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Modeling open quantum system device operation with multivalley effective mass theory

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Introduction

To faithfully model the operation of a qubit in Si, we must capture the complex static and dynamic valley-orbit physics of the high-dimensional system into which this effective two-level system is embedded. We've developed a framework for CAD to gate fidelity modeling of a device:

- CAD design of the device (including device stack and gate electrodes)
- Poisson solve for electrostatics (e.g. QCAD [1] or COMSOL)
- Multivalley effective mass theory [2] for valley-orbital sector, solve generalized eigenvalue problem $H|\psi\rangle = ES|\psi\rangle$
- Description of coupling to the environment, master equation
- Integrate master equation to obtain device dynamics
- Evaluate gate operation w.r.t. qubit degrees of freedom

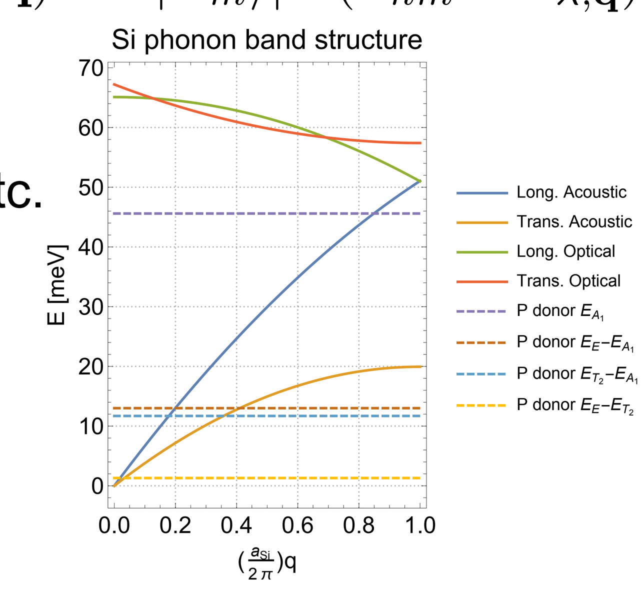
Electron-phonon coupling
$$H_{\text{e-ph}} = \sum_{\lambda,\mathbf{q}} \mathbf{A}(\lambda,\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}}b^{\dagger}_{\lambda,\mathbf{q}} + \mathbf{A}^{\dagger}(\lambda,\mathbf{q})e^{-i\mathbf{q}\cdot\mathbf{r}}b_{\lambda,\mathbf{q}}$$

Inelastic transition rates
$$\Gamma_{nm} \propto \sum_{\lambda} \int \mathrm{d}^3\mathbf{q} |\langle E_n|\mathbf{A}(\lambda,\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}}|E_m\rangle|^2 \delta(\omega_{nm} - \omega_{\lambda,\mathbf{q}})$$

