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Towards analog quantum simulation of strongly correlated electron systems with lithographic quantum dots

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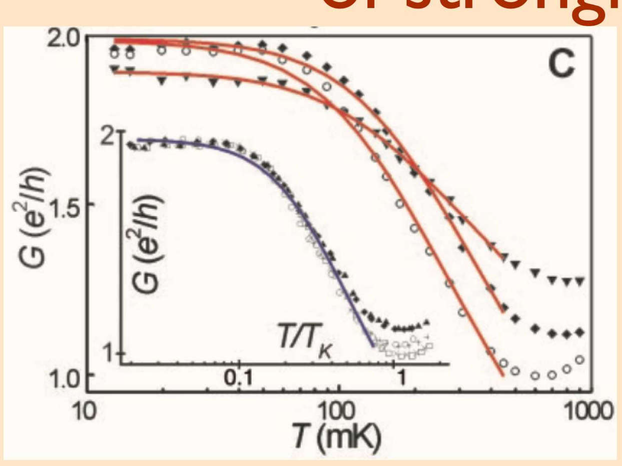
Motivation

Analog Quantum Simulation

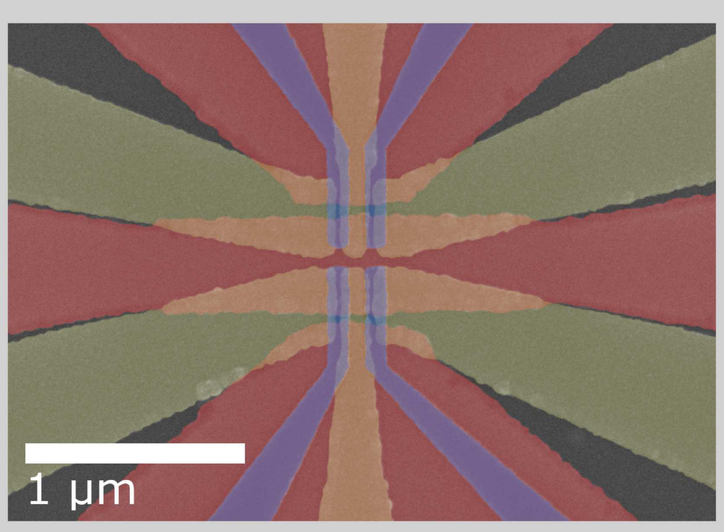
Exact simulation of correlated quantum systems can be prohibitively difficult. However, fabrication and control of quantum systems has come to the point where we can consider attempting to imitate one quantum system with a precisely controllable engineered one that has a similar Hamiltonian – this is known as analog quantum simulation. [1]

Could quantum dots (QDs) be used for analog simulation of strongly correlated electron systems?



- QDs have already been shown to exhibit the Kondo effect in transport experiments (left, [2])
- This exemplifies their relation to the Anderson impurity model (AIM)
- Can we combine measurement and feedback to simulate the AIM for dynamical mean-field theory?

Model



Devices being modeled

- Calculations here are based on a Ge hole QD design developed at Sandia (left, [3])
- We are developing tools to model these devices so we can implement analog quantum simulation

Effective mass equations and simulation of quantum dots

The wavefunction of a quantum dot is calculated using an effective mass equation, which encodes details of the underlying material.

$$\left(\sum_{\mu,\nu} \frac{\hat{p}_\mu \hat{p}_\nu}{2m_{\mu\nu}} + \hat{V}\right) F = EF$$

These equations are solved using a discontinuous Galerkin (DG) discretization in our code, Laconic. DG methods use localized basis functions that can differ between mesh elements based on local physics, e.g. evanescent tails at a material interface.

Infinite elements in Discontinuous Galerkin methods

Simulation of open systems can be done using infinite elements. These elements can accurately encode complex bath modes without a large increase in computational difficulty.

