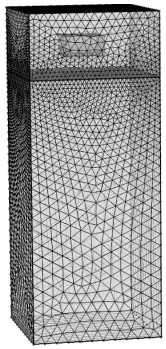
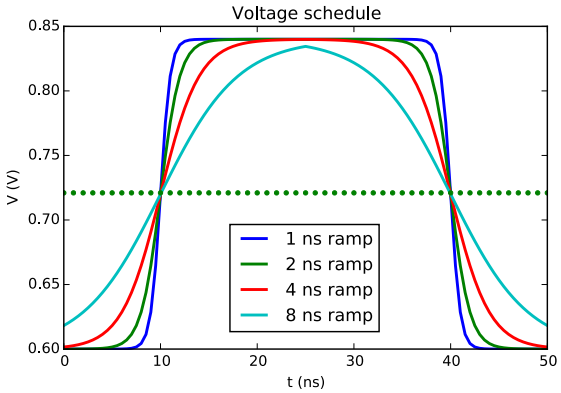
SAND2015-1315C

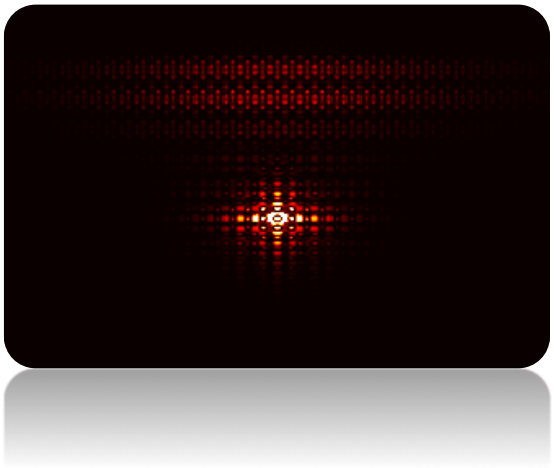
Exceptional service in the national interest

Sandia National Laboratories

Multi-valley effective mass theory for device-level modeling of open quantum dynamics







Collaborators:
John K. Gamble, Andrew Baczewski,
Wayne Witzel, Inès Montaño, Erik Nielsen, Rick Muller – *Sandia*
Adam Frees – *Univ. Wisconsin-Madison*

Toby Jacobson
Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration

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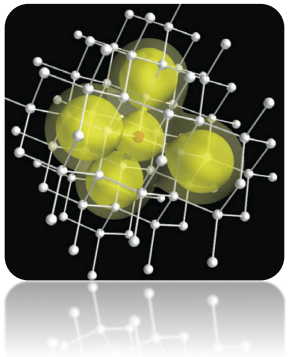
Modeling device *operation* requires dynamics

Multi-valley effective mass theory: [Gamble, et al. **arXiv:1408.3159**]
Cartesian Gaussian basis
Central cell correction tuned-up for P in Si
Inhomogeneous strain (a la [Herring & Vogt, Phys Rev 1956])
Realistic electrostatic potentials (from e.g. QCAD, COMSOL)
Electron-phonon coupling



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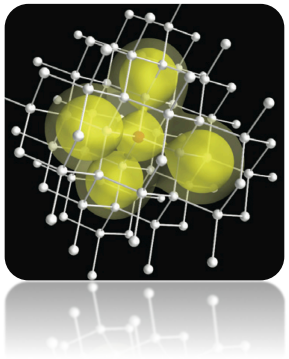
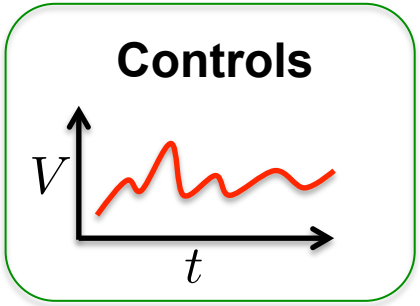


extending this framework into the time domain…



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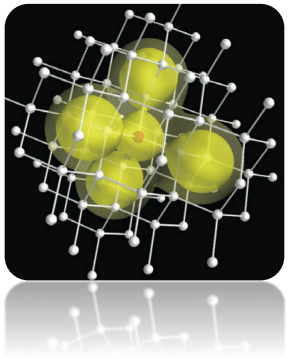

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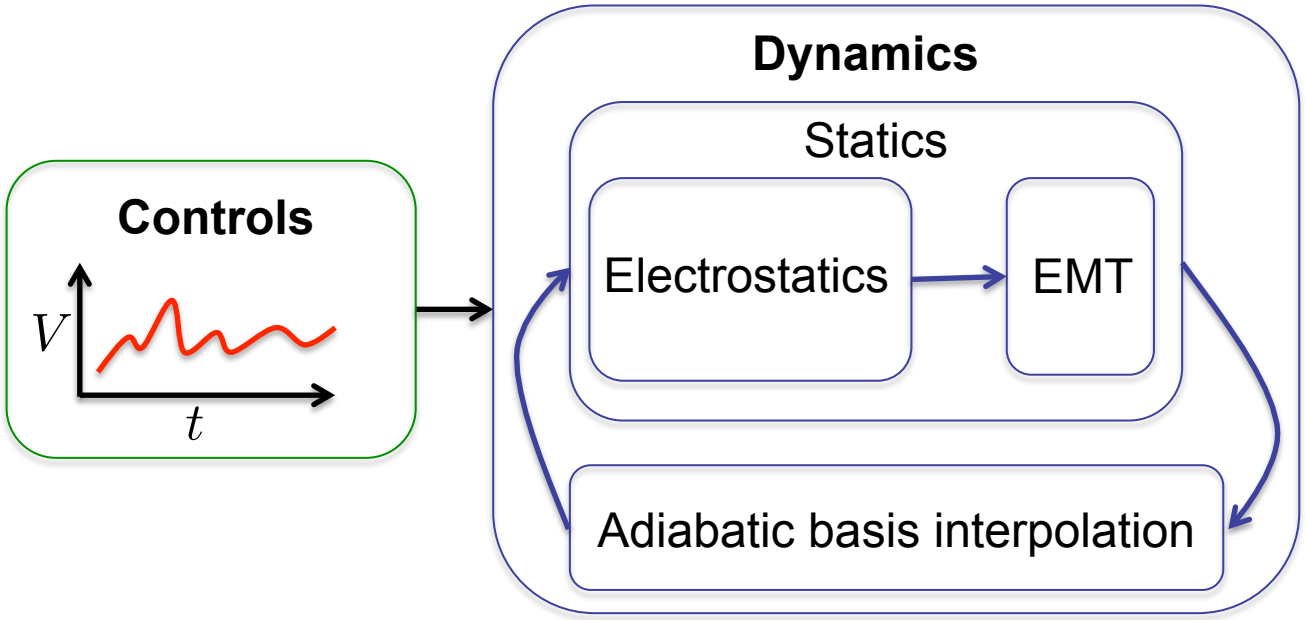

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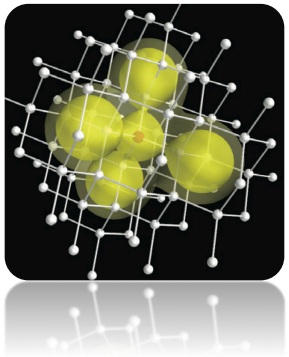

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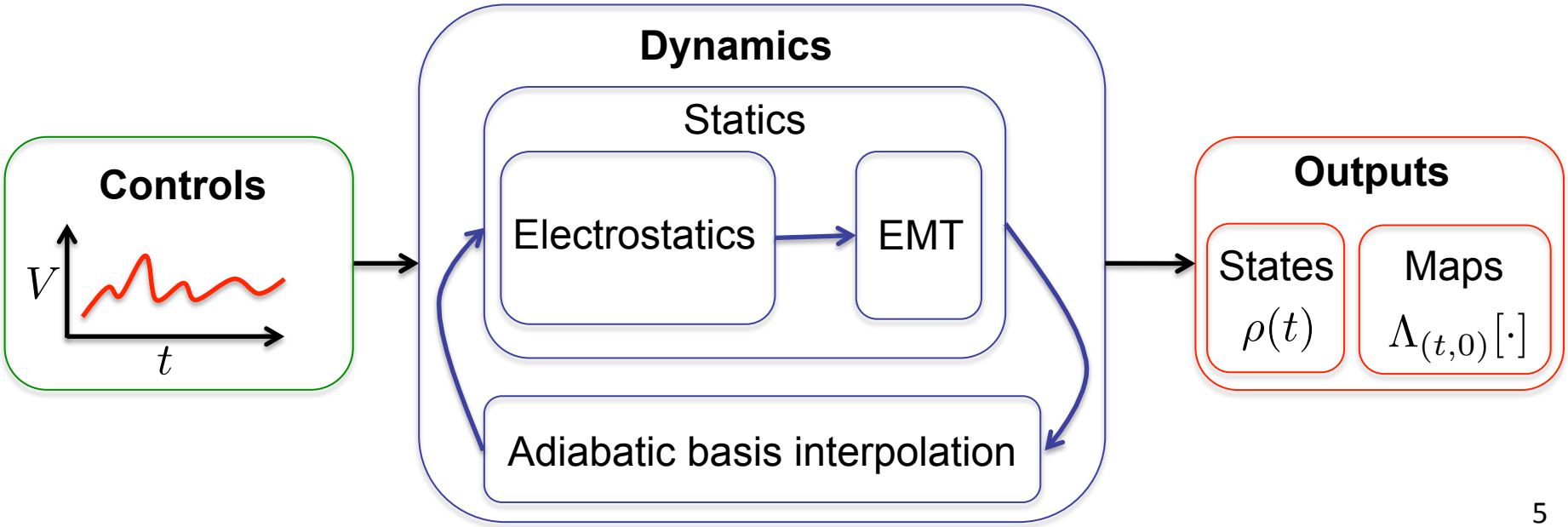
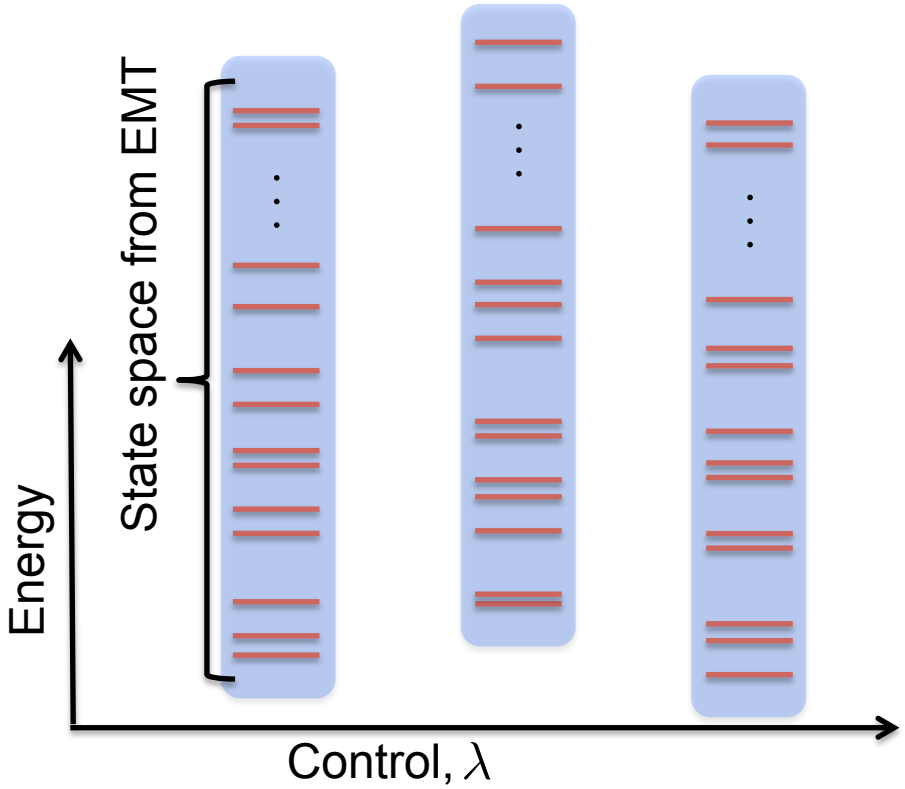


