# Optimizing Josephson junction performance and nonlinear effects in “smart” electronics

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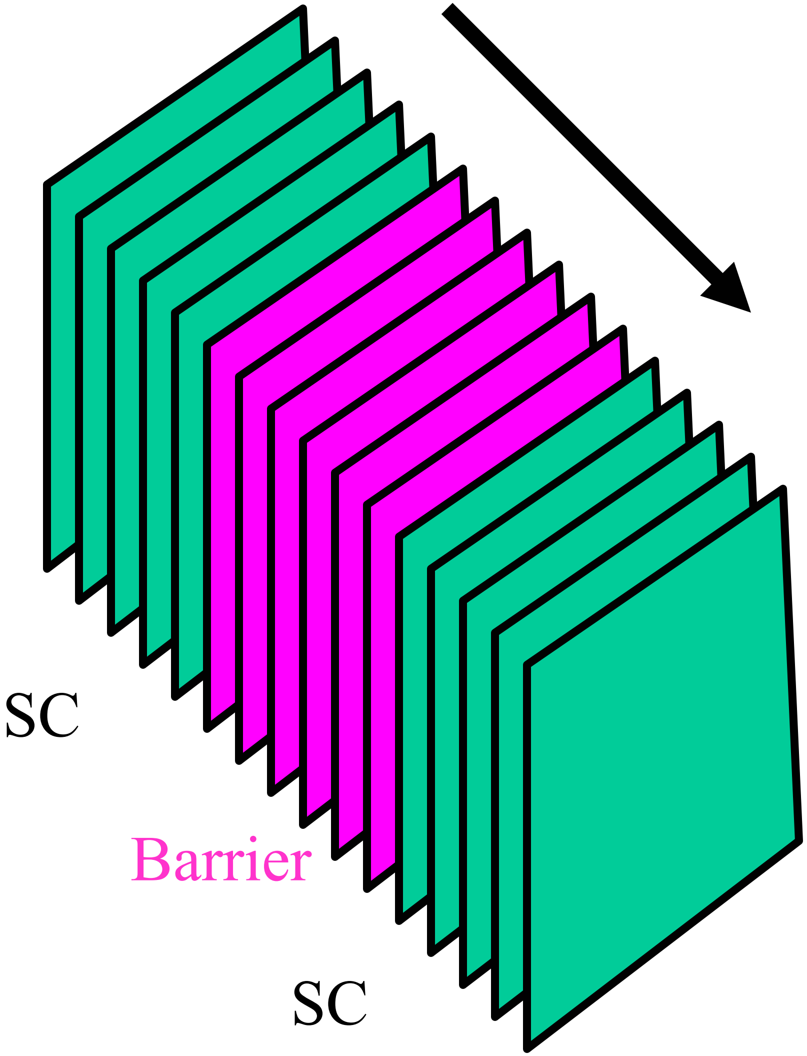
# Overall goals of project

- Provide a theoretical framework to describe Josephson junctions with barriers tuned close to the **metal-insulator transition**, with the goal of **minimizing** the junction switching speed and maintaining a **nonhysteretic** current-voltage characteristic.
- Examine **nonlinear** effects in “smart” electronics to understand how nonlinearities determine the **ultimate device performance**.

# Current research problems

- Examining a new way to **classify** Josephson junctions by determining the **Thouless energy** of the junction.
- Determining a microscopic model for the MIT in **$Ta_xN$** to incorporate in the JJ modelling.
- Developing a **nonequilibrium formalism** that can investigate nonlinear response.
- Testing numerical algorithms by **applying to model systems** before porting them to real materials situations.

