SAND2021-9300C

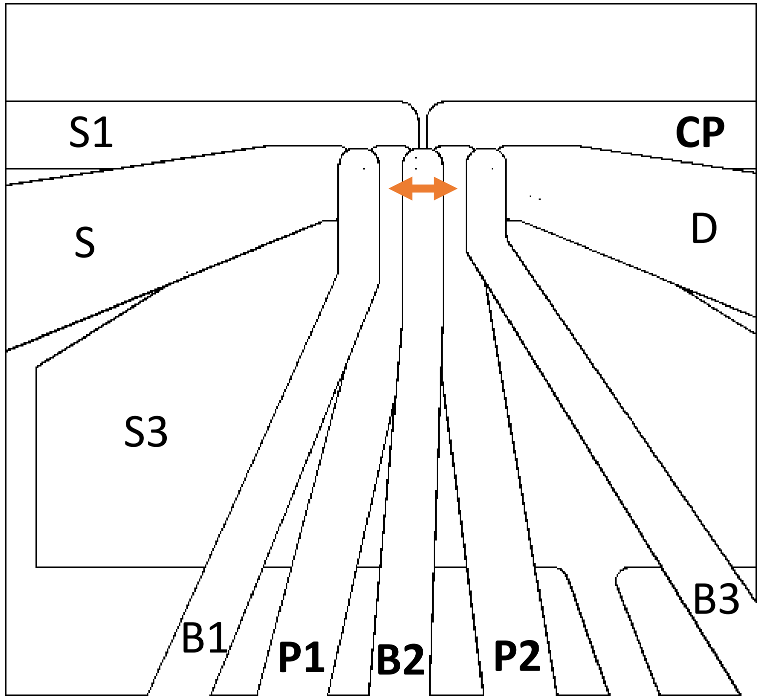
PI: **Steve Young**

Sandia/Princeton collaboration:
Multivalley effective mass theory modeling of Princeton SiGe devices

Presenter: **Toby Jacobson**

Results:

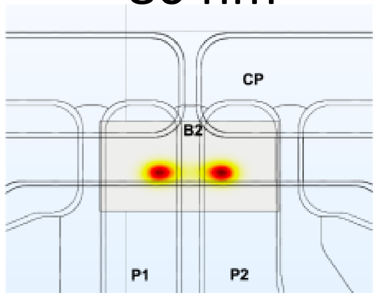
- CAD modeling of Princeton double dot devices
- Estimates of differential lever arm to resonator-coupled gate
- Multi-valley effective mass theory modeling of a double dot with realistic alloy disorder



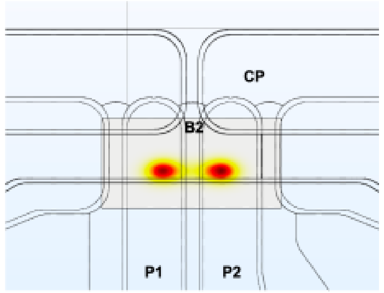
SiGe cap: 50 nm
Si well: 8 nm
SiGe substrate: 1.2 µm

Two gate pitches modeled:

80 nm



60 nm



Gate labeling convention from [Borjans, et al. APL 116, 234001 (2020)]

ARO/LPS Quantum Computing Program Review, August 2-5, 2021

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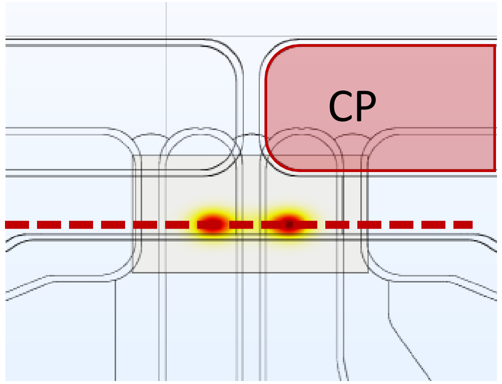
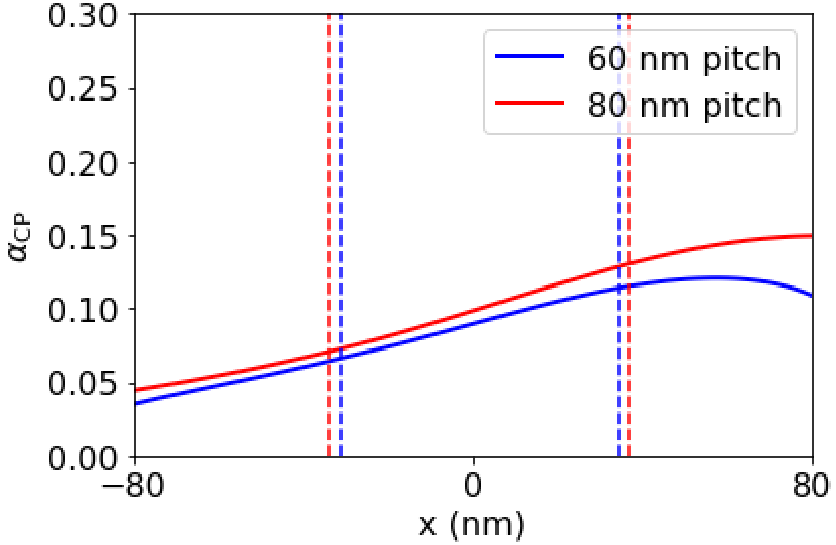
Cut through center line of formed double dot