Dynamics framework

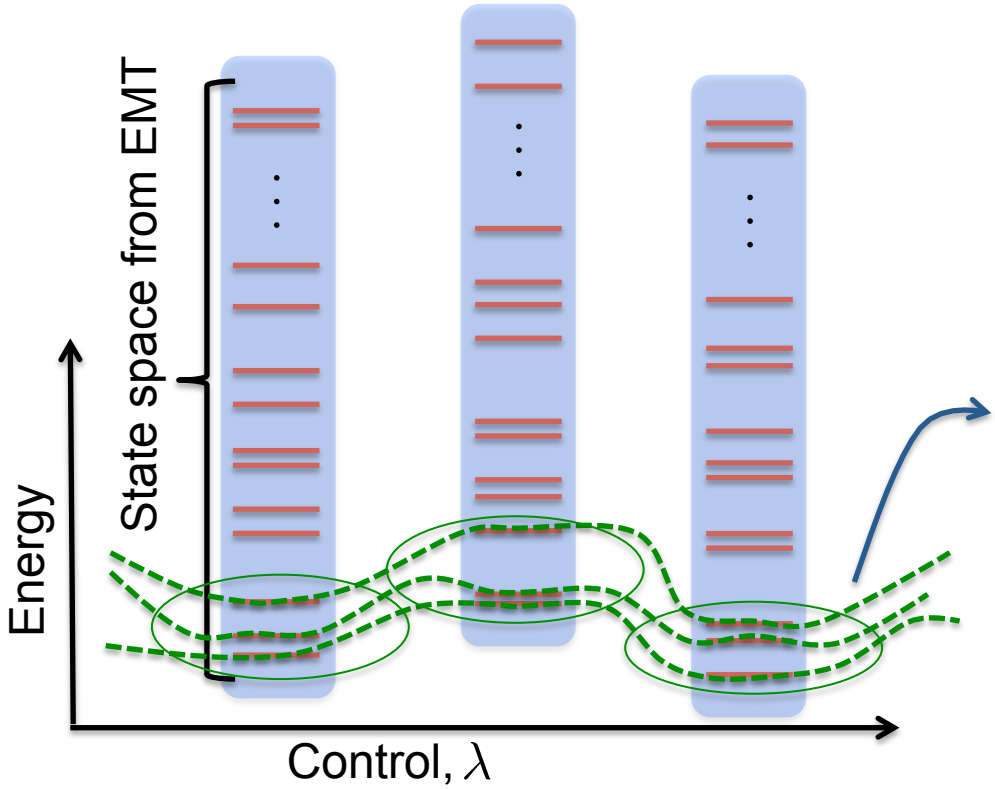


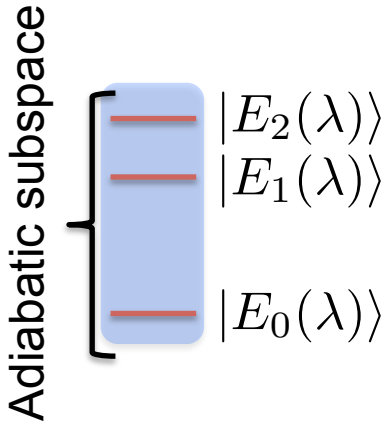
Equation of motion:

Time-local master equation

$$\dot{\rho} = -\frac{i}{\hbar}\left[H(t), \rho\right] + \mathcal{D}_t\{\rho\}$$

Dynamics framework





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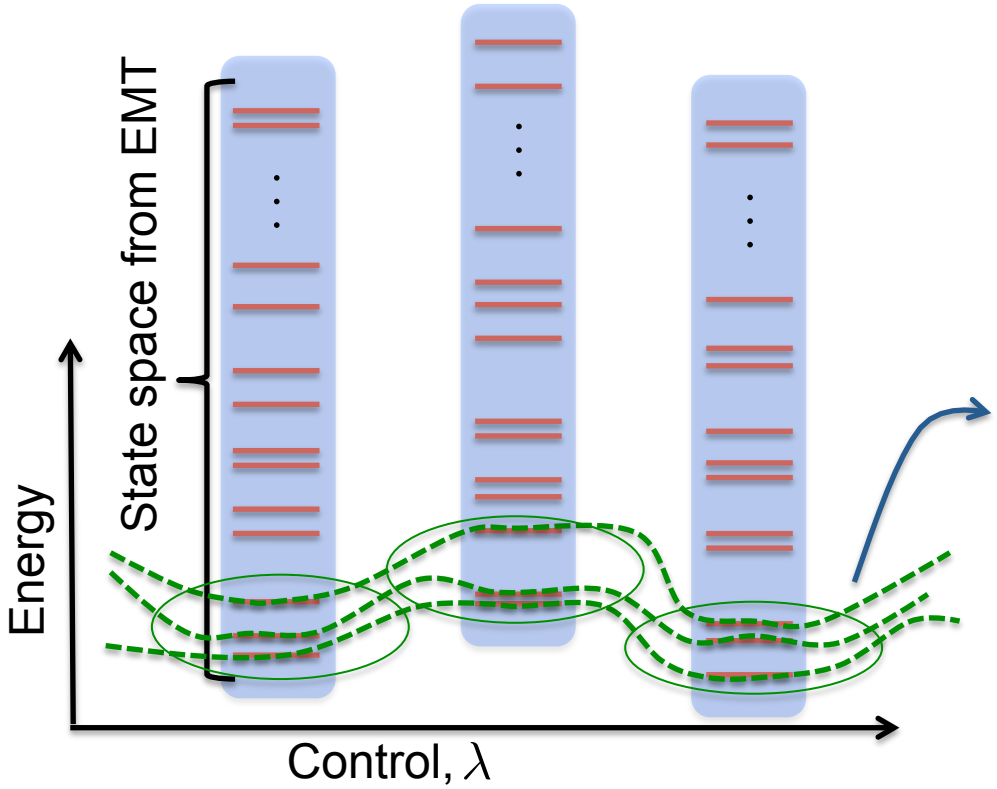
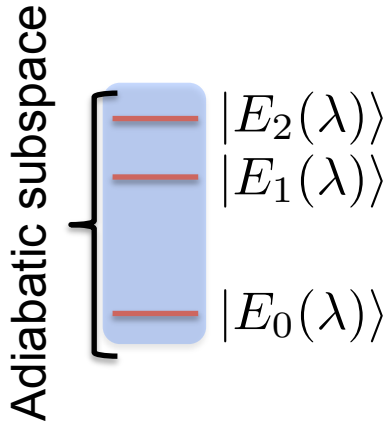
→ …within instantaneous low-energy subspace

$$\dot{\tilde{\rho}} = -\frac{i}{\hbar}\left[\mathbf{E}(t), \tilde{\rho}\right] + \{\dot{\lambda}(t)\cdot\mathbf{B}(t), \tilde{\rho}\} + \mathcal{D}_t\{\tilde{\rho}\}$$

Dynamics framework





dynamical phase

basis connection

Equation of motion:

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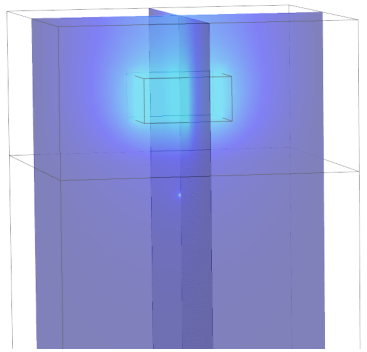
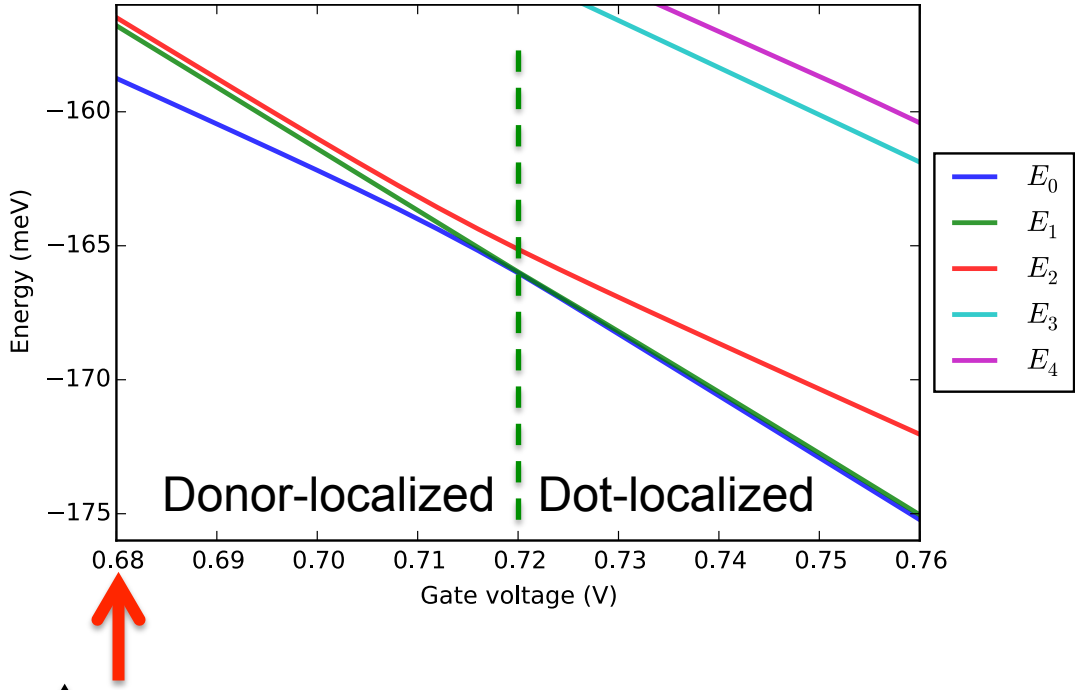
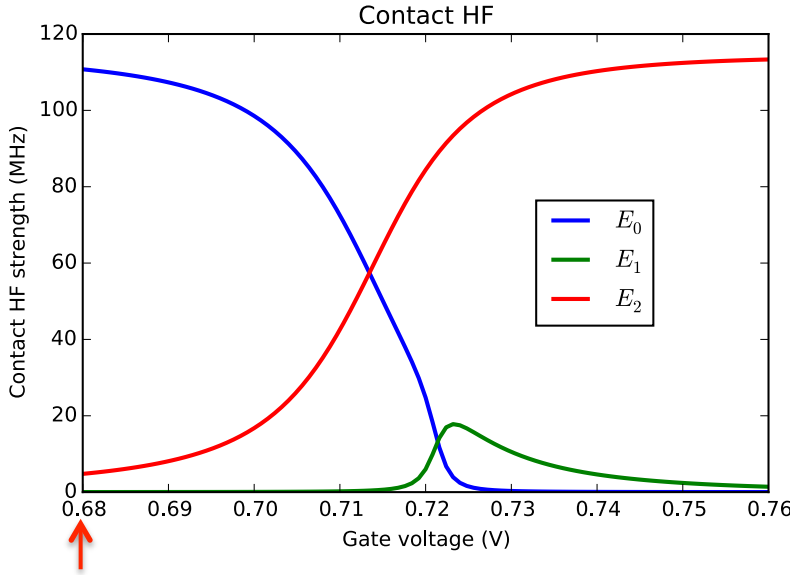
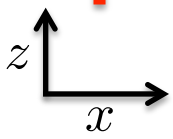
Shuttling between donor and interface dot



