Computational design and optimization of nanoscale spintronic and thermoelectric devices

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Overall goals of project

- **Integrate** first principles DFT calculations with many-body physics to provide a **self-consistent** description of transport in devices composed of multilayers of metals, semiconductors, insulators and correlated materials.
- Interested in **equilibrium** and **nonequilibrium** situations.
- Goal is to create a robust computational engine useful in **designing** and **testing** novel device ideas.
- Current applications are to **spintronic** and **thermoelectric** systems, but the methodology is quite general and could be applied to virtually any multilayered system.

Current research problems

- Developing linear response transport codes.
- Performing DFT calculations on magnetic nanoscale systems and interfaces.
- Constructing nonequilibrium formalisms.
- Examining Landauer-based approaches to current-induced magnetization reversal.
- Developing a theoretical description of inelastic light scattering from correlated nanostructures.

Research Personnel

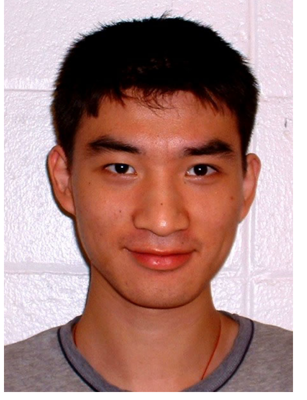
- PI’s: Jim Freericks and Amy Liu (Georgetown) and Barbara Jones (IBM)
- Postdoctoral fellows: Denis Demchenko and Volodomyr Turkowski
- Graduate Students: Ling Chen and Alexander Joura
- Domestic experimental collaborators: Stuart Parkin (IBM)
- Foreign partners: Veljko Zlatic (Croatia), Frank Steglich (Germany), Alex Hewson (England), Ralf Bulla (Germany), Tom Devereaux (Canada), and Andrij Shvaika (Ukraine)

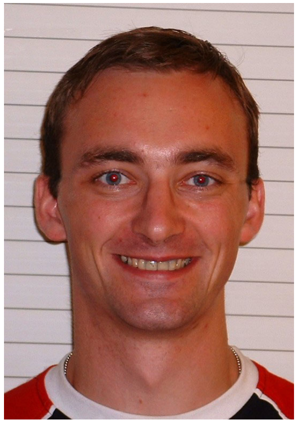
Industrial Leadership in Physics

- New Ph.D. level graduate program, started in 2001.
- Focus is on students interested in working in **industry**.
- **Physics** coursework is combined with **Business** coursework.
- A 12-month **industrial apprenticeship** is required of all students.
- Program currently has 14 students, with two involved in this NIRT project.

Industrial Apprenticeship at IBM

- Ling Chen has been working at IBM's Almaden Research Center on current-driven magnetization reversal with Barbara Jones during the 2003 calendar year.
- Alexander Joura will start working at IBM in the summer of 2004. His project will entail transport in magnetic multilayer structures useful for spintronics applications.

