Crossover from quantum mechanical tunneling to incoherent (Ohmic) transport in a strongly correlated multilayer nanostructure

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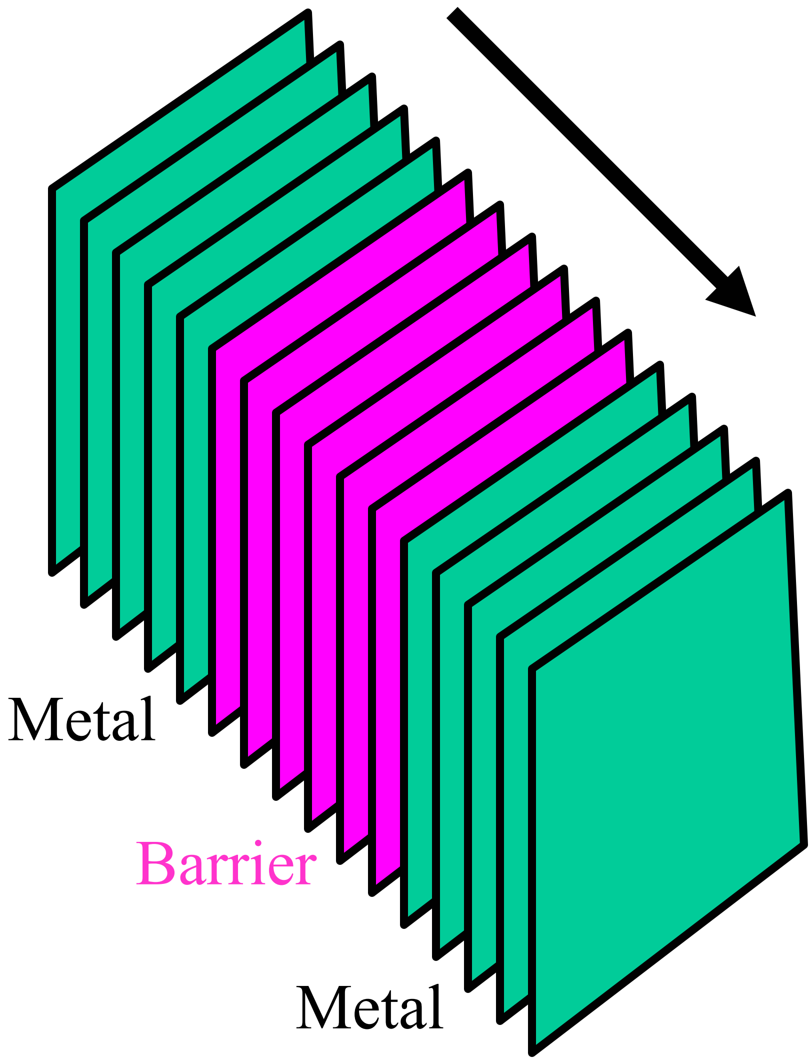
Tunnel junctions in electronics



- 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

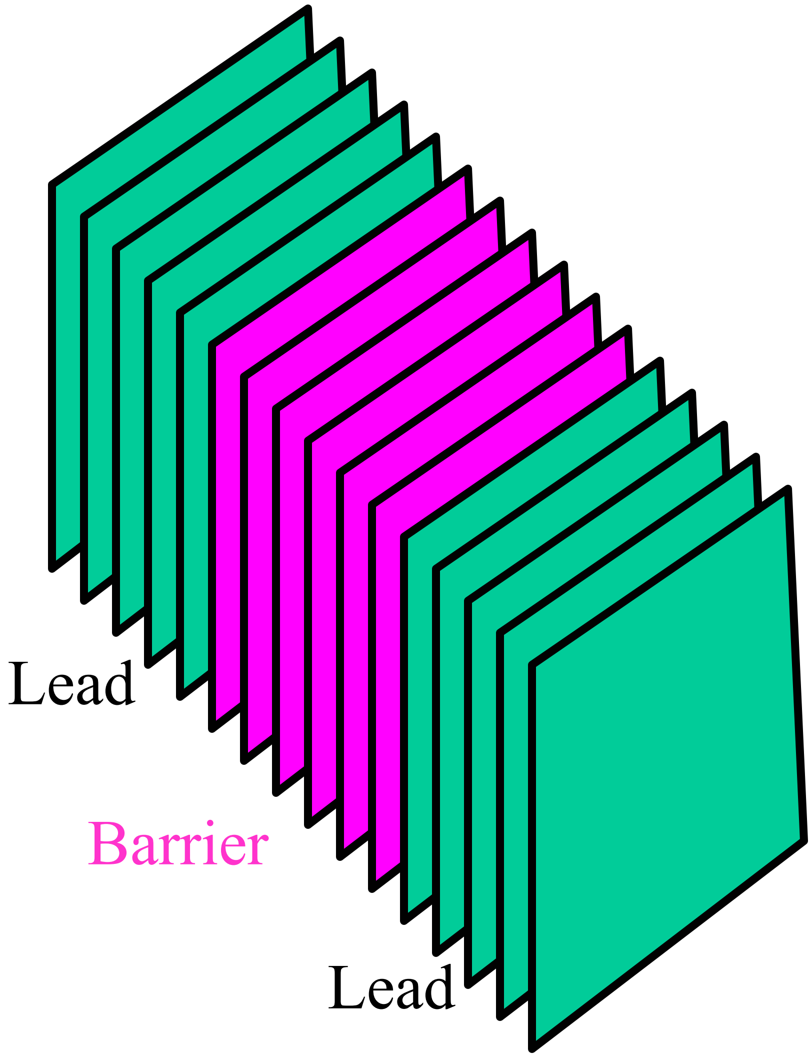
Theoretical Approaches

- Ohm's law: $R_n = \rho L/A$, holds for bulk materials
- Landauer approach: calculate resistance by determining the reflection and transmission coefficients for quasiparticles moving through the inhomogeneous device ($R_n = h[1-T]/2e^2 T$)
- Works well for ballistic metals, diffusive metals, and infinitesimally thin tunnel barriers ("delta functions").
- Real tunnel barriers have finite thickness---quasiparticle picture breaks down inside the insulating barrier.
- As the barrier thickness approaches the bulk limit, the transport becomes incoherent (thermally activated) in an insulator and is not governed by tunneling.

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

- A self-consistent recursive Green’s function approach called inhomogeneous dynamical mean field theory (developed by Potthoff and Nolting) can handle all of these wrinkles.

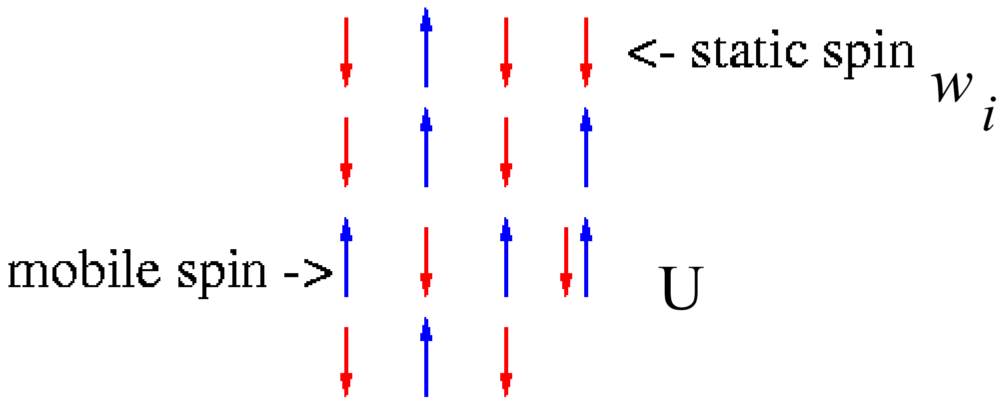
Our model



- 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, but we don't do so here.

Spinless Falicov-Kimball Model

$$H = -\frac{t}{2\sqrt{d}}\sum_{<i,j>} c_i^\dagger c_j + E\sum_i w_i + U\sum_i c_i^\dagger c_i w_i$$

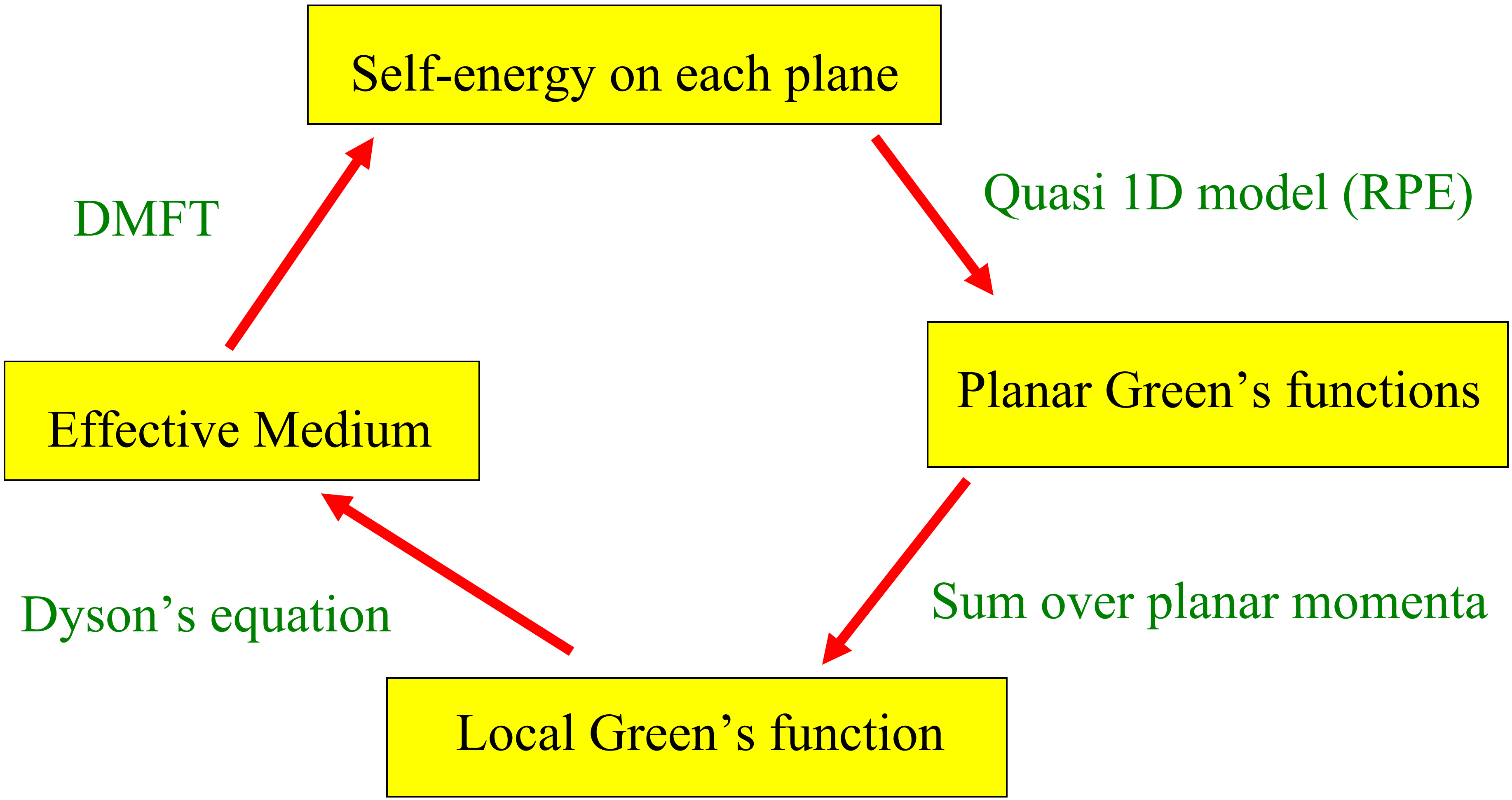


•**exactly solvable model** in the local approximation using dynamical mean field theory.

