Analytic Model for Electron Confinement in a Layered Material

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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 $\phi_{\text{top}}$ away from gates
  
  – layer of material A of thickness $d_{z_1}$ (in units of nm)

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- δ-doped interface of charge density $\rho_1$ (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 $\rho_2$ (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
    \[ \nabla \cdot \epsilon \nabla \phi = \rho_1 \delta_1 + \rho_2 \delta_2 - \rho_{\phi} \] (2.1)
    in which \( \epsilon \) is scaled dielectric constant, \( \delta_i \) is \( \delta \)-function on \( i \)-th \( \delta \)-doped interface and \( \rho_{\phi} \) 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
    \[ -\nabla \cdot \left( \frac{\hbar^2}{2m} \nabla \psi \right) = -(\phi + U) \psi + \lambda \psi \] (2.2)
    - \( m \) is effective mass, \( U \) is conduction band offset, \( \lambda \) is energy level (eigenvalue), \( \psi \) is wave function (eigenfunction)
    - eigenvalue and eigenfunction in confinement layer are \( \lambda^{cf}, \psi^{cf} \)
    - eigenvalue and eigenfunction in channel are \( \lambda^{ch}, \psi^{ch} \)
    - 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 \( \rho_{\phi} = \sum |\psi|^2 \), summed over all \( \lambda < E_F \)

- Material parameters and physical constants

<table>
<thead>
<tr>
<th>Parameter</th>
<th>InP</th>
<th>InGaAs</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k )</td>
<td>12.61</td>
<td>13.9</td>
<td>1</td>
</tr>
<tr>
<td>( \epsilon = k \epsilon_0 / e^2 )</td>
<td>.697</td>
<td>.769</td>
<td>1/(eV nm)</td>
</tr>
<tr>
<td>( m )</td>
<td>.079</td>
<td>.041</td>
<td>( m_0 )</td>
</tr>
<tr>
<td>( \hbar^2 / 2m )</td>
<td>.484</td>
<td>.94</td>
<td>eV/( nm^2 )</td>
</tr>
<tr>
<td>( U )</td>
<td>0</td>
<td>.224</td>
<td>eV</td>
</tr>
</tbody>
</table>
Constant value units
\( \hbar^2/2m_0 \) 0.0382 eV/nm²
\( \epsilon_0/e^2 \) 0.0553 1/(eV nm)

Note that since the potential \( \phi \) is potential energy measured in eV, rather than electrostatic potential, the coefficient \( \epsilon \) in the Poisson equations has units of \( 1/(eV \text{ nm}) \). 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
    \[
    \lambda_{1f}^{cf}(\phi_g) < 0 < \lambda_{2f}^{cf}(\phi_g)
    \]
    \[
    0 < \lambda_{1f}^{cf}(\phi_g = 0)
    \] (2.3)
  
  - Channel layer: single confined electron under gate, single wire (i.e. 2D) electron states away from gate
    \[
    \lambda_{1h}^{ch}(\phi_g) < 0 < \lambda_{2h}^{ch}(\phi_g)
    \]
    \[
    \lambda_{1h}^{ch}(\phi_g = 0) < 0 < \lambda_{2h}^{ch}(\phi_g = 0)
    \] (2.5)
  
  - Since \( \lambda_{1h}^{ch}(\phi_g) < \lambda_{1h}^{ch}(\phi_g = 0) \), it is enough to check that
    \[
    \lambda_{1f}^{cf}(\phi_g) < 0 < \min(\lambda_{2f}^{cf}(\phi_g), \lambda_{1f}^{cf}(\phi_g = 0))
    \]
    \[
    \lambda_{1h}^{ch}(\phi_g = 0) < 0 < \lambda_{2h}^{ch}(\phi_g)
    \] (2.7)

3 Approximations for Electrostatics

- no BCs on sides
- bottom boundary at \( \infty \)
- 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

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

(3.1)

in which $z_1 = d z_1$ and $z_2 = d z_1 + d z_2 + d z_3 + d z_4 + d z_5 + d z_6$ are the positions of the $\delta$-doped layers.

- potential $\phi = \phi^{2D}_L$ 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
    $$\phi^{2D}_L (x, z) = \pi^{-1} (\arctan \left( \frac{x + L/2}{z} \right) - \arctan \left( \frac{x - L/2}{z} \right))$$
    (3.2)
  - value and second derivative on central axis $x = 0$
    $$\phi^{2D}_L (x = 0, z) = 2 \pi^{-1} \arctan (L/2z)$$
    (3.3)
    $$\phi^{2D}_{Lxx} (x = 0, z) = -\pi^{-1} z^{-2} \frac{2L/z}{(1 + L^2/4z^2)^2}$$
    (3.4)

