QUANTUM DOTS

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w opracowaniu internetowej wersji wykładów.

1 Theory: Poisson-Schrődinger Problem

The potential confining the electrons in electrostatic QD originates from electric charges on the gates and ionized impurities (usually donors). Moreover, the net confinement potential includes the self-consistent Hartree-type component, which results from the electrons in the dot (each electron interacts with themselves in a indirect way). If we know the charge density and appropriate boundary conditions, we can find the confinement potential by solving the Poisson equation. The confinement potential leads to the localization of electrons in the QD. The localized quantum states of electrons can be found by solving the Schrődinger equation (with the confinement potential). Knowing the wave functions of QD confined electrons we can determine the charge density in the QD that – in turn – determines the confinement potential via the Poisson equation.

$\Longrightarrow$ **self-consistent Poisson-Schrődinger problem**

1.1 Electrostatic Field in the QD

Sources of electron confinement in electrostatic QD's

(1) gates

(2) source and drain electrodes

(2) band offsets
(discontinuities of the conduction band at semiconductor heterojunctions)

(3) Schottky barriers at metal-semiconductor junctions

(4) ionized donors and acceptors

(5) excess electrons confined in the QD

1.2 Computational Method

Potential energy of electron confined in the QD

$$U_{conf}(\mathbf{r}) = U_{band}(z) - e\Phi(\mathbf{r}) \ , \qquad (1)$$

$U_{band}(z)$ = band offset energy (resulting from the conduction band discontinuity in the z direction)

In two-terminal nanodevice, U_{band} is described by the potential of the single potential well and barrier.

In three-terminal nanodevice, U_{band} corresponds to the single potential well surrounded by two potential barriers.

$\Phi(\mathbf{r})$ = potential of the resultant (total) electrostatic field

According to the superposition principle, potential $\Phi(\mathbf{r})$ of the total electrostatic field is given by

$$\Phi(\mathbf{r}) = \varphi_1(\mathbf{r}) + \varphi_2(\mathbf{r}) \; , \tag{2}$$

$\varphi_1(\mathbf{r})$ = potential of the electrostatic field created by all charges in the nanosystem excluding of the QD confined electrons

$\varphi_2(\mathbf{r})$ = potential of the electrostatic field created by the electrons confined in the QD

We introduce

$U_{elst}(\mathbf{r})$ = potential energy of the electron in the electrostatic field with potential $\varphi_1(\mathbf{r})$

$$U_{elst}(\mathbf{r}) = -e\varphi_1(\mathbf{r}) \; . \tag{3}$$

Potential $\varphi_1(\mathbf{r})$ is a solution of Poisson equation

$$\nabla^2\varphi_1(\mathbf{r}) = -\frac{\varrho_D(\mathbf{r})}{\varepsilon_0\varepsilon_s} \; , \tag{4}$$

$\varrho_D(\mathbf{r})$ = charge density of ionized donors

ε_0 = electric permittivity of vacuum

ε_s = relative static electric permittivity of nanostructure material (for GaAs based nanodevices: $\varepsilon_s = 13.2$)

Potential $\varphi_2(\mathbf{r})$, which stems from the QD confined electrons, can be calculated in a Hartree approximation as follows:

$$\varphi_2(\mathbf{r}) = -\frac{\kappa e}{\varepsilon_s}\sum_{\nu=1}^{N}\int d^3r' \frac{|\psi_\nu(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|} \; , \tag{5}$$

where $\kappa = 1/(4\pi\varepsilon_0)$.

$\psi_\nu(\mathbf{r})$ = one-electron wave functions calculated by the Hartree-Fock method

The summation in Eq. (5) runs over all occupied one-electron states.

1.2.1 Calculation of charge density

(1) In the two-terminal nanodevice (Ashoori, MIT), all donors are ionized since they are localized in the barrier AlGaAs layer with the higher energy than the GaAs minimum conduction band energy.

For this layer

$$\varrho_D(\mathbf{r}) = +en_D \tag{6}$$

n_D = donor concentration

(2) The three-terminal nanodevice (Tarucha, NTT) consists of several n-type GaAs layers with different donor concentration.

For the non-degenerate n-type semiconductor at $T = 0$ and $V_{sd} = 0$ the Fermi energy F is determined by the ground-state donor energy E_D

$$F = E_D \ .$$

We can assume [1] that E_D also determines the Fermi energy of the source and drain.

$\Longrightarrow$ The ionization of the donor can only be caused by the electrostatic field acting at the donor center position $\mathbf{r}$.

1.2.2 Donor ionization condition

The donor in position $\mathbf{r}$ becomes ionized if the total potential energy of electron in the electrostatic field, i.e.,

$$U_{tot}(\mathbf{r}) = -e\Phi(\mathbf{r}) \ , \tag{7}$$

is larger than the electrochemical potential of the nearest electron reservoir (source or drain), i.e.,

$$U_{tot}(\mathbf{r}) > -eV_{s(d)} \tag{8}$$

$V_{s(d)}$ = source (drain) voltage

After the ionization process the liberated electron flows from the donor center to the source or drain.

For a convenience we can take on the common Fermi energy F as a reference energy. This can be realized by putting $F = 0$.

$\Longrightarrow$ **donor ionization condition**

$$\varrho_D(\mathbf{r}) = \begin{cases} +en_D(\mathbf{r}) & \text{if } U_{tot}(\mathbf{r}) > -eV_{s(d)} \ , \\ 0 & \text{otherwise} \ , \end{cases} \tag{9}$$

The charge density used in the Poisson equation is calculated according to condition (9).

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[1] This assumption is not true in the case of the degenerate n-type semiconductor.

1.2.3 Boundary conditions

The Poisson problem is uniquely formulated if we put the boundary conditions on the surface that surrounds the integration region.

Putting the boundary conditions on the total potential $\Phi(\mathbf{r})$ allows us to take into account all charges in the nanodevice.

In order to solve the Poisson equation we need the boundary conditions for potential $\varphi_1(\mathbf{r})$. They are calculated using the formula

$$\varphi_1(\mathbf{r}_{boundary}) = \Phi(\mathbf{r}_{boundary}) - \varphi_2(\mathbf{r}_{boundary}) \tag{10}$$

The boundary conditions on the surfaces of electrodes are determined by the voltages applied to these electrodes.