$0.68\ V$







[Calderón, et al. PRL 2006, PRB 2007, PRB 2008]
[Baena, et al. PRB 2012]

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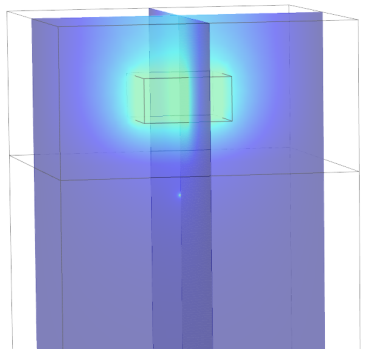
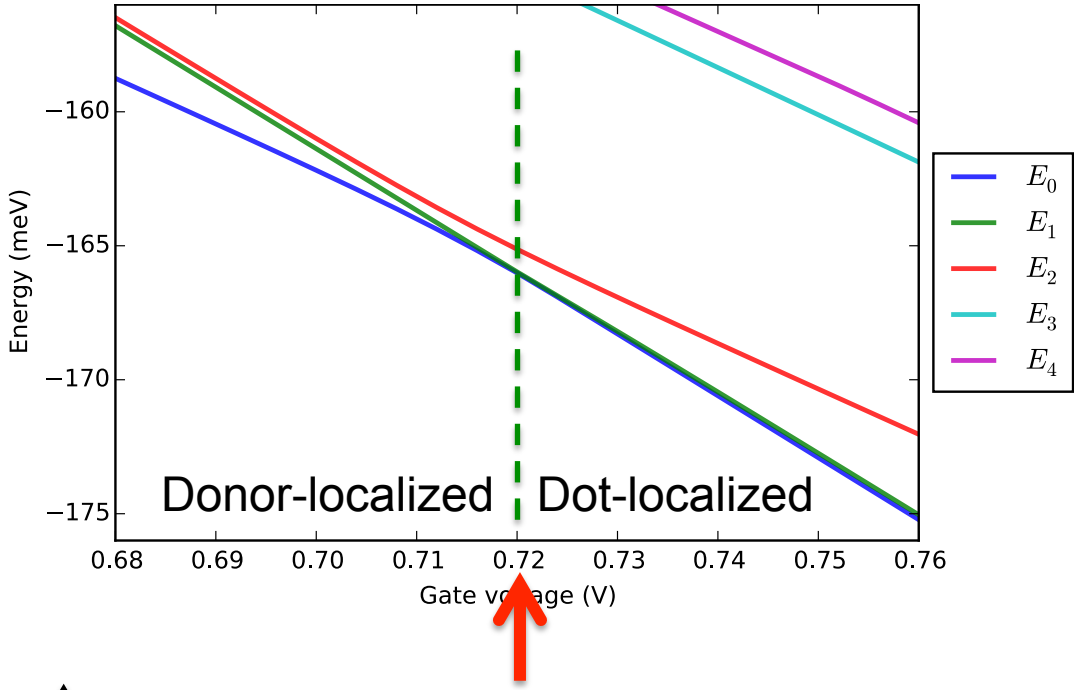
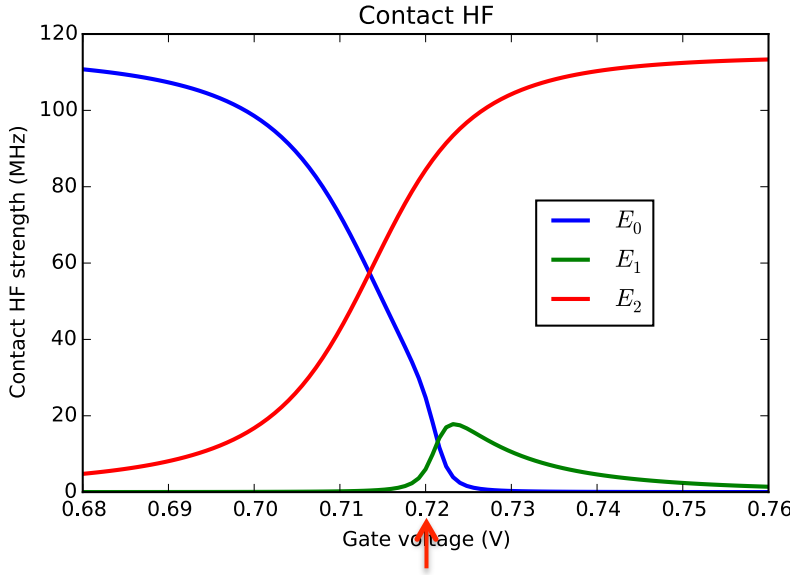
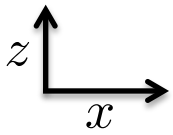


$0.72\ V$







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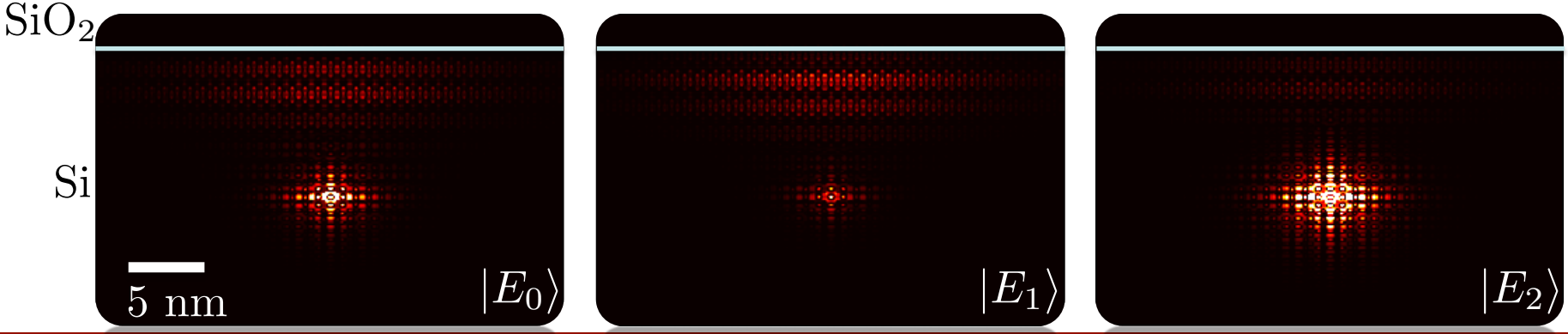

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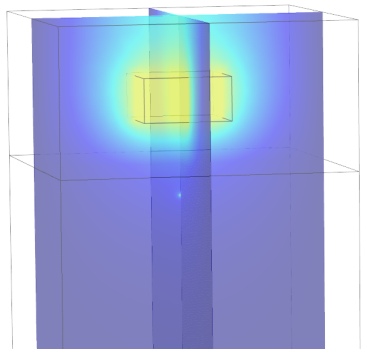
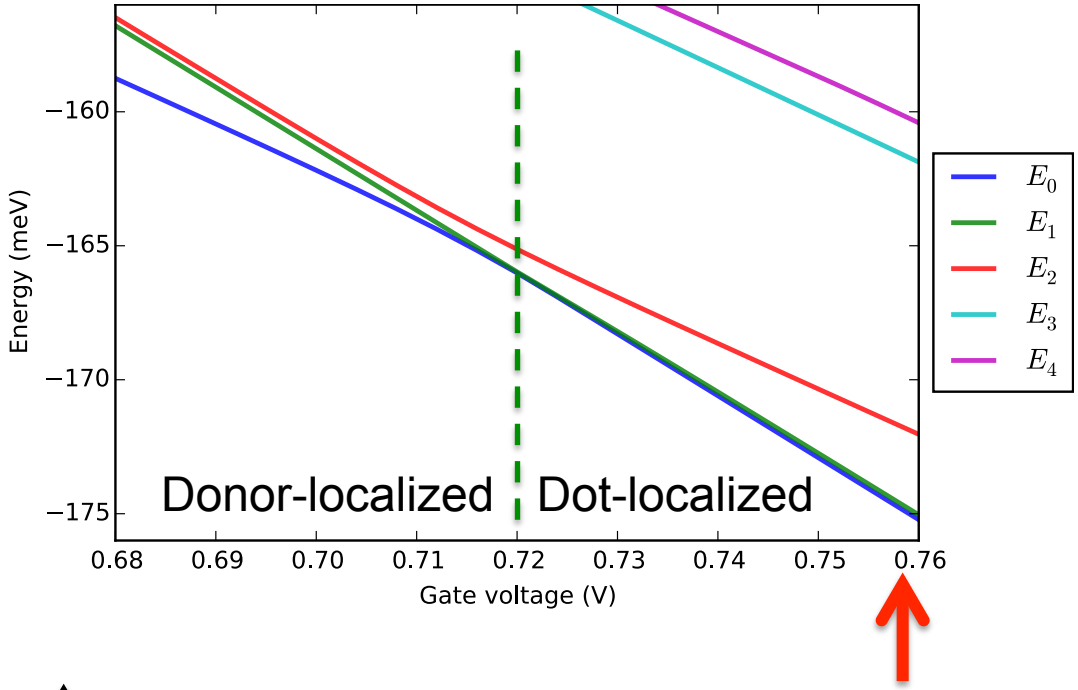
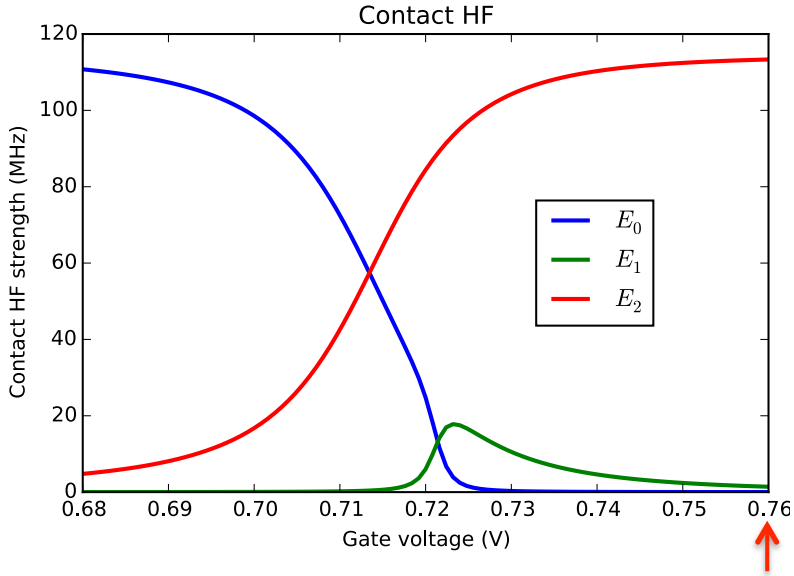
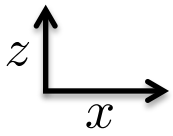


