Simulation of Silicon Nanodevices at Cryogenic Temperatures for Quantum Computing

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Contents

- Silicon Quantum Computing
- Computational Workflow
- Modeling Qubit Devices with COMSOL
Quantum Computation

Qubit → Two level system obeying quantum mechanics

Examples
- Spins in Silicon
- Flux in Superconductors
- Electronic states of ions
- Photon Polarization

Encodes information of 2 complex numbers - $C_1$ & $C_2$

Quantum Computer → An array of several interacting qubits

Encodes information of $2^N$ numbers

Quantum mechanical laws allow qubits to represent & process exponentially more information than bits!

Information on 300 qubits → Number of particles in the entire universe!
Silicon Quantum Computation – Modeling Parameters

Donor electron

Electrostatic solver

Electronic Structure Solver

Magnetic Field From MW Antenna

Gate Performance Simulator

Electron & Nuclear Donor Spins in Silicon

$|\uparrow\rangle + |\downarrow\rangle$

Magnetic Field


Muhonen et. al, NAT. NANOTECH. 9, 968 (2014)
Contents

Silicon Quantum Computing

Computational Workflow

Modeling Qubit Devices with COMSOL
Computational Workflow for Designing Silicon Donor Qubits

Input: Device Geometry, Gate Voltages, Magnetic Fields, Material Model

Output: Spin States, Coherence/Relaxation times, Quantum Gate Fidelity

T. S. Humble et. al, Nanotechnology, 27, 42 (2016)
Test Device Model & Equations

Device to readout the spin of donor electron

Poisson & Current Continuity:
\[ n, p, V \]

Dependent Variables:
\[ E_c, E_v, E_{fn}, E_{fp}, n_i \]

Ohmic Boundary Condition

\[
\nabla \cdot (\varepsilon \nabla V) = -q (p - n + N_{D+} - N_{A-}) \\
\frac{\partial n}{\partial t} = \frac{1}{q} (\nabla \cdot J_n) - U_n \\
\frac{\partial p}{\partial t} = -\frac{1}{q} (\nabla \cdot J_p) - U_p \\
\]

\[
n = N_C F_{1/2} \left( \frac{E_{F_n} - E_c}{k_B T} \right) \quad N_{D+} = \frac{N_D}{1 + g_D \exp \left( \frac{E_{F_n} - E_D}{k_B T} \right)} \\
p = N_V F_{1/2} \left( \frac{E_v - E_{F_p}}{k_B T} \right) \quad N_{A-} = \frac{N_A}{1 + g_A \exp \left( \frac{E_v - E_A}{k_B T} \right)} \\
E_c = -\chi - qV \quad E_v = -\chi - E_g - qV \\
n_i = \sqrt{N_v N_c \exp \left( -E_g / 2k_B T \right)} \\
n_{eq} - p_{eq} + N_{a-} - N_{d+} = 0 \\
n_{eq} = \frac{1}{2} (N_{d+} - N_{a-}) + \frac{1}{2} \sqrt{(N_{d+} - N_{a-})^2 + 4n_i p_i n_i} \\
p_{eq} = \frac{1}{2} (N_{d+} - N_{a-}) - \frac{1}{2} \sqrt{(N_{d+} - N_{a-})^2 + 4n_i p_i n_i} \\
V_{eq} = V_0 - \chi - \frac{E_g}{2q} \log \left( \frac{n_{eq}}{n_i} \right) + \frac{1}{2} \log \left( \frac{n_v}{N_v} \right) \\
\]

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Challenges at Low Temperature

Exponential dependence of densities with temperature

\[ n = N_C F_{1/2} \left( \frac{E_F - E_C}{k_B T} \right) \]

\[ p = N_V F_{1/2} \left( \frac{E_V - E_F}{k_B T} \right) \]

\[ N_D^+ = \frac{N_D}{1 + g_D \exp \left( \frac{E_F - E_D}{k_B T} \right)} \]

\[ N_A^- = \frac{N_A}{1 + g_A \exp \left( \frac{E_A - E_F}{k_B T} \right)} \]

\[ E_C = -\chi - qV \quad E_V = -\chi - E_g - qV \]

\[ n_i = \sqrt{N_C N_V \exp \left( -E_g / 2 k_B T \right)} \]

Huge spatial gradients in electron density

Convergence Plots

Finite Element Linear Solver

Error

Iterations for Different Temperatures

15K  50K  100K  300K
Guidelines for Low Temperature Convergence

1. Approximate hole densities \( p = \frac{n_i^2}{n} \)
   Reduce number of degrees of freedom to be solved for

2. Use Finite Element Log Discretization
   Solve for the Log of electron density which has smaller spatial gradients than electron density

3. Modify equations appropriately
   Minimize divide-by-zero-errors
   e.g. \( n_i = \sqrt{N_c N_v} \exp (-E_g / 2k_BT) \)
   \( V_{eq} = V_0 - \frac{E_g}{2q} + \frac{k_BT}{q} \log \left( \frac{n_{eq}}{N_c N_v} \right) + \frac{1}{2} \log \left( \frac{N_c}{N_v} \right) \)
   \( V_{eq} = V_0 - \chi + \frac{k_BT}{q} \left( \log \left( \frac{n_{eq}}{\gamma n_i} \right) \right) \)

4. Choose appropriate meshing
   High densities near gates & swept mesh across domains

5. Use proper initial guesses for electron density
   Set appropriate scaling factors in the Jacobian matrix
Device electrostatics ($n, E_c$ and $F$) from COMSOL can (a) simulate locations for spin-readout and (b) electric fields experienced by $^{31}\text{P}$ electron qubits, and is consistent with our understanding and other semiconductor packages.
Comparison with Higher Temperatures

300 K – 15 K

20 K – 15 K

Gradients over 5K

Conduction Band Energy

Electric Field

Over 5 K, typical accuracies of conduction band energy is ~ 1 meV and electric field ~ 0.1 MV/m
Summary

• Electrostatic calculations are an integral part of a computational workflow needed to design silicon donor qubits for quantum computing.

• Simulating electrostatics at low temperature poses convergence issues as several parameters such as carrier densities scale exponentially at low temperature.

• We have provided a guideline of simulating electrostatics at low temperatures and have achieved convergence down to 15 K for a test nanostructure.

• The electrostatics at 15 K with COMSOL yield expected results for the position of charge reservoirs, donors, conduction band and electric fields.

• We then compared the results at 15 K to higher temperatures to quantify the accuracy of device electrostatics with temperature.

F.A. Mohiyaddin et. al, COMSOL Conference 2017 (2017)
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