# Josephson junctions for digital electronics

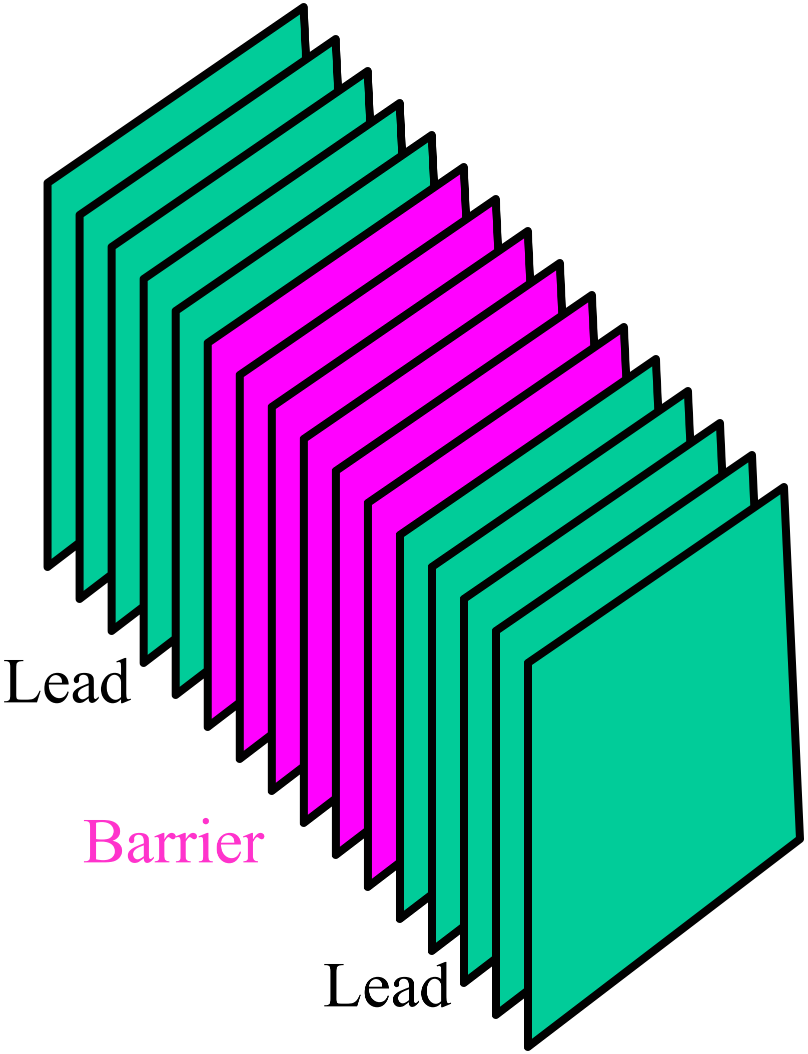


- Sandwich of superconductor-barrier-superconductor with current moving perpendicular to the planes
- Nonlinear current-voltage characteristics used for electronics
- Band insulator barriers: $AlO_x$ MgO
- Correlated material barriers: FeSi, $SrTiO_3$
- Barriers near the MIT: $V_2O_3$, $Ta_xN$

# Have a theory that incorporates all forms of transport (ballistic, diffusive, incoherent, and correlated) on an equal footing