•possesses homogeneous, commensurate/incommensurate CDW phases, phase segregation, and **metal-insulator transitions**.

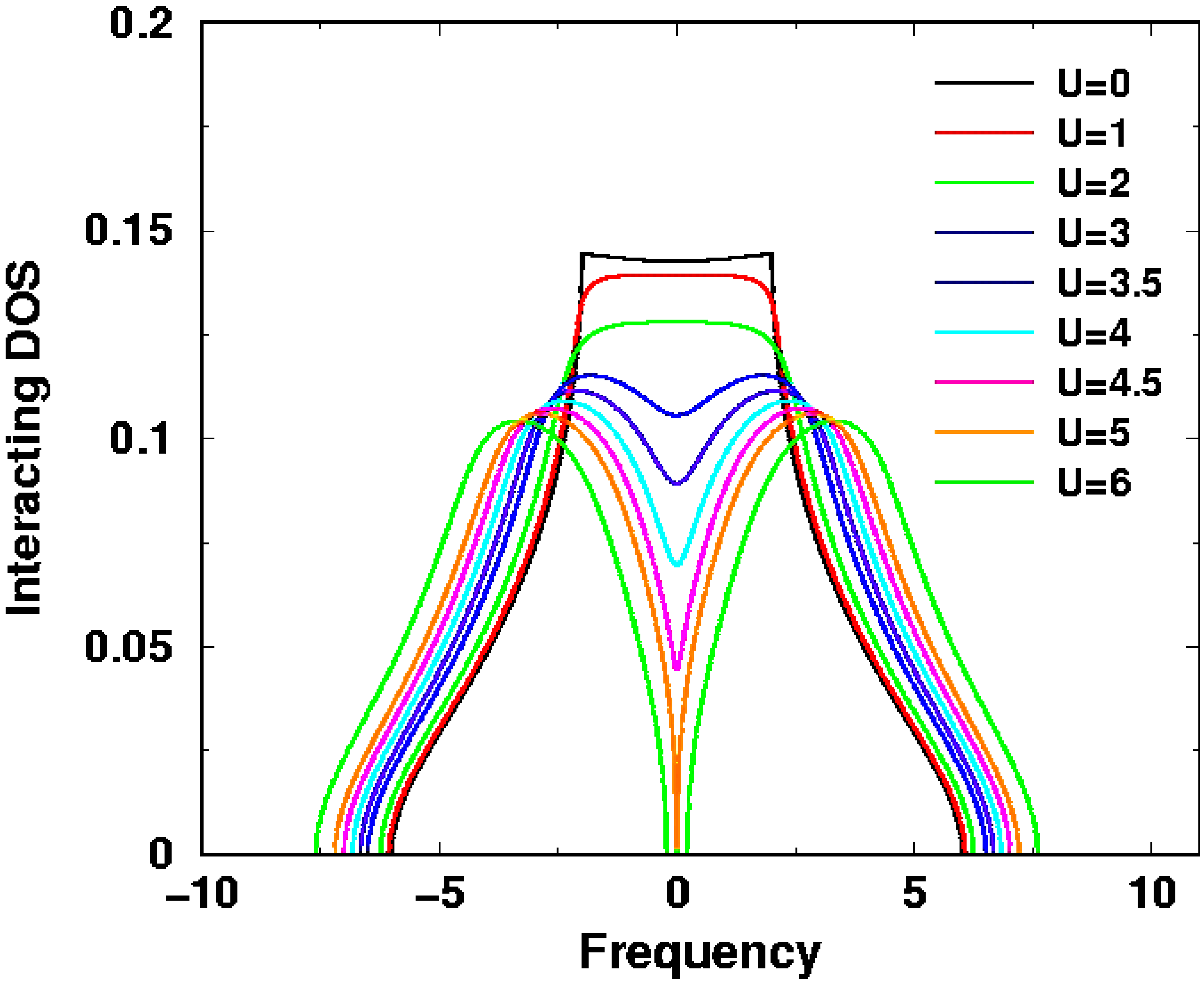
•*A self-consistent recursive Green's function approach solves the inhomogeneous many-body problem (Potthoff-Nolting algorithm).*

Computational Algorithm



Algorithm is iterated until a self-consistent solution is achieved

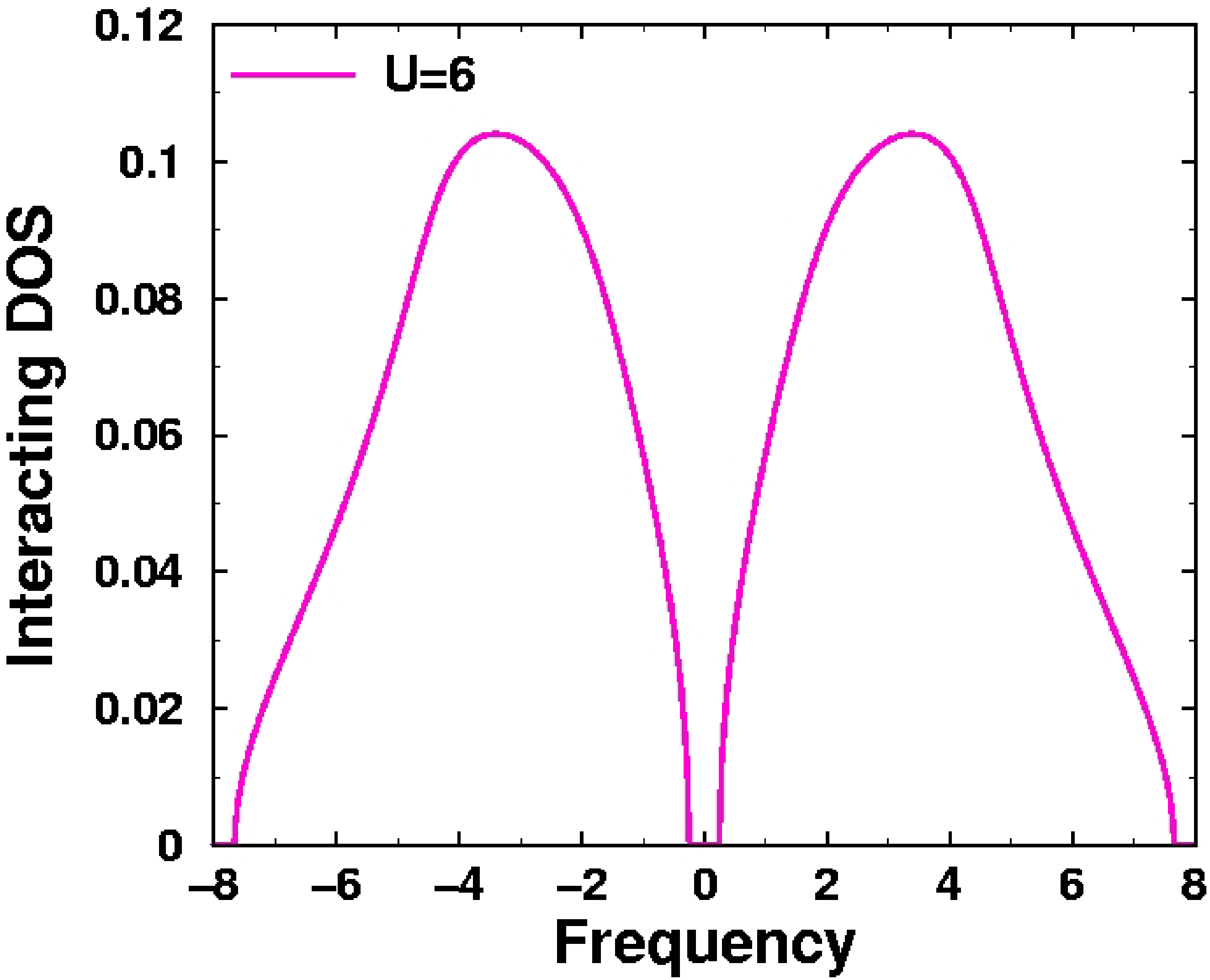
Metal-insulator transition (half-filling)



The Falicov-Kimball model has a **metal-insulator transition** that occurs as the correlation energy U is increased. The bulk interacting DOS shows that a **pseudogap** phase first develops followed by the opening of a **true gap** above U=4.9 (in the bulk).

Note: the FK model is **not a Fermi liquid** in its metallic state since the lifetime of excitations is finite.