$\lambda =$ phonon mode

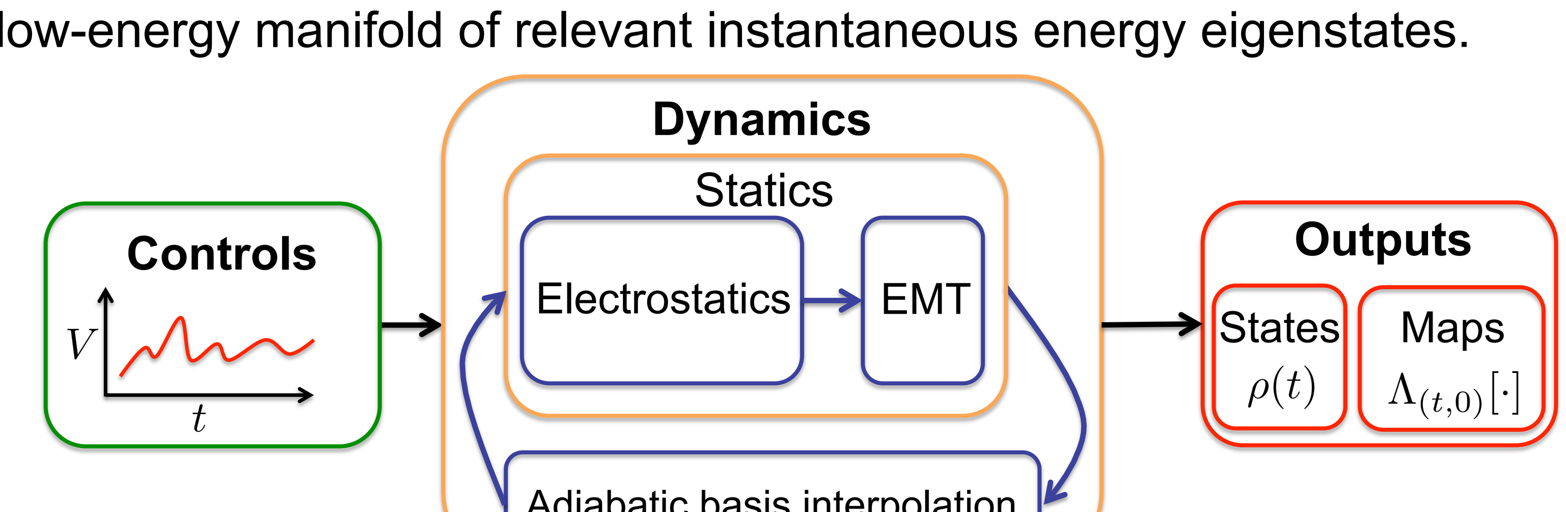
$\mathbf{A}(\lambda,\mathbf{q})$ contains deformation potentials, etc.

Time-local master equation for density matrix evolution
$$\dot{\rho} = -\frac{i}{\hbar}[H(t),\rho] + \mathcal{D}_t\{\rho\}$$