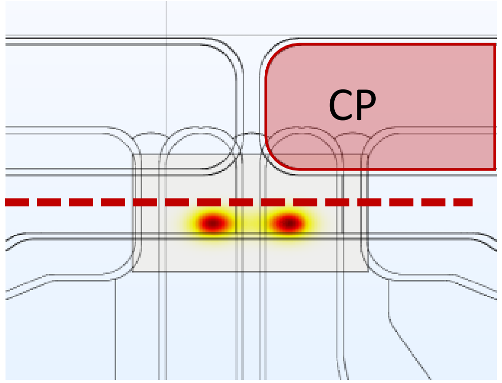
Differential lever arm:

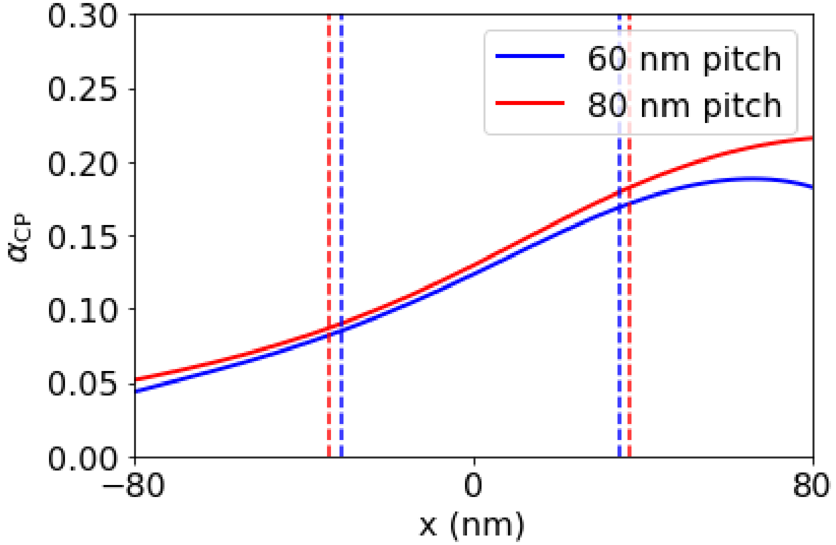
60 nm pitch: β_{CP}=0.05e

80 nm pitch: β_{CP}=0.06e

Using β estimation technique of [Borjans, et al. APL 116, 234001 (2020)]