$0.76\ V$







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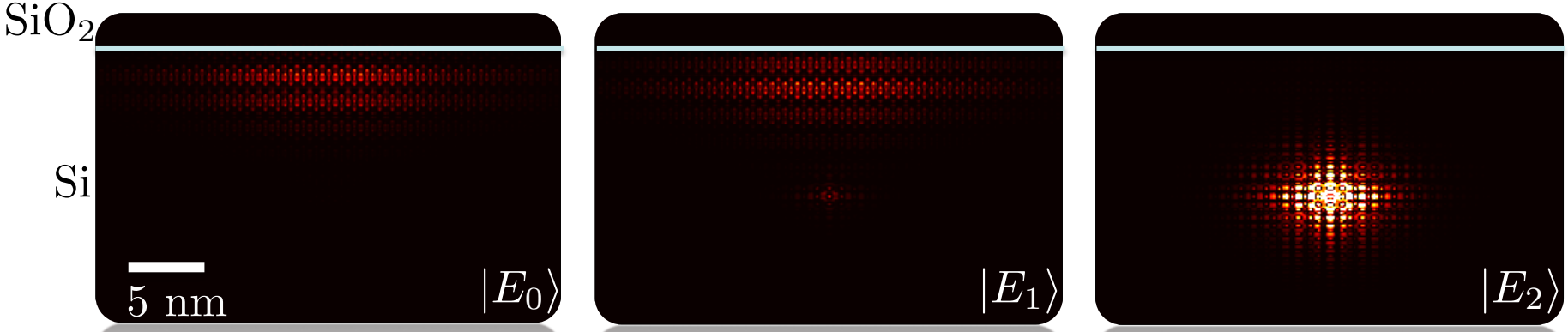
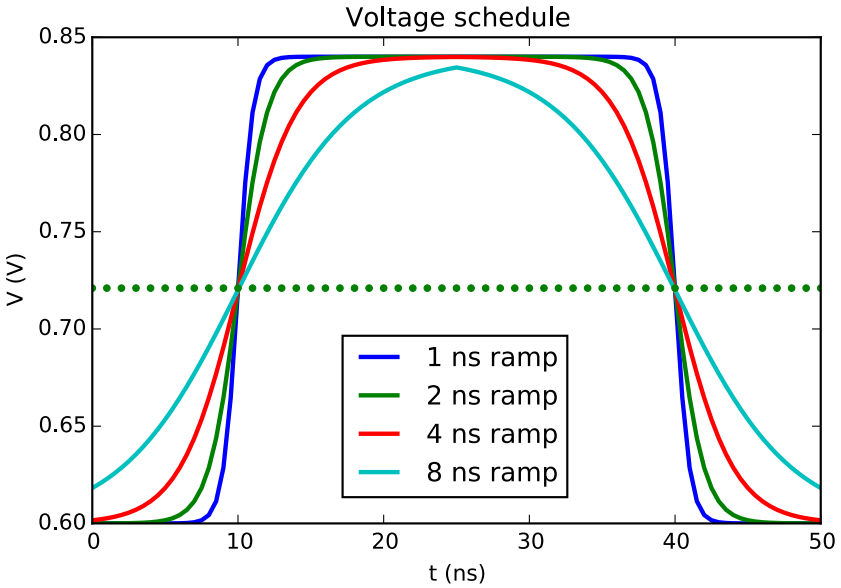


Closed/open dynamics



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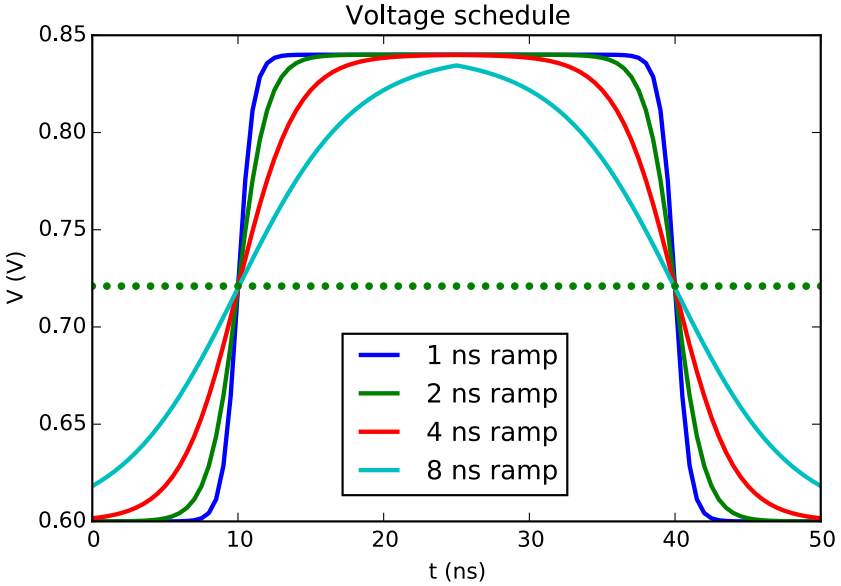

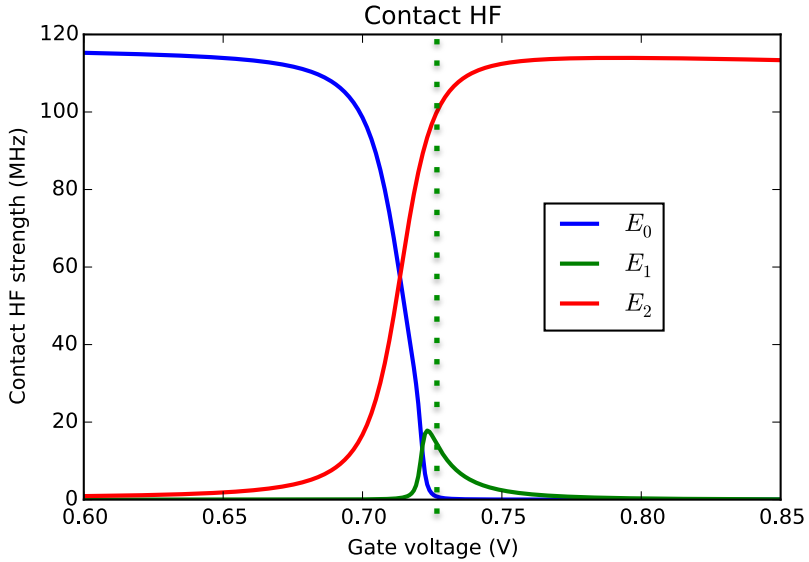

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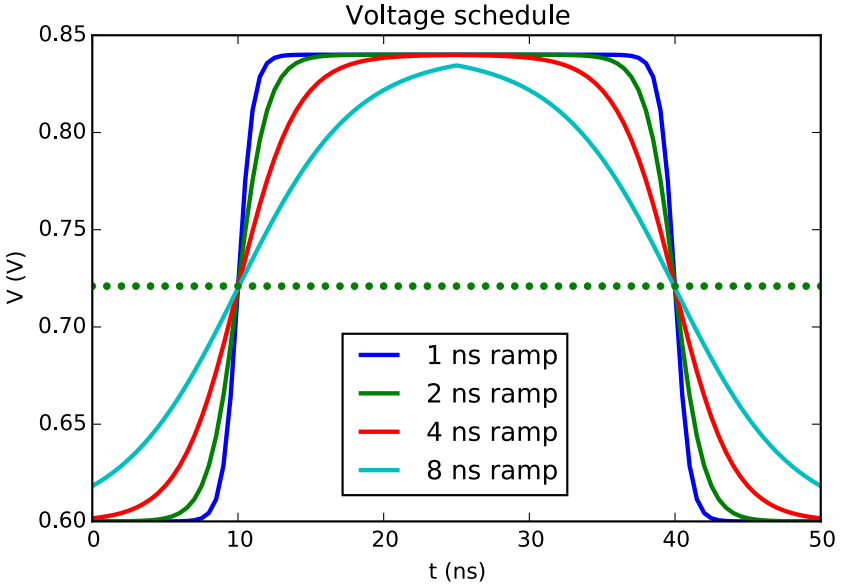