- potential $\phi = \phi^{3D}_d$ 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
    $$\phi^{3D}_d (x) = \phi (r, z)$$
    $$= \frac{|z|}{2\pi} \int_0^{2\pi} \int_0^{d/2} |x' - x|^{-3} r' dr' d\theta'$$
    (3.5)
    $$= \frac{|z|}{2\pi} \int_0^{2\pi} \int_0^{d/2} \left( z^2 + (r - r' \cos \theta')^2 + r'^2 \sin^2 \theta' \right)^{-3/2} r' dr' d\theta'$$
  - value and second derivative on central axis $r = 0$
    $$\phi^{3D}_d (r = 0, z) = 1 - (1 + d/2z)^{-1/2}$$
    (3.6)
    $$\phi^{3D}_{drr} (r = 0, z) = -\frac{3}{2} |z| (d/2)^2 (z^2 + (d/2)^2)^{-5/2}$$
    (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

\[
\begin{align*}
\phi_{xx} &= \begin{cases} 
-\phi_{b}\phi_{d}^{2D} - \phi_{g}\phi_{L}^{2D} & \text{if dimgate} = 2 \\
-\phi_{b}\phi_{d}^{2D} - \phi_{g}\phi_{L}^{3D} & \text{if dimgate} = 3
\end{cases} \tag{3.9} \\
\phi_{yy} &= \begin{cases} 
0 & \text{if dimgate} = 2 \\
-\phi_{g}\phi_{L}^{3D} & \text{if dimgate} = 3
\end{cases} \tag{3.10}
\end{align*}
\]

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

\[
\begin{align*}
\lambda &= \lambda^{x} + \lambda^{y} + \lambda^{z} \tag{4.1} \\
\psi(x, y, z) &= \psi^{x}(x)\psi^{y}(y)\psi^{z}(z) \tag{4.2}
\end{align*}
\]

in which

\[
\begin{align*}
-(\hbar^{2}/2m)\psi^{x}_{xx} &= -\phi^{x}\psi^{x} + \lambda^{x}\psi^{x} \tag{4.3} \\
-(\hbar^{2}/2m)\psi^{y}_{yy} &= -\phi^{y}\psi^{y} + \lambda^{y}\psi^{y} \tag{4.4} \\
-(\hbar^{2}/2m)\psi^{z}_{zz} &= -\phi^{z}\psi^{z} + \lambda^{z}\psi^{z} \tag{4.5}
\end{align*}
\]

• use separation to find eigenvalues in channel of width \( w \) and center \( z \)

• for 2D (half plane) gates, neglect variation of \( \phi \) 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 $\phi$ across wells and approximate $(x,y)$ dependence by second derivative as,
\[
\phi \approx .5\phi_{rr}(r = 0, z)r^2 \\
= \phi^x(x) + \phi^y(y) \\
\phi^x(x) = .5\phi_{rr}(r = 0, z)x^2 \\
\phi^y(y) = .5\phi_{rr}(r = 0, z)y^2
\]
(4.7)  (4.8)  (4.9)  (4.10)

• eigenvalue and eigenvalue spacing for 1D parabolic potential $\phi(x) = \phi_2 x^2$ are
\[
\lambda_1^p = (\phi_{xx}\hbar^2/4m)^{1/2} \\
d\lambda^p = 2\lambda_1^p
\]
(4.11)  (4.12)

• denote $\lambda^{P_x}$ and $\lambda^{P_y}$ for the eigenvalues due to the parabolic potential in the x- and y-directions, respectively.

• denote $d\lambda^{P_x}$ and $d\lambda^{P_y}$ 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
\[
\phi(z) = \begin{cases} 
0 & |z - z_0| > L/2 \\
-U & |z - z_0| < L/2
\end{cases}
\]
(4.13)

• eigenvalues for this square well are solutions of
\[
\lambda_{sw} = c_1 k_1^2 - U \\
k_1^2(1 + (c_1/c_0)\tan^2(k_1 w/2)) = U/c_1
\]
(4.14)  (4.15)
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

$$
\psi = \psi^{sw}(z)\psi^{P_x}(x)\psi^{P_y}(y) \\
\lambda = \lambda^{sw} + \lambda^{P_x} + \lambda^{P_y} \\
d\lambda = \begin{cases} 
\min(d\lambda^{P_x}, d\lambda^{P_y}) & \text{if dimgate} = 2 \\
\frac{d\lambda^{P_x}}{} & \text{if dimgate} = 3 
\end{cases}
$$

$$
\tag{4.16} \\
\tag{4.17} \\
\tag{4.18}
$$

5 Matlab Programs

- gateChanWireSim
  - for given set of parameters computes potential $\phi$ and eigenvalues for channel and confining layer

- gateChanWireSimRSearch
  - searches for parameter sets that satisfy goals

- gateChanWireSimSample
  - for fixed geometry and charge, draws curves in $\phi_g, \phi_b$ 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).