In the case of the three-terminal nanodevice we put on the following boundary conditions:

$$\Phi(\mathbf{r}_{source}) = V_s = 0 \ , \tag{11}$$

$$\Phi(\mathbf{r}_{drain}) = V_d \equiv V_{ds} \ , \tag{12}$$

$$\Phi(\mathbf{r}_{gate}) = V_g - \phi_B/e \ , \tag{13}$$

where
V_g = gate voltage,
ϕ_B = Schottky barrier at the metal-semiconductor interface

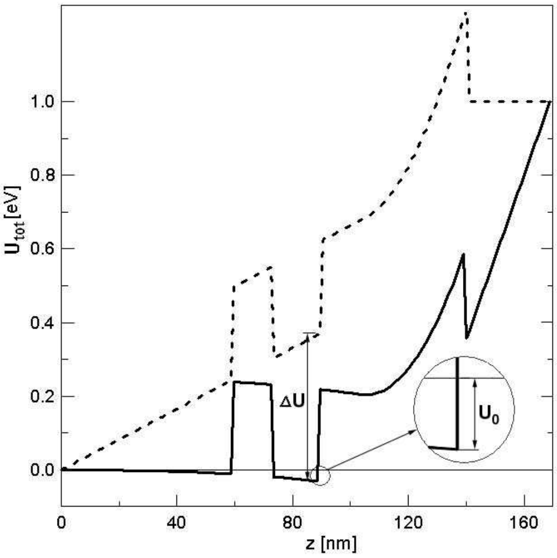

Figure 1: Boundary conditions for total potential energy $U_{tot} = -e\Phi$ at $r = R_c$ (dotted curve) and potential energy U_{tot} calculated along the cylinder axis (solid curve) for the two-terminal nanodevice (Ashoori, MIT). U_0 and ΔU denote the depths of the vertical and lateral confinement potentials, respectively.

1.2.4 Self-consistent solution of the Poisson-Schrődinger problem

Initial charge density $\varrho_{D,initial}(\mathbf{r})$

$\Longrightarrow$ Poisson equation

$\Longrightarrow$ electrostatic potential $\varphi_1(\mathbf{r})$

$\Longrightarrow$ confinement potential

$$-e\varphi_{conf}(\mathbf{r}) = U_{band}(z) - e[\varphi_1(\mathbf{r}) + \varphi_2(\mathbf{r})]$$

$\Longrightarrow$ Schrődinger equation

$\Longrightarrow$ one-electron wave functions $\psi_\nu(\mathbf{r})$

$\Longrightarrow$ electron charge density

$\Longrightarrow$ modified charge density $\varrho_D(\mathbf{r})$

$\Longrightarrow$ Poisson equation

$\Longrightarrow$ modified electrostatic potential $\varphi_1(\mathbf{r})$

$\Longrightarrow \ldots$

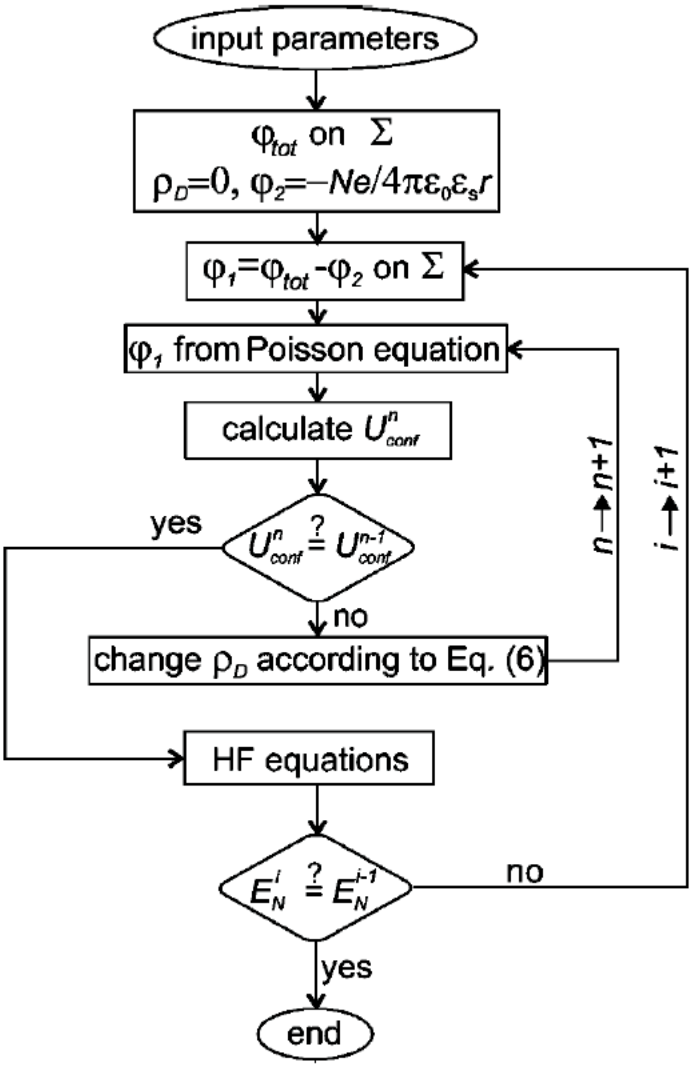

Figure 2: Block diagram of self-consistent procedure for solving the Poisson-Schrődinger problem. Total electrostatic potential $\varphi_{tot} \equiv \Phi$.

1.2.5 Solutions of Poisson equation

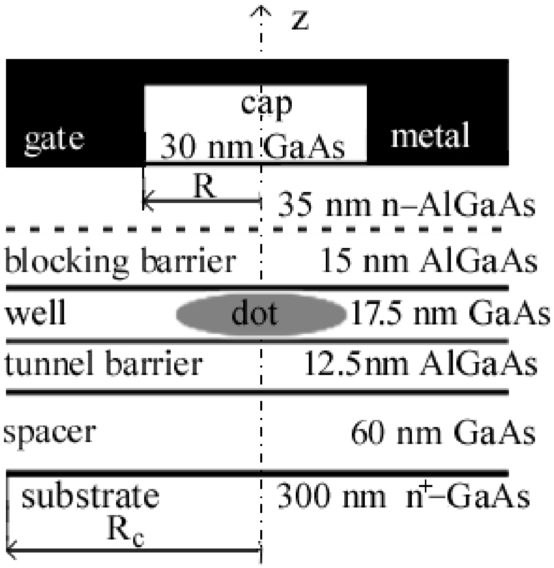

Figure 3: Schematic of two-terminal nanodevice (R.C. Ashoori et al., MIT). $R =$ radius of GaAs cap covered by metal gate, $R_c =$ radius of cylindrical surface, on which we put the boundary conditions for Poisson equation.