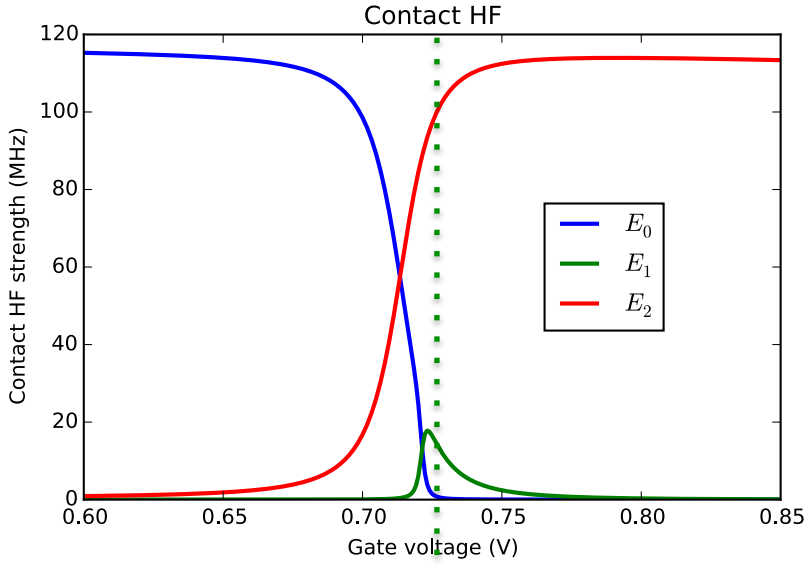

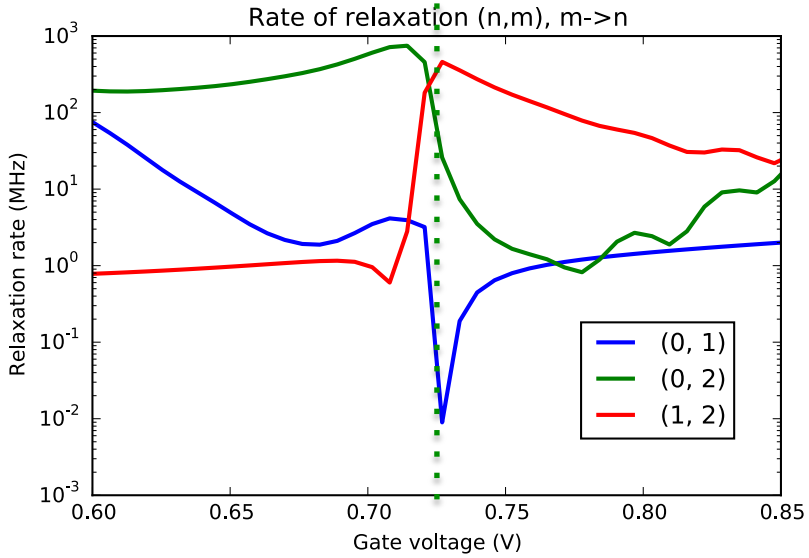

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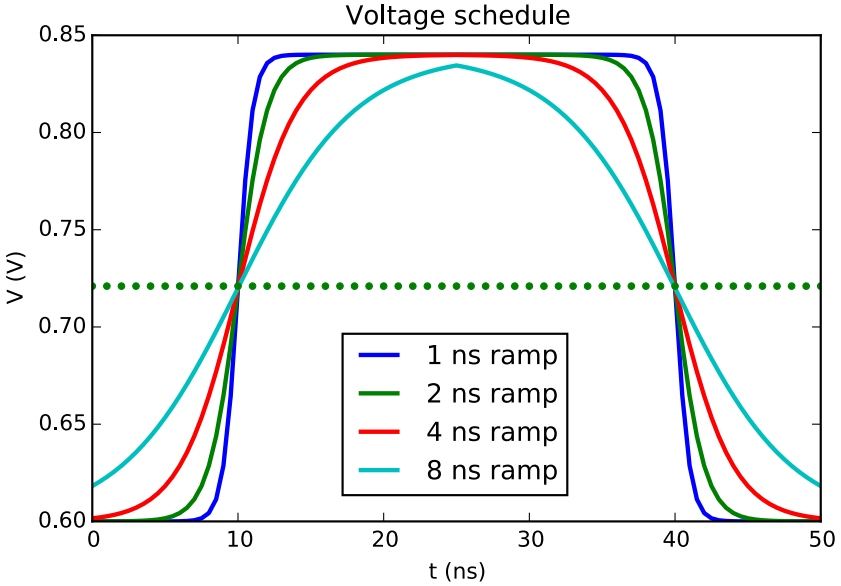

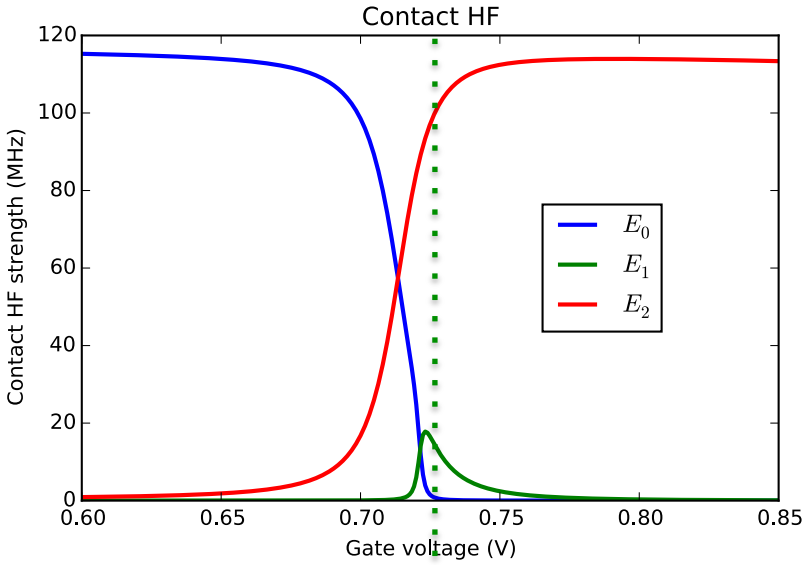

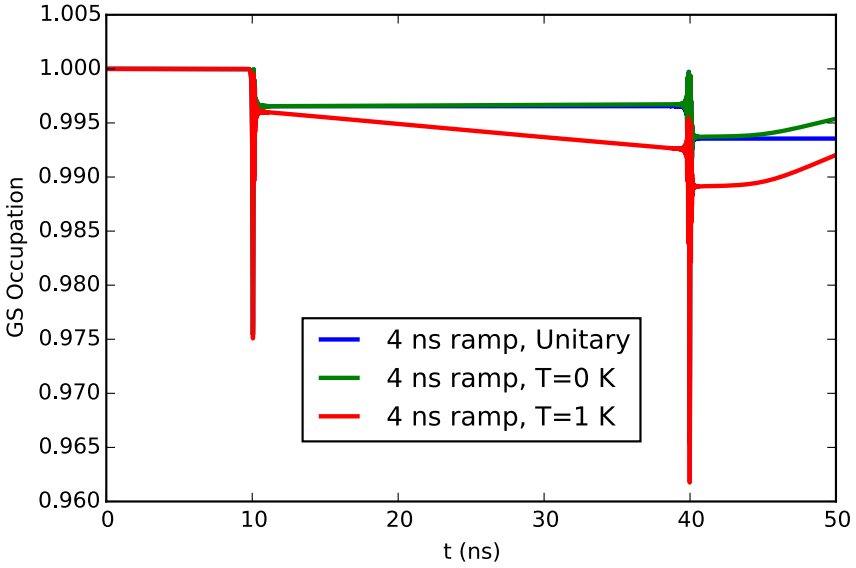

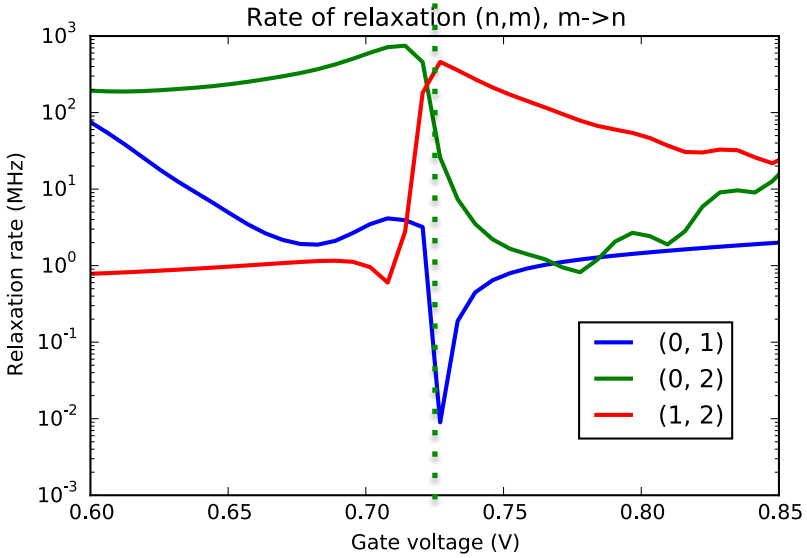

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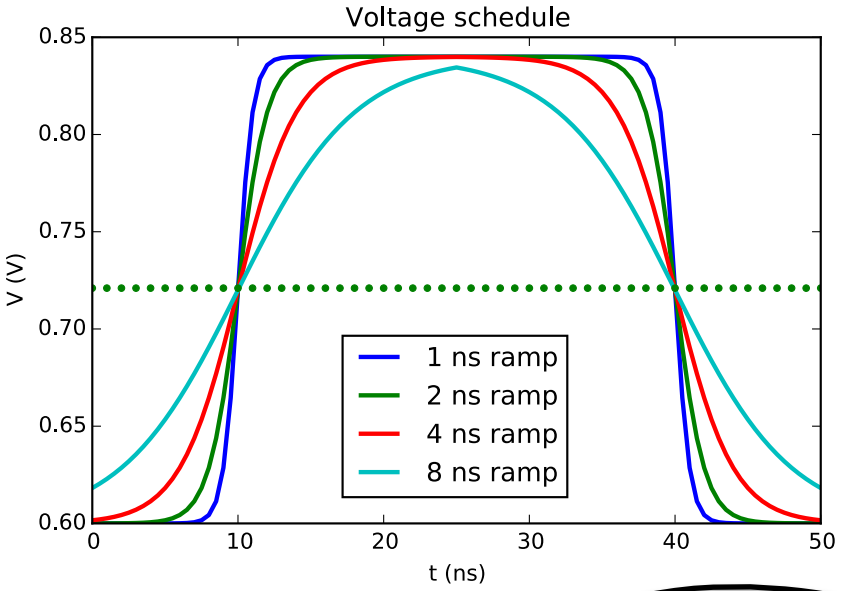