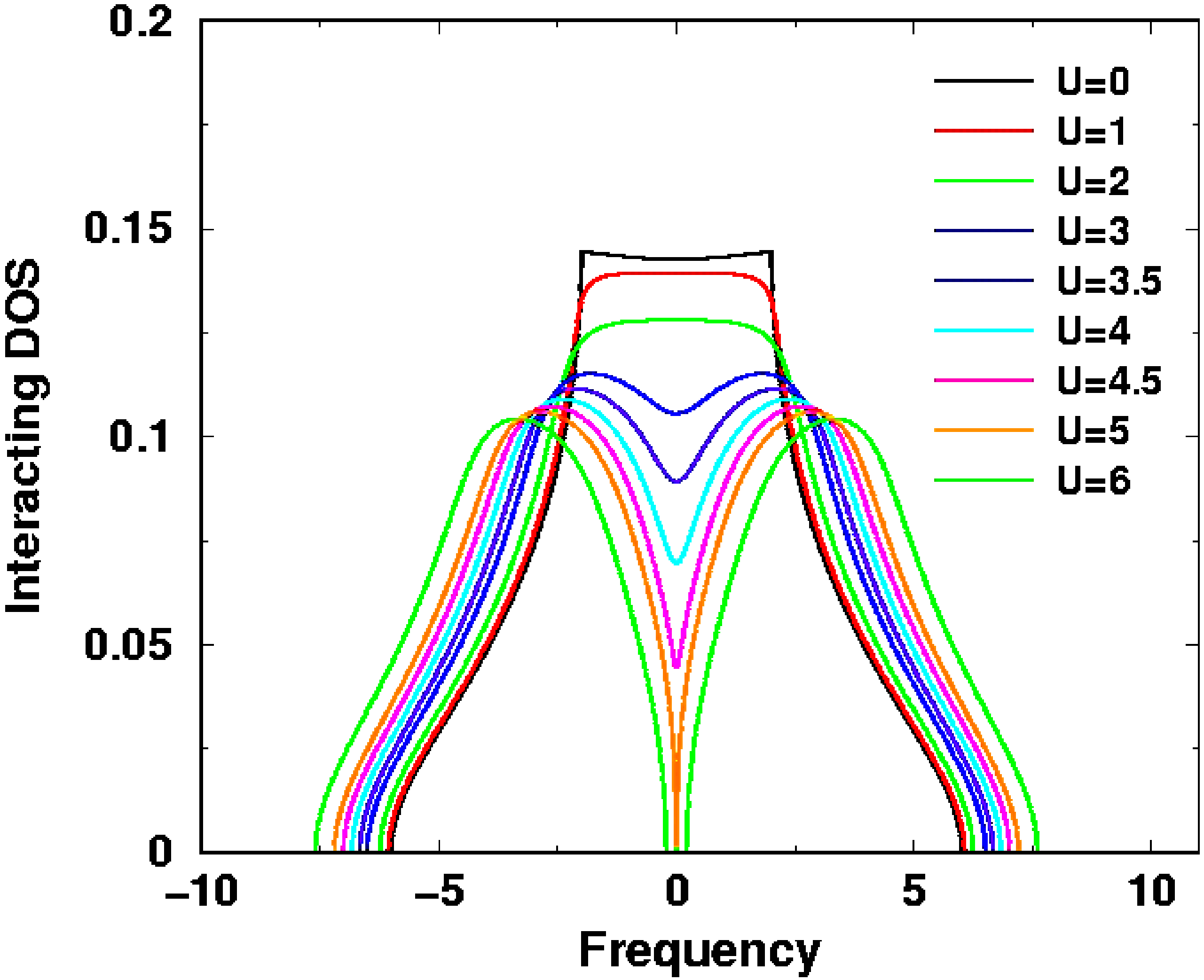
- We evaluate the **figure of merit** in a linear-response formalism by calculating the junction resistance in the normal state $R_n$ and the critical current $I_c$ to yield $I_cR_n$.

# Our model



- The superconducting leads are composed of a **ballistic metal** that **superconducts** via a BCS mechanism.
- 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.

