Project Q5.2

Exchange Energy and Tunnel Coupling of Hole Qubits in a 5-Gate FinFET – Simulation Study

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Abstract - We performed 3D TCAD simulations of exchange energy and tunnel coupling of hole spin qubits in the 5-gate Si FinFET fabricated at University of Basel. Self-consistent Schrödinger-Poisson calculations with S-BAND (Synopsys) at T = 3K and 1K yield wave functions, energy spectra, and split energies due to dot coupling. The exchange energy is obtained by post-processing the hole density distributions using LDA. It is found to be in the order of 10 meV and to increase with plunger gate voltage as a result of increasing confinement. The dependence of exchange energy on gate length and gate distance is demonstrated for a corresponding 4-gate FinFET. The computed split energies are a direct measure of the tunnel coupling. They strongly depend on the wave function symmetry and amount to ~13 µeV for the ground state and ~5 µeV for the first excited state. The tunnel barrier transmission is estimated from the split energies using a rectangular potential model.

Device Structure & Simulation Methods

Device Structure:

- We studied the 5-gate Si FinFET fabricated at Uni Basel [1] (Fig. 1(a)) using the 3D domain shown in Figs. 1 (b,c) for self-consistent k·p Schrödinger-Poisson simulations.

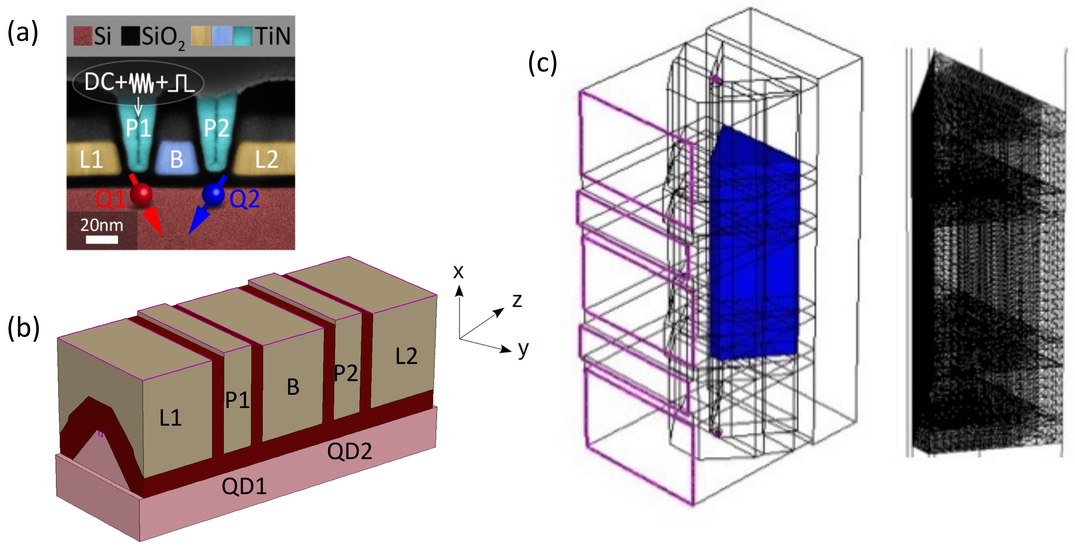


Figure 1: (a) 2D cross section of fabricated 5-gate Si FinFET device along fin direction, with double QDs formed under P-gates. (b) 3D device structure for electrostatics simulations. (c) 3D domain and mesh for self-consistent k·p Schrödinger-Poisson simulations.

Simulation Methods:

- Self-consistent 6-band k·p Schrödinger-Poisson using S-BAND of Synopsys [2].
- Quantum domain with 190'974 elements, Fermi statistics, no Coulomb blockade.
- Perfect convergence down to T = 3K, partial convergence at T = 1K.
- Total CPU time for one bias point at 1K: 53 h on Intel(R) Xeon(R) E5-2680 v4 @ 2.40GHz.
- Exchange energy and tunnel coupling obtained by post-processing using S-VISUAL [2].

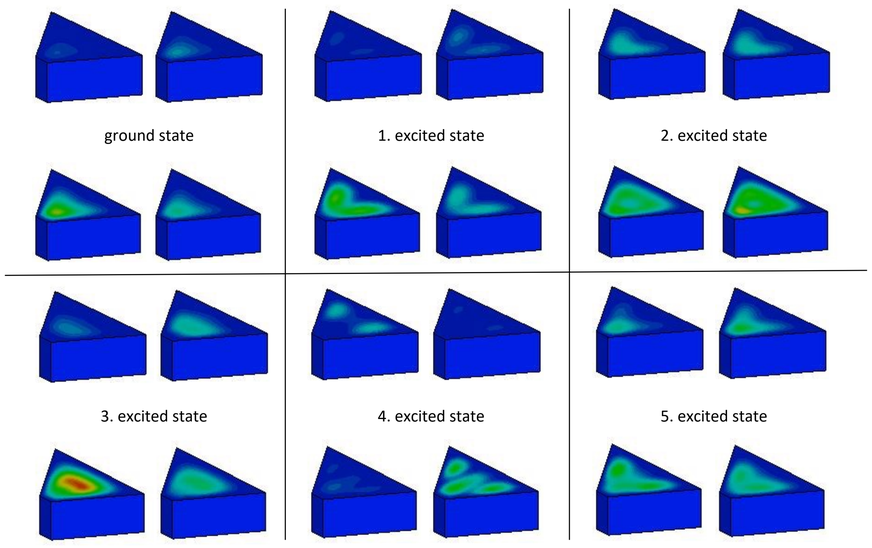


Figure 2: Probability density (square of wave function) of the six lowest states under the plunger gates $P_{1/2}$ at T = 1K. Each state is two-fold due to the dot coupling. Gate voltage as indicated in Fig. 3 (a).