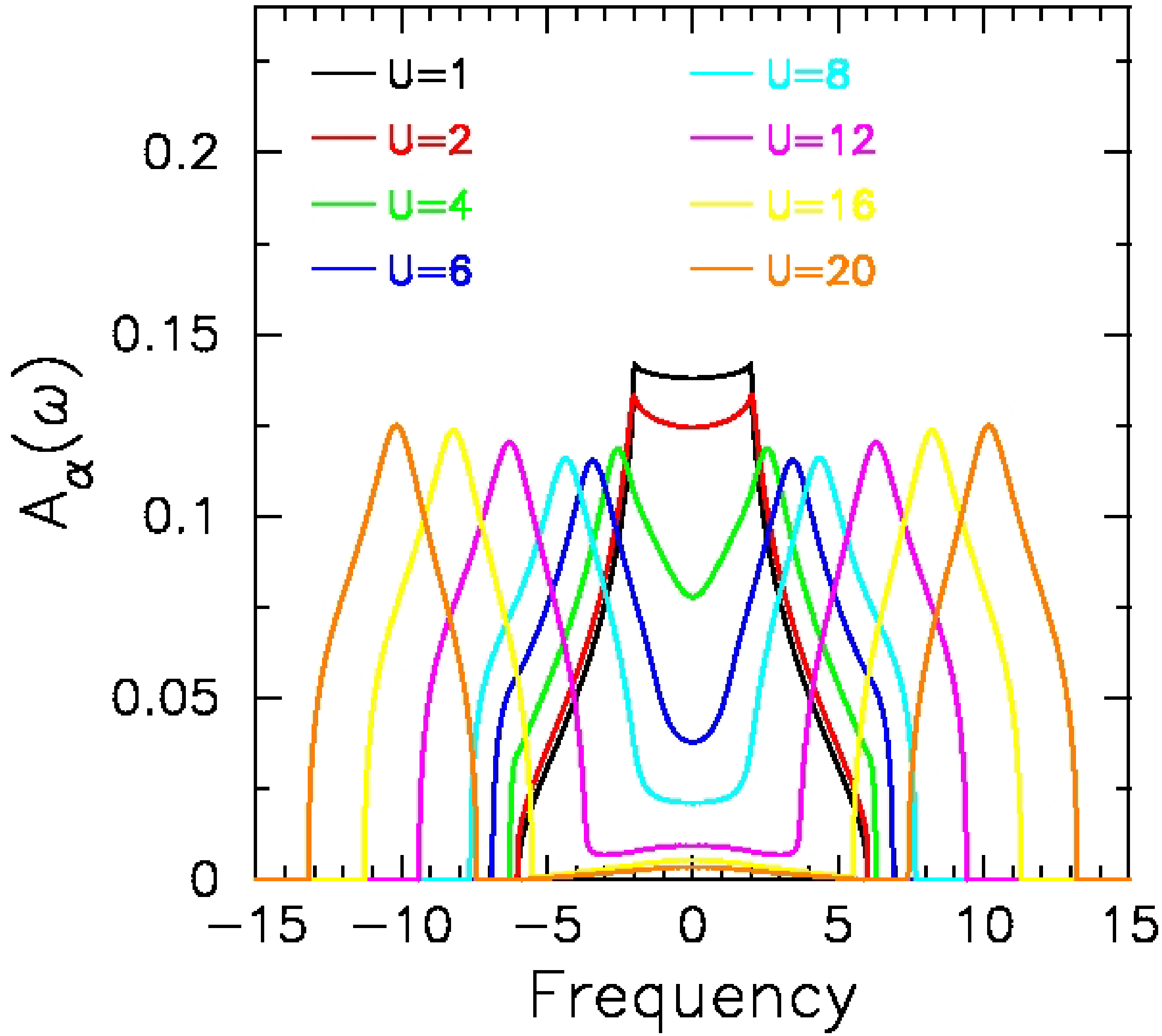
Near the MIT (U=6)



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.

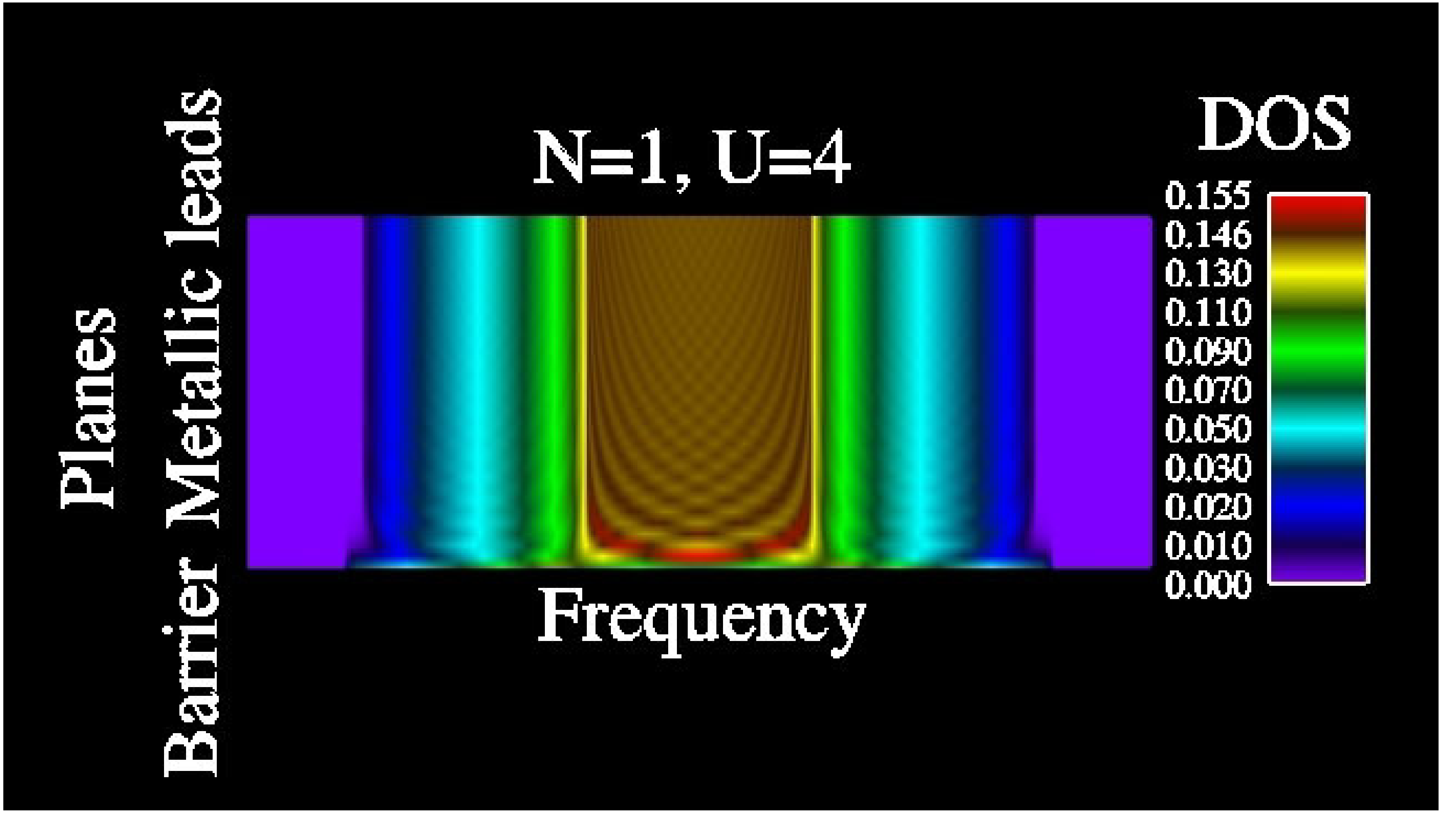
L=a (Single plane barrier)



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 and has a metallic shape.