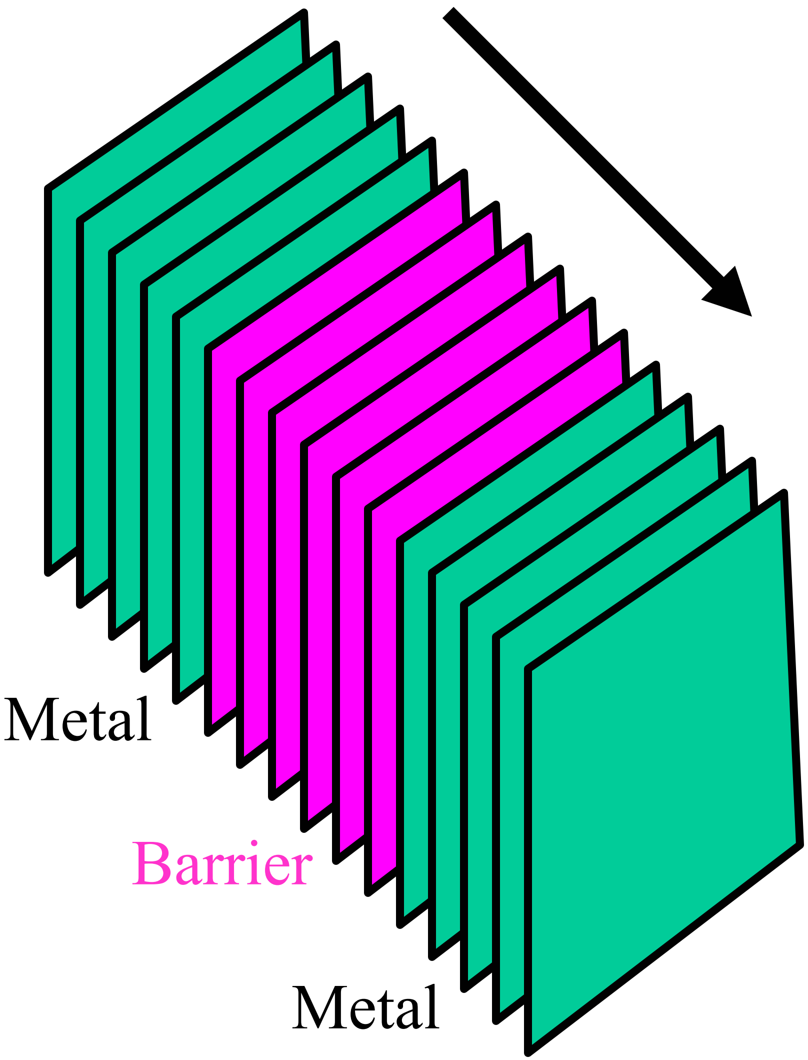




Quantum World Around Us

- A course in quantum mechanics and materials science taught to nonscientists at Georgetown.
- The curriculum is modeled on Richard Feynman's book QED, which introduces a methodology for teaching quantum mechanics using stopwatch hands and combining arrows.
- Students read materials-science-based Scientific American articles on quantum mechanics and they write a paper on Tom Stoppard's *Hapgood* (a two-slit experiment analogy made with spies).
- We are engaging in an **assessment case-study** to measure long-term learning in the course.
- Working with undergraduate researchers, we will test the understanding of the 1996 Scientific American article "Quantum Seeing in the Dark" loosely based on the two-slit experiment.

Tunnel junctions in electronics

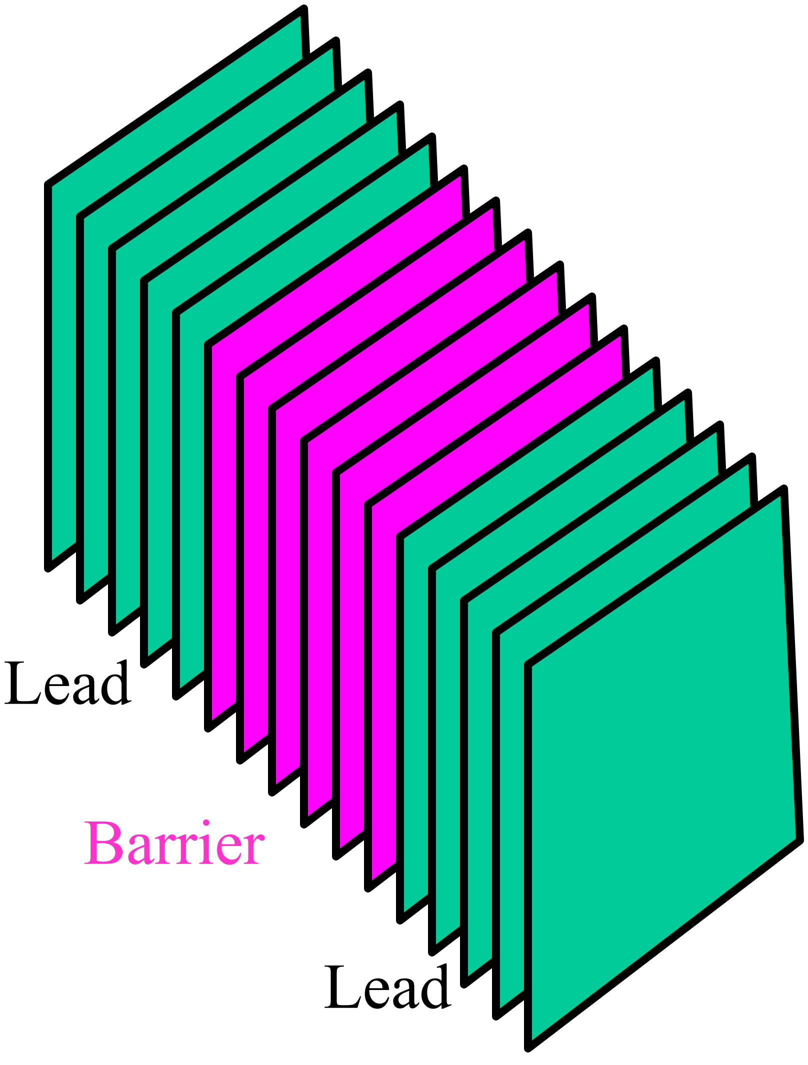


- Sandwich of metal-barrier-metal with current moving perpendicular to the planes
- Nonlinear current-voltage characteristics
- Josephson junctions, diodes, spintronic devices, etc.
- Band insulators: AlO_x MgO
- Correlated materials: FeSi, $SrTiO_3$
- Near MIT: V_2O_3, Ta_xN

Need a theory that can incorporate all forms of transport (ballistic, diffusive, incoherent, and correlated) on an equal footing