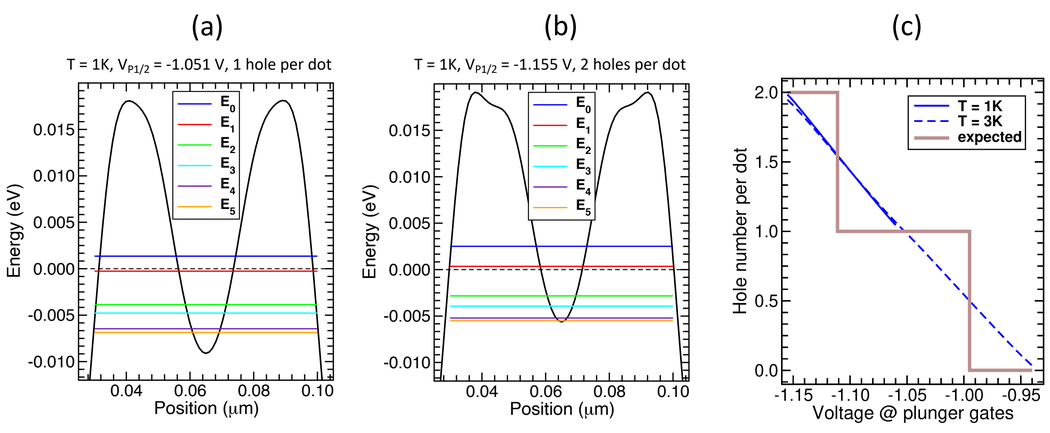


Figure 3: (a) Valence band edge along fin direction (black) and energy level spectrum wrt Fermi energy (dashed) for exactly one hole in the QD. Each level is split (split energy of the lowest two levels shown in Fig. 6 (b).) (b) The case of exactly two holes in each QD. From the change of the level spacing the corresponding Hartree energy can be estimated to be ~1 meV. (c) Simulated charging curves (blue) versus expected charging curve (brown) when Coulomb blockade in the leads would be included. The thermal smearing at T = 1K would be comparable to the line width of the brown line.

Simulation Results: Exchange Energy

- Exact exchange energy of homogeneous hole gas in Si [3]:

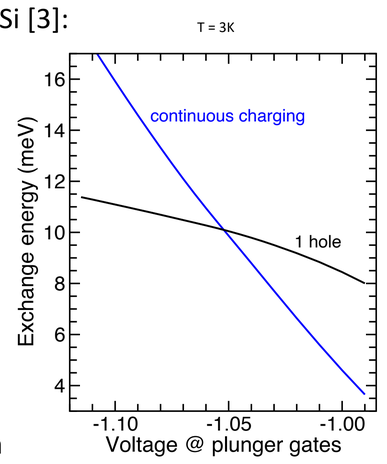
$$e_{\mathrm{X}} = -\frac{E_{\mathrm{X}}[p]}{N} = -\frac{3}{2}\left(\frac{3}{2\pi}\right)^{1/3} a_{\mathrm{B}}\, p^{1/3}\,[\mathrm{Ry}] = -\frac{3}{2}\left(\frac{3}{2\pi}\right)^{1/3} \frac{7.2}{\epsilon_{\mathrm{s}}} 10^{-8}\, p^{1/3}\,[\mathrm{eV}]$$

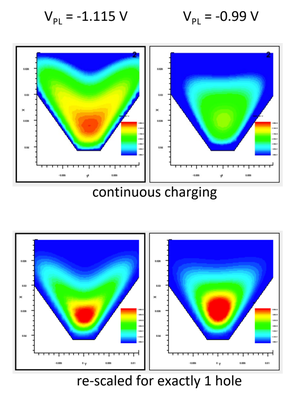
$$\textbf{LDA}: \quad E_{\mathrm{X}}[p] = \int d^3\mathbf{r}\, p(\mathbf{r})\, e_{\mathrm{X}}\,[p(\mathbf{r})]$$

$$\textbf{average p}: \quad E_{\mathrm{X}}[\langle p\rangle] = -0.721\,\langle p\rangle^{1/3}\, 10^{-8}\,[\mathrm{eV}]$$