U=4 (anomalous metal) DOS



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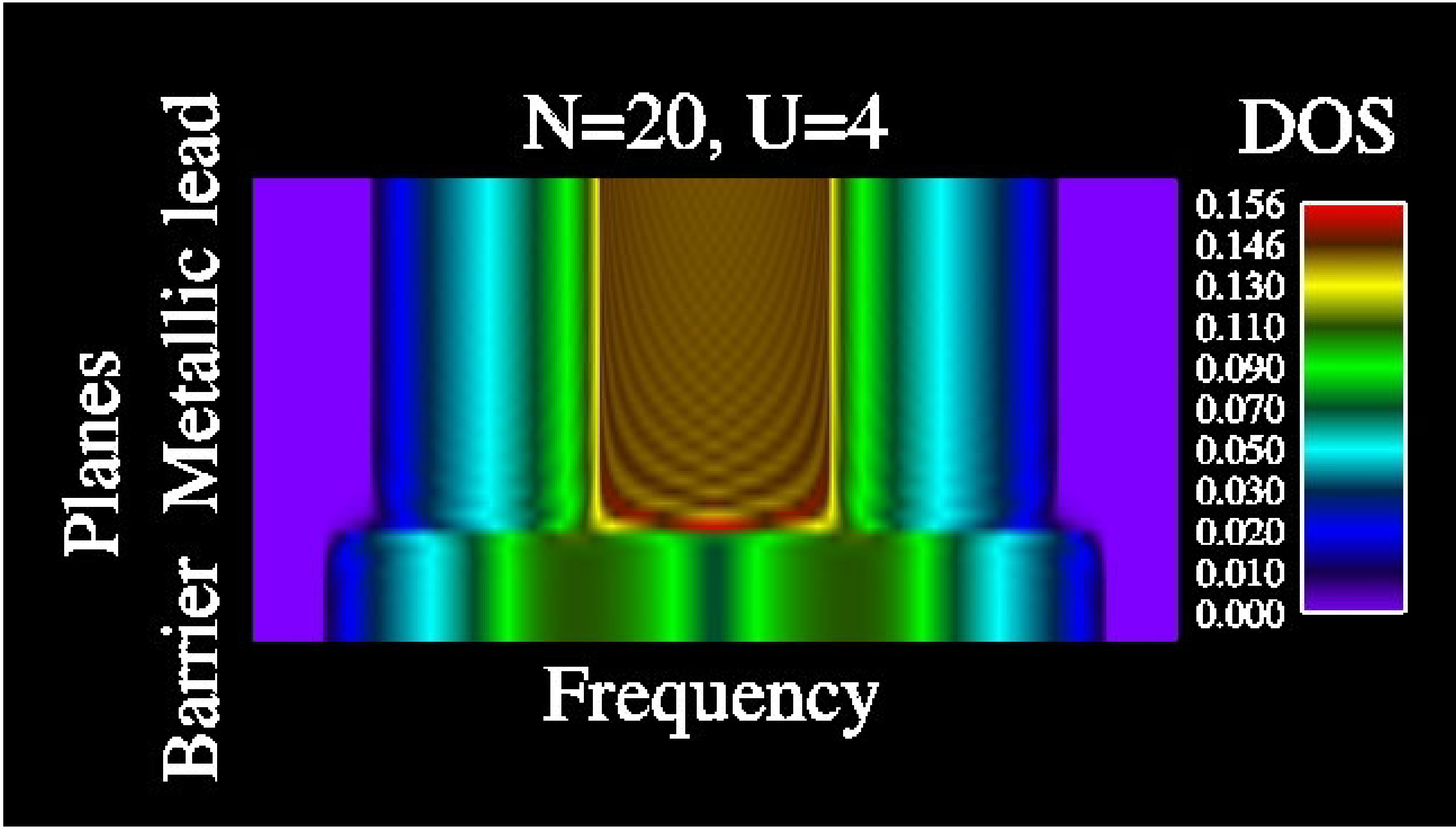
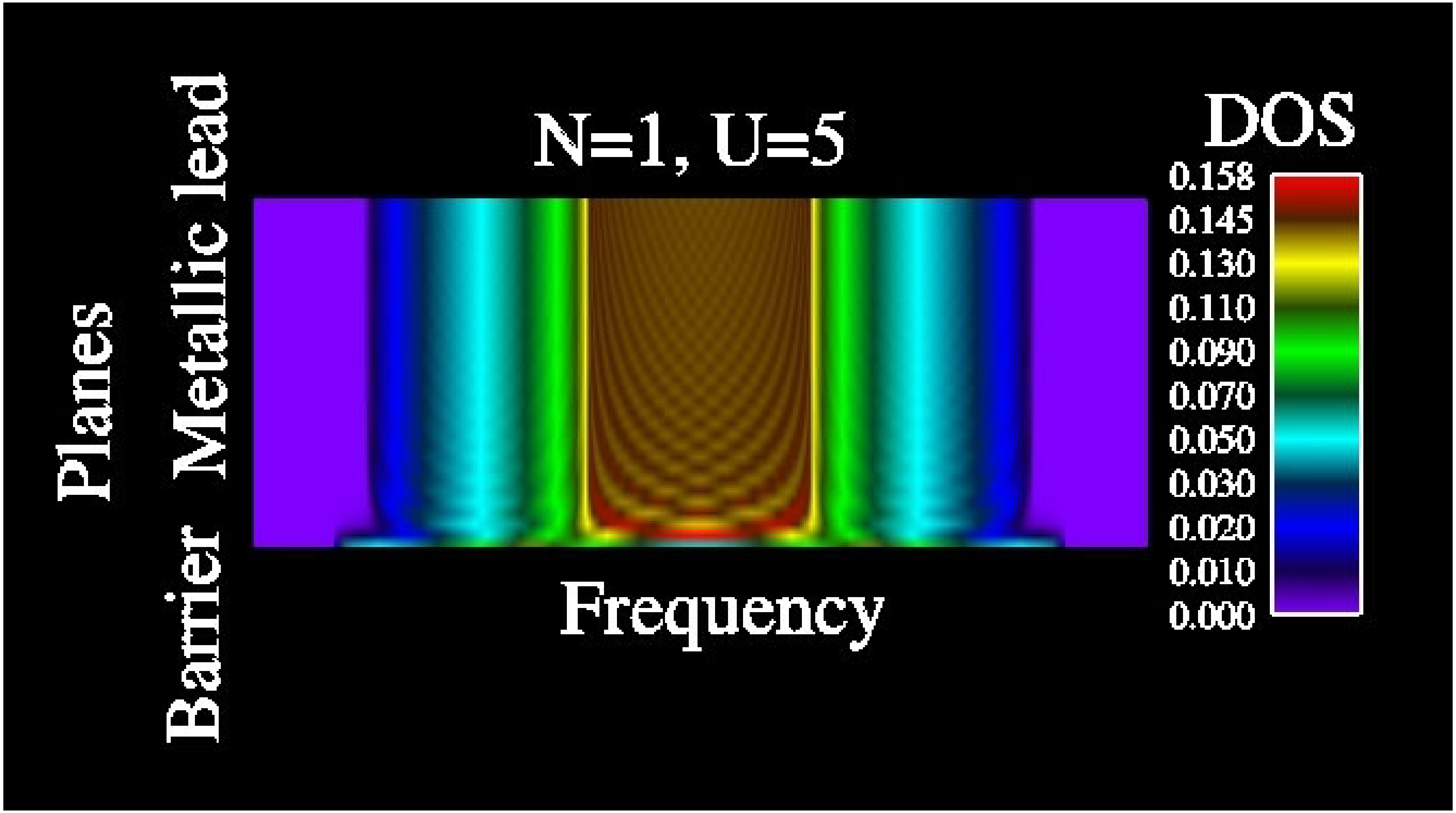