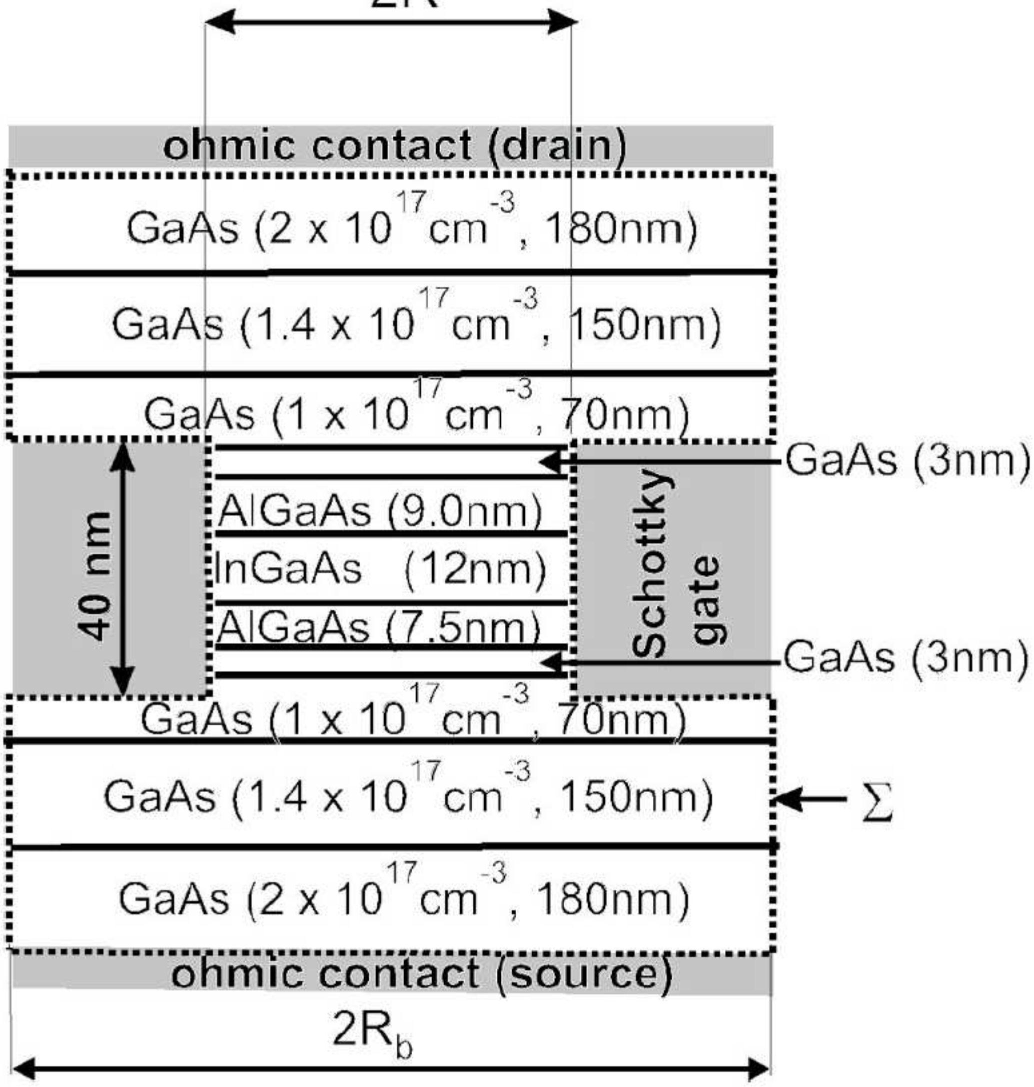

Figure 4: Schematic of three-terminal nanodevice (S. Tarucha et al., NTT). Given are donor concentrations and layer thicknesses. Dotted line corresponds to cylindrical surfaces with radii R i R_b, on which we put the boundary conditions for Poisson equation.

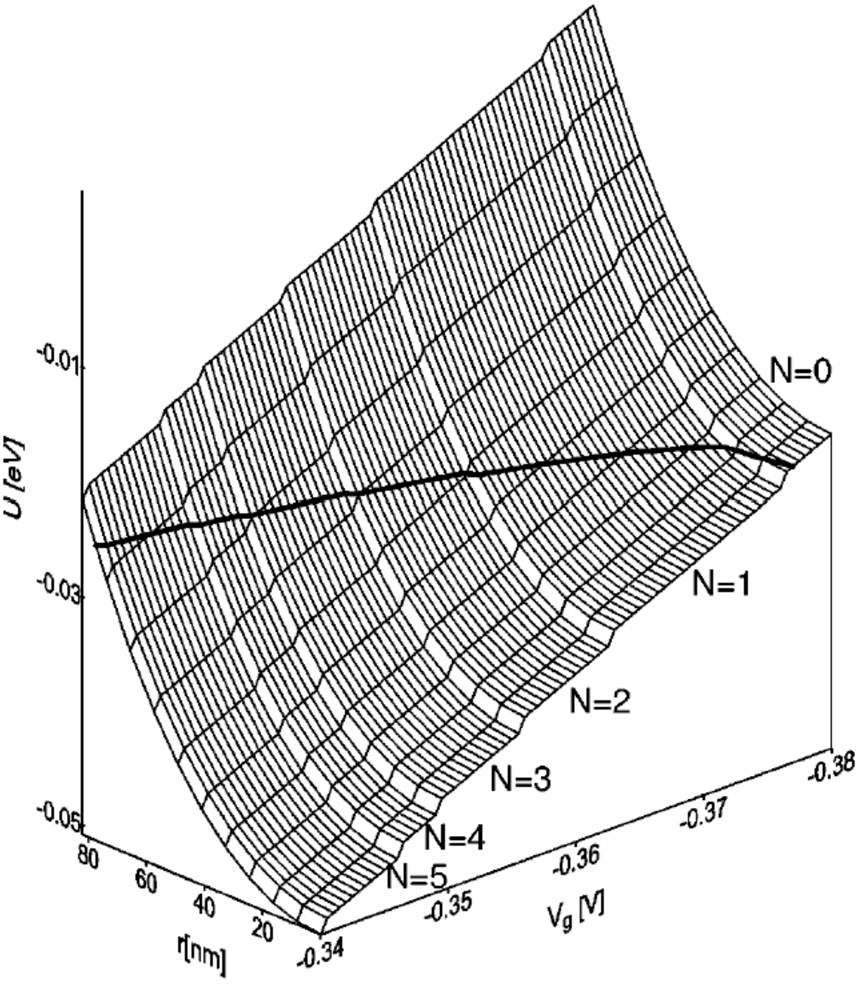

Figure 5: Electrostatic potential energy U of lateral confinement in two-terminal nanodevice (Ashoori, MIT) as a function of radial coordinate r, gate voltage V_g, and number of QD-confined electrons N. Thick solid curve shows the Fermi energy.