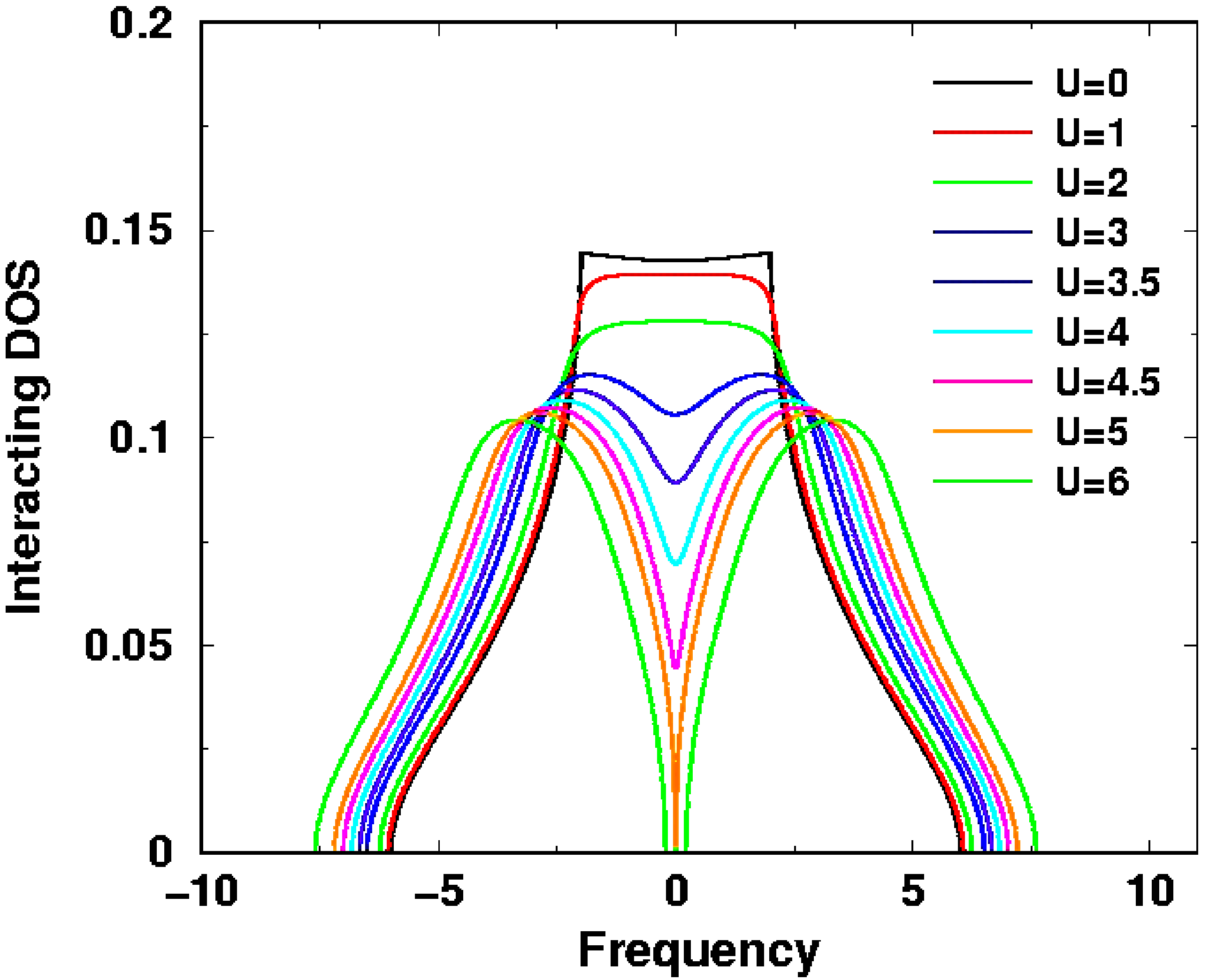
- A self-consistent recursive Green’s function approach called **dynamical mean field theory** can handle all of these wrinkles.