U=5 (near critical) DOS



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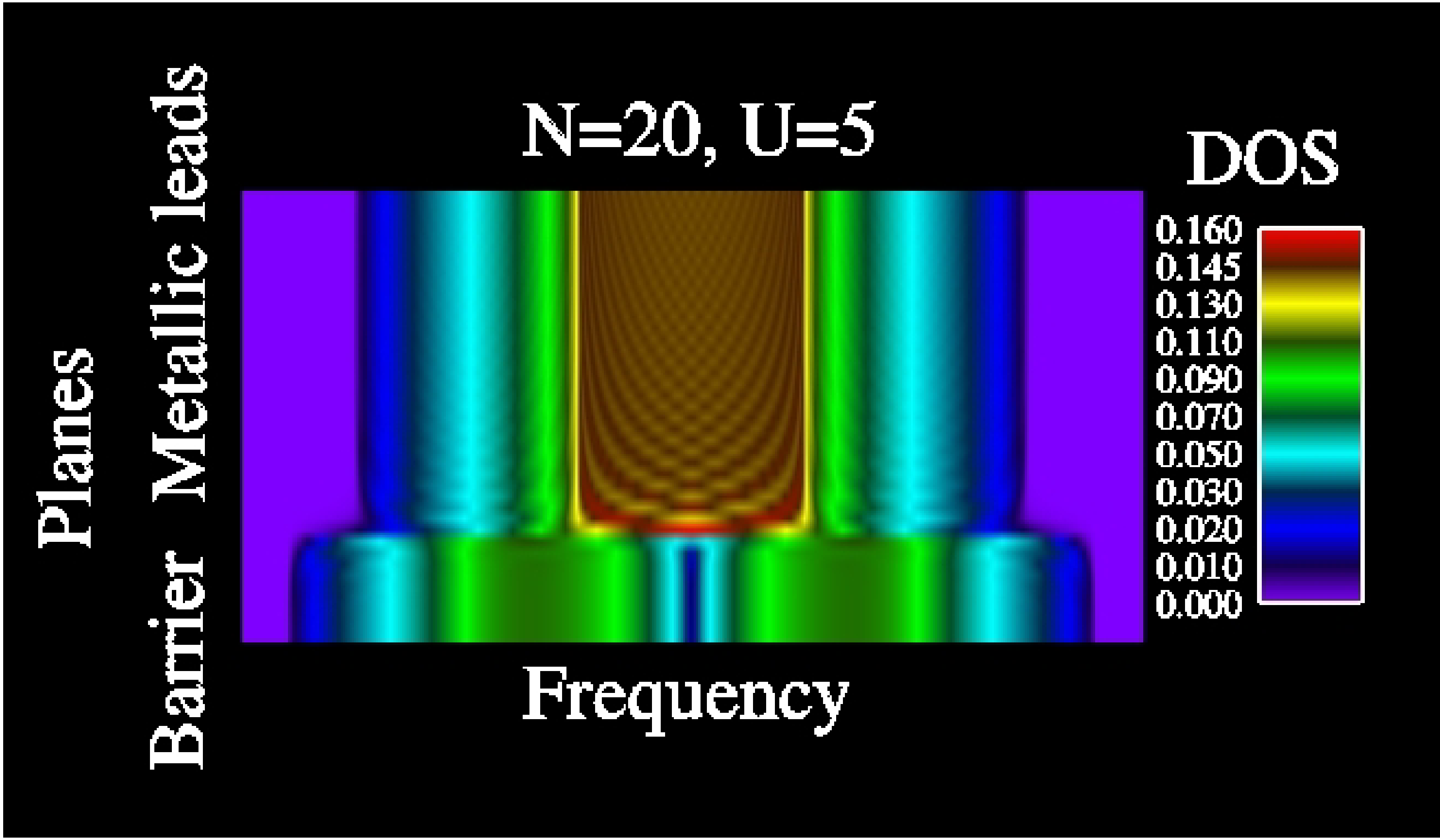
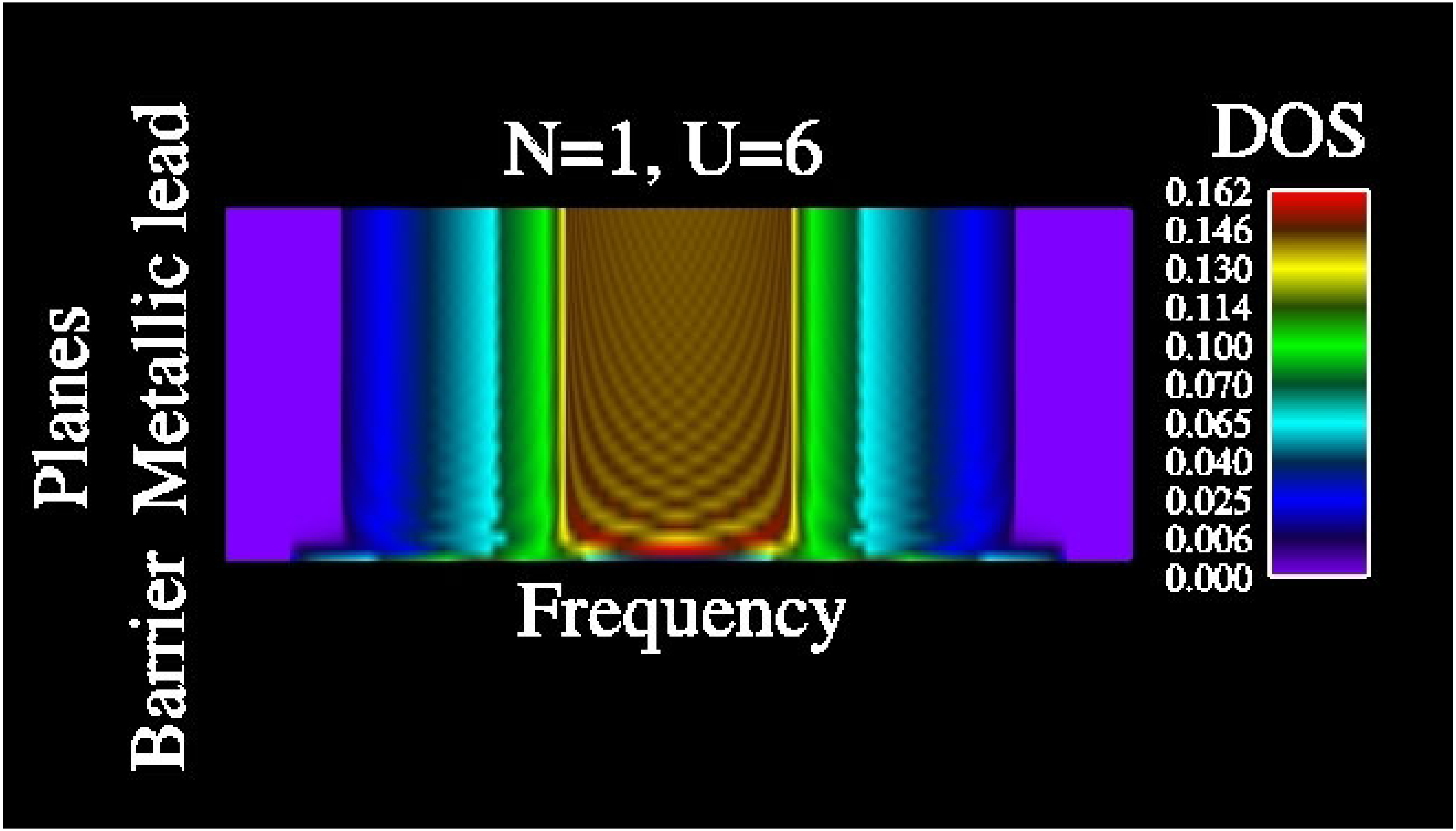
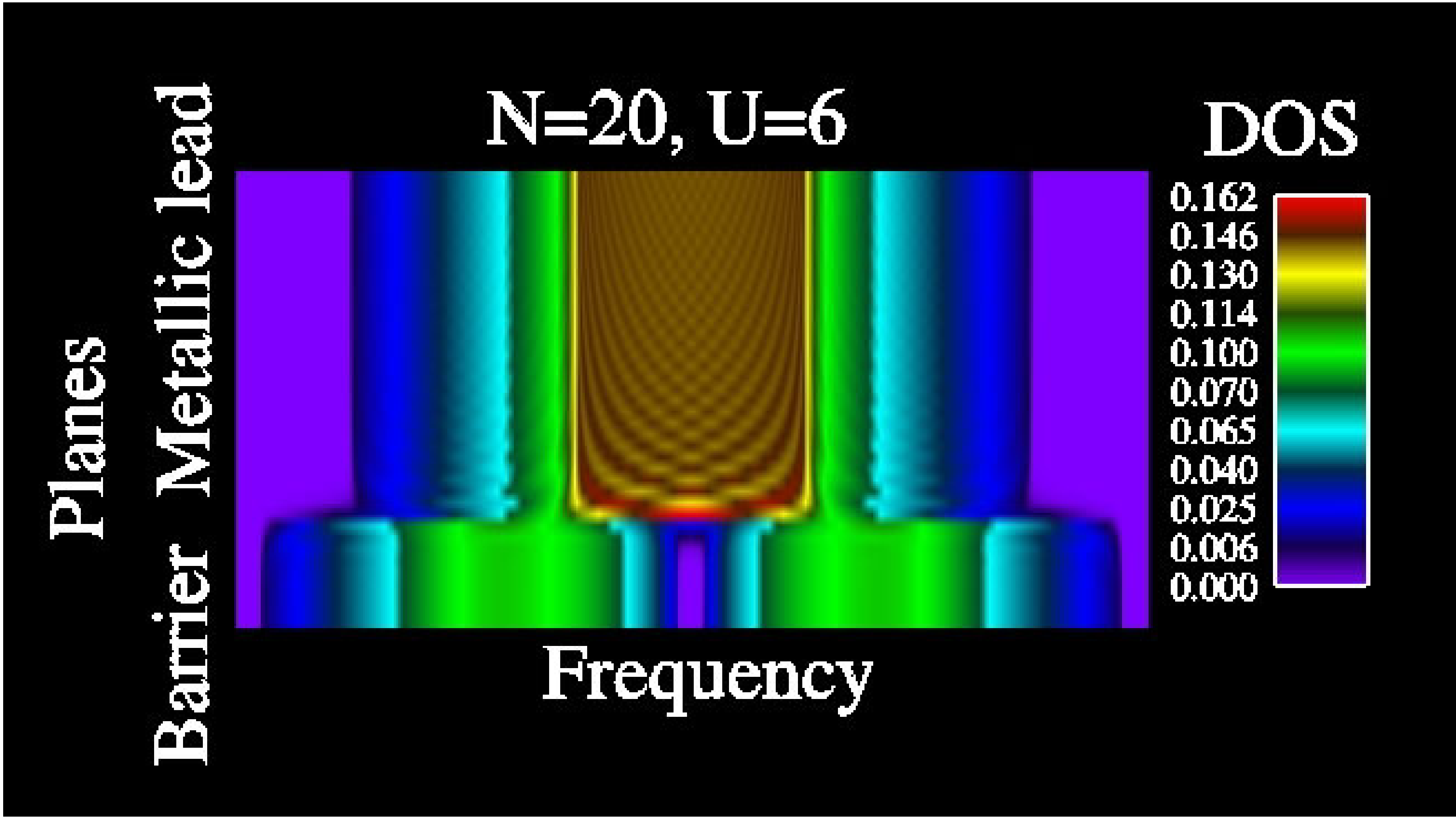


U=6 (small-gap insulator) DOS

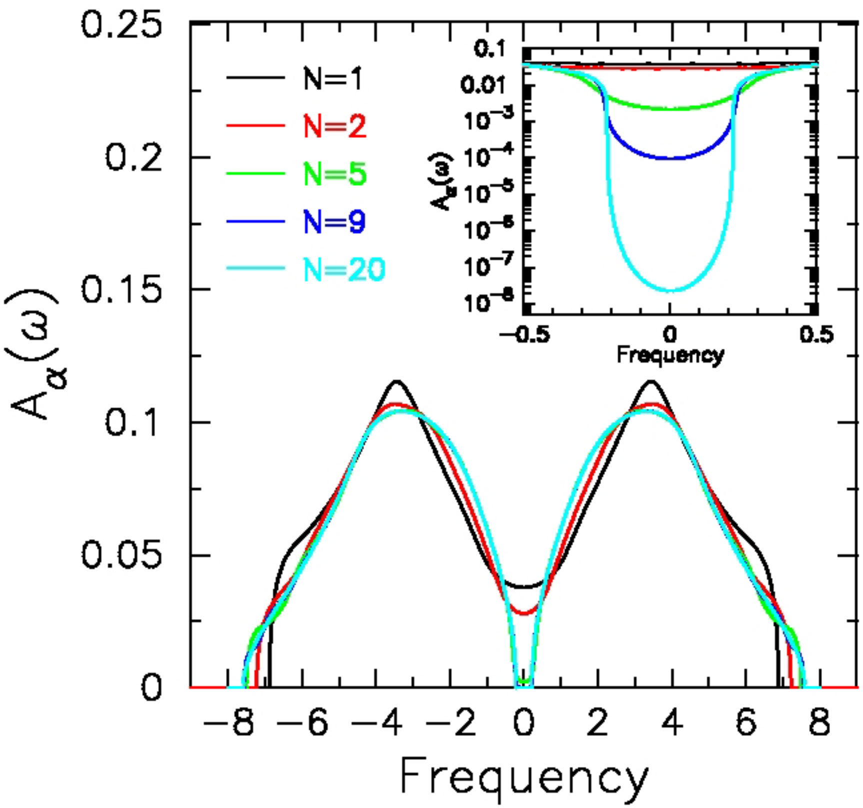


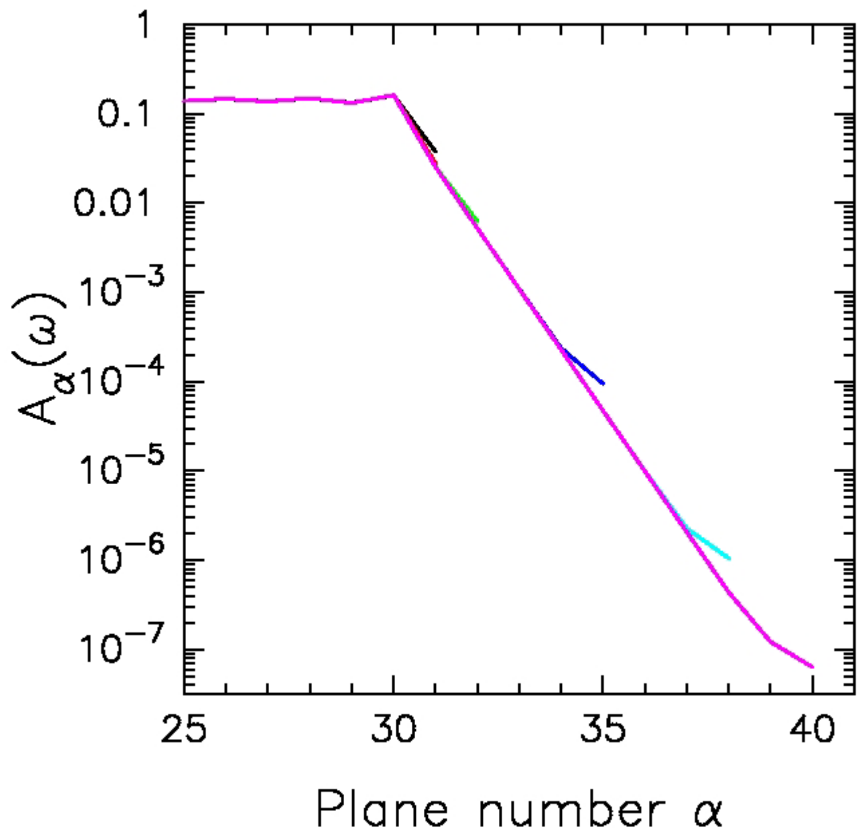
U=6 (small-gap insulator) DOS



U=6 Correlated insulator

DOS has exponential tails, but never vanishes in the “gap”; the exponential decay has the same characteristic length for all barrier thicknesses.