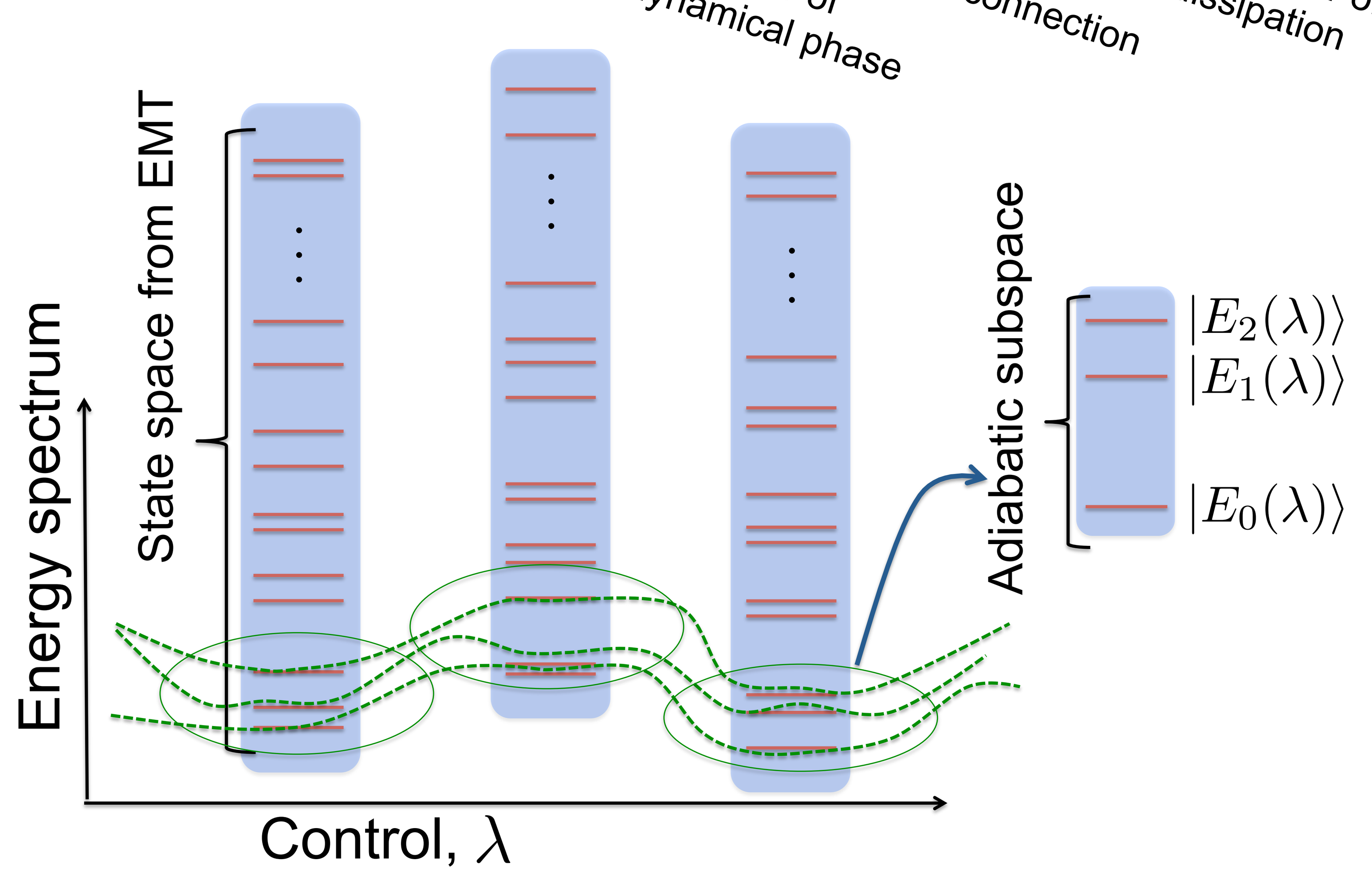


Model reduction

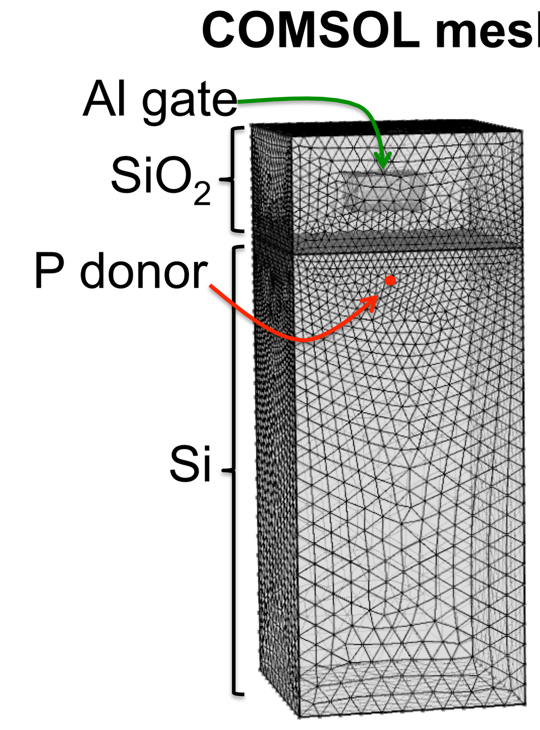
We're interested mainly in the lowest-energy states of the valley-orbit sector. To reduce the number of states we need to track while simulating dynamics, we perform a projective model reduction to a low-energy manifold of relevant instantaneous energy eigenstates.