Our model



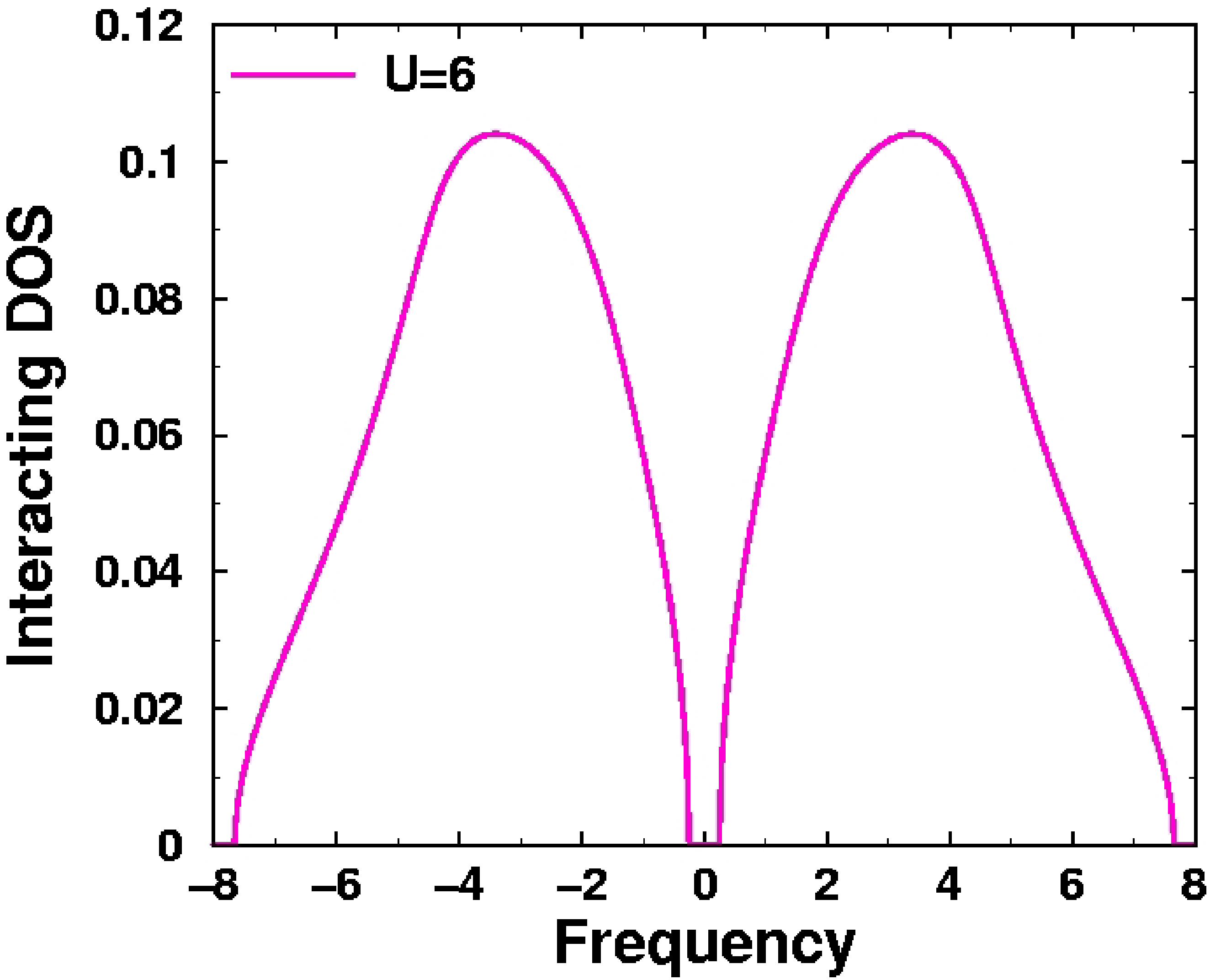
- The metallic leads can be ballistic normal metals, mean-field theory ferromagnets, or BCS superconductors.
- Scattering in the barrier is included via charge scattering with "defects" (Falicov-Kimball model)
- Scattering can also be included in the leads if desired.

Metal-insulator transition



The Falicov-Kimball model has a **metal-insulator transition** that occurs as the correlation energy U is increased. Note: the FK model is **not a Fermi liquid** in its metallic state since the lifetime of excitations is always finite.