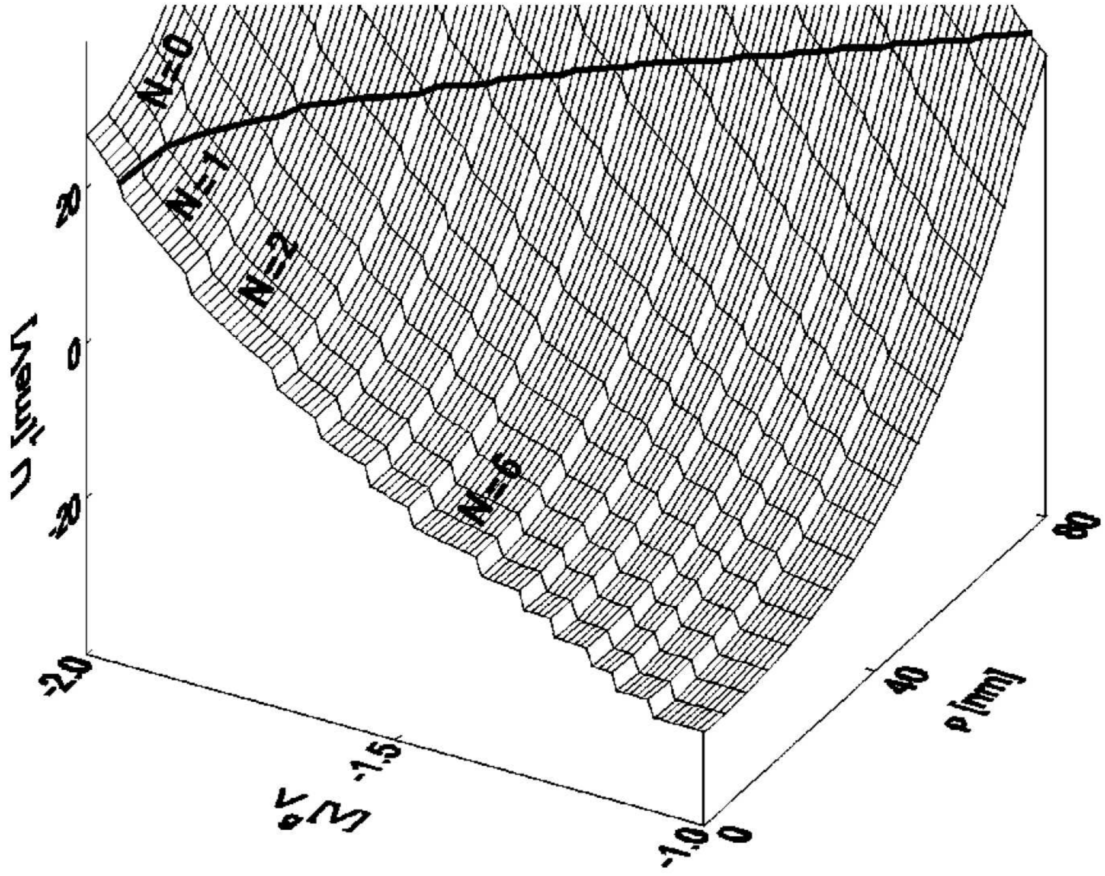

Figure 6: Electrostatic potential energy $U_1 \equiv U$ of lateral confinement in three-terminal nanodevice (Tarucha, NTT) as a function of radial coordinate $\rho \equiv r$, gate voltage V_g, and number N of QD-confined electrons. Thick solid line shows the Fermi energy.

1.2.6 Hartree-Fock method for N-electron Schrődinger equation

The Hamiltonian of N-electron system confined in the QD

$$H = \sum_{i=1}^{N} \left[h(\mathbf{r}_i) + \sum_{j>i}^{N} \frac{\kappa e^2}{\varepsilon_\infty r_{ij}} \right] . \tag{14}$$

The one-electron Hamiltonian

$$h(\mathbf{r}) = -\frac{\hbar^2}{2m_e}\nabla^2 + U_{conf}(\mathbf{r}) \ , \tag{15}$$

where
m_e = electron conduction band mass
$r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ = electron-electron distance
ε_∞ = high-frequency relative electric permittivity, which is responsible for a screening of Coulomb interactions at small distances r_{ij}.

For the cylindrical symmetry the one-electron wave functions can be expanded as follows:

$$\psi_{ns}(\mathbf{r}) = \sum_{k_x k_y} c^{ns}_{k_x k_y} g_{k_x k_y}(\mathbf{r}) \ , \tag{16}$$

where we introduce the polynomial-Gaussian basis

$$g_{k_x k_y}(\mathbf{r}) = x^{k_x} y^{k_y} \exp[-\alpha(x^2 + y^2) - \beta z^2] \ , \tag{17}$$

$c^{ns}_{k_x k_y}$ = linear variational parameters
α, β = non-linear variational parameters
n = set of orbital quantum numbers, s = spin quantum number
$\nu = (n, s)$

2 Quantum Coulomb blockade: theory and experiment

2.1 Voltage-to-energy conversion factor

$$\alpha_N(V_g) = \left.\frac{\partial \mu_N}{\partial V_g}\right|_{V_{ds}=0} \tag{18}$$

Unit of $\alpha_N = e =$ elementary charge

Knowing the conversion factor we can convert the measured change of gate voltage ΔV_g to the change of energy of electron system according to