# 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 or a generalized Einstein relation).

$$E_{Th} = \hbar / t_{Dwell} ; R_N = \frac{h}{2e^2} \frac{E_{ls}}{E_{Th}}$$

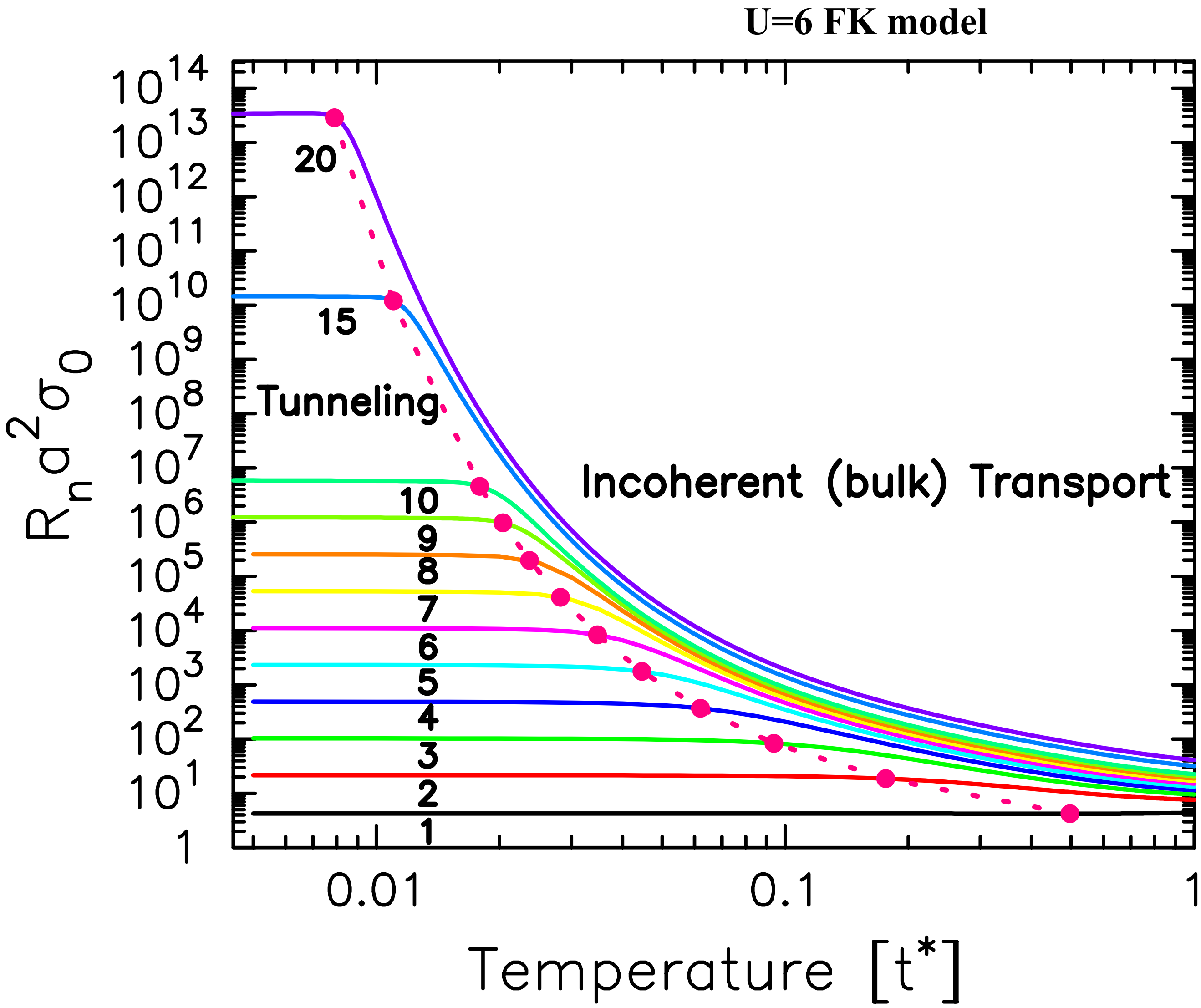
- A **unifying form** for the Thouless energy can be determined from the resistance of the barrier region and its electronic density of states:

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

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

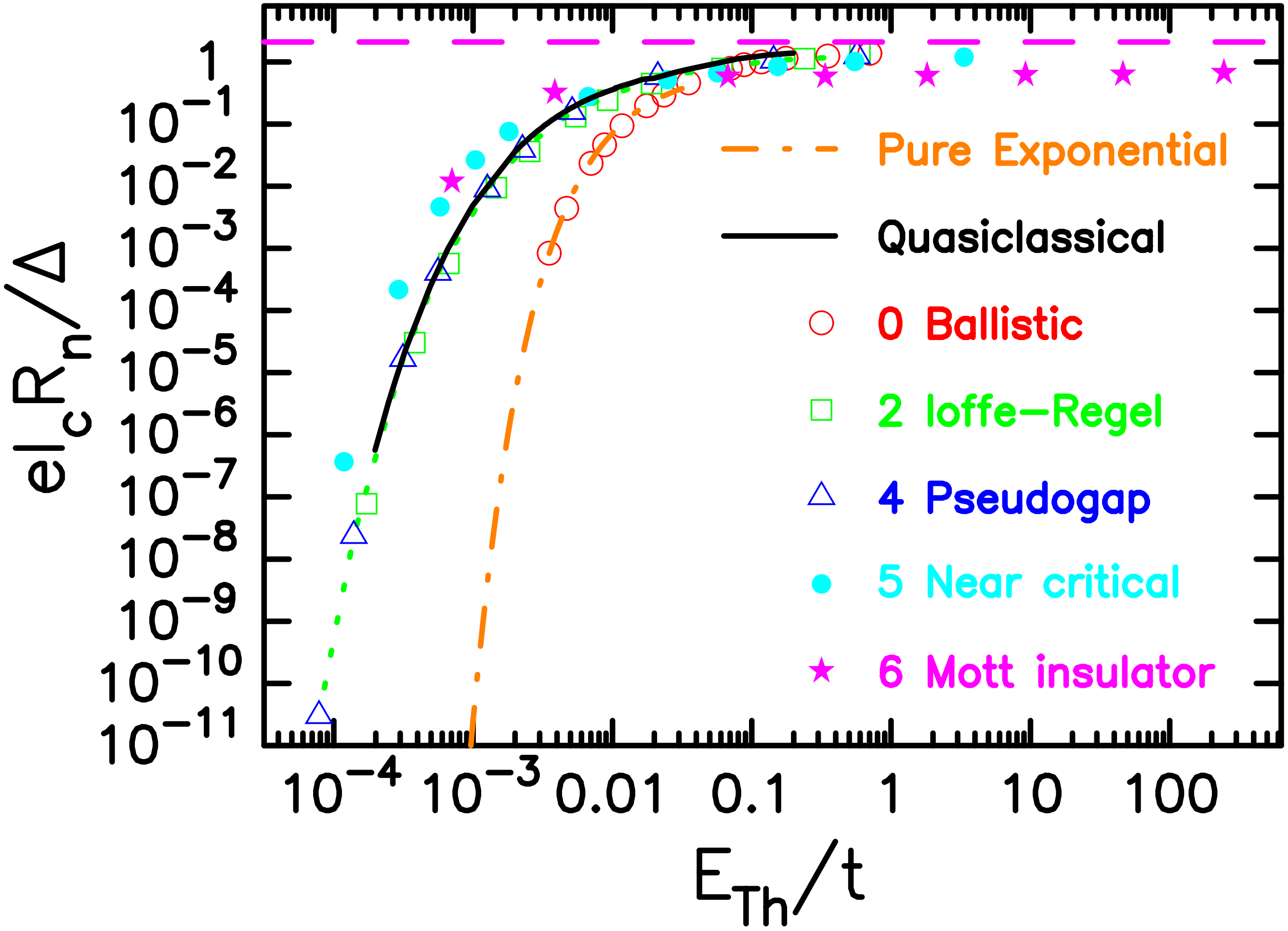
# Crossover from tunneling to Ohmic transport

The Thouless energy **determines 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!



# Figure of Merit

- The Thouless energy determines the figure of merit once it becomes the **smallest energy scale** in the problem. The quasiclassical approach seems to hold **all they way up to the MIT**. Beyond that, the behavior seems to become **nonuniversal**.



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Hence the Thouless energy is an important diagnostic energy for Josephson junctions!

We hope experimentalists can incorporate it into their analysis.