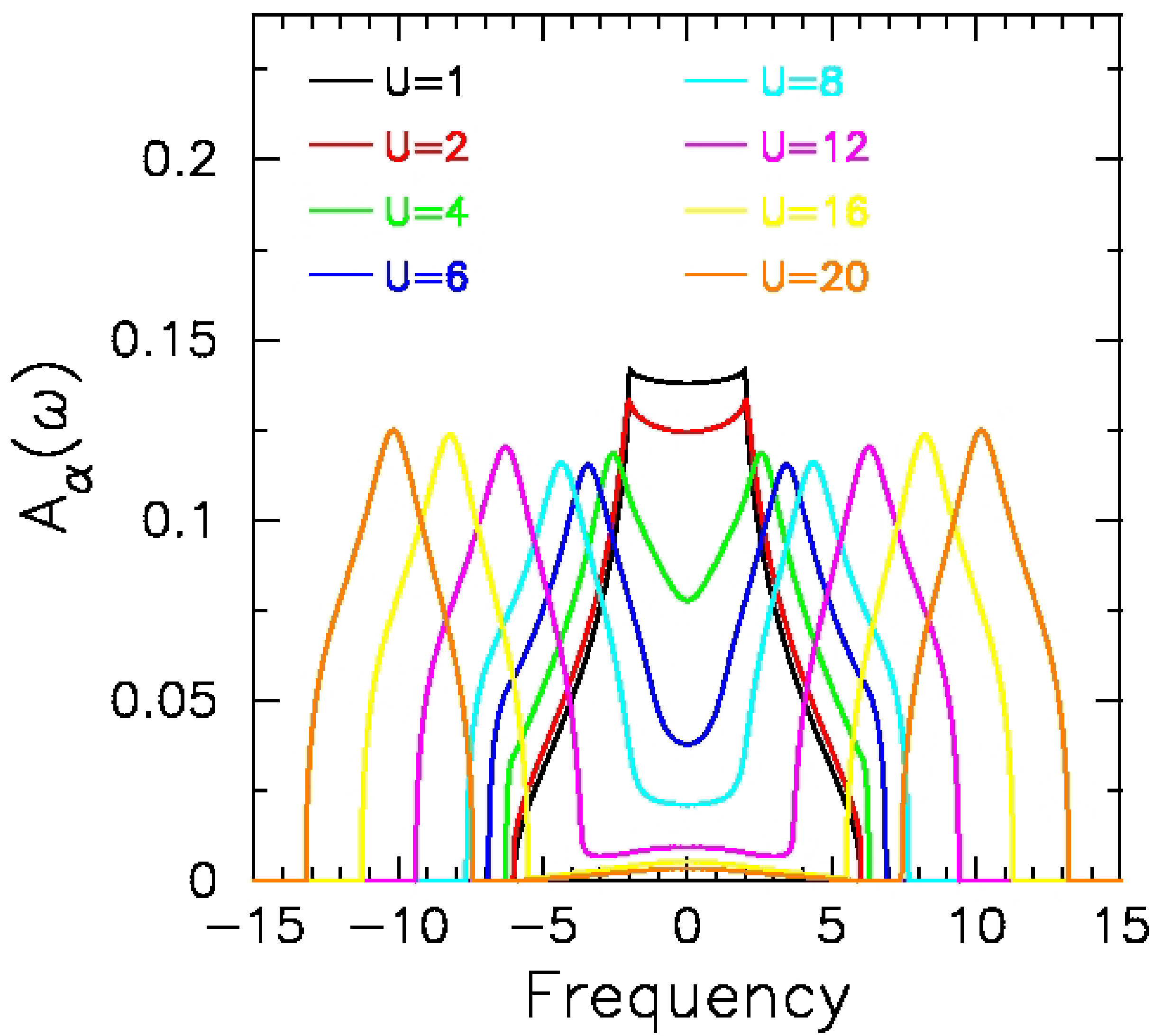
Near the MIT (U=6)



If we take t=0.25ev then W=3ev, and the gap size is about 100mev.

This is a correlated insulator with a small gap, close to the MIT.

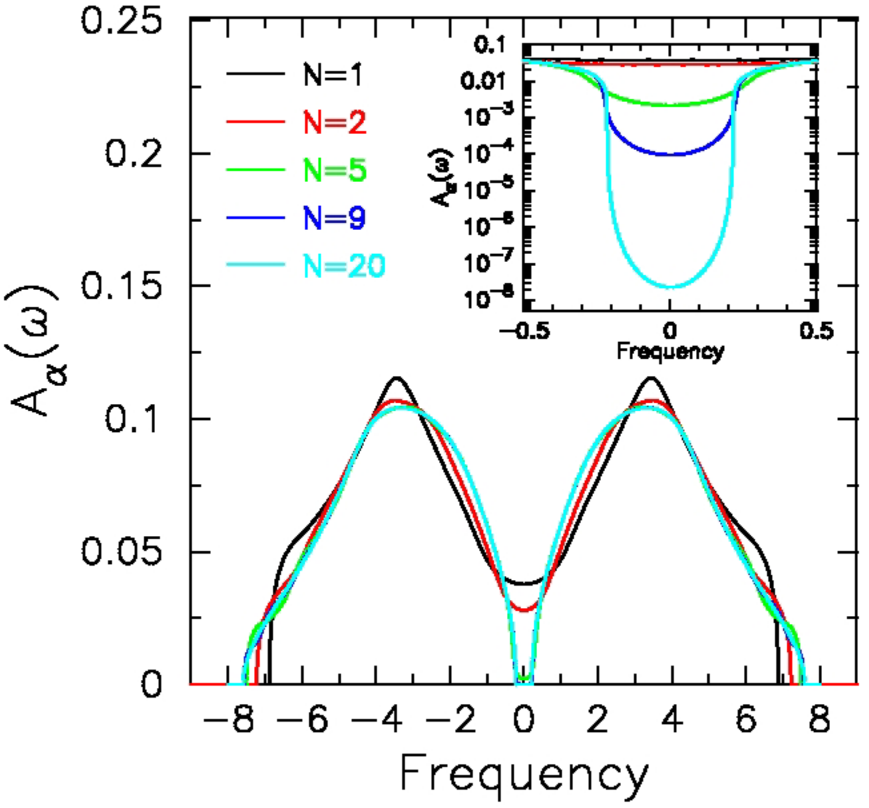
L=a (single plane barrier)