Complex exponentials with Laguerre polynomials can represent many different plane waves using a single basis. [6,7]

$$u_n(x) = \sqrt{-2i\kappa_\circ}\, e^{i\kappa_\circ x} L_n(-2i\kappa_\circ x)$$

$$e^{ikx} \propto \sum_{n=0}^{\infty} \left(\frac{k-\kappa_\circ}{k+\kappa_\circ}\right)^n u_n(x)$$

Anderson Impurity Model

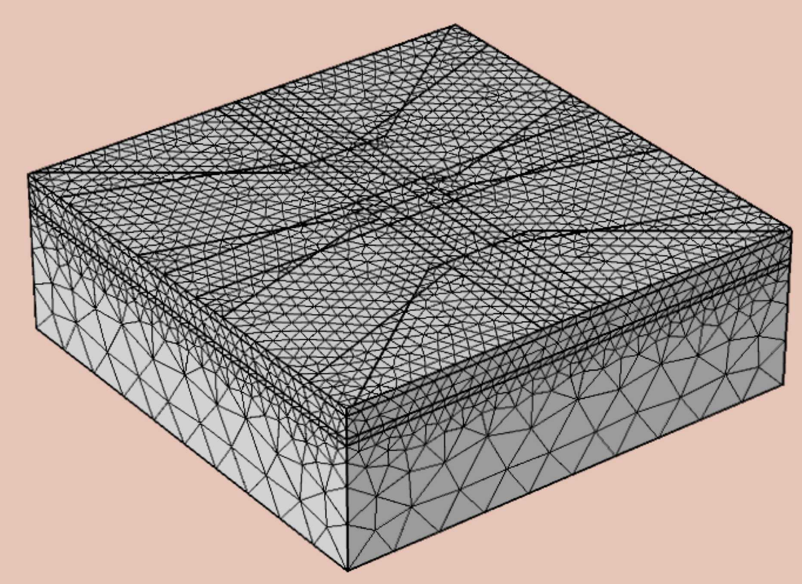
$$\hat{H}_{AIM} = \sum_{\sigma j} \epsilon_{\sigma j} \hat{c}_{\sigma j}^\dagger \hat{c}_{\sigma j} + \sum_j U_j \hat{n}_{\uparrow j} \hat{n}_{\downarrow j} + \sum_{\sigma j k} t_{\sigma j k} \hat{c}_{\sigma j}^\dagger \hat{c}_{\sigma k} + \sum_{\sigma j k} \left(V_{\sigma j k} \hat{c}_{\sigma j}^\dagger \hat{d}_{\sigma k} + h.c.\right)$$

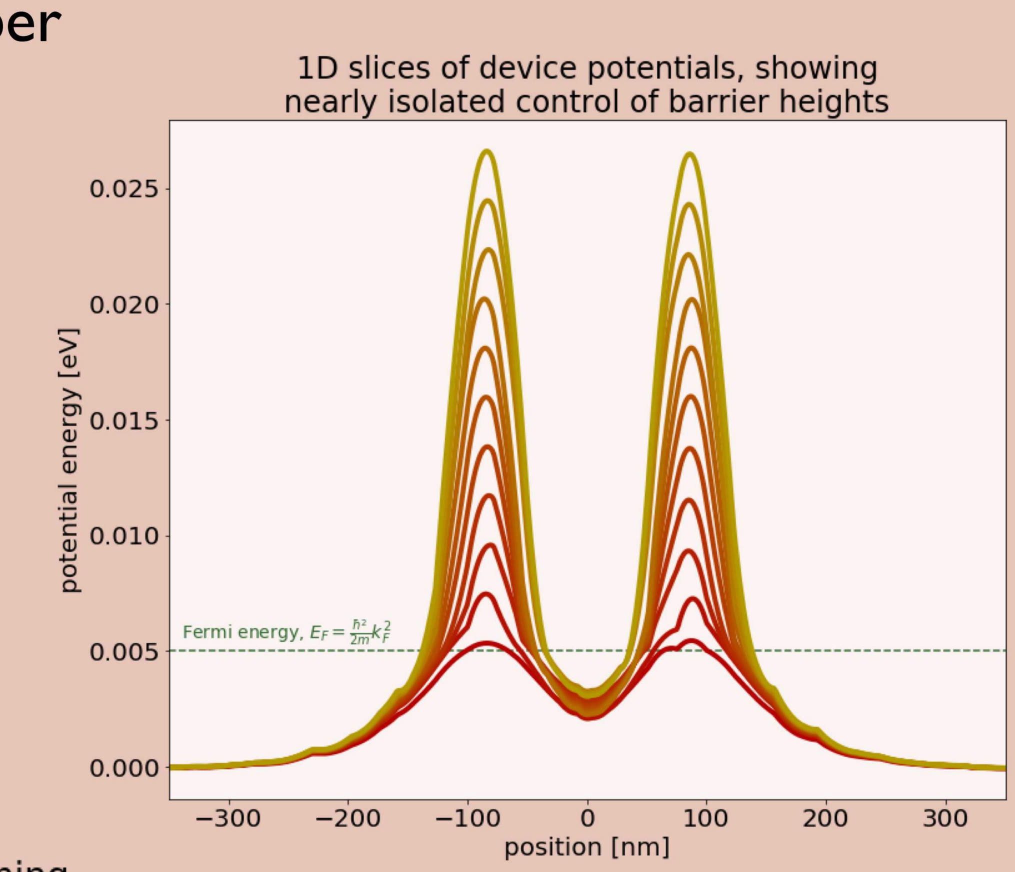
The AIM is a natural way to describe quantum dot systems, with fermionic operators of the impurity corresponding to the electrons on the dot, the $\hat{c}_{\sigma j}$s, and the bath operators corresponding to the leads, the $\hat{d}_{\sigma j}$s. Prior to this work, Laconic could compute all the coefficients but the $V_{\sigma jk}$s for most systems – the infinite elements will give it this functionality.

