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Abstract

This report describes a simple analytic model that has been developed to simulate the electron wave function in a layered material. Some optimization has been performed using this model to find system parameters for which there is a single confined electron in the confinement layer and a single state quantum wire in the channel layer.

1 Problem Statement

- Goals: Find a set of system parameters resulting in
  - a quantum dot containing a single confined electron in the confinement layer
  - a quantum wire with a single state in the channel layer
- Layered structure
  - top interface on which gates are positioned, potential ϕ_{top} away from gates
  - layer of material A of thickness dz_1 (in units of nm)

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- δ-doped interface of charge density ρ_1 (in units of electrons nm^{-2})
- layer of material A of thickness dz_2 (in units of nm)
- layer of material B of thickness dz_3 (in units of nm)
- layer of material A of thickness dz_4 (in units of nm)
- layer of material B of thickness dz_5 (in units of nm)
- layer of material A of thickness dz_6 (in units of nm)
- δ-doped interface of charge density ρ_2 (in units of electrons nm^{-2})
- layer of material A of thickness dz_7 (in units of nm)
- bottom interface

- Gates
  - central gate of diameter *dgate* (in units of nm) and potential $\phi_{top} - \phi_g$ (in units of eV); the geometry of the central gate is
    - a circle, if $dimgate = 3$
    - an infinite strip, if $dimgate = 2$
  - blocking gates, consisting of parallel infinite half planes
    - parallel to the central gate if $dimgate = 2$
    - distance between the central gate and the blocking gate on each side is *dgap*
    - potential on the blocking gates is $\phi_{top} + \phi_b$ (in units of eV)

- Material
  - A is InP
  - B is InGaAs

- Approximations
  - no intrinsic doping
  - no temperature effects ($T = 0$)

2 Equations

- Electrostatics
  - Poisson equation

$$\nabla \cdot \epsilon \nabla \phi = \rho_1 \delta_1 + \rho_2 \delta_2 - \rho_\psi \tag{2.1}$$

    in which ϵ is scaled dielectric constant, δ_i is δ-function on i-th δ-doped interface and ρ_ψ is the self-consistent charge density
  - Dirichlet boundary conditions at the top
  - Neumann boundary conditions at the bottom
  - periodic boundary conditions on the sides
- Wave function
  - single particle Schrodinger equation

$$-\nabla \cdot (\frac{\hbar^2}{2m} \nabla \psi) = -(\phi + U)\psi + \lambda \psi \tag{2.2}$$

  - m is effective mass, U is conduction band offset, λ is energy level (eigenvalue), ψ is wave function (eigenfunction)
  - eigenvalue and eigenfunction in confinement layer are λ^{cf}, ψ^{cf}
  - eigenvalue and eigenfunction in channel are λ^{ch}, ψ^{ch}
  - eigenvalue space $d\lambda = \lambda_2 - \lambda_1$ is the difference between the first two eigenvalues
  - normalized so that $\int \psi dx = 1$
  - Fermi energy E_F set to $E_F = 0$
  - self-consistent charge density is $\rho_\psi = \sum |\psi|^2$, summed over all $\lambda < E_F$
- Material parameters and physical constants

Parameter	InP	InGaAs	Units
k	12.61	13.9	1
$\epsilon = k\epsilon_0/e^2$	.697	.769	1/(eV nm)
m	.079	.041	m_0
$\hbar^2/2m$	.484	.94	eV/nm^2
U	0	.224	eV

Constant	value	units
$\hbar^2/2m_0$	.0382	eV/nm^2
ϵ_0/e^2	.0553	1/(eV nm)

Note that since the potential ϕ is potential energy measured in eV, rather than electrostatic potential, the coefficient ϵ in the Poisson equations has units of 1/(eV nm). The dielectric constant for a vacuum is $\epsilon_0 = 8.854 \times 10^{-12} C^2 N^{-1} m^{-2}$.

- Goals
  - Confinement layer: single confined electron under gate, no wire (i.e. 2D) electron states away from gate

$$\lambda_1^{cf}(\phi_g) < 0 < \lambda_2^{cf}(\phi_g) \tag{2.3}$$
$$0 < \lambda_1^{cf}(\phi_g = 0) \tag{2.4}$$

  - Channel layer: single confined electron under gate, single wire (i.e. 2D) electron states away from gate

$$\lambda_1^{ch}(\phi_g) < 0 < \lambda_2^{ch}(\phi_g) \tag{2.5}$$
$$\lambda_1^{ch}(\phi_g = 0) < 0 < \lambda_2^{ch}(\phi_g = 0) \tag{2.6}$$