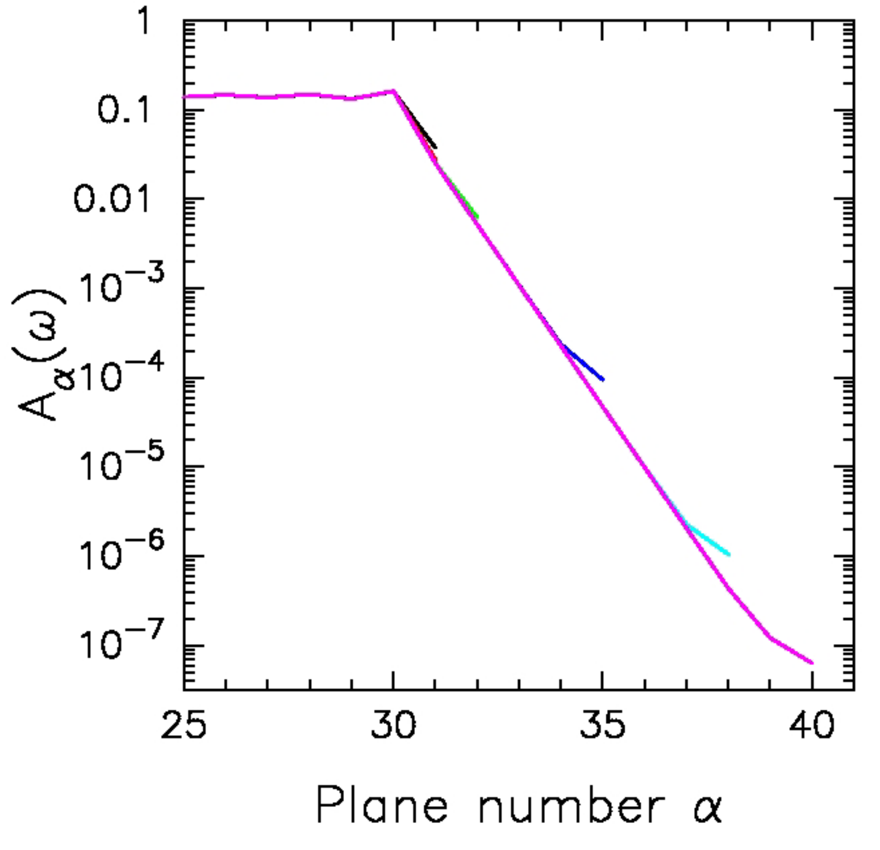


Local DOS on the central barrier plane. Note how the upper and lower Hubbard bands form for the Mott transition, but there is always substantial subgap DOS from the localized barrier states. This DOS arises from quantum-mechanical tunneling.