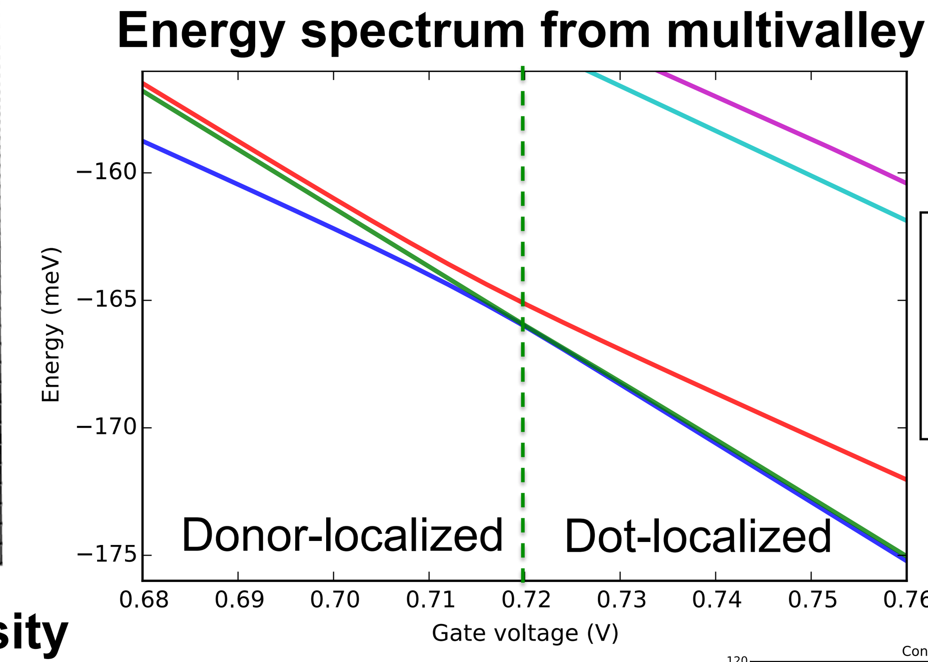
Master equation for subspace dynamics
$$\dot{\tilde{\rho}} = -\frac{i}{\hbar}[\mathbf{E}(t),\tilde{\rho}] + \{\dot{\lambda}(t)\cdot\mathbf{B}(t),\tilde{\rho}\} + \mathcal{D}_t\{\tilde{\rho}\}$$
generator of dynamical phase; basis connection; generator of dissipation