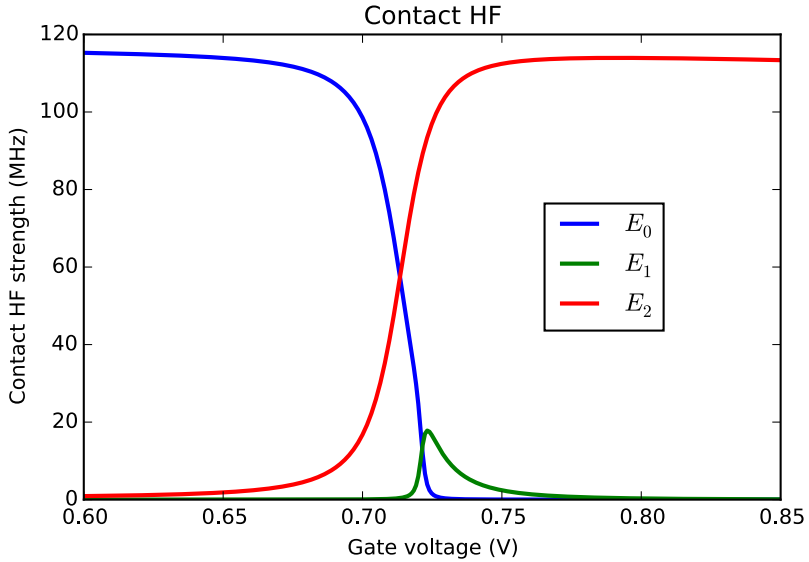

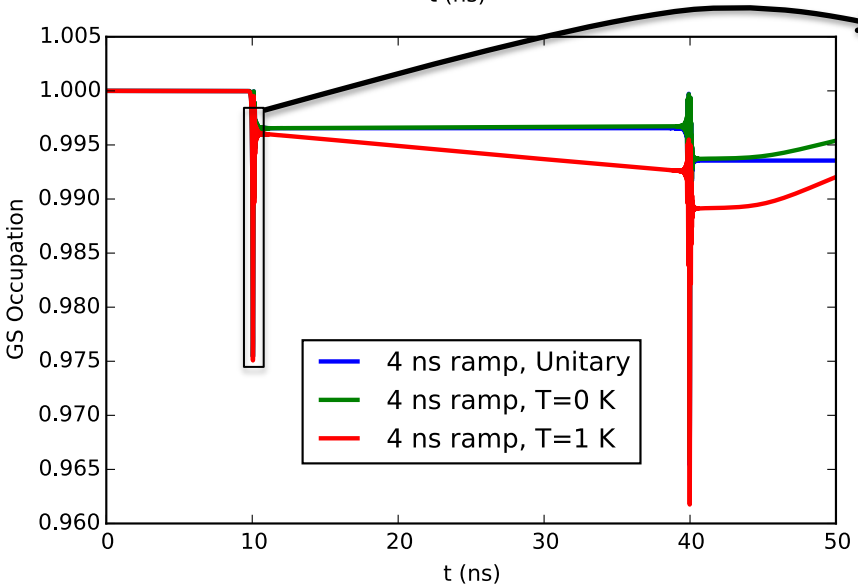

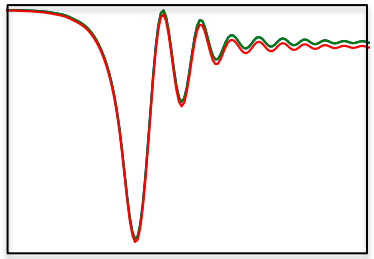

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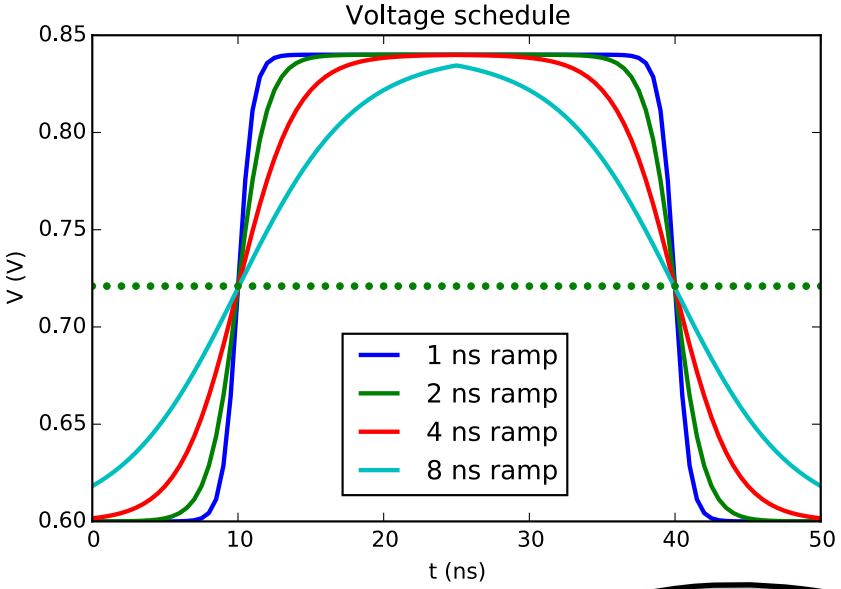

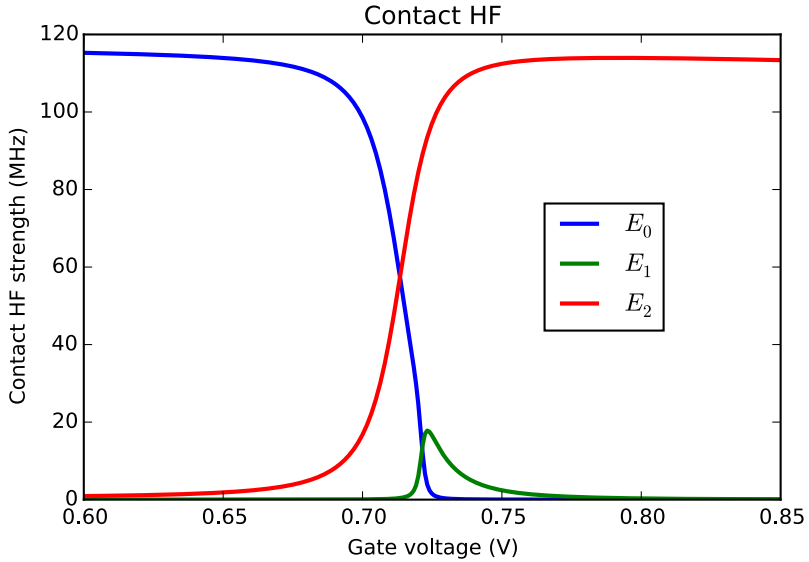

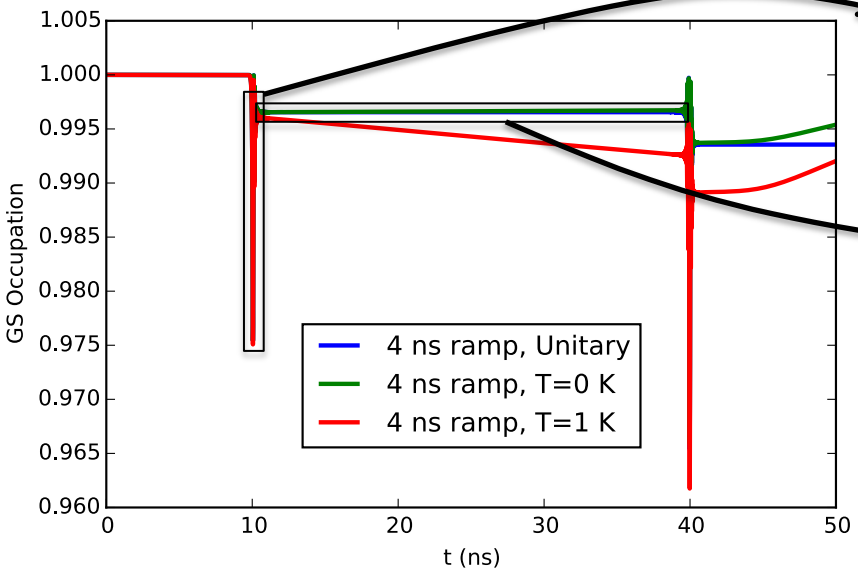

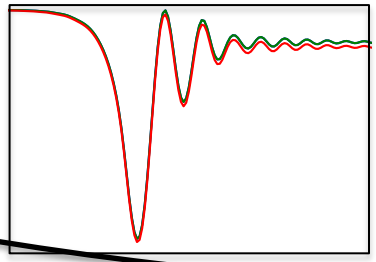

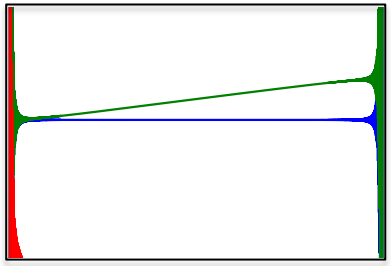

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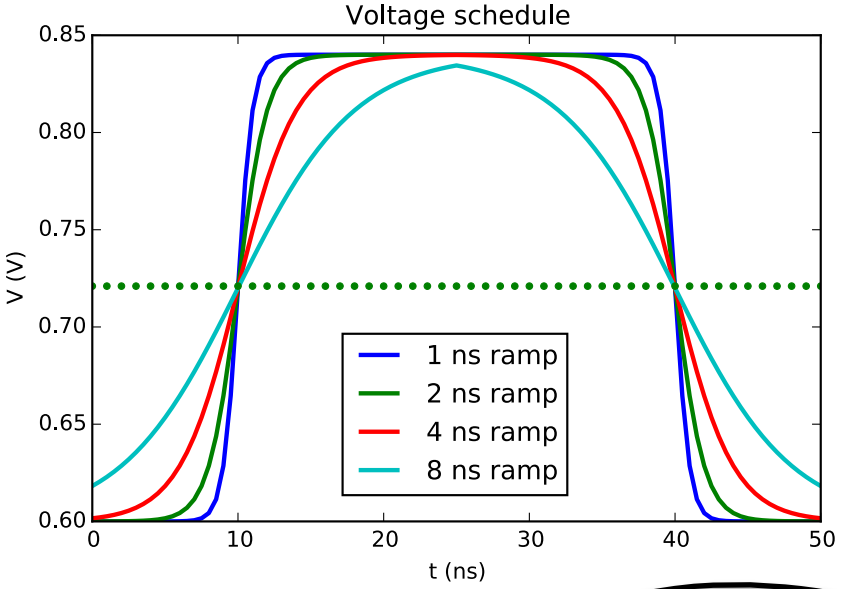
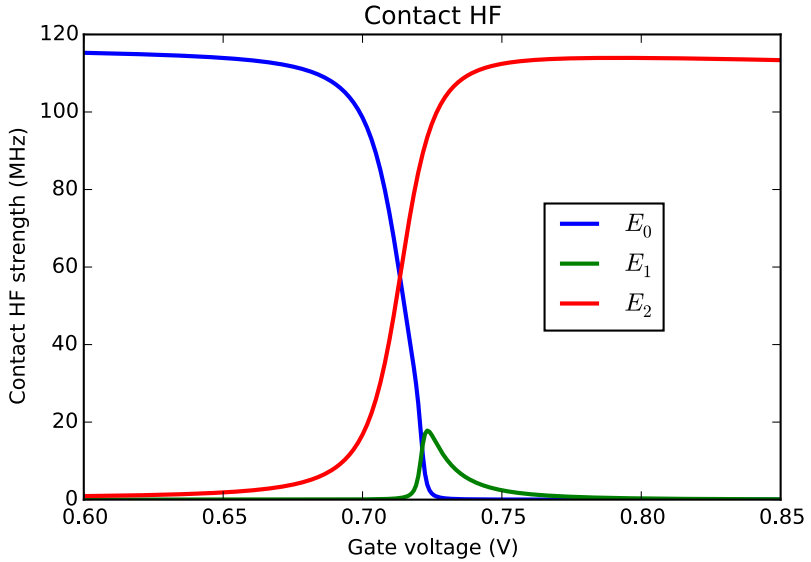
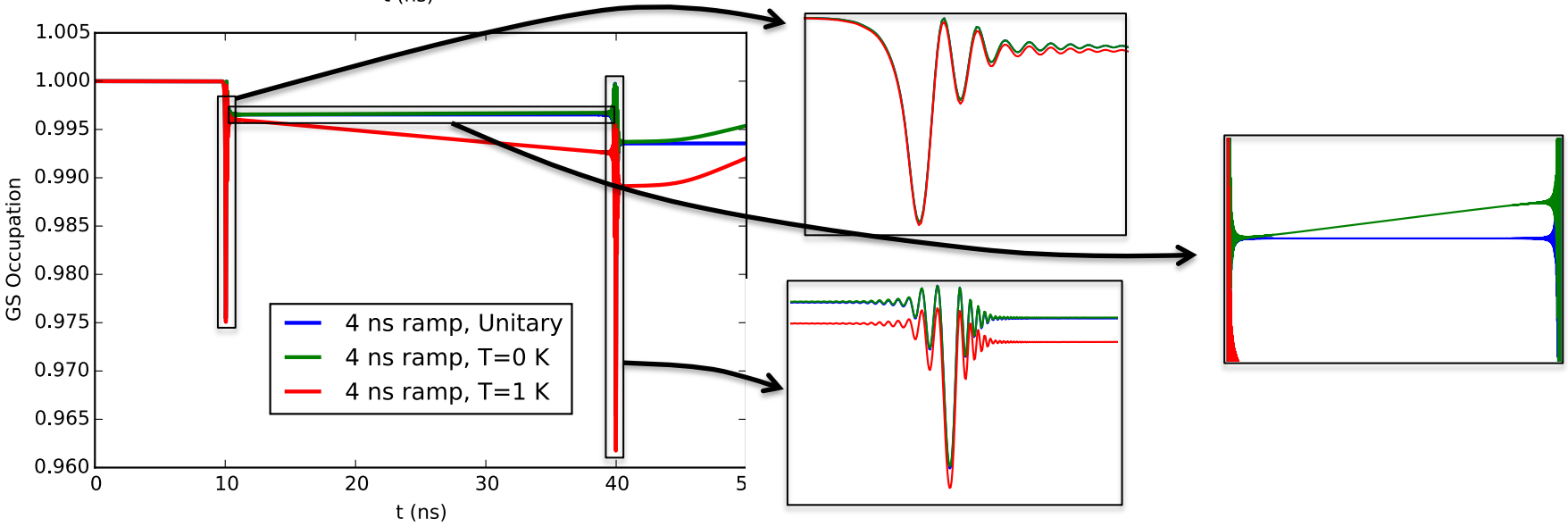
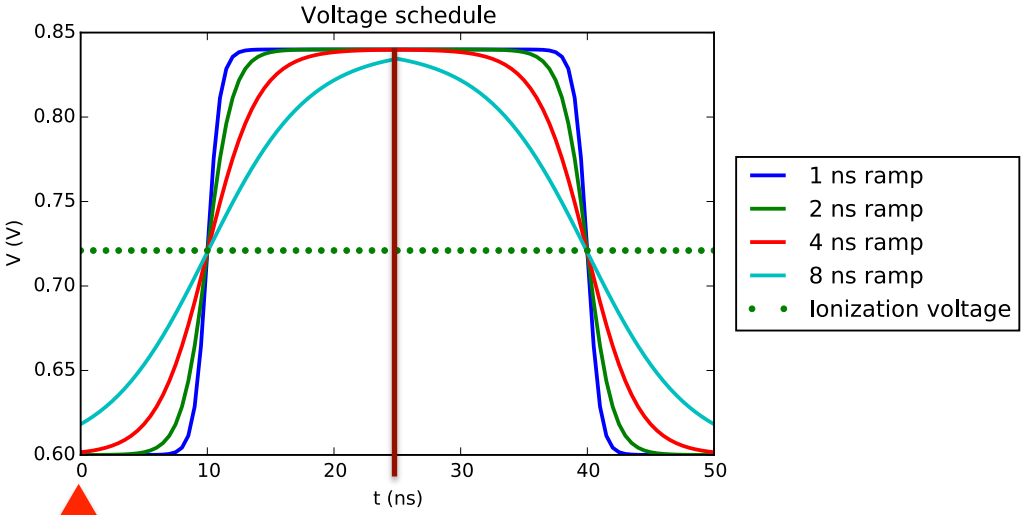