  - Since $\lambda_i^{ch}(\phi_g) < \lambda_i^{ch}(\phi_g = 0)$, it is enough to check that

$$\lambda_1^{cf}(\phi_g) < 0 < \min(\lambda_2^{cf}(\phi_g), \lambda_1^{cf}(\phi_g = 0)) \tag{2.7}$$
$$\lambda_1^{ch}(\phi_g = 0) < 0 < \lambda_2^{ch}(\phi_g) \tag{2.8}$$

3 Approximations for Electrostatics

- no BCs on sides
- bottom boundary at ∞
- no self-consistent term
- variation in dielectric constant is neglected; value for InP used throughout (easy to correct)

- potential $\phi = \phi^{1D}$ due to charges in modulationally doped layers

$$\phi^{1D} = \begin{cases} \phi_{top} - \epsilon_A^{-1}(\rho_1 + \rho_2)(z - z_{top}) & z_{top} < z < z_1 \\ \phi_{top} - \epsilon_A^{-1}\rho_2(z - z_{top}) & z_1 < z < z_2 \\ \phi_{top} - \epsilon_A^{-1}\rho_2(z_2 - z_{top}) & z_2 < z < z_{bottom} \end{cases} \tag{3.1}$$

  in which $z_1 = dz_1$ and $z_2 = dz_1 + dz_2 + dz_3 + dz_4 + dz_5 + dz_6$ are the positions of the δ-doped layers.

- potential $\phi = \phi_L^{2D}$ for gate that is on a line (in 2D) or a strip (in 3D) $|x| < L/2$ with potential $\phi = 1$ on gate and $\phi = 0$ away from gate

  - full solution

$$\phi_L^{2D}(x, z) = \pi^{-1}(\arctan(\frac{x + L/2}{z}) - \arctan(\frac{x - L/2}{z})) \tag{3.2}$$

  - value and second derivative on central axis $x = 0$

$$\phi_L^{2D}(x = 0, z) = 2\pi^{-1}\arctan(L/2z) \tag{3.3}$$

$$\phi_{Lxx}^{2D}(x = 0, z) = -\pi^{-1}z^{-2}\frac{2L/z}{(1 + L^2/4z^2)^2} \tag{3.4}$$

- potential $\phi = \phi_d^{3D}$ for gate that is circle $r < d/2$, for $r = |(x, y)|$, with potential $\phi = 1$ on gate and $\phi = 0$ away from gate

  - full solution

$$\begin{aligned} \phi_d^{3D}(\boldsymbol{x}\ ) &= \phi(r, z) \\ &= \frac{|z|}{2\pi}\int_0^{2\pi}\int_0^{d/2} |\boldsymbol{x}\ - \boldsymbol{x}\ '|^{-3} r' dr' d\theta' \\ &= \frac{|z|}{2\pi}\int_0^{2\pi}\int_0^{d/2} (z^2 + (r - r'\cos\theta')^2 + r'^2\sin^2\theta')^{-3/2} r' dr' d\theta' \end{aligned} \tag{3.5}$$

  - value and second derivative on central axis $r = 0$

$$\phi_d^{3D}(r = 0, z) = 1 - (1 + d/2z)^2)^{-1/2} \tag{3.6}$$

$$\phi_{drr}^{3D}(r = 0, z) = -\frac{3}{2}|z|(d/2)^2(z^2 + (d/2)^2)^{-5/2} \tag{3.7}$$

- Summary
  - The total potential is

$$\phi = \begin{cases} \phi^{1D} + \phi_b(1 - \phi_d^{2D}) - \phi_g \phi_L^{2D} & \text{if dimgate} = 2 \\ \phi^{1D} + \phi_b(1 - \phi_d^{2D}) - \phi_g \phi_L^{3D} & \text{if dimgate} = 3 \end{cases} \tag{3.8}$$

  - The second derivatives of the total potential on the central axis are

$$\phi_{xx} = \begin{cases} -\phi_b \phi_{dxx}^{2D} - \phi_g \phi_{Lxx}^{2D} & \text{if dimgate} = 2 \\ -\phi_b \phi_{dxx}^{2D} - \phi_g \phi_{Lrr}^{3D} & \text{if dimgate} = 3 \end{cases} \tag{3.9}$$

$$\phi_{yy} = \begin{cases} 0 & \text{if dimgate} = 2 \\ -\phi_g \phi_{Lrr}^{3D} & \text{if dimgate} = 3 \end{cases} \tag{3.10}$$