$$\Delta E_N = \alpha_N \Delta V_g \ . \tag{19}$$

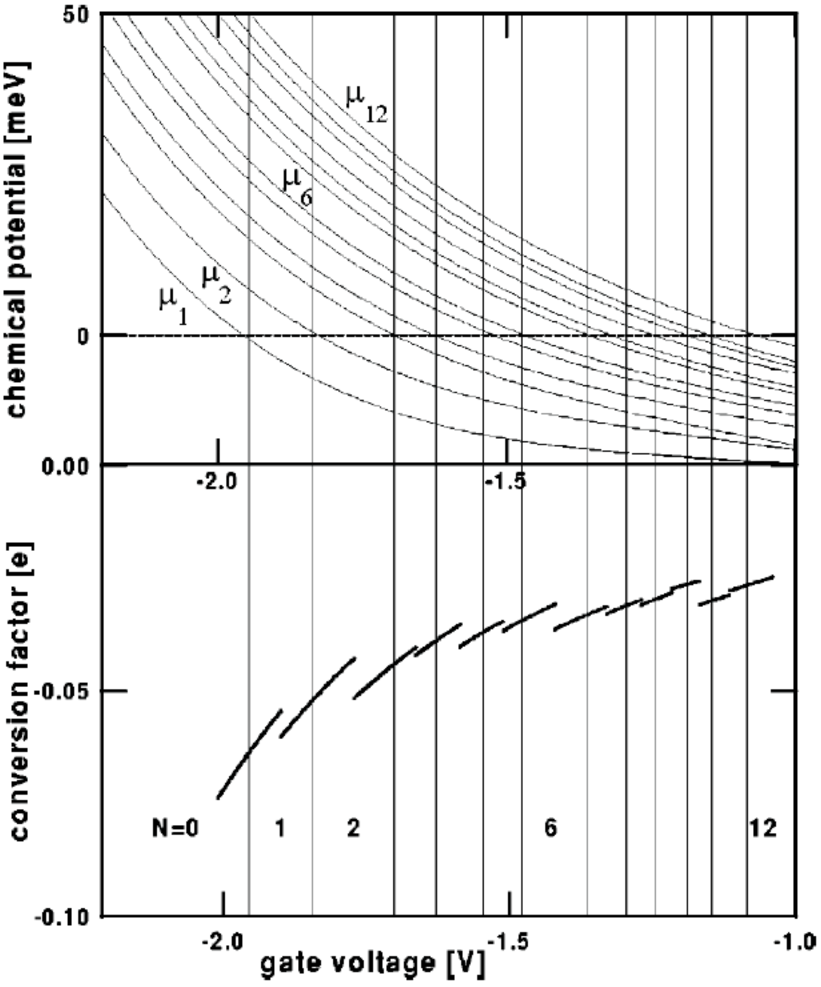

Figure 7: Chemical potential μ_N (upper panel) and conversion factor α_N (lower panel) for three-terminal nanodevice (Tarucha, NTT) at $V_{ds} = 0$ as functions of gate voltage and number N of electrons confined in the QD. Vertical lines correspond to the measured source-drain current peaks.

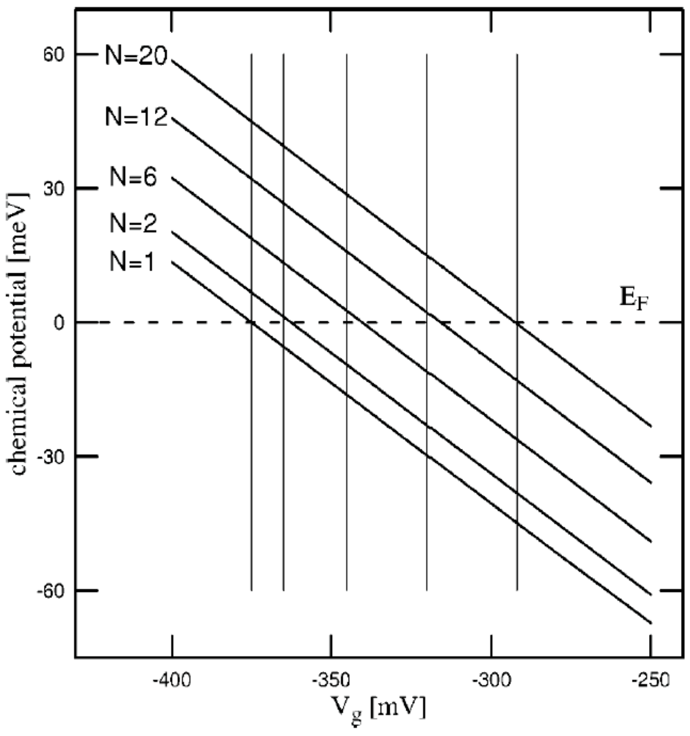

Figure 8: Chemical potential for two-terminal nanodevice (Ashoori, MIT) as a function of gate voltage V_g and number N of electrons confined in the QD. Vertical lines correspond to the measured capacitance peaks.

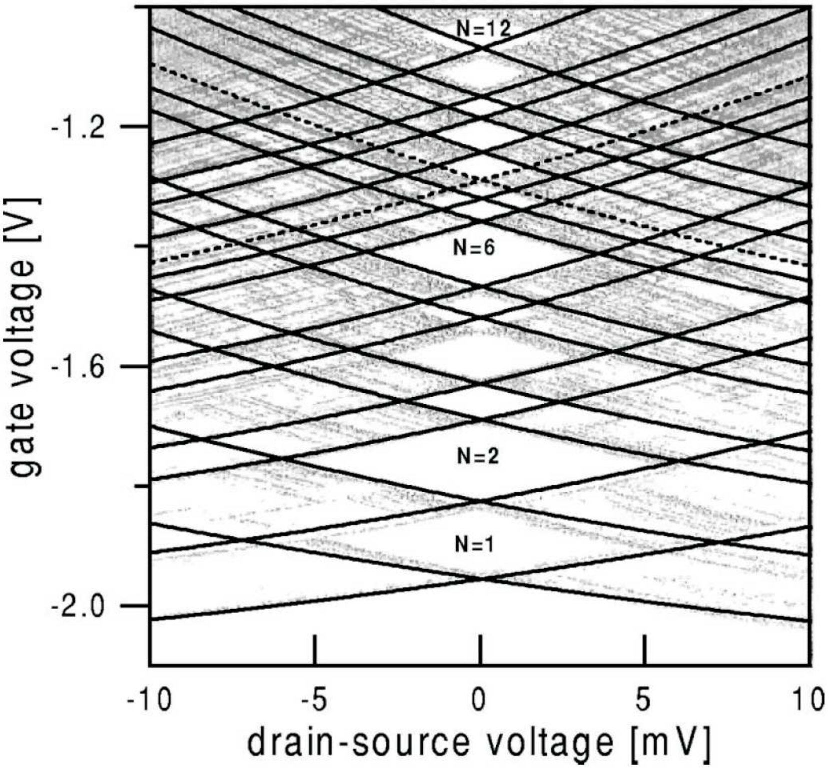

Figure 9: Stability diagram with Coulomb diamonds for three-terminal vertical QD. Solid (dashed) curves display the boundaries of single-electron tunnelling via the N-electron ground state (first excited state). In white regions, number N of electrons confined in the QD is constant.