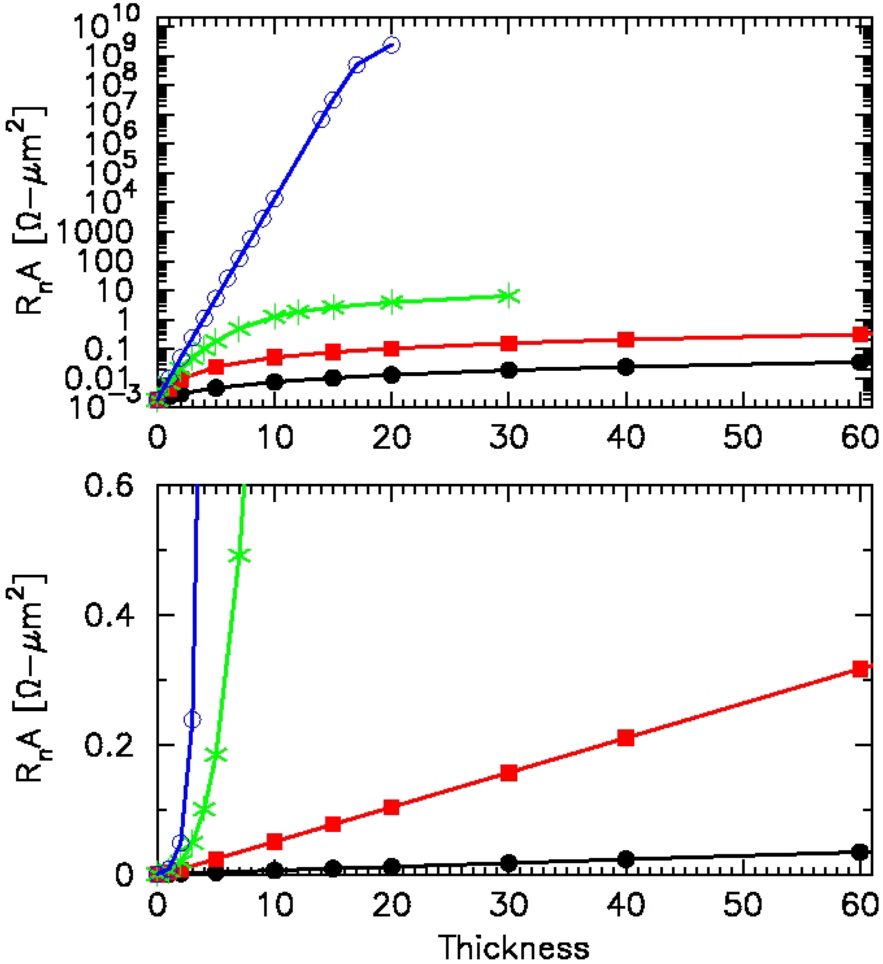


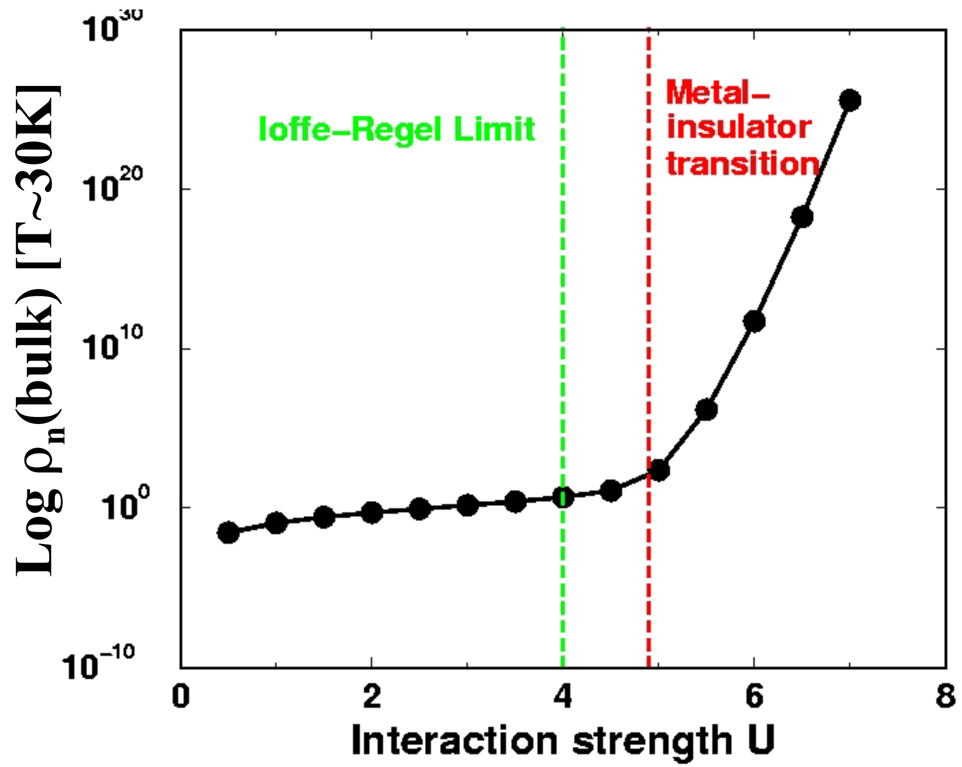


Junction resistance

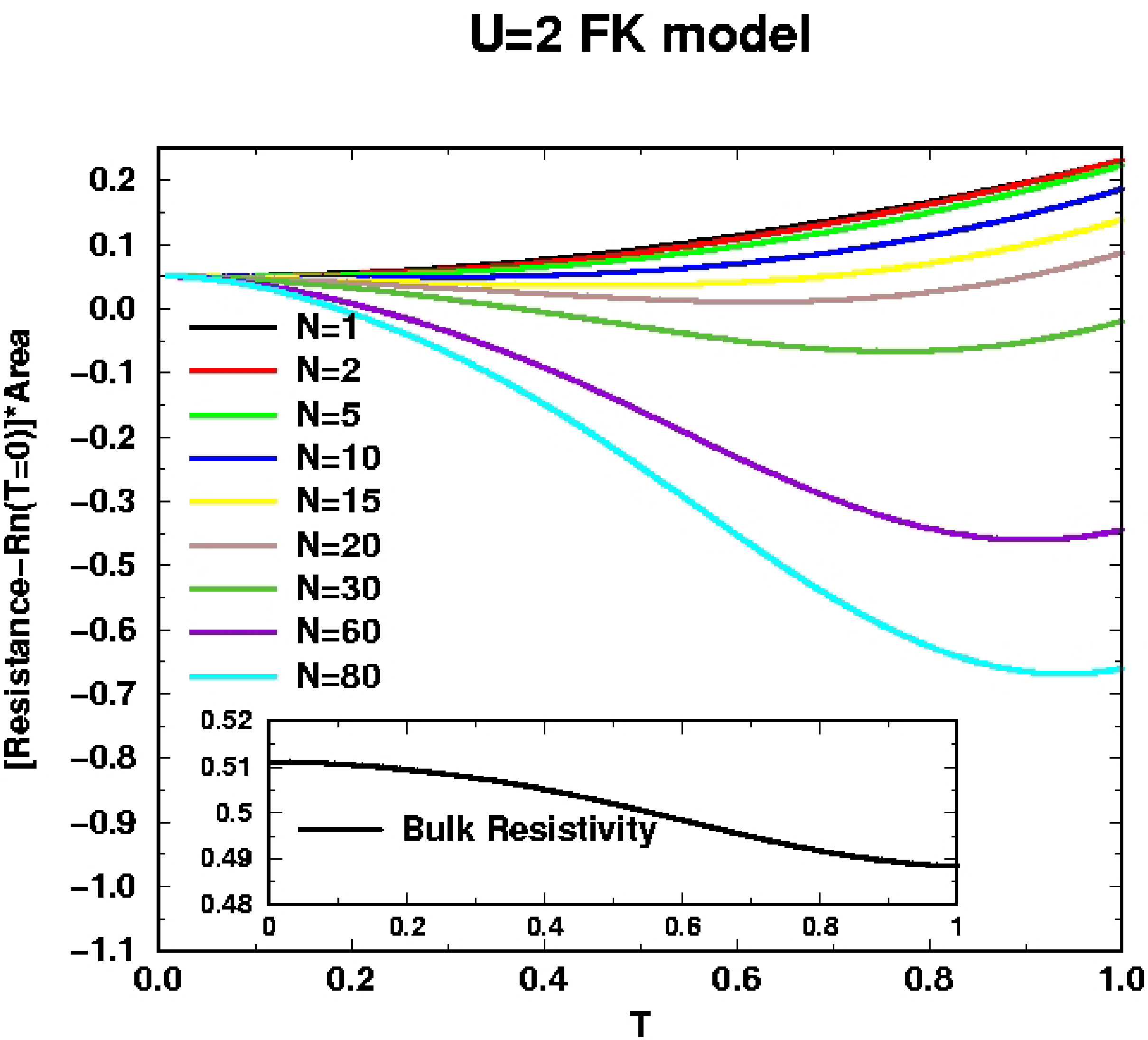
- The linear-response resistance can be calculated in equilibrium using a Kubo-Greenwood approach.
- We must work in real space because there is no translational symmetry.
- R_n is calculated by inverting the conductivity matrix and summing all matrix elements of the inverse.