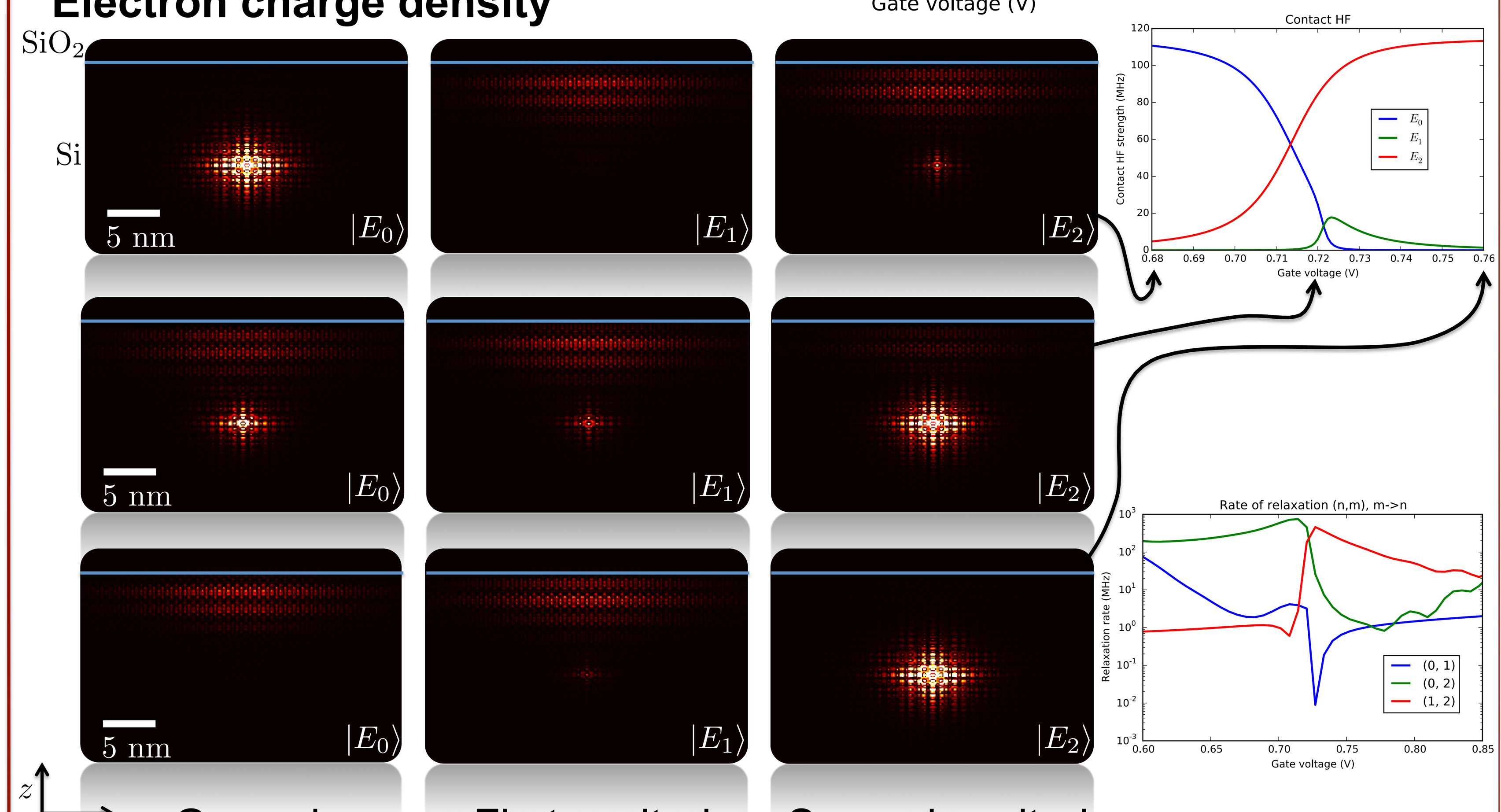


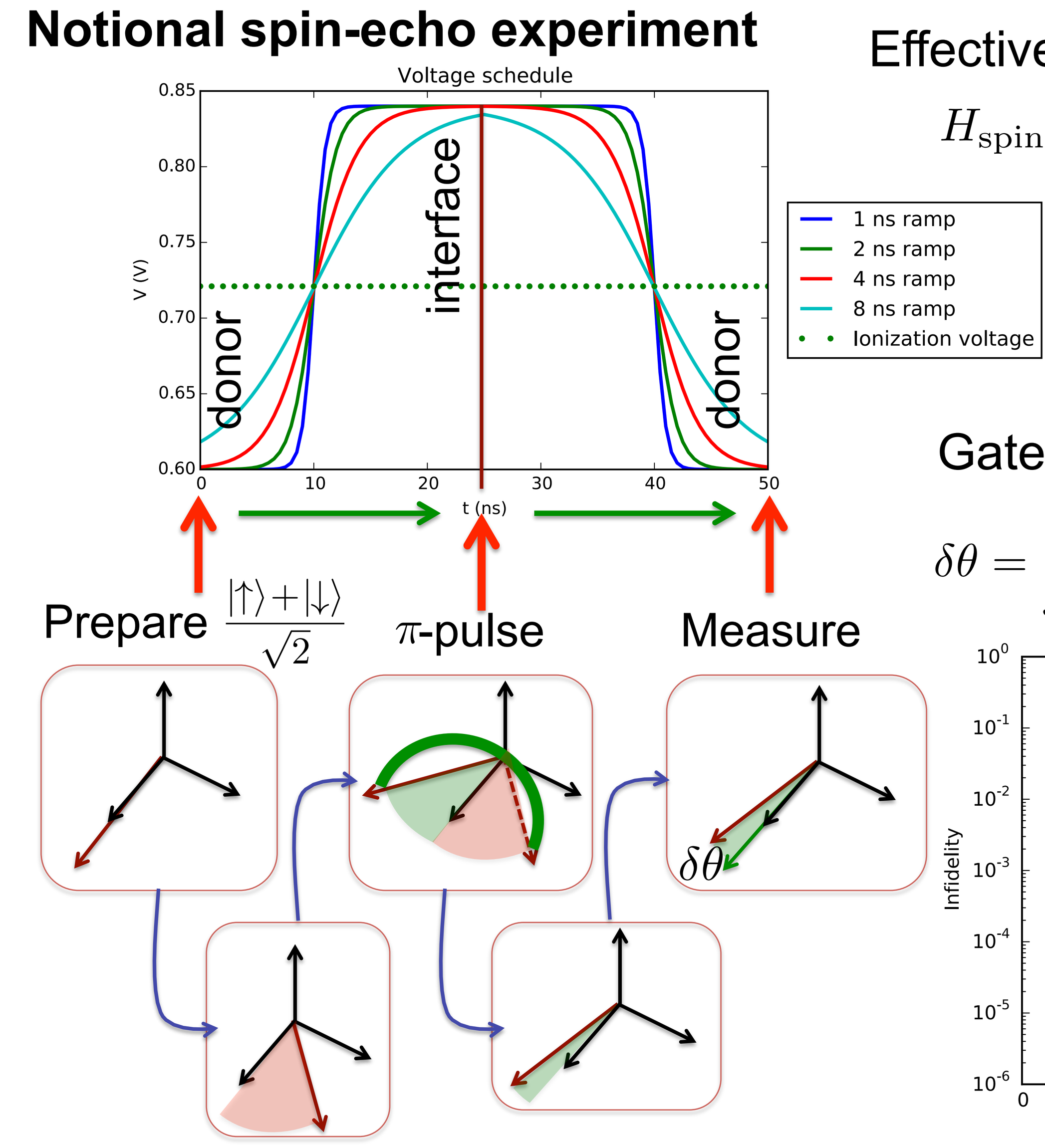
Example



Shuttling an electron between a P donor and a quantum dot at a Si/SiO_2 interface



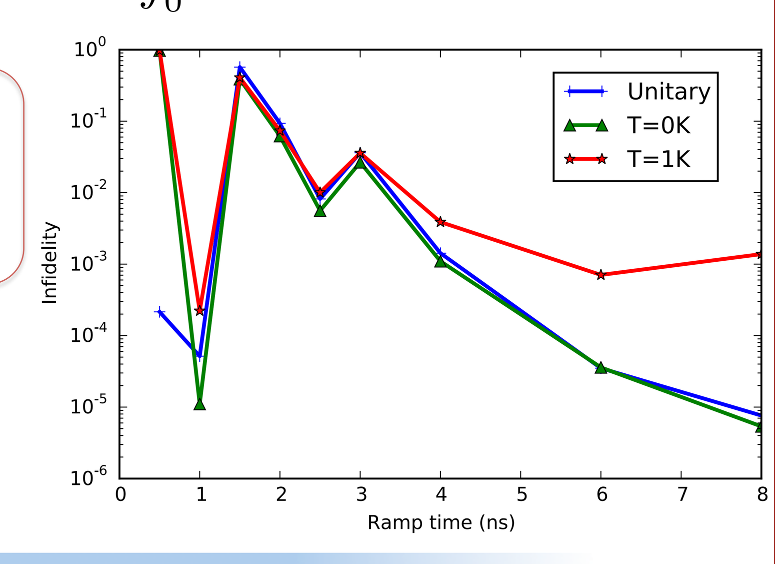




Effective qubit Hamiltonian
$$H_{\text{spin}}(t) = A(t)\vec{\sigma_e}\cdot\vec{\sigma_n}$$

Depending on underlying processes in the valley-orbital sector, $A(t)$ may not be deterministic

Gate infidelity: $\mathcal{I} = 1 - \cos(\delta\theta)^2$
$$\delta\theta = \int_0^{T/2} \mathrm{d}t\left[A(t) - A(t+T/2)\right]/\hbar$$



Summary

Given a CAD design for a device, we solve for the electrostatics and describe the valley-orbit physics of the device. We then describe the dynamics of a relevant low-energy subspace, deriving an effective (potentially stochastic) qubit Hamiltonian. Having solved for this dynamics, we can evaluate gate fidelity.

References:

[1] X. Gao, et al., J. App. Phys. **114**, 164302 (2013)
[2] Gamble, Jacobson, et al. Phys. Rev. B **91**, 235318 (2015)

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