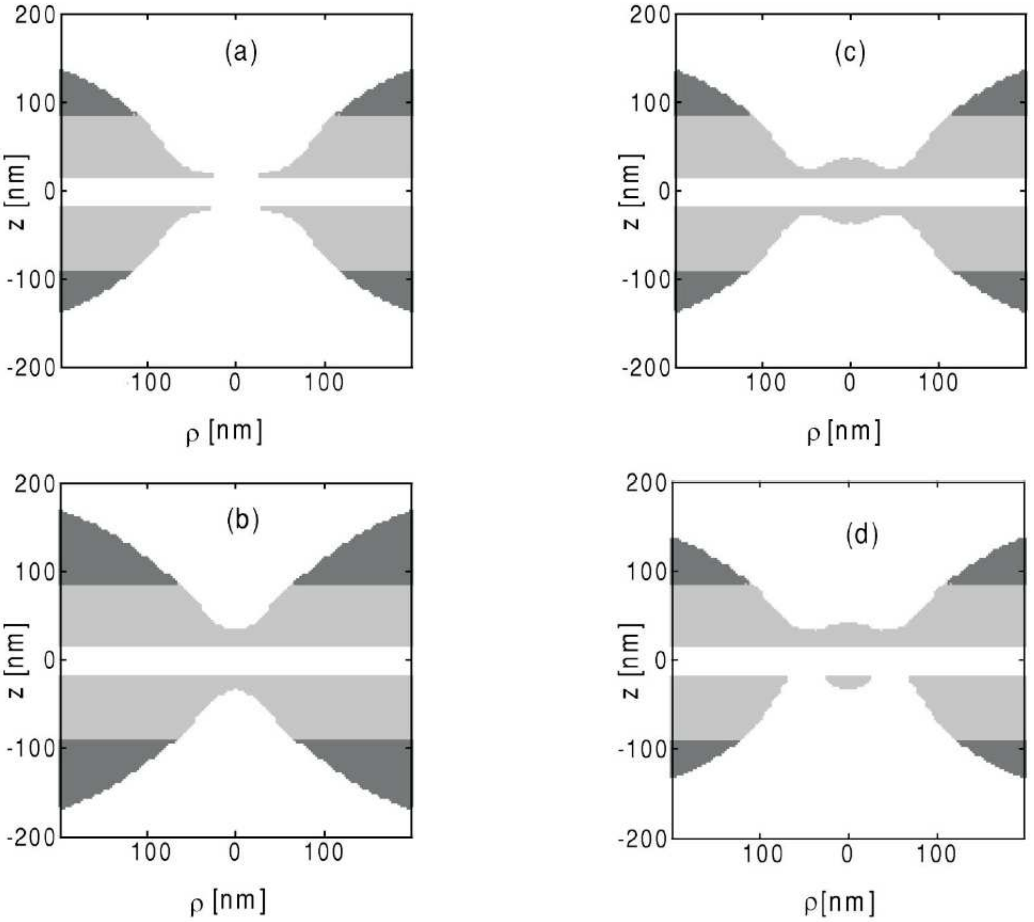

Figure 10: Charge density for ionized donors in n-GaAs layers in three-terminal nanodevice (Tarucha, NTT) as a function of cylindrical coordinates $\rho \equiv r$ and z. White, gray, and dark gray regions correspond to $\varrho_D = 0, 10^{17}$, and 1.4×10^{17} [e/cm^3], respectively. (a) $V_g = -1$ V, $V_{ds} = 0$, $N = 0$, (b) $V_g = -2$ V, $V_{ds} = 0$, $N = 0$, (c) $V_g = -1$ V, $V_{ds} = 0$, $N = 12$, (d) $V_g = -1$ V, $V_{ds} = 50$ mV, $N = 12$.

3 Modelling the confinement potential shape

3.1 Three-dimensional profiles of confinement potential

confinement potential energy (for QD with cylindrical symmetry)

$$U_{tot}(r,z) \equiv U_{conf}(r,z)$$

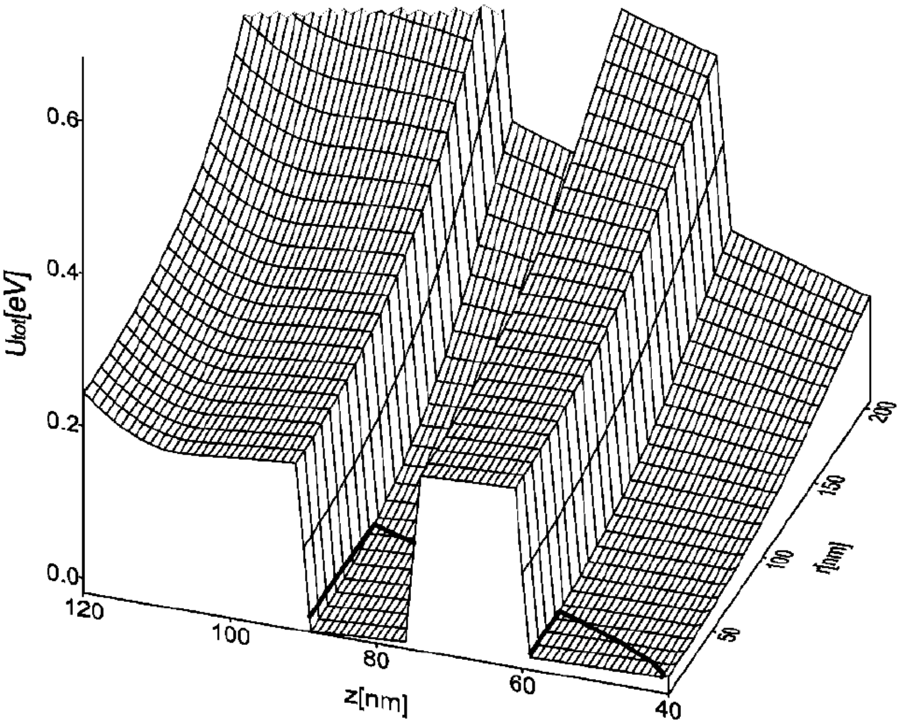

Figure 11: Total potential energy $U_{tot} \equiv U_{conf}$ of electron confinement in two-terminal nanosystem (Ashoori, MIT) as a function of cylindrical coordinates r i z. Thick solid line corresponds to the Fermi energy.