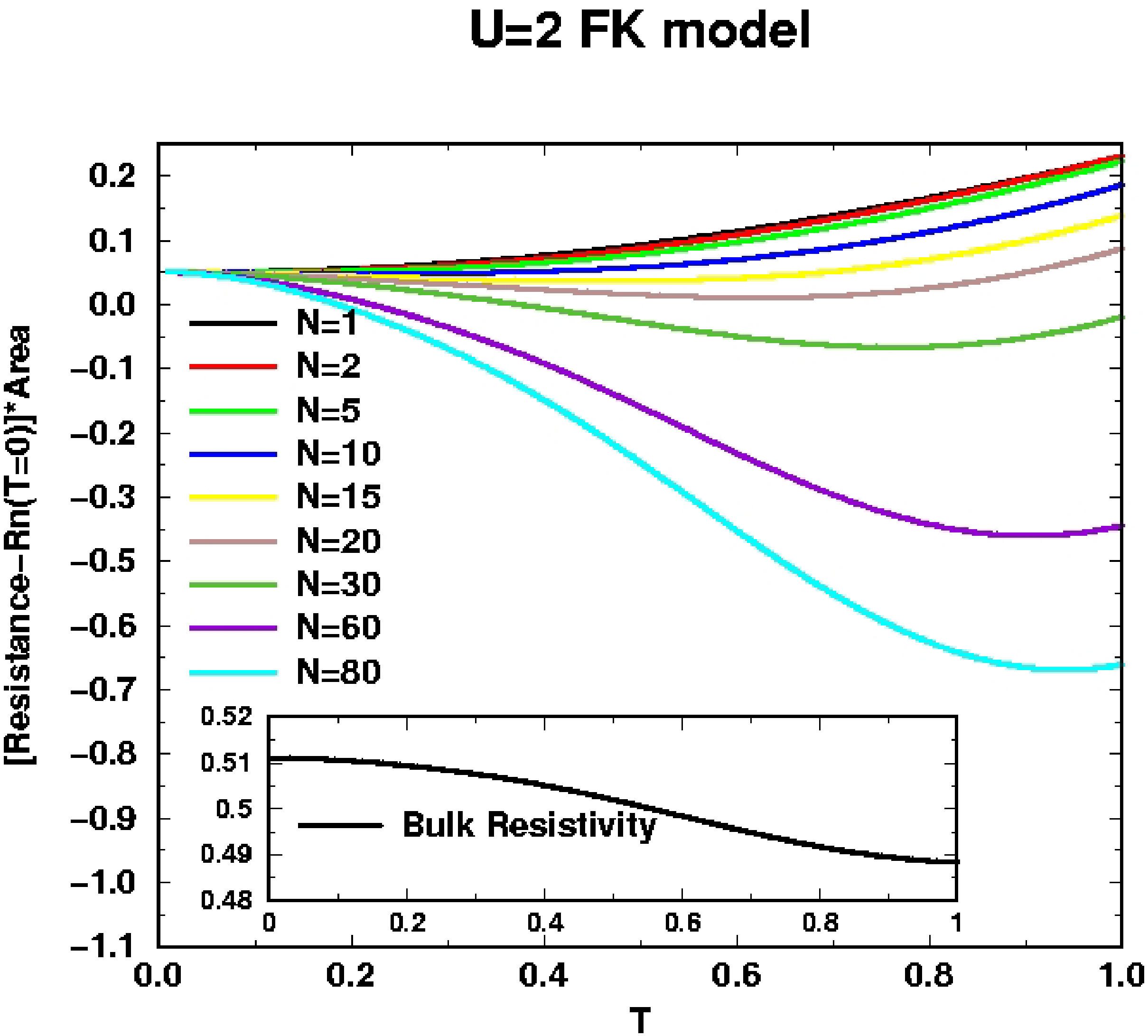
U=6 Correlated insulator

DOS has exponential tails, but never vanishes in the “gap”.





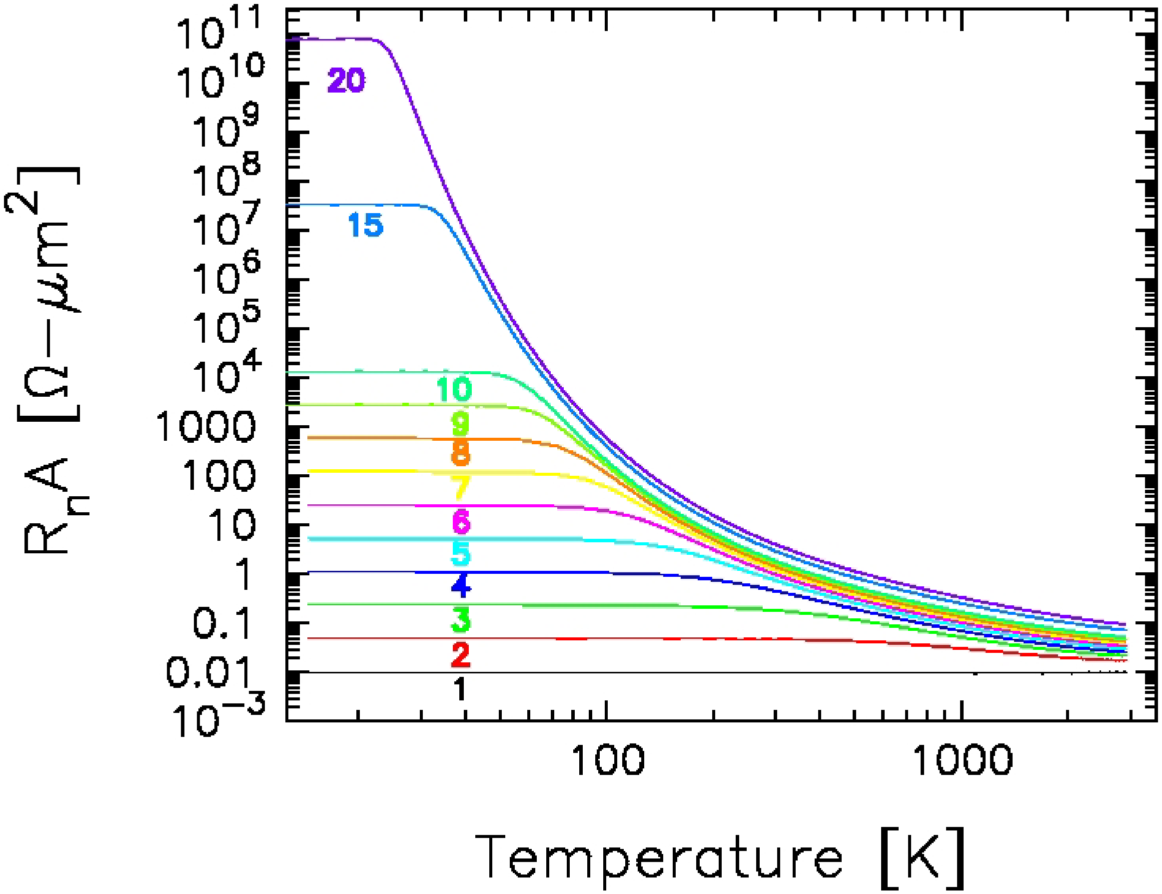
Temperature dependence (correlated metal)



- The thin barrier appears more “metallic”; as the barrier is made thicker, the resistance is equal to a contact resistance plus an Ohmic contribution, proportional to the bulk resistivity.

Resistance for U=6 (correlated insulator)

- Resistance here shows tunneling plateaus, and a strong temperature dependence in the incoherent regime.