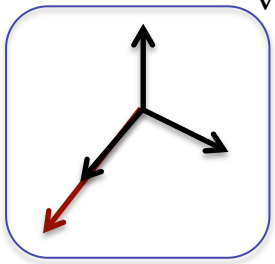




Spin-echo fidelity during shuttling



Prepare $\frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}}$



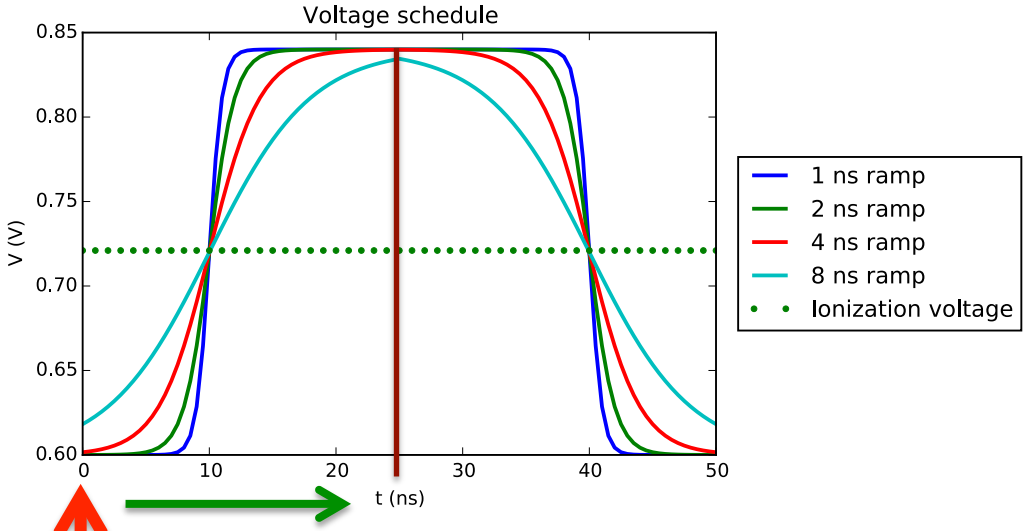
Errors:
Non-adiabaticity
Thermalization

$$H_{\text{spin}}(t) = A(t)\overrightarrow{\sigma_e} \cdot \overrightarrow{\sigma_n}$$

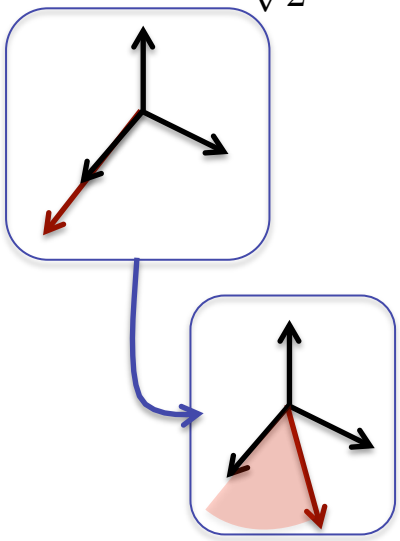
$$\delta\theta = \int_0^{T/2} \mathrm{d}t\big[A(t) - A(t+T/2)\big]/\hbar$$

$$\mathcal{I} = 1 - \cos(\delta\theta)^2$$

Spin-echo fidelity during shuttling



Prepare $\frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}}$



Errors:
Non-adiabaticity
Thermalization

$$H_{\text{spin}}(t) = A(t)\overrightarrow{\sigma_e} \cdot \overrightarrow{\sigma_n}$$

$$\delta\theta = \int_0^{T/2} \mathrm{d}t\big[A(t) - A(t+T/2)\big]/\hbar$$

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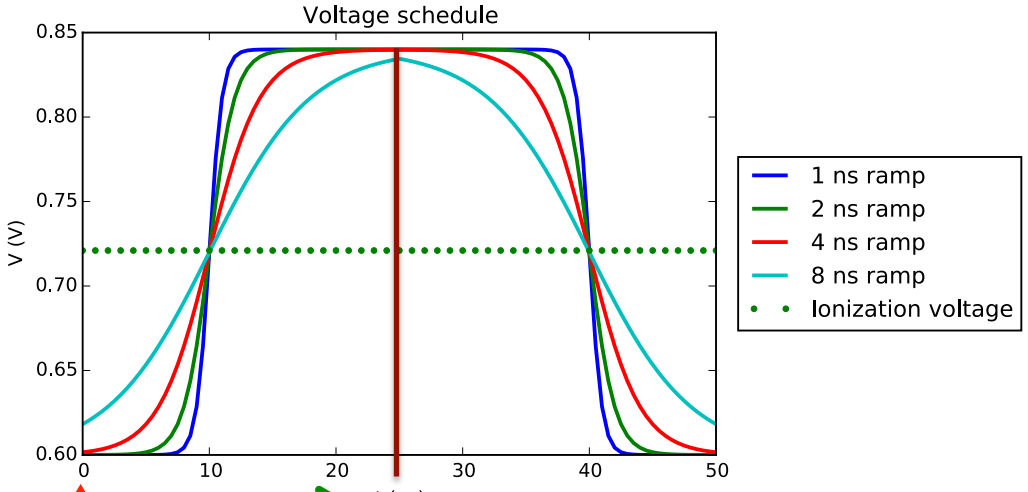
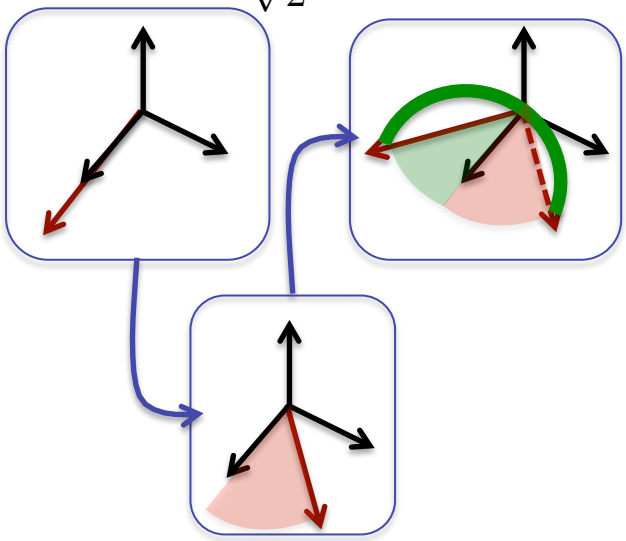
Spin-echo fidelity during shuttling



Prepare $\frac{|\uparrow\rangle+|\downarrow\rangle}{\sqrt{2}}$ π-pulse



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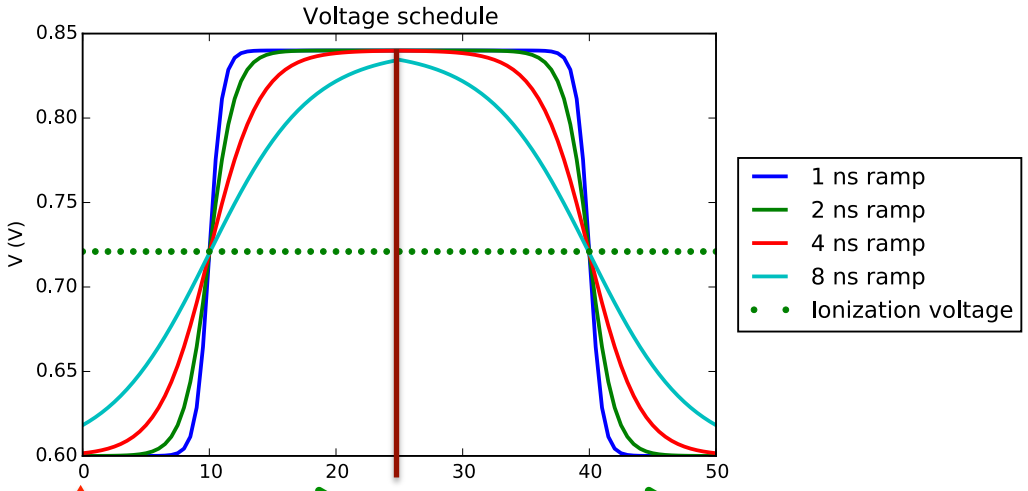
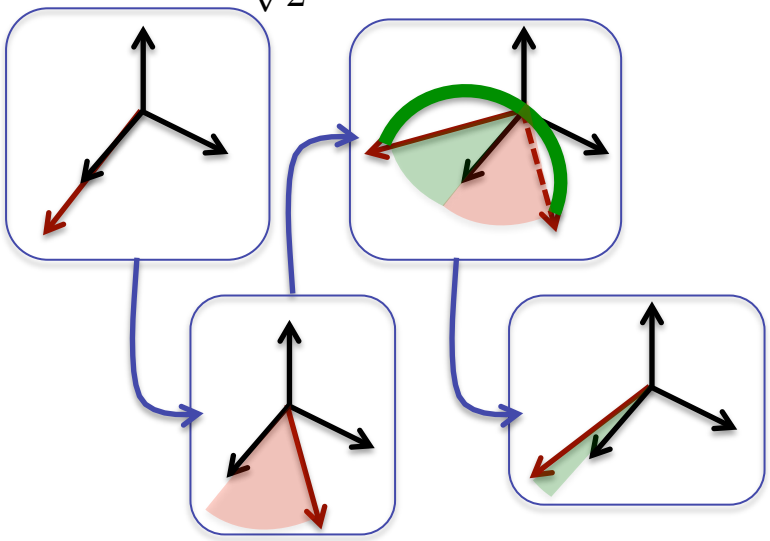
Spin-echo fidelity during shuttling