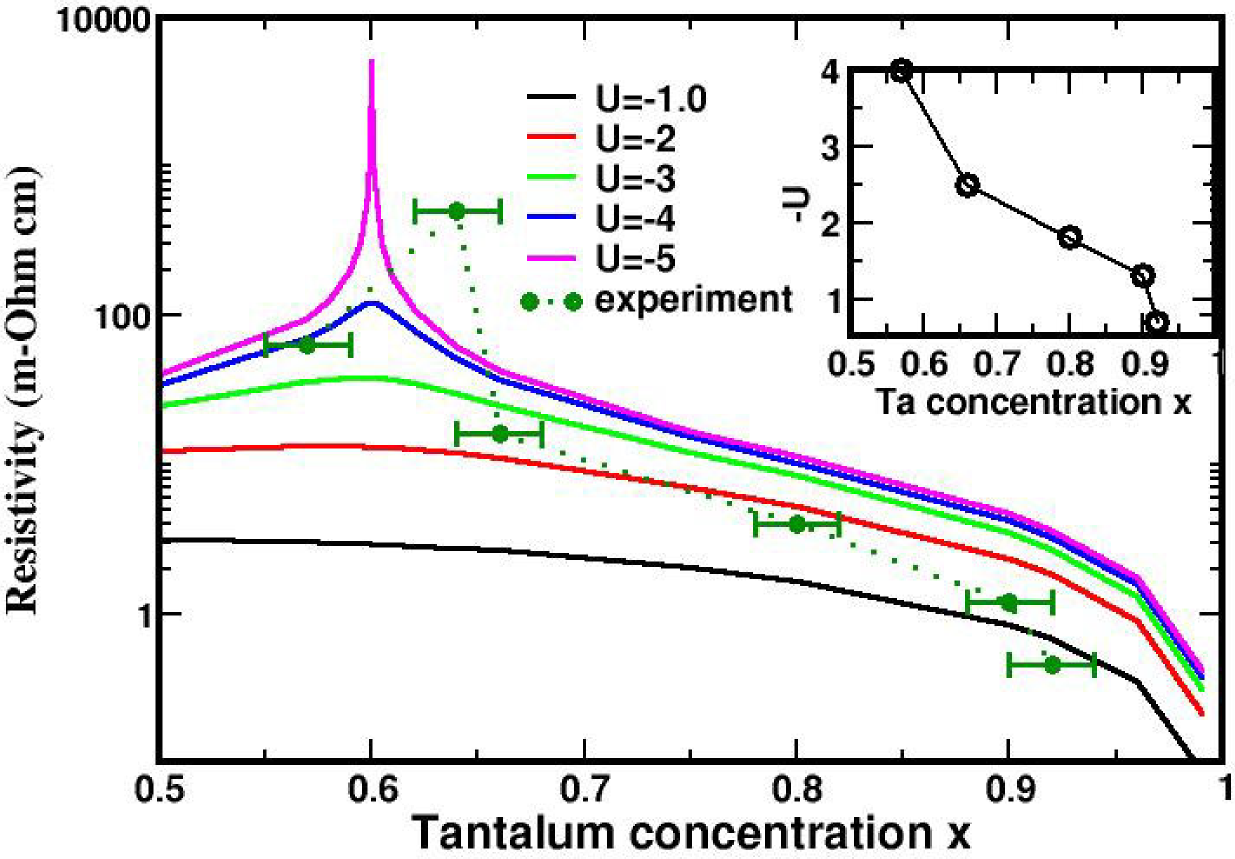
# Tantalum-nitride barrier junctions

- Can $Ta_xN$ barriers be employed as a “drop-in” technology to increase the **operating temperature** and **switching speed** of Josephson junctions in digital electronics?
- Tantalum defects **bind five electrons** (removing free electrons from the system) and they act as scattering centers for the remaining conduction electrons.
- $Ta_3N_5$ is a **band insulator** with a gap of at least 1.5eV.
- As x approaches 0.6, $Ta_xN$ becomes **more and more** insulating in character.
- **Is it possible to model this system with the Falicov-Kimball model?**

