Accurate Simulation of 2-Well Quantum Devices

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The Target Device

- Creates and confines a quantum dot electrostatically
- Senses dot using a quantum wire.

Device Structure

- Side Gate
- Center Gate
- Side Gate

- AlInAs
- InP
- δ-doping
- InGaAs
- InP
- InP
- γ-doping

Device Structure
Device Operation

Side voltage applied
quantum wire
Multiple states in the lower well.
Confinement in 2 directions.

Side and dot voltage applied
quantum wire + quantum dot
Single state in the upper well.
Confinement in 3 directions
Multiple states in the lower well.
Confinement in 2 directions
Operational Behavior Discrepancy

*The predicted side gate bias required to pinch off the lower well quantum wire is too high.*

\[
\text{Pinchoff } V_{\text{side}} = \begin{cases} 
\sim 10 \text{ V (simulation)} \\
\sim 1 \text{ V (experiment)} 
\end{cases}
\]
Use a fixed charge boundary condition rather than a fixed potential boundary condition on the ungated surface.

Specify

\[ \kappa_1 \frac{\partial \phi_1}{\partial n} - \kappa_2 \frac{\partial \phi_2}{\partial n} = \sigma_{\text{surface charge}} \]

\( \phi_1 = \text{potential inside device} \)

\( \phi_2 = \text{potential outside device} \)
Boundary Condition Comparison (2D)

Fixed Charge BC

Fixed Potential BC

Using fixed charge boundary conditions at the ungated surface “narrows” the potential between the side gates.
Using a fixed charge boundary condition at the ungated surface lowers the pinchoff voltage.
Boundary Condition Comparison (3D)

Fixed potential boundary conditions

Fixed charge boundary conditions

- Top potential (transverse slice)
- Lower well potential (transverse slice)
Boundary Condition Comparison (3D)

Lower well pinchoff comparison*

Lower well potential minimum (V)

Using a fixed charge boundary condition at the ungated surface lowers the pinchoff voltage.

* Calculations done using “local” density of states calculation
Consequences

- The simulation results with fixed charge boundary conditions more accurately reflect experimental results (See E. Croke and M. Gyure poster)

- The use of fixed charge boundary conditions leads to a problem for the potential that is no longer separable.
Handling the Numerical Consequences

**Problem:** How to solve a non-separable elliptic PDE using a solver* that explicitly depends upon separability?

**Solution:** Transform the non-separable boundary conditions into separable boundary conditions.

Handling the Numerical Consequences

Transform mixed boundary conditions to equivalent Neumann boundary conditions.

\( \kappa \frac{\partial \phi}{\partial n} \) specified

\( \phi \) specified

\( \frac{\partial \phi}{\partial n} \) specified
Transforming boundary conditions ...

Equations to be solved:

$$L \begin{pmatrix} \frac{\partial \phi_{\text{gates}}}{\partial n} \end{pmatrix} = \phi_{\text{gates}}$$

Neumann data at gates

Neumann - Dirichlet operator: evaluated using FFT’s

The critical aspect for efficiency

The transformation equations are solved iteratively using pre-conditioned conjugate gradients (4-5 iterations).
Conclusions

• The simulation results with fixed charge boundary conditions on the ungated surface more accurately reflect experimental results.

• The non-separable nature of the new boundary conditions does not impact the use of FFT’s to evaluate the Neumann-Dirichlet operator.

• The Neumann-Dirichlet operator can be efficiently inverted to obtain equivalent separable boundary conditions.

• The non-separable potential calculation takes only 2x the time of the separable problem!