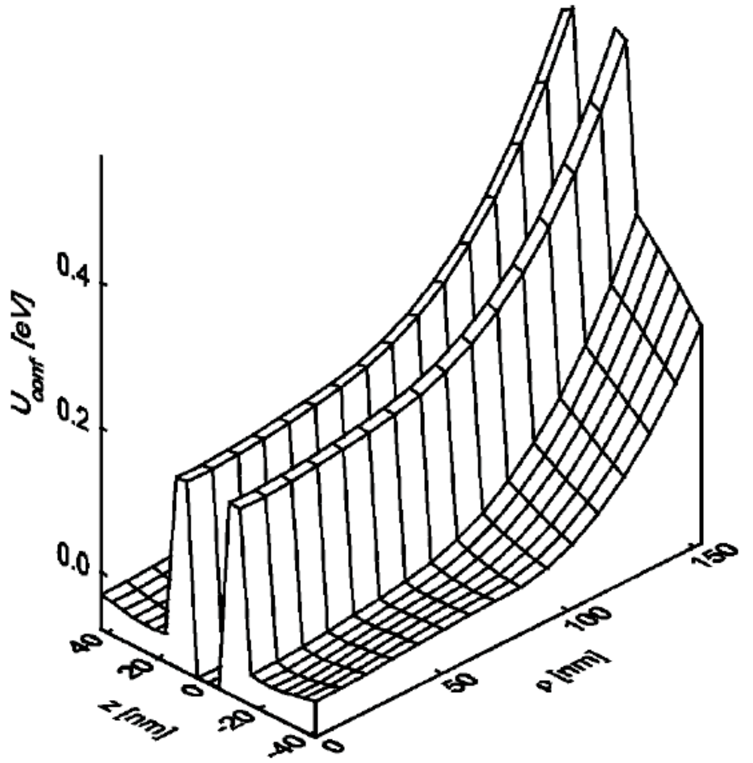

Figure 12: Total potential energy U_{conf} of electron confinement in three-treminal nanosystem (Tarucha, NTT) as a function of cylindrical coordinates $\rho \equiv r$ i z.

3.2 Lateral confinement potential

Confinement potential energy (for QD with cylindrical symmetry, $z = z_0 = const$)

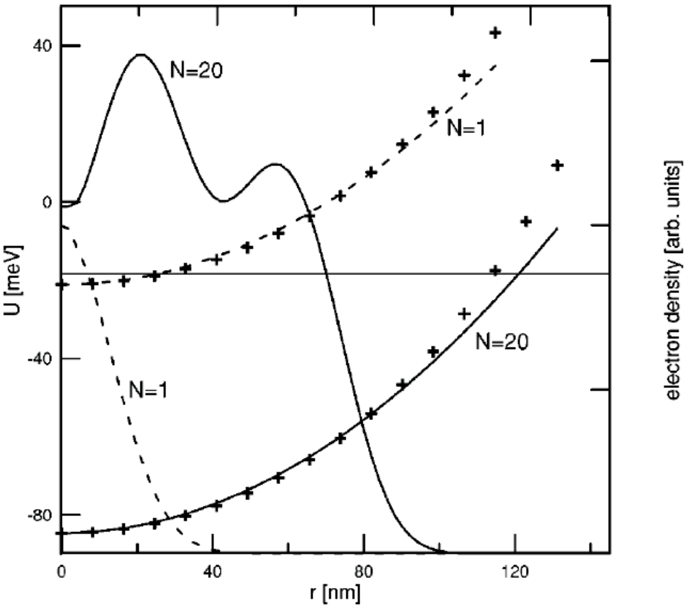

Figure 13: Electrostatic potential energy $U \equiv U_{elst}$ (left scale) of the lateral confinement of electron in two-terminal nanodevice (Ashoori, MIT) as a function of radial coordinate r for z fixed inside the quantum well. N = number of QD confined electrons. Crosses show the solutions to the Poisson equation, solid and dashed curves show the fitted parabolas. Electron density (right scale) is depicted by the dashed curve ($N = 1$) and solid curve ($N = 20$). Horizontal line correspond to the Fermi energy.

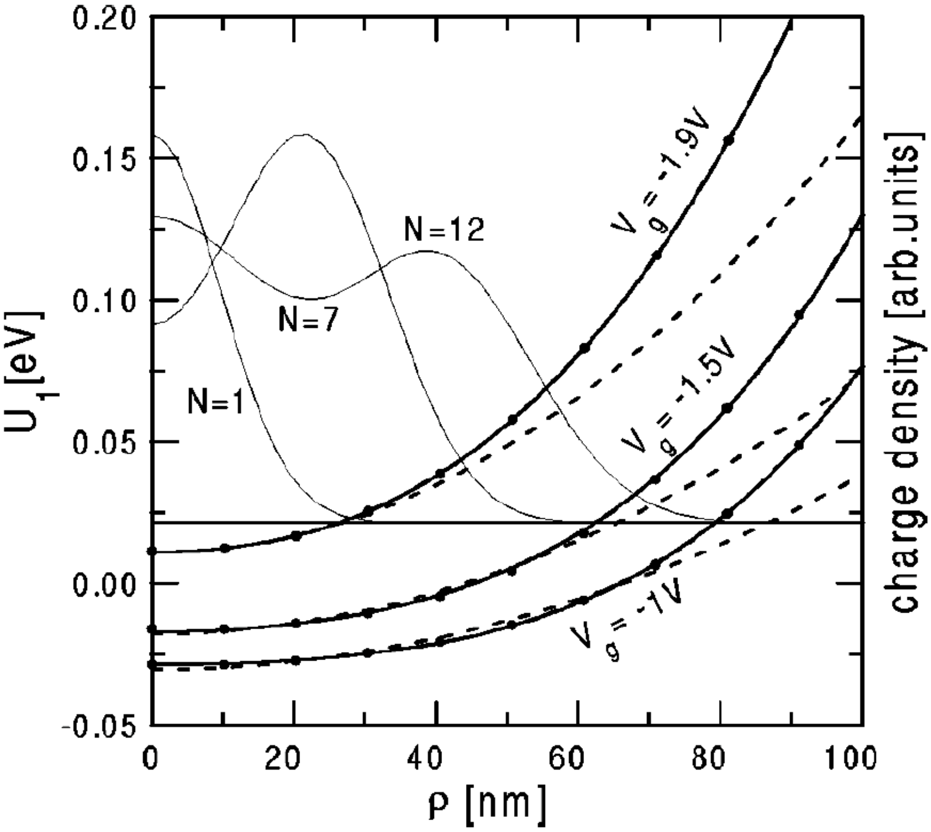

Figure 14: Electrostatic potential energy $U_1 \equiv U_{elst}$ (left scale) of the lateral confinement of electron in three-terminal nanodevice as a function of $\rho \equiv r$ and gate voltage V_g for $z = 0$, $V_{sd} = 0$, and $N = 1$, 7 i 12. Dots show the solutions to the Poisson equation, solid lines – the fitted 6th degree polynomials, dashed curves – the fitted parabolas, thin lines – electron densities (right scale). Horizontal line corresponds to the Fermi energy.