4 Approximations for Schrodinger

- Separable solutions: If m is constant and $\phi(x,y,z) = \phi^x(x) + \phi^y(y) + \phi^z(z)$, then

$$\lambda = \lambda^x + \lambda^y + \lambda^z \tag{4.1}$$

$$\psi(x,y,z) = \psi^x(x)\psi^y(y)\psi^z(z) \tag{4.2}$$

  in which

$$-(\hbar^2/2m)\psi_x^x x = -\phi^x\psi^x + \lambda^x\psi^x \tag{4.3}$$

$$-(\hbar^2/2m)\psi_y^y y = -\phi^y\psi^y + \lambda^y\psi^y \tag{4.4}$$

$$-(\hbar^2/2m)\psi_z^z z = -\phi^z\psi^z + \lambda^z\psi^z \tag{4.5}$$

- use separation to find eigenvalues in channel of width w and center z
- for 2D (half plane) gates, neglect variation of ϕ across wells and approximate x dependence by second derivative as

$$\phi = \phi^x(x) = .5\phi_{xx}(x = 0, z)x^2 \tag{4.6}$$

- for 3D (circular) gates, neglect variation of ϕ across wells and approximate (x, y) dependence by second derivative as,

$$\begin{aligned} \phi &\approx .5\phi_{rr}(r=0,z)r^2 && (4.7)\\ &= \phi^x(x) + \phi^y(y) && (4.8)\\ \phi^x(x) &= .5\phi_{rr}(r=0,z)x^2 && (4.9)\\ \phi^y(y) &= .5\phi_{rr}(r=0,z)y^2 && (4.10) \end{aligned}$$

- eigenvalue and eigenvalue spacing for 1D parabolic potential $\phi(x) = \phi_2 x^2$ are

$$\begin{aligned} \lambda_1^p &= (\phi_{xx}\hbar^2/4m)^{1/2} && (4.11)\\ d\lambda^p &= 2\lambda_1^p && (4.12) \end{aligned}$$

- denote λ^{Px} and λ^{Px} for the eigenvalues due to the parabolic potential in the x- and y-directions, respectively.

- denote $d\lambda^{Px}$ and $d\lambda^{Px}$ for the eigenvalue eigenvalue spacing due to the parabolic potential in the x- and y-directions, respectively.

- for offset in wells, neglect variation across the well, and use

$$\phi(z) = \begin{cases} 0 & |z - z_0| > L/2 \\ -U & |z - z_0| < L/2 \end{cases} \qquad (4.13)$$

- eigenvalues for this square well are solutions of

$$\begin{aligned} \lambda^{sw} &= c_1 k_1^2 - U && (4.14)\\ k_1^2(1 + (c_1/c_0)\tan^2(k_1 w/2)) &= U/c_1 && (4.15) \end{aligned}$$

  in which c_0 and c_1 are the values of $\hbar^2/2m$ outside the well and in the well, respectively; i.e. c_0 is the value for InP and c_1 is the value for InGaAs.

- Summary
  - We want a single eigenvalue in the quantum dot formed in the confined layer, and a single transverse state for the quantum wire in the channel.

- The lowest eigenvalue comes from the z-eigenvalue of the well, plus the x- and y-eigenvalues from the parabolic potential formed by the gates.
- The spacing between the first and second eigenvalues comes from the spacing of the x- or y-eigenvalues, since the spacing for the z-eigenvalues is much larger.
- For the channel layer, only the spacing from the x-eigenvalue is used, since the objective is to have only a single state that is transverse to the quantum wire. There should be multiple states in the y-direction along the wire.
- For the confining layer, the spacing in the minimum of the spacing of x- and y-eigenvalues.
- The eigenfunctions, lowest eigenvalue and eigenvalue spacing are

$$\psi = \psi^{sw}(z)\psi^{Px}(x)\psi^{Py}(y) \tag{4.16}$$

$$\lambda = \lambda^{sw} + \lambda^{Px} + \lambda^{Py} \tag{4.17}$$

$$d\lambda = \begin{cases} \min(d\lambda^{Px}, d\lambda^{Py}) & \text{if dimgate} = 2 \\ d\lambda^{Px} & \text{if dimgate} = 3 \end{cases} \tag{4.18}$$

5 Matlab Programs

- gateChanWireSim
  - for given set of parameters computes potential ϕ and eigenvalues for channel and confining layer
- gateChanWireSimRSearch
  - searches for parameter sets that satisfy goals
- gateChanWireSimSample
  - for fixed geometry and charge, draws curves in ϕ_g, ϕ_b plane on which the inequalities of (2.7), (2.8) are equalities; i.e. the curves where energies cross the Fermi energy

6 Results

- random search of large volume in parameter space yielded a small number of parameter sets satisfying bounds (2.7), (2.8).