algorithms

Final Formulas Step-by-Step

$$I(V) = \frac{e}{2\tau}\int_{-\infty}^{\infty} d\,E\,D(E-U)(f_1(E) - f_2(E))$$

$$N = \frac{1}{2}\int_{-\infty}^{\infty} d\,E\,D(E-U)(f_1(E) + f_2(E))$$

$$f_1(E) = \frac{1}{1+\exp\left(\frac{E-eV}{kT}\right)}, \quad f_2(E) = \frac{1}{1+\exp\left(\frac{E}{kT}\right)}$$

$$D(E) = \frac{1}{\pi}\cdot\frac{\gamma}{(E-E_0)^2+\gamma^2}$$

$$\tau = \frac{\gamma}{2\hbar}$$

$$U = \frac{1}{2}eV + U_0\Delta N$$

$$\Delta N = N - N_0$$

If we assume that N_0 corresponds to zero bias, we get:

$$N_0 = \int_{-\infty}^{\infty} d\,E\,D(E)f_2(E)$$

U_0 is taken as a constant depending on the size and shape of the quantum dot.

For a spherical quantum dot with radius R (in nanometers):

$$U_0 \approx \frac{A}{R}$$

Then we get:

$$U = \frac{1}{2}eV - U_0N_0 + U_0N$$

The algorithm is as follows:

1. First, calculate U_0 and N_0 for the given quantum dot radius and energy level E_0.
2. Next, vary the bias V, and for each value solve for ΔN:

$$\Delta N = -N_0 + \frac{1}{2}\int_{-\infty}^{\infty} d\,E\,D\left(E - \frac{1}{2}eV - U_0\Delta N\right)(f_1(E) + f_2(E))$$

We solve this equation with either simple iterations or Newton's method, starting with $\Delta N = 0$.

We rewrite the equation so that the right side equals zero:

$$G(x) := x + N_0 - \frac{1}{2}\int_{-\infty}^{\infty} d\,E\,D\left(E - \frac{1}{2}eV - U_0x\right)(f_1(E) + f_2(E)) = 0$$

The derivative of $G(x)$ is:

$$\frac{\partial G}{\partial x} = 1 - \frac{\gamma}{\pi} U_0 \int_{-\infty}^{\infty} d\,E \, \frac{E - E_0 - \frac{1}{2}eV - U_0 x}{\left[\left(E - E_0 - \frac{1}{2}eV - U_0 x\right)^2 + \gamma^2\right]^2} (f_1(E) + f_2(E))$$

Newton's Method Algorithm

We start with $x_0 = 0$ and compute:

$$x_1 = x_0 - \frac{G(x_0)}{\frac{\partial G}{\partial x}(x_0)}$$

Then:

$$x_{n+1} = x_n - \frac{G(x_n)}{\frac{\partial G}{\partial x}(x_n)}$$

We stop when $|x_{n+1} - x_n| < 10^{-6}$ or after 20 iterations.

(3) Using the calculated $\Delta N = x$, we compute the current:

$$I(V) = \frac{e}{2\tau} \int_{-\infty}^{\infty} d\,E\, D(E - U)(f_1(E) - f_2(E))$$

$$U = \frac{1}{2}eV + U_0 \Delta N$$

We repeat steps 2 and 3 for each voltage value.

Step-by-Step Solution

First, compute U_0 and N_0 for the given radius and energy level:

$$U_0 \approx \frac{0.3}{R}$$

For $R = 3$ nm:

$$U_0 \approx \frac{0.3}{3} \approx 0.1 \text{ eV}$$

Now calculate:

$$N_0 = \int_{-\infty}^{\infty} d\,E \cdot D(E) f_2(E)$$

with:

$$D(E) = \frac{1}{\pi} \cdot \frac{\gamma}{(E - E_0)^2 + \gamma^2}, \quad f_2(E) = \frac{1}{1 + \exp\left(\frac{E}{kT}\right)}$$

$$N_0 = \int_{-\infty}^{\infty} d\,E \cdot \frac{1}{\pi} \cdot \frac{\gamma}{(E - E_0)^2 + \gamma^2} \cdot \frac{1}{1 + \exp\left(\frac{E}{kT}\right)}$$

MATLAB results for N_0. The calculated result: $N_0 \approx 0.0064196$.

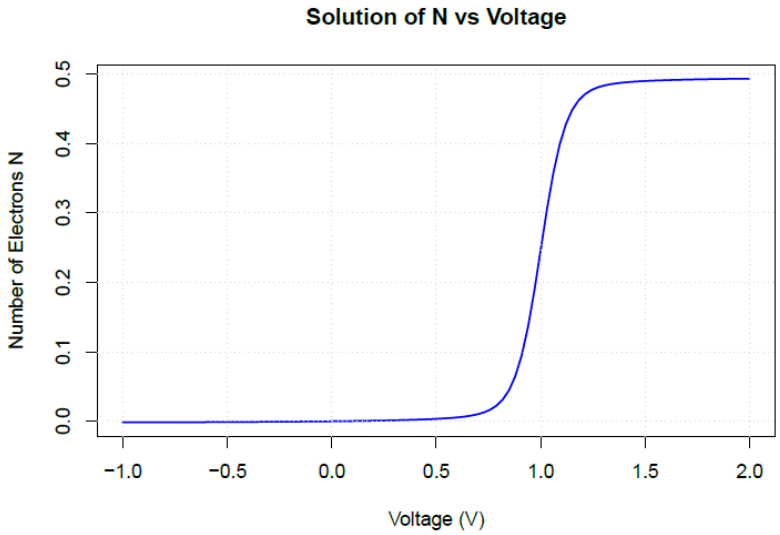

Figure 4:Computed $N(V)$ from R code

Results and Discussion

Further investigation and modeling of the transistor's charge transport characteristics are greatly facilitated by the discovery that the parameter N is roughly zero. This value is close to zero, which makes it easier to analyze and solve related equations by allowing us to concentrate on other important features.

The crucial impact of energy broadening and quantum dot size distribution on the electronic transport in quantum dot-based field-effect transistors was demonstrated by our numerical simulation. According to the rule of large numbers, the size distribution of quantum dots tends to become more symmetric as their number rises.

In line with theoretical predictions, it was demonstrated that important physical phenomena as resonant tunneling, Coulomb blockade, and quantum confinement significantly affected the current-voltage characteristics. By adjusting variables such as temperature, dispersion, and quantum dot size, important information on how to maximize device performance was discovered.

These results offer useful avenues for enhancing the stability and effectiveness of next-generation quantum dot FETs while also advancing nanoelectronic devices. To further improve device performance and dependability, future research will concentrate on improving quantum transport models, examining more intricate quantum dot distributions, and tackling the consequences of disorder and inhomogeneity.

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