Thouless energy

- The **Thouless energy** measures the quantum energy associated with the time that an electron spends inside the barrier region of width L (Energy extracted from the resistance).

$$E_{Th} = \hbar / t_{Dwell}$$

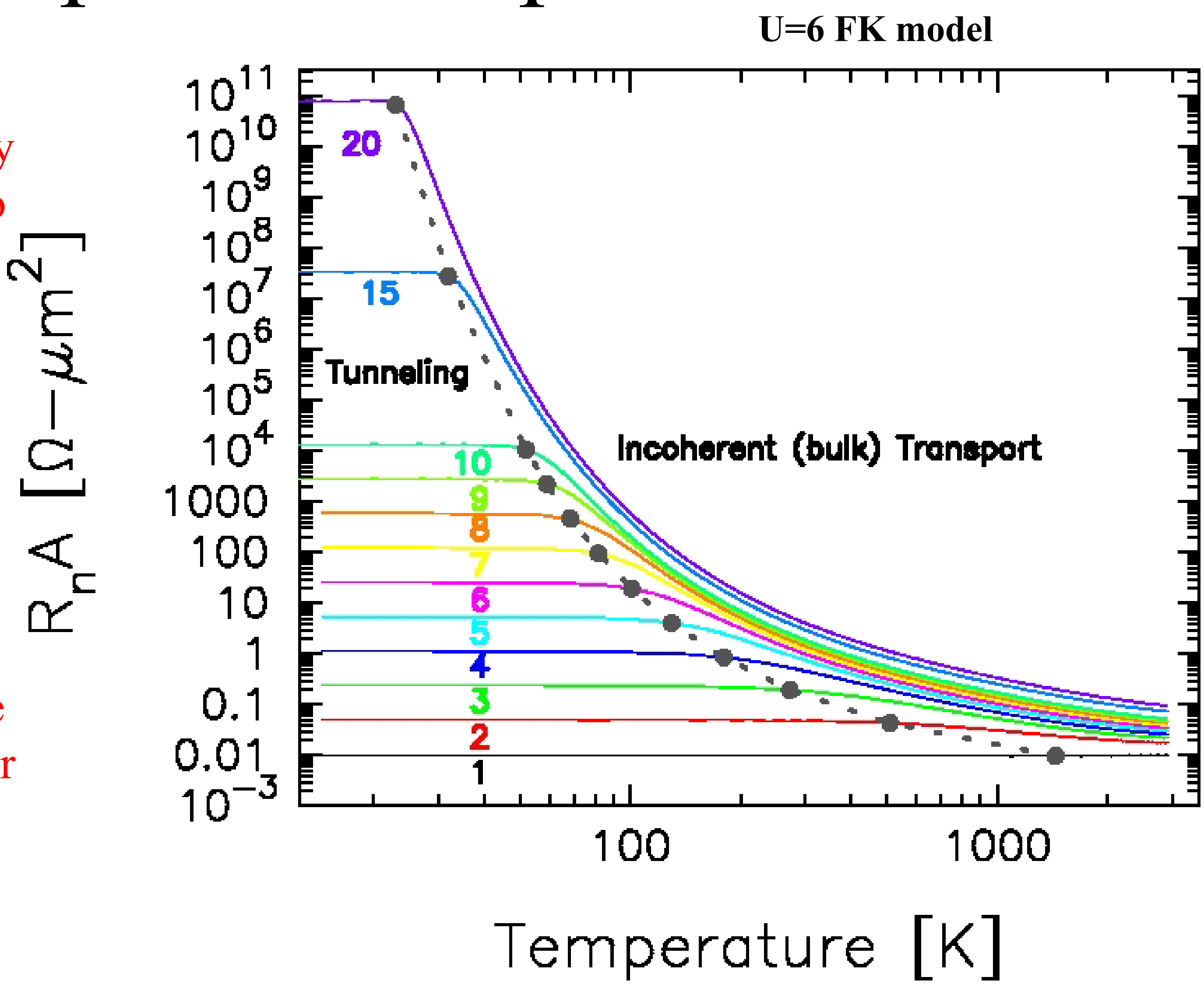
- A **unifying form** for the Thouless energy can be determined from the resistance of the barrier region and the electronic density of states:

$$E_{Th} = \frac{\hbar}{2e^2 \int d\omega N_{Bulk}(\omega) \frac{-df(\omega)}{d\omega} R_N A L}$$

- This form produces both the **ballistic** $E_{Th} = \hbar v_F^N / \pi L$ and the **diffusive** $E_{Th} = \hbar D / L^2$ forms of the Thouless energy.

Temperature dependence

The Thouless energy appears to be able to determine the transition
from tunneling to incoherent transport as a function of temperature.
Note that this temperature is not simply related to the energy gap or barrier thickness!



Future work

- Schottky barriers/charge accumulation regions.
- Magnetic leads/barriers.
- Multiband models (d-electrons/transition metals).
- Nonequilibrium formulation for current-voltage characteristics and switching dynamics.
- We can benefit from interesting data on devices like these, especially from systems constructed out of correlated materials.