- Charge distribution re-scaled by continuous hole number for exactly one hole per QD.
- A more negative PL-gate bias confines density to Fin tip → Exchange energy increases with increasing confinement.
- Example Gaussian:

$$p(x) = \sqrt{a/\pi}\exp(-ax^2) \rightarrow \int dx\, p^{4/3}(x) \sim a^{1/6}$$





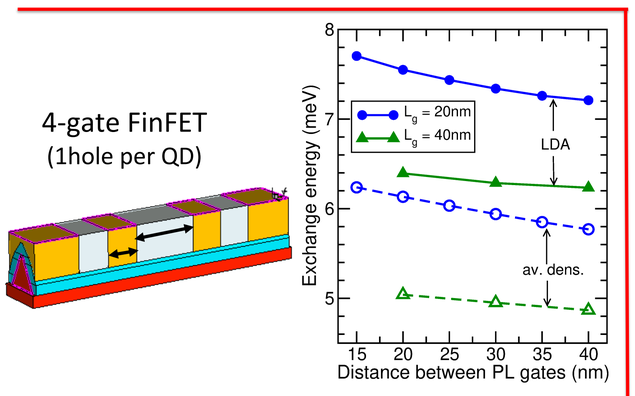


Figure 5: Exchange energy as function of gate distance for different gate lengths (20nm - blue, 40nm - green).

Figure 4 (a): Exchange energy as function of plunger gate voltage for continuous charging (blue) and for re-scaled hole number equal to one at all voltages (black). (b) Comparison of charge distribution at highest and lowest plunger gate voltage.

Simulation Results: Tunnel Coupling

- Extracted split energies from S-BAND: $\Delta E_0 \sim 13$ µeV, $\Delta E_1 \sim 5$ µeV.
- ΔE_0 increases with more negative plunger gate bias as tunnel barrier reduces.
- $\Delta E_1 < \Delta E_0$ because of p-like symmetry of first excited states.
- ΔE_1 not monotonous due to voltage-dependent wave function overlap.

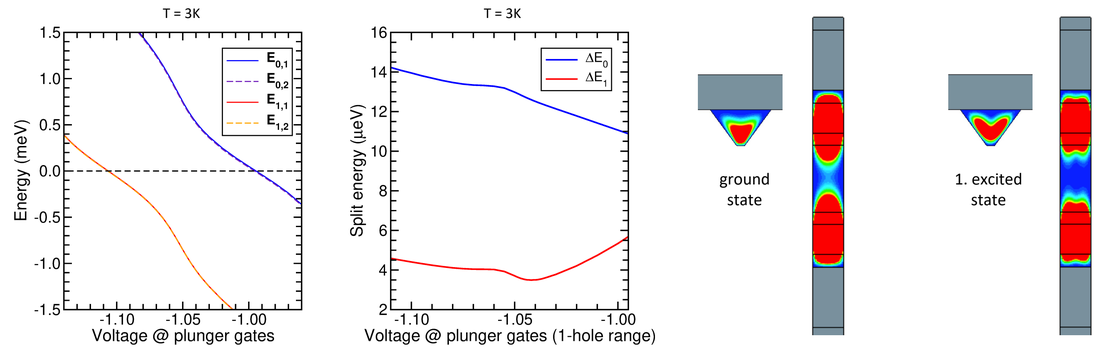
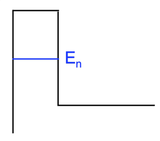
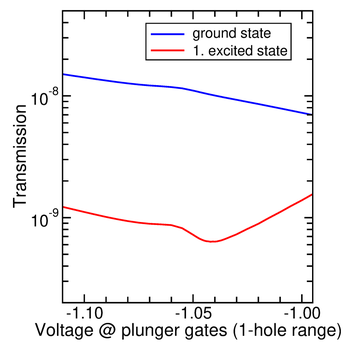


Figure 6 (a): Variation of lowest two energy levels with plunger gate voltage. Split energy is the difference between solid and dashed curves. (b) Extracted split energies. (c) Wave function overlap. (d) Transmission.

$$\Delta E_{\mathrm{n}} = 8(E_{\mathrm{V,max}} - E_{\mathrm{n}})\exp(-b\kappa_{\mathrm{n}}) \quad \text{with } E_{\mathrm{n}} \text{ solution of}$$
$$= 8(E_{\mathrm{V,max}} - E_{\mathrm{n}})\sqrt{T_{\mathrm{n}}} \quad (T_{\mathrm{n}} \text{ transmission prob.})$$



$$T_{\mathrm{n}} = \left[\frac{\Delta E_{\mathrm{n}}}{8(E_{\mathrm{V,max}} - E_{\mathrm{n}})}\right]^2$$



Conclusion

- S-BAND and S-VISUAL (Synopsys) can be used to compute and post-process LDA exchange energy and tunnel coupling of hole qubits in 5-gate FinFETs (within certain limits).
- Exchange energy increases with increasing confinement (bias dependence).
- Conservation of integer charge was mimicked by re-scaling density globally.
- Tunnel coupling strongly depends on symmetry of wave functions.

Acknowledgement

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References

1. Camenzind et al., Nature Electronics 5 (2022)
2. Sentaurus Band Structure and Sentaurus Visual Manuals, ver. 2023.12, Synopsys Inc.
3. R. Zimmermann, Many Particle Theory of Highly Excited Semiconductors,Teubner Leipzig, 1988