3.3 Approximations for the lateral confinement potential

(1) parabolic approximation

$$U(r) = \frac{m_e \omega_0^2}{2} r^2 \tag{20}$$

(2) polynomial of 6th degree

$$U(r) = \sum_{m=0}^{3} v_m r^{2m} \tag{21}$$

(3) power-exponential function (spherical symmetry)

$$U(r) = -U_0 \exp[-(r/L)^p] \tag{22}$$

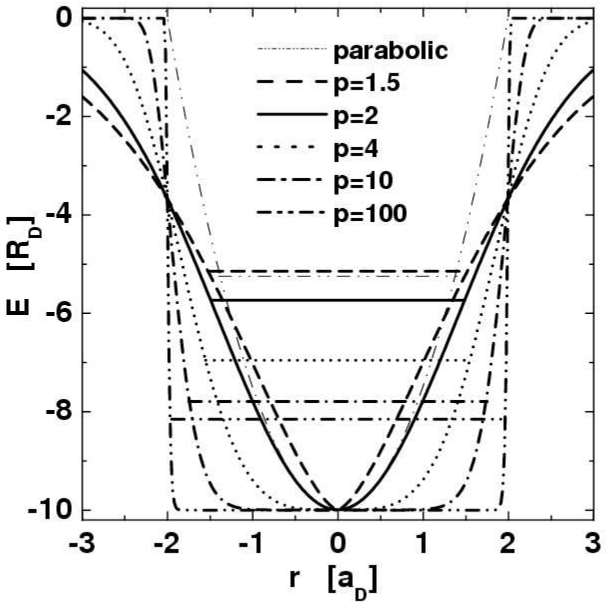

Figure 15: Power-exponential potential (22) for $L = 2a_D$, $U_0 = 10R_D$ and different values of softness parameter p. Shown is the parabolic approximation of (22). $a_D =$ donor Bohr radius, $R_D=$ donor rydberg. Horizontal lines correspond to the ground state energy of electron in potential (22).

Power-exponential potential for the cylindrically symmetric QD

$$U(r,z) = -U_0 \exp[-(r/R_\perp)^{p_\perp} - (|z|/R_\|)^{p_\|}] \tag{23}$$

U_0 = depth of potential well
$R_\perp$ = range of potential in perpendicular directions (x, y)
$R_\|$ = range of potential in parallel direction (z)
$p_\perp$ and $p_\|$ = softness parameters for perpendicular and parallel directions, respectively

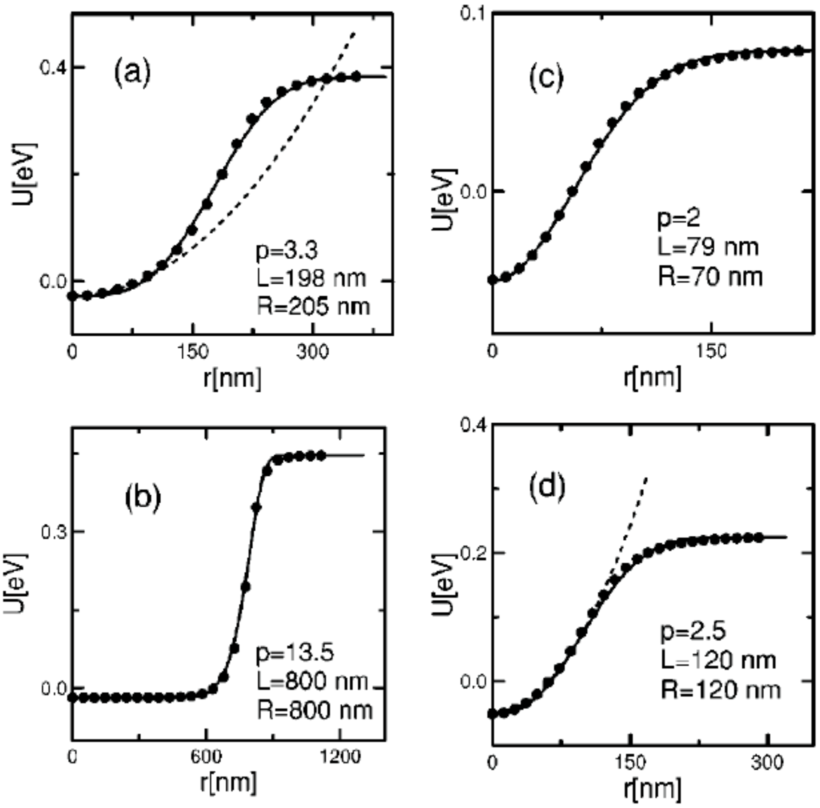

Figure 16: Electron potential energy of lateral confinement in two-terminal nanodevice with cap radius $R \equiv R_c$. Dots = numerical solutions to the Poisson equation, dashed curves = fitted parabolas, solid curves = fitted power-exponential functions. (a) QD studied by Ashoori el al., (b) large QD, (c) small QD, (d) best parabolic fit.

3.4 Natural and artificial atoms: similarities and differences

Natural atoms:

- electrons are bound by the Coulomb binding potential created by a nucleus (note that the Coulomb potential is divergent at origin, i.e., at the center of the nucleus)
- bound localized electron states with discrete energy levels
  - spatial extension of electron probability density $\sim 0.1 \div 1$ nm
  - energy level separations $\Delta E_{mn} \simeq 0.1 \div 1$ eV
  - continuum edge energy is well defined ($E = 0$ at infinity)
    $\Longrightarrow$ stable bound states with infinite lifetime
- electrons are moving in vacuum

Artificial atoms (electrostatic QD's):

- electrons are confined by the confinement potential
  (smooth potential well of finite depth created by electrodes and heterojunctions)
- localized quasi-bound states of electrons with discrete energy levels
  - spatial extension of electron probability density $\sim 10 \div 100$ nm
  - energy level separations $\Delta E_{mn} \simeq 1 \div 10$ meV
  - continuum edge energy is badly defined
    (usually there are regions in nanostructure, in which the energy of the electron is lower than that in the QD)
    $\Longrightarrow$ unstable quasi-bound states with finite lifetime
- electrons are moving in atomic environment
  $\Longrightarrow$ phonons

3.5 Confinement potential acting on nucleons in atomic nucleus

Woods-Saxon model potential

$$U(r) = \frac{-U_0}{e^{p(r-R)} + 1} \tag{24}$$

U_0 = depth of potential well
R = radius of nucleus
p determines the steepness of the potential-well boundary
(remind: Fermi distribution function)

Due to a similarity of spherically symmetric power-exponential potential (22) and Woods-Saxon potential (24) we could rather use the notion ”artificial nucleus” to the QD.