Cut through center line of S/D gates





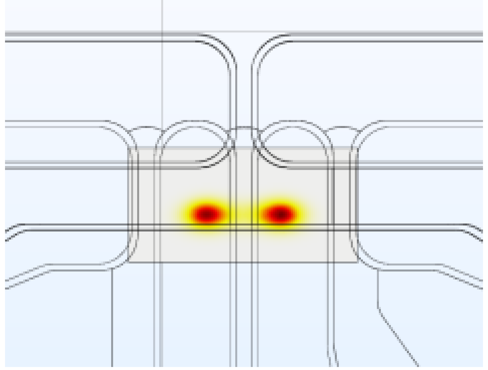
60 nm pitch: β_{CP}=0.08e

80 nm pitch: β_{CP}=0.09e

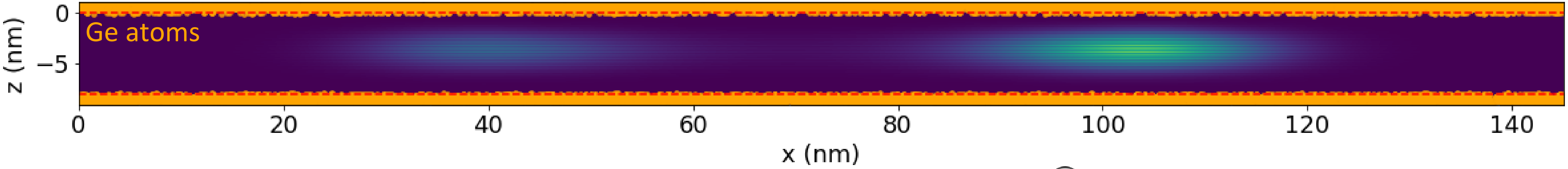
- Suggests that differential lever arm may be electrostatically tunable
- Similar values for both gate pitches (for similarly-tuned inter-dot tunnel coupling)

Disorder model:

- Interface softness: 0.9 Å sigmoidal Ge concentration $f(z) \propto 1 + \tanh(z/\sigma)$
- Alloy disorder: 500 [μeV][nm^3] δ-perturbation for each Ge atom
- Intra- and inter-valley coupling computed with Bloch functions derived from DFT

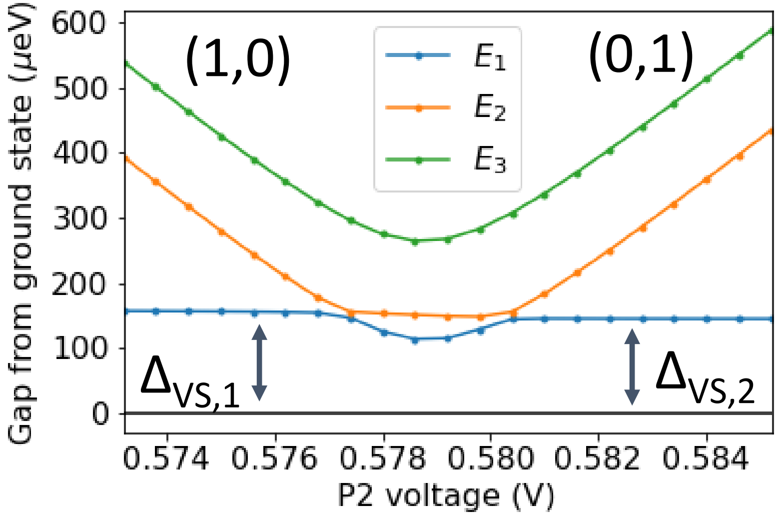


Princeton 60/25 design near charge-hybridized detuning



Software used to generate these results: *Laconic*

- A mesh-based PDE solver we have developed with collaborators at Sandia
- Nodal/modal discontinuous Galerkin finite element method
- Facilitates effective mass theory treatment at an atomistic level and high-accuracy representation of wavefunctions near abrupt interfaces



Here, $\Delta_{VS,1}$=157 μeV, $\Delta_{VS,2}$=145 μeV

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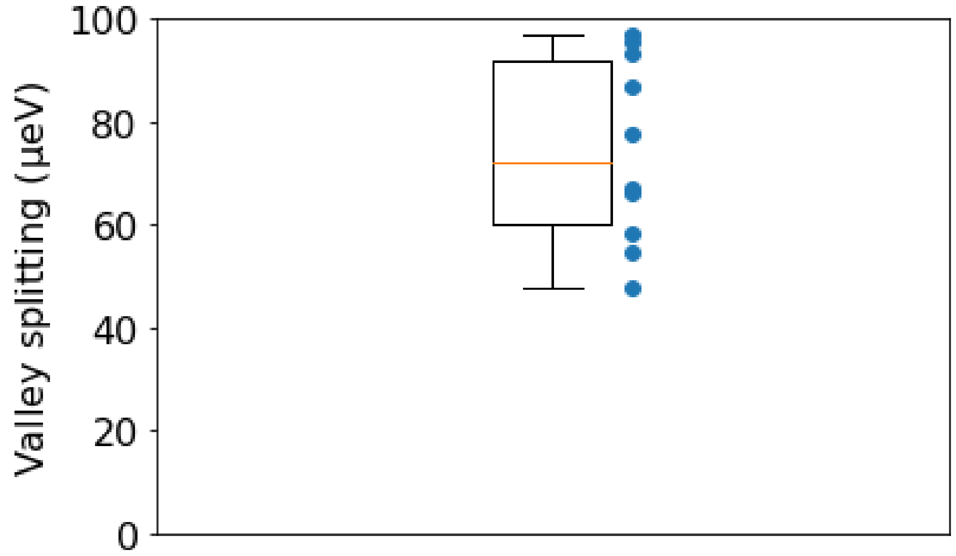
Simulated distribution of valley splittings for $\sigma_{interface}$=0.9 Å