Resistance versus resistivity





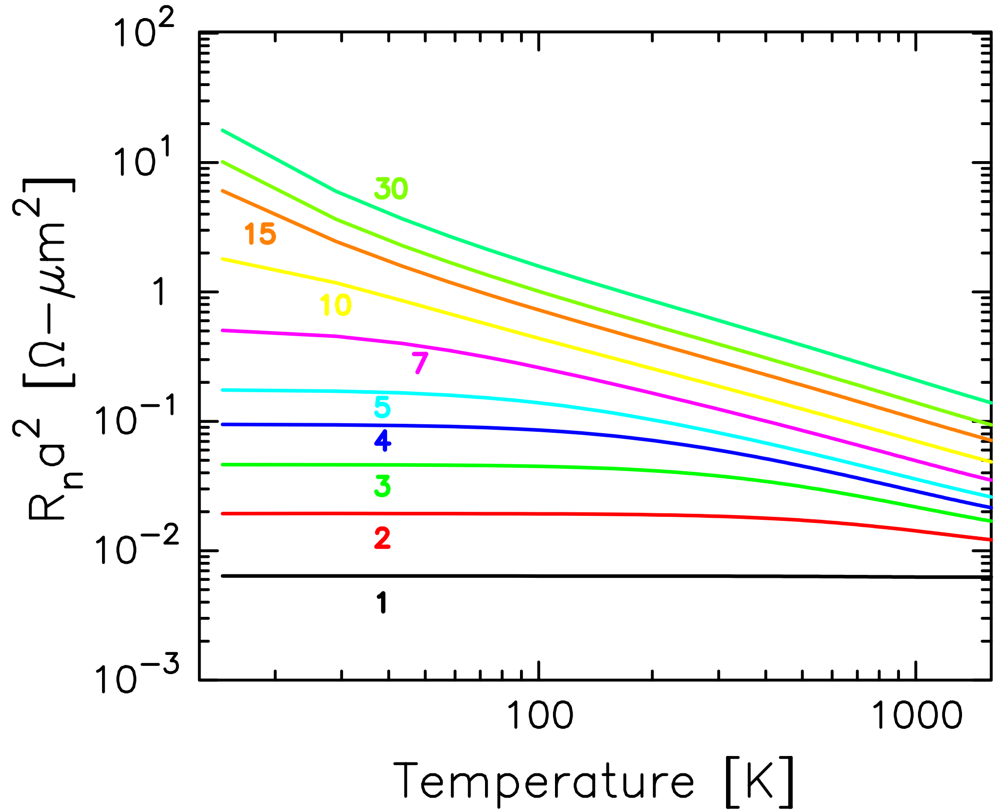
Temperature dependence (correlated metal)



- 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.

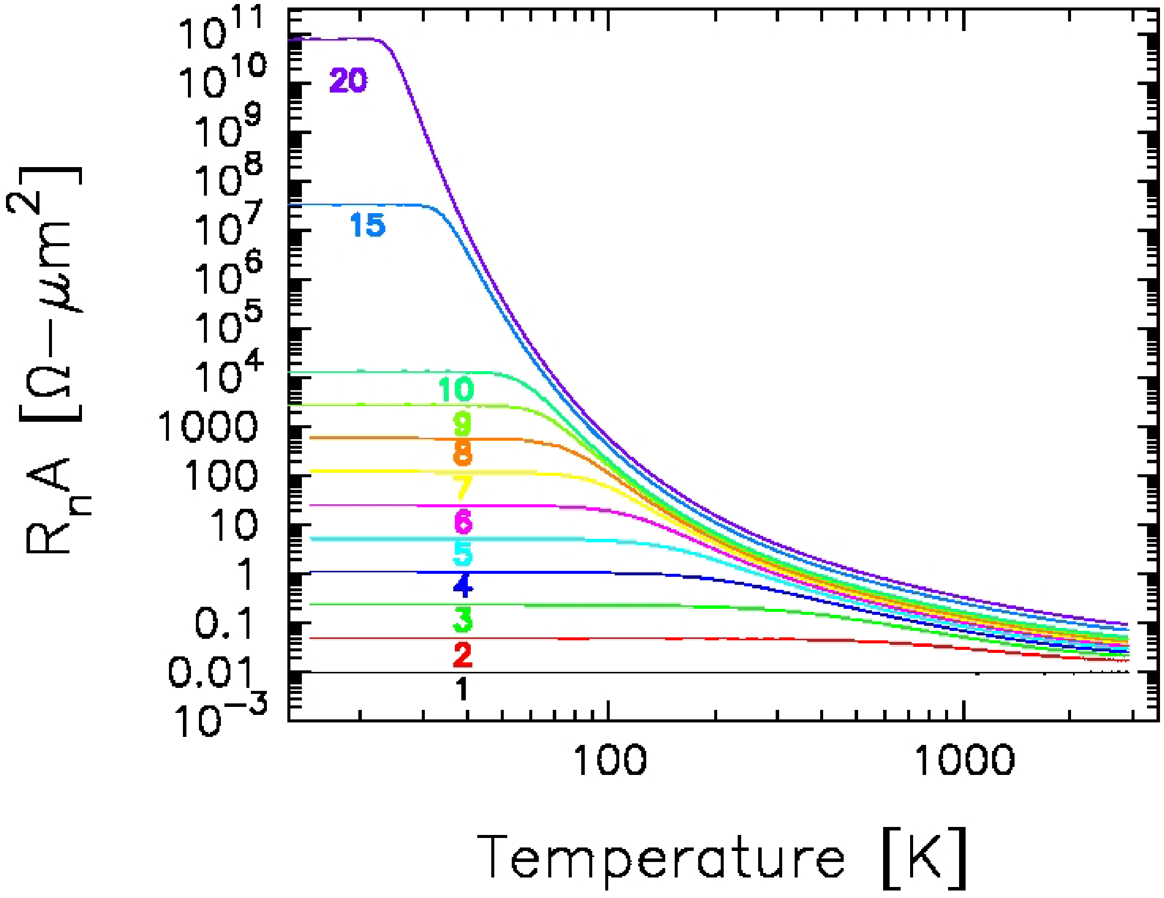
Resistance for U=5 (near critical)

- Tunneling occurs when the junction resistance has little temperature dependence.
- Incoherent transport occurs when the temperature dependence becomes strong.



Resistance for U=6 (correlated insulator)

- Resistance here shows the tunneling plateaus more clearly, and a stronger 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:

$$E_{Th} = \frac{\hbar}{2e^2 \int d\omega N(\omega) \frac{-df(\omega)}{d\omega} R_N AL}$$

- 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.

Thouless energy II

- The **resistance** can be considered as the **ratio** of the Thouless energy to the quantum-mechanical level spacing Δ_E (with $R_Q=h/2e^2$ the quantum unit of resistance)

$$R_n = R_Q \frac{\Delta_E}{2\pi E_{Th}}$$

- The inverse of the level spacing is related to the density of states of the barrier via

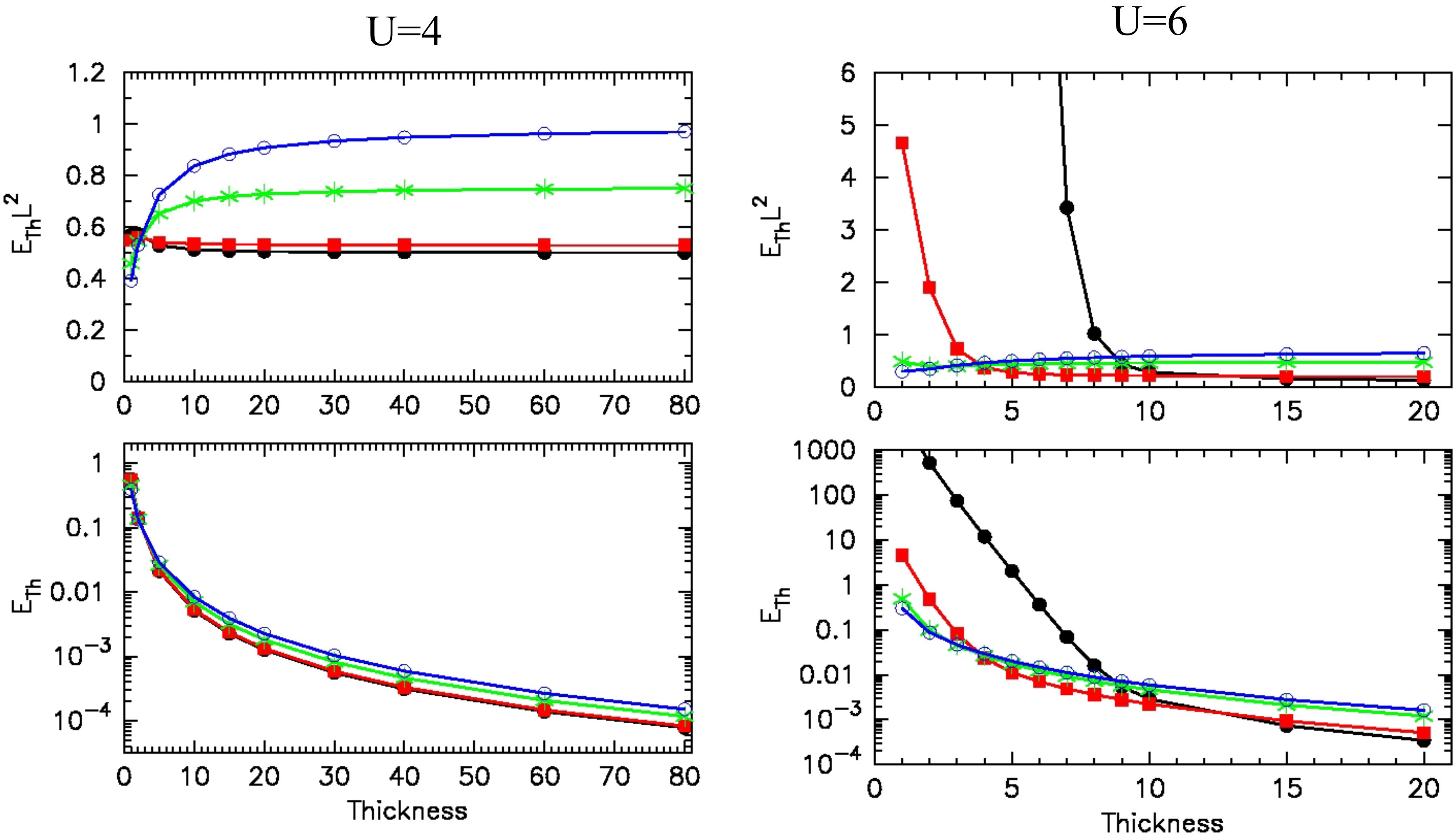
$$\Delta_E^{-1} = VN(\mu)$$

- Generalizing the above relation to an insulator by

$$\Delta_E^{-1} = AL\int d\omega N(\omega)\left[-\frac{df(\omega)}{d\omega}\right]$$