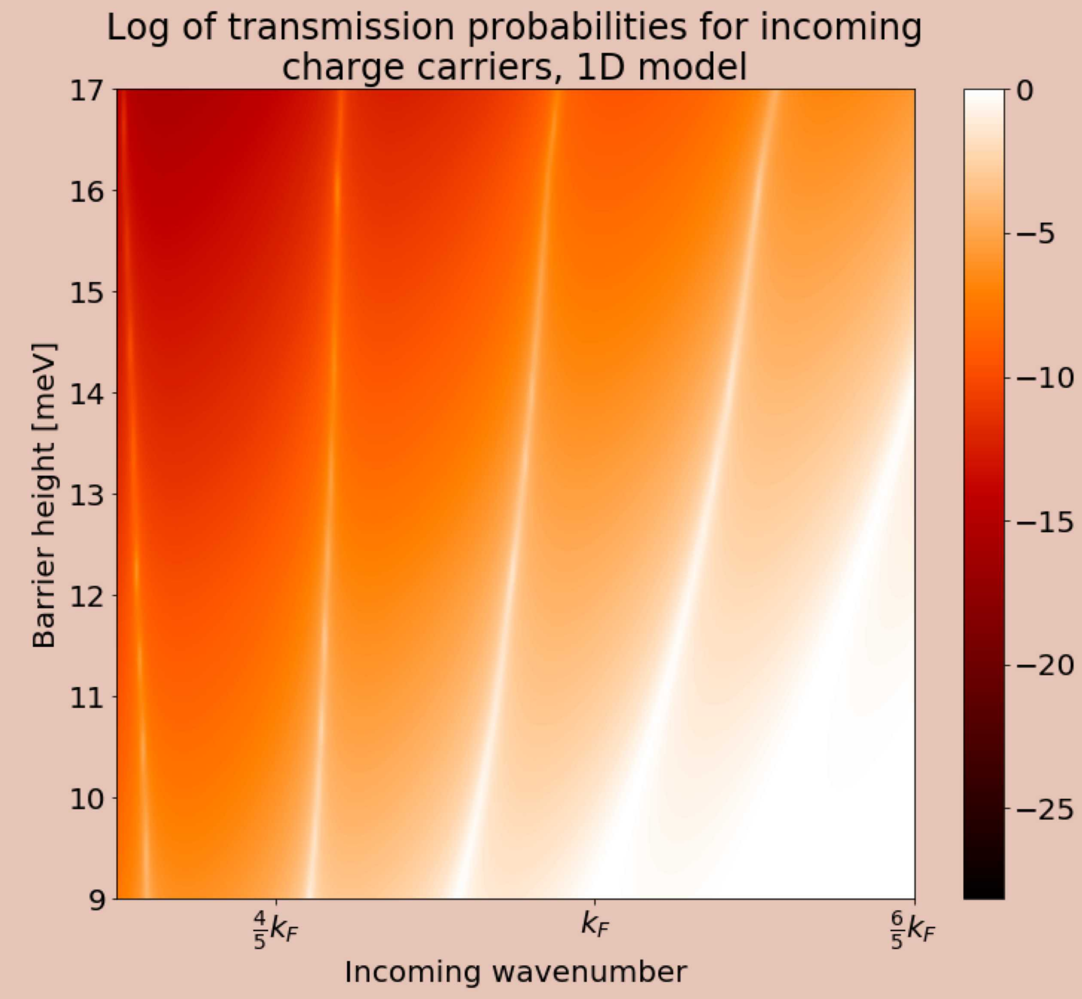
Results

Device control

- Can we adjust AIM parameters of a quantum dot separately?
- Device potentials are calculated using COMSOL
- Sweeps of gate voltages showed aspects of the potential could be controlled nearly independently
  - Dot to lead potential difference
  - Dot occupation number
  - Barrier heights





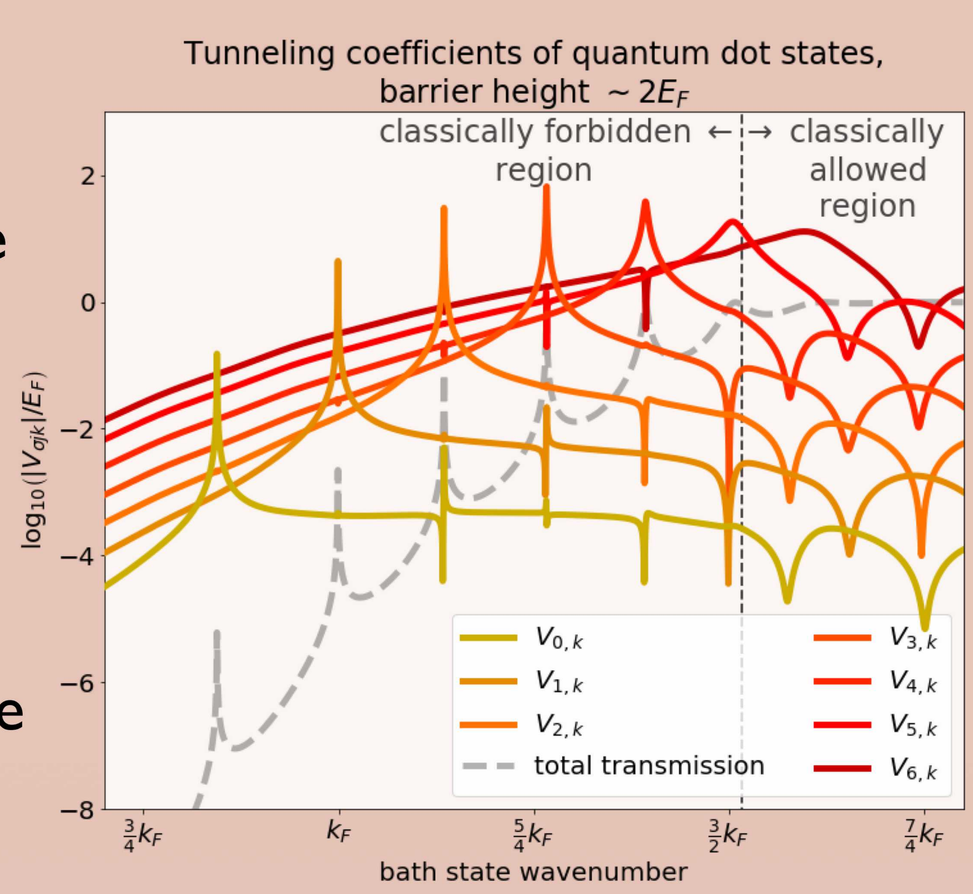


Transmissions through the quantum dot

- Infinite elements are used to calculate transmission probabilities for electrons through the QD potential
- Calculations show an exponential sensitivity of transmission probability to the barrier heights

Tunneling coefficients for quasi-bound states

- Transmission calculations can be extended to get tunneling between QD and leads ($V_{\sigma jk}$)
- Spikes in transmission correspond to resonances with specific states
- Dips in tunneling coefficients line up with resonances of higher level states of similar parity



References

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