Prepare $\frac{|\uparrow\rangle+|\downarrow\rangle}{\sqrt{2}}$ π-pulse



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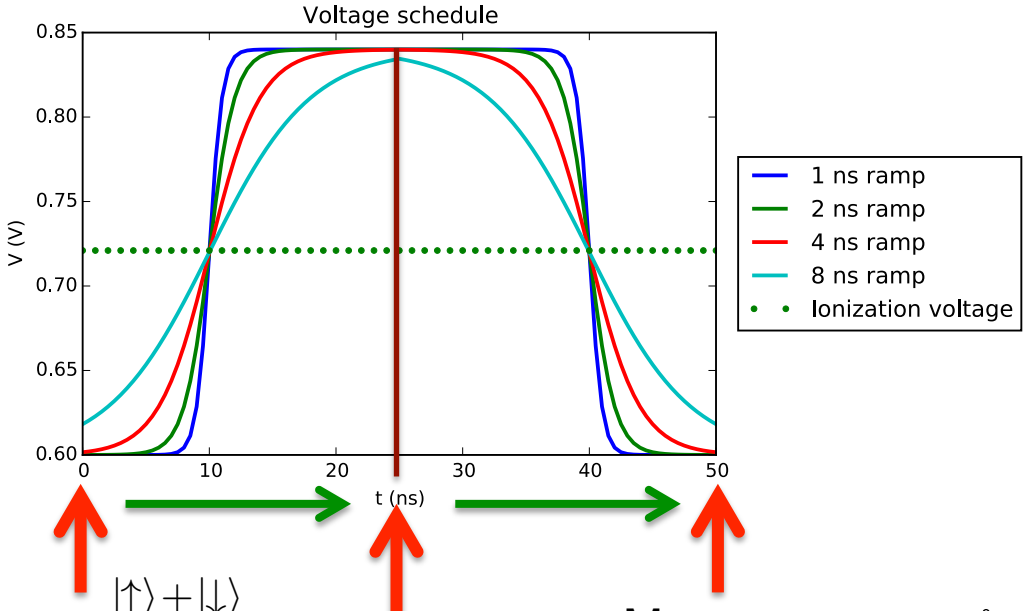
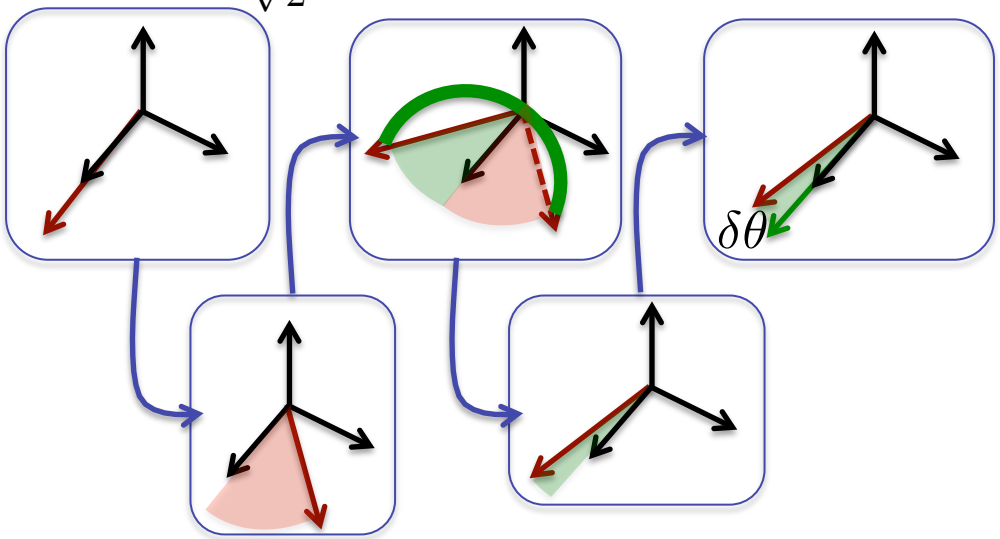
Spin-echo fidelity during shuttling





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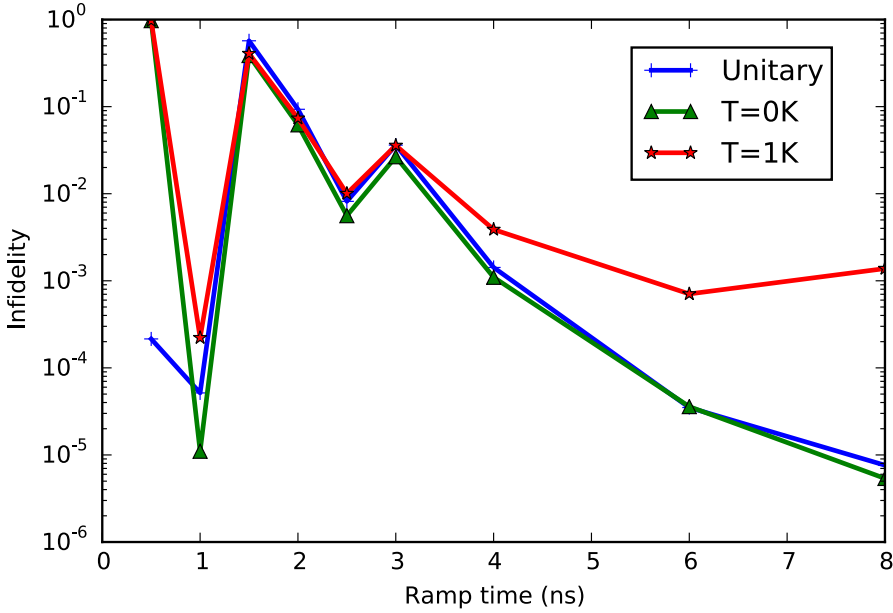
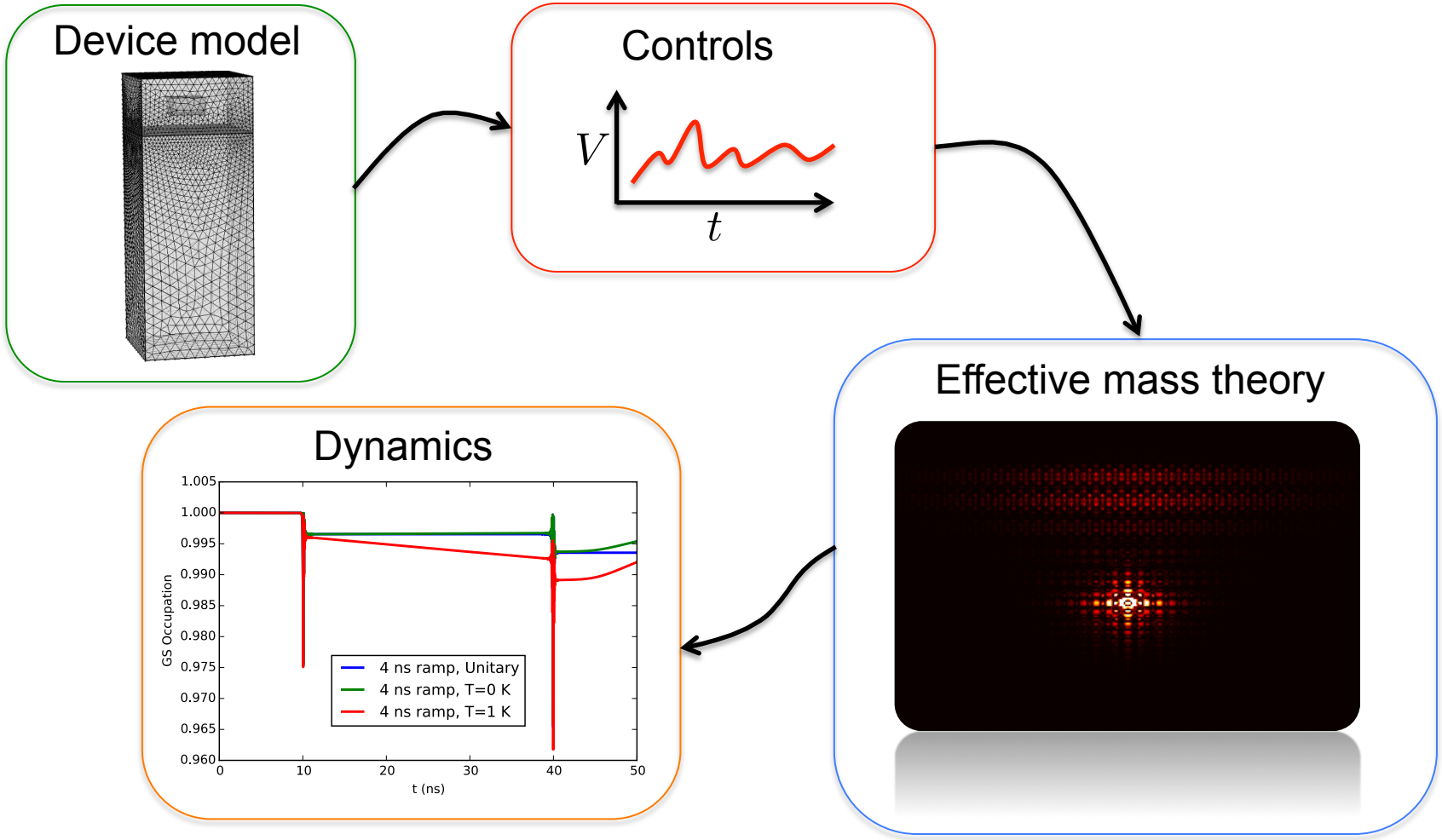


Summary



Collaborators:

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Adam Frees – *Univ. Wisconsin-Madison*

Thank you!