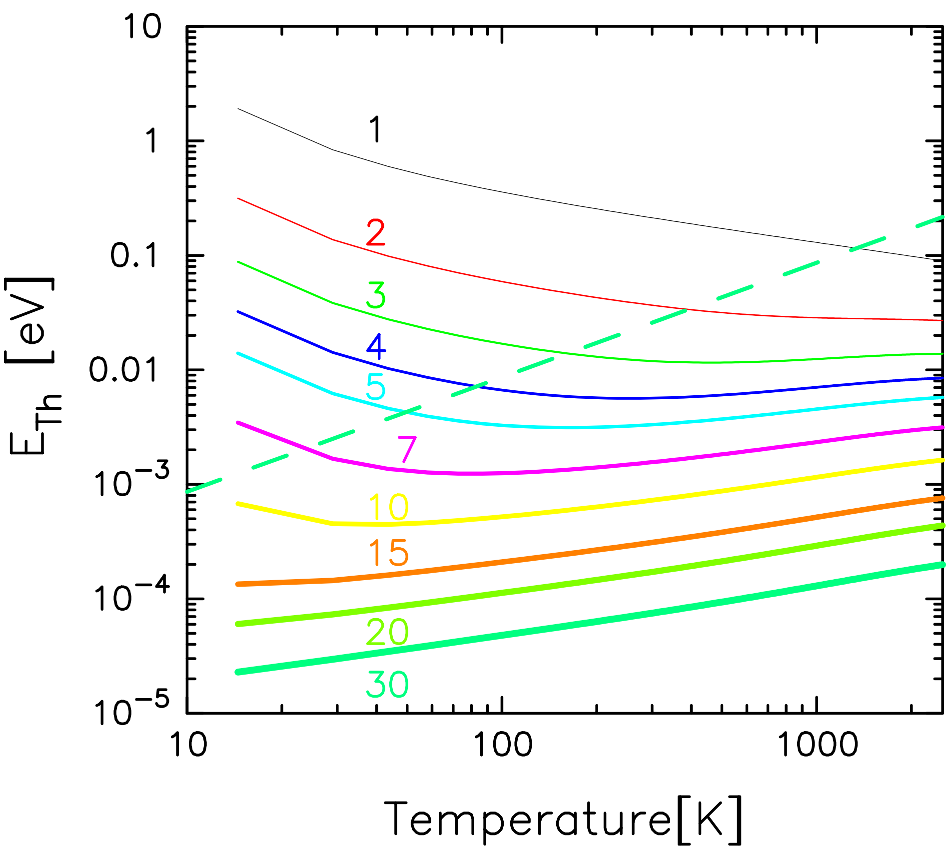
- gives the general form for the Thouless energy.

Thickness dependence

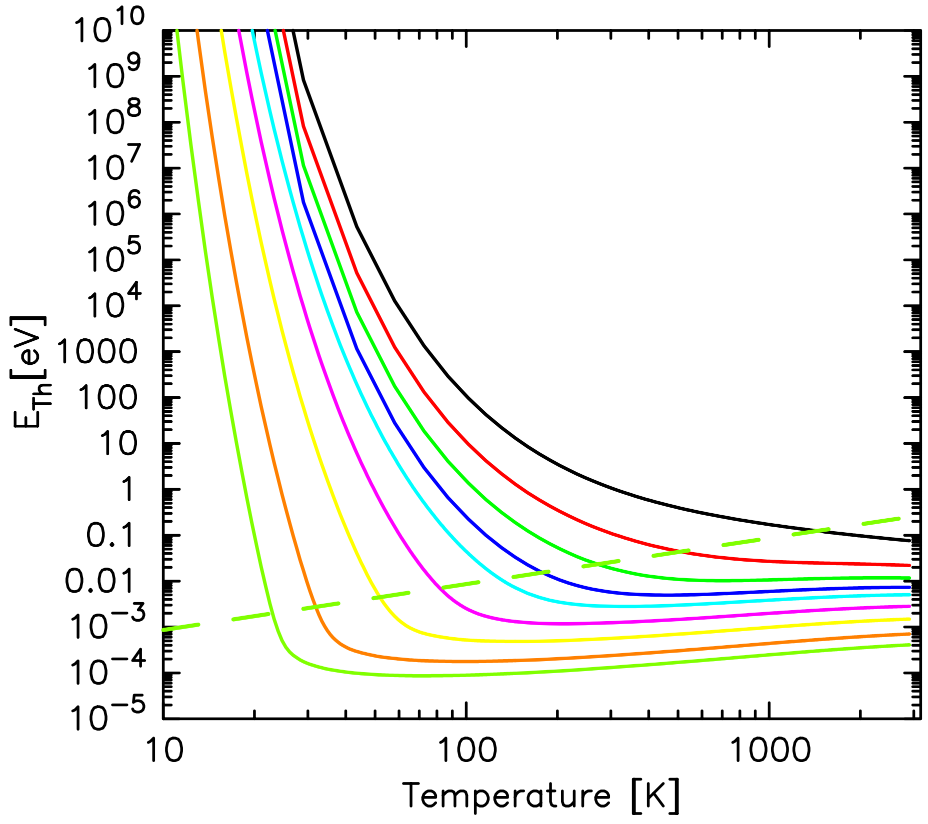


Temperature dependence

U=5

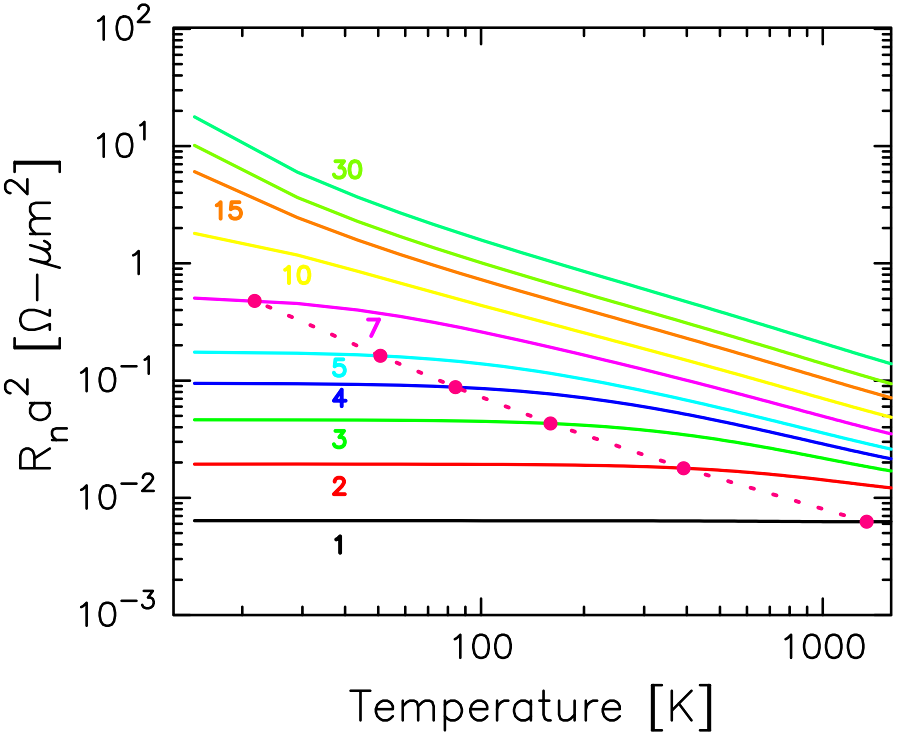


U=6

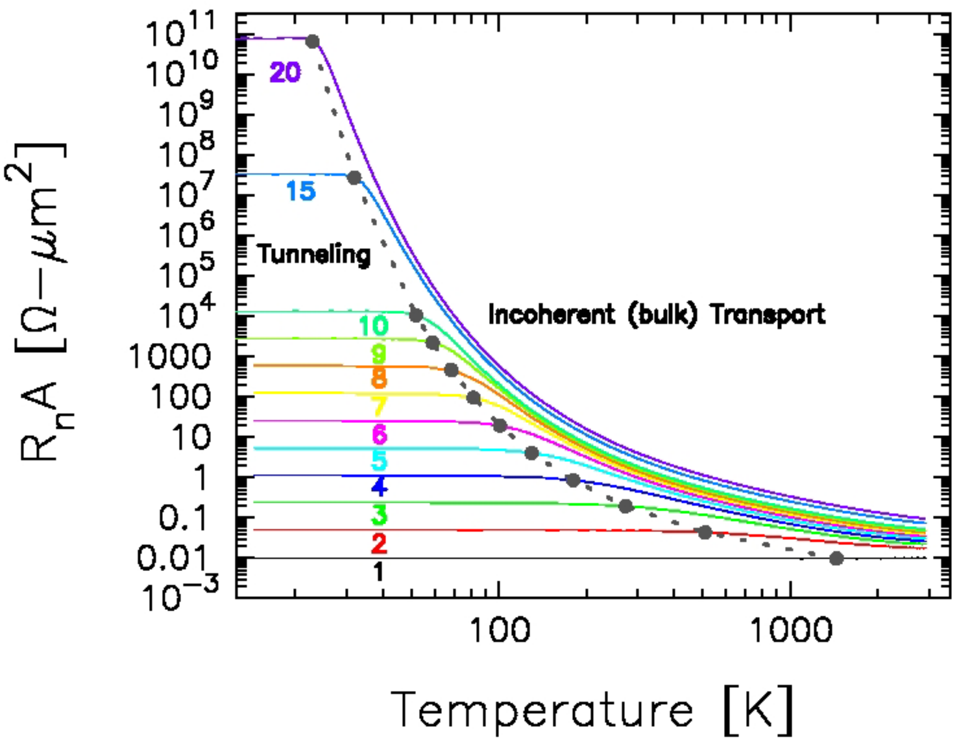


Temperature dependence (II)

U=5 FK model



U=6 FK model



The Thouless energy determines the transition from tunneling to incoherent transport as a function of temperature!

Note that the crossover temperature is not simply related to the energy gap!

Tunnel diagnostic/engineering

- The Thouless energy and the crossover point can be estimated with the low temperature resistance and the bulk DOS of the insulator, since R_n has weak temperature dependence in the tunneling regime.
- The junction can be optimized for tunneling properties if the operating temperature and barrier properties are known.
- It may be possible to use the Thouless energy to investigate the presence of pinholes as well.

Benefits of junctions near a MIT

- Thicker barriers are likely less susceptible to pinholes, and may not require as flat interfaces.
- Junction reproducibility on a chip may be easier with a thicker barrier.
- Likely to have a smaller junction capacitance (faster switching for the same value of the resistance).

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.