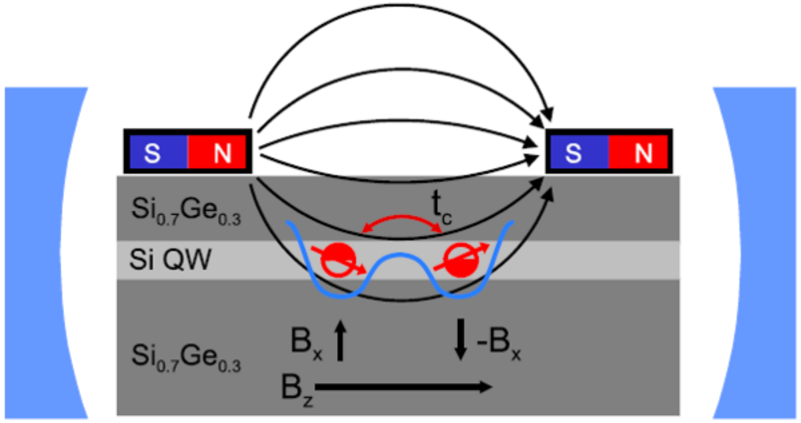


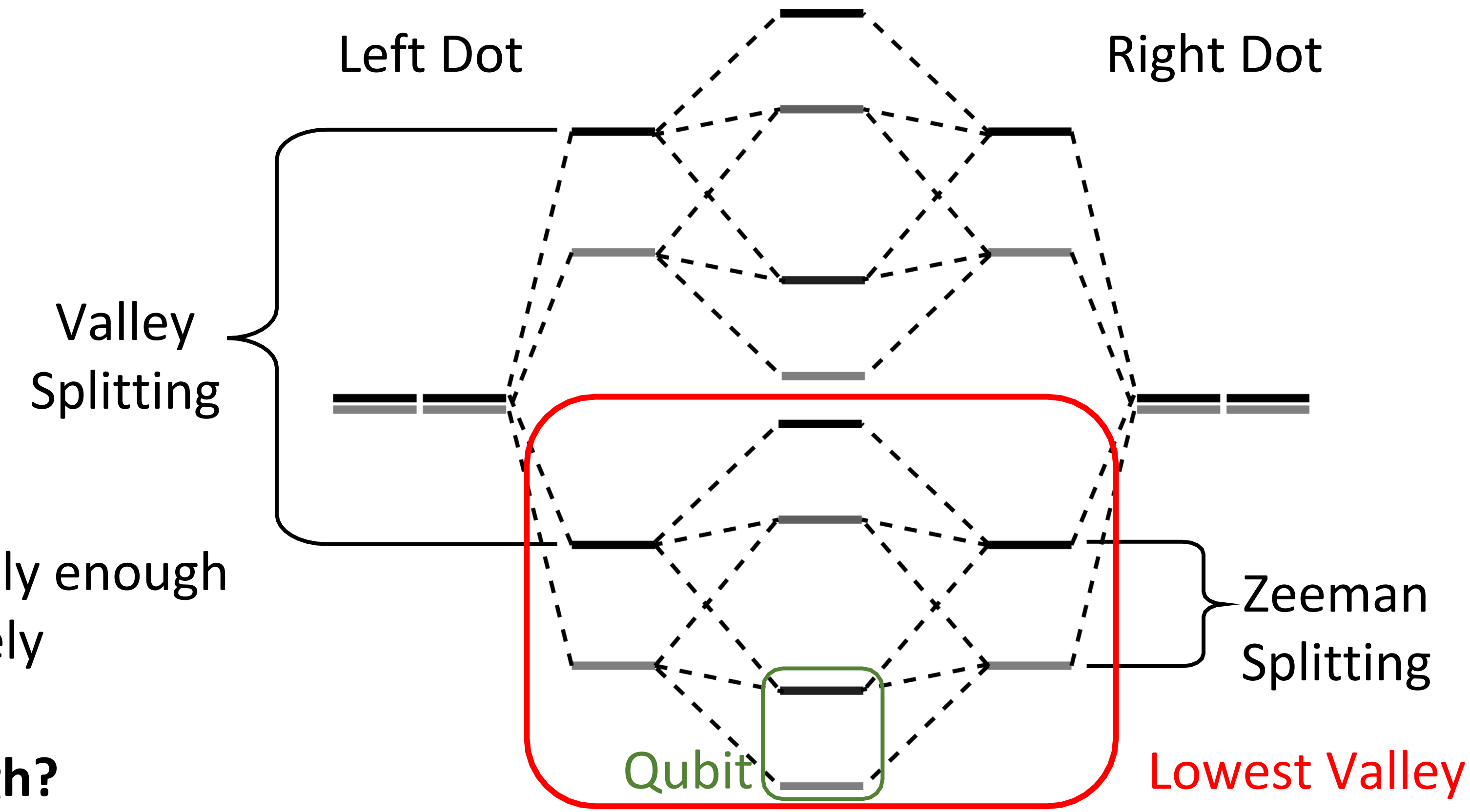
Next steps:

- Calibrate electrostatic model to better match in-practice tune-up voltages/thresholds
- Calibrate disorder model to agree with observed valley splitting statistics
  - Critical parameter: interface alloy diffusion width $\sigma_{interface}$ for upper and lower interfaces
- Integrate microscopic model into effective Hamiltonian modeling at level of input-output theory
  - Charge noise coupling to valley degrees of freedom through inter-valley dipole

Sandia/Princeton collaboration:
Expanding Dynamic Open-System Model of Semiconductor Spin Qubits

Presenter: **Steve Young**



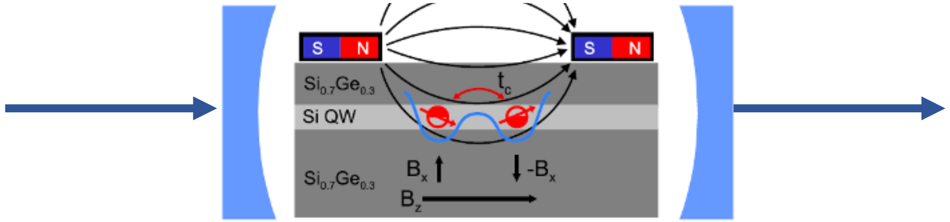


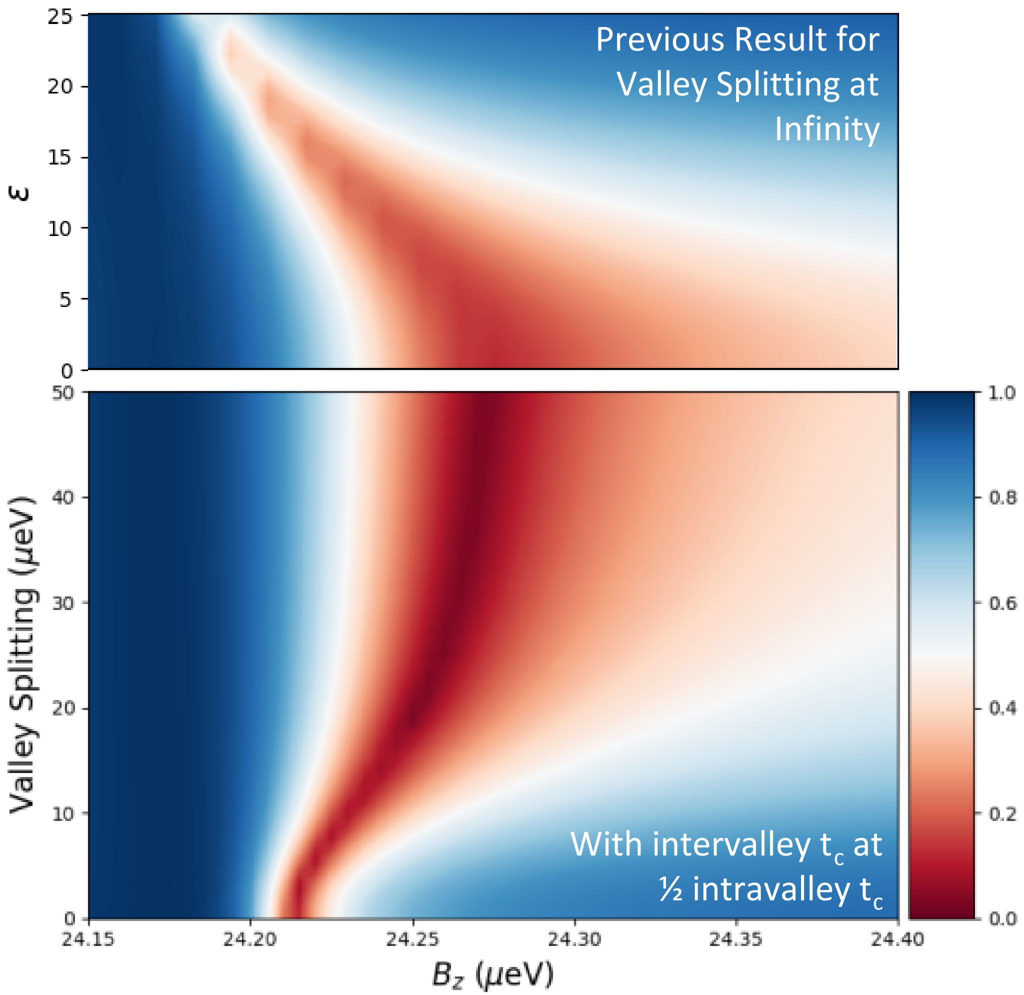
Ideally, the valley degeneracy is split widely enough that we can ignore the upper valley entirely

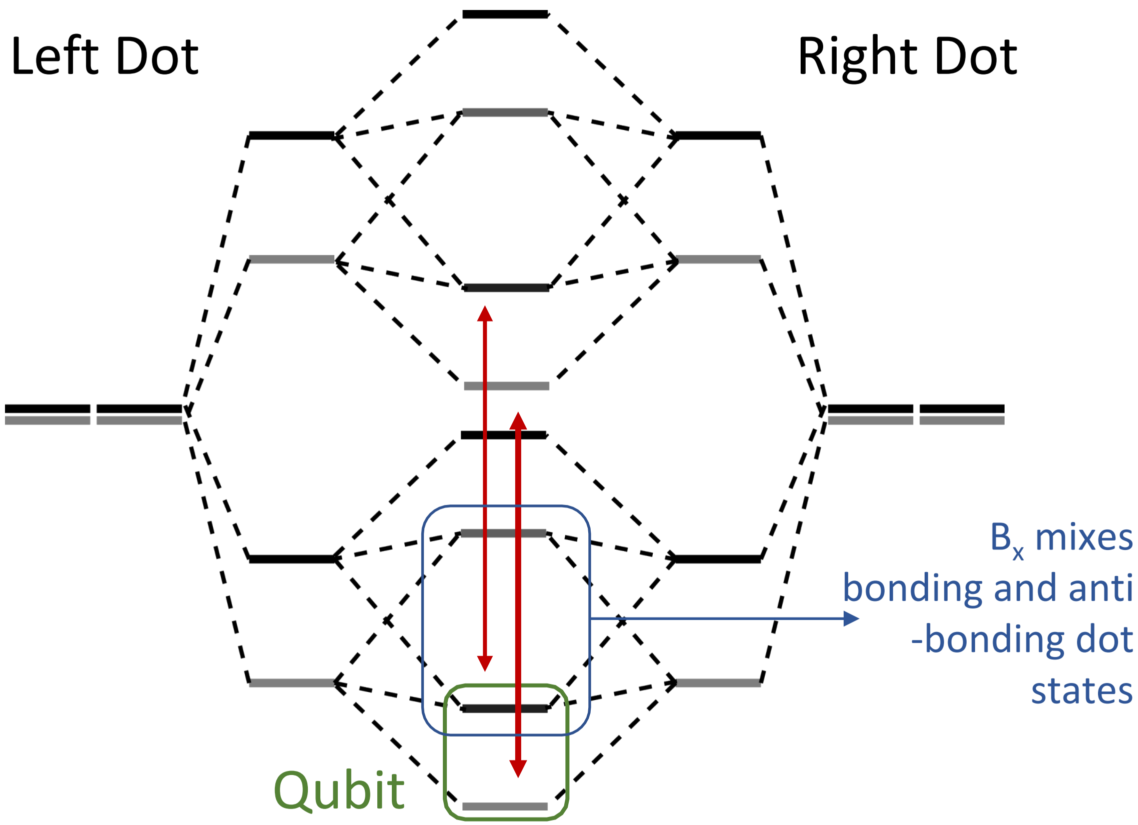
However, what constitutes widely enough?

Small Valley Splitting Impact on Single Dots

Transmission Through Cavity







Intervalley tunnel coupling effect is weaker on B_x-mixed states, shifting them less. **Qubit energy splitting increases**

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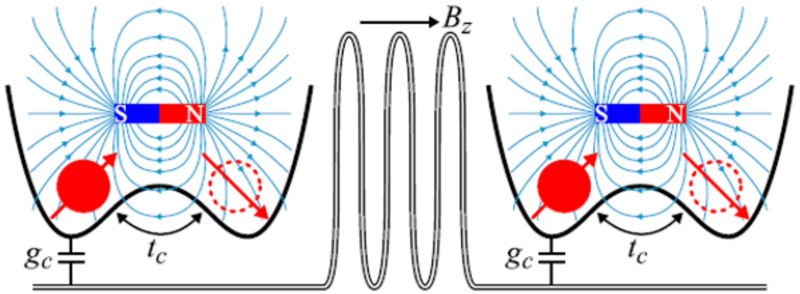
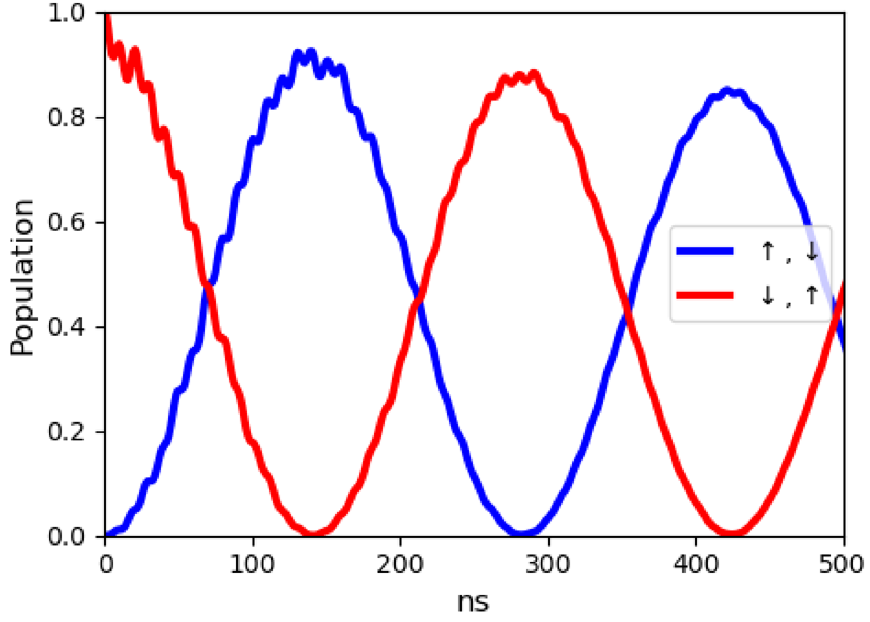
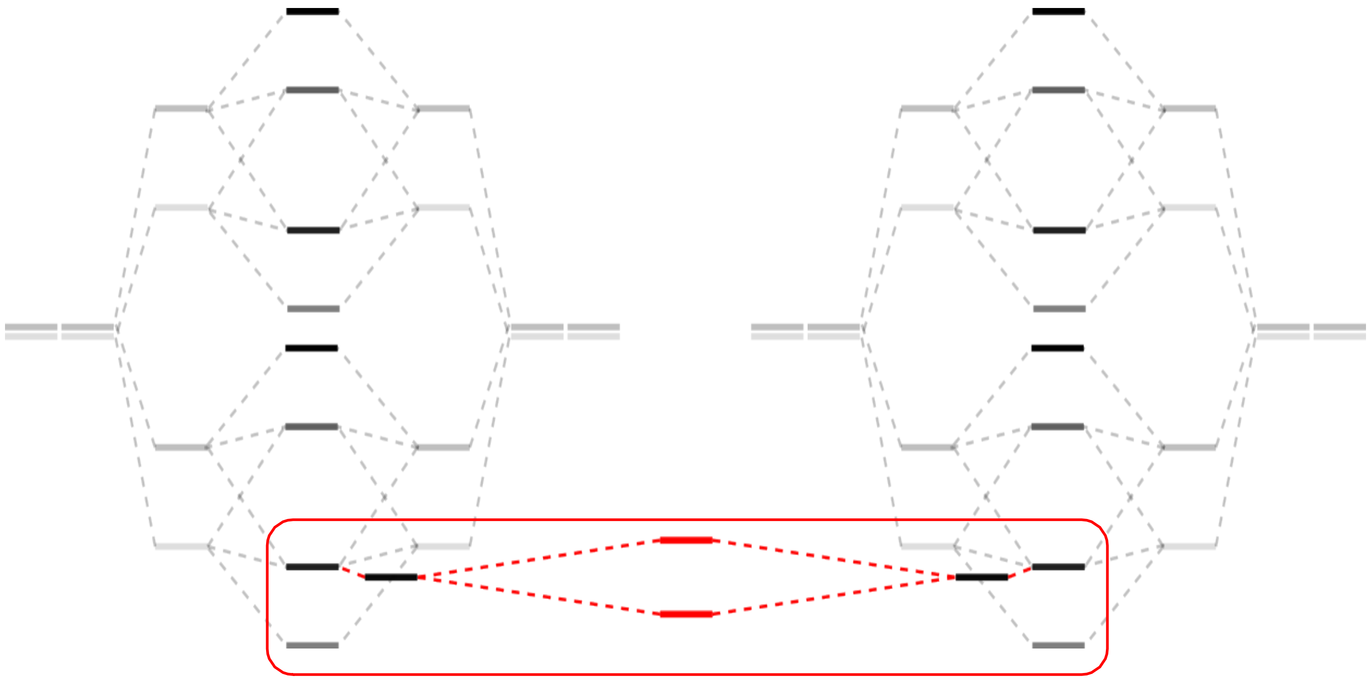
Small Valley Splitting Impact on Gate Fidelity



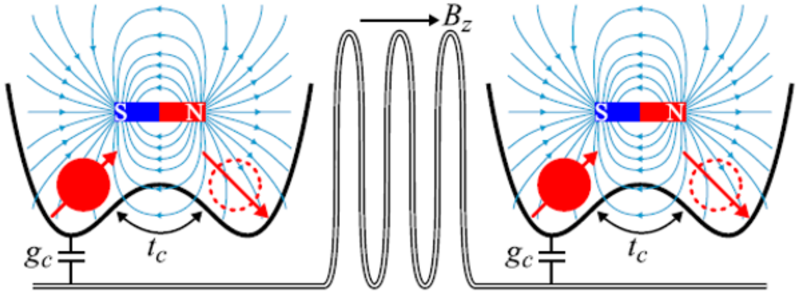


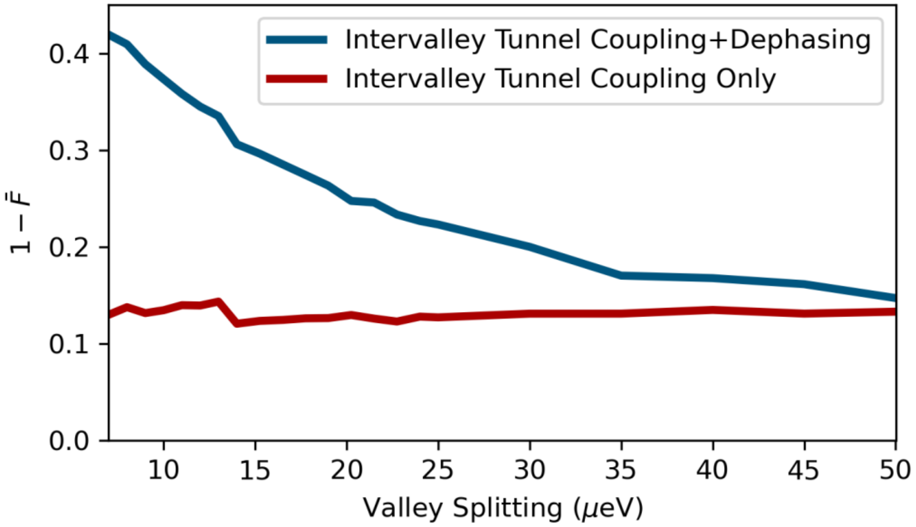


Field coupling mixes singly excited states of two qubits
Forms basis for iSWAP gate

How do valley interactions (tunnel coupling, phonon coupling, spin-orbit coupling, charge noise, *etc.*) affect gate fidelity?

Small Valley Splitting Impact on Gate Fidelity





Valley splitting + intervalley tunnel coupling is not itself problem

Intervalley decoherence (commensurate with intravalley decoherence) affects fidelity even at relatively large valley splittings

Ongoing and Future Work

- Parameters generated from microscopic device modeling:
    - Intra- and inter-valley tunnel couplings
    - Electron-phonon coupling
    - Spin-orbit coupling
    - Inter-valley dipoles
    - Frequency-dependent charge noise

  What ranges of various parameters are possible given device structure and design?
- Parameter optimization tolerance

  What parameters are best or most important to get right?
- Time-dependent parameters (model device operations)
- Search for favorable operating regimes outside assumptions underlying previous models

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