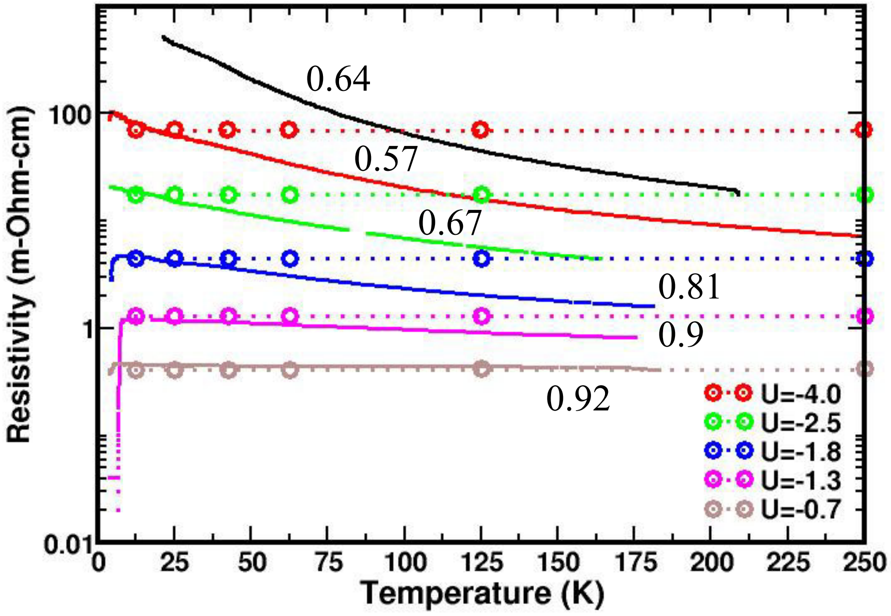
# What kind of MIT occurs in $Ta_xN$?

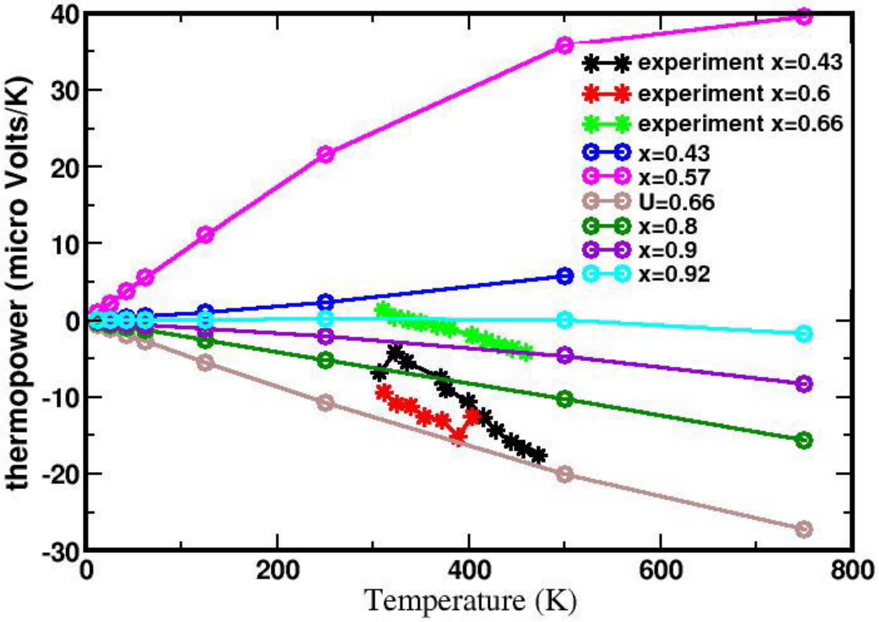
- Band structure calculations indicate that the commensurate insulator is **analogous to a charge-density-wave insulator**. This can be insulating away from x=0.6 if the CDW becomes incommensurate.
- The FK model predicts an insulator only at x=0.6, but a bad metal near x=0.6; the MIT is a **Mott-like transition**, where the DOS is suppressed to zero at the chemical potential.
- If disorder and localization effects are included, then the MIT can be an Anderson transition, **driven by the localization of the electrons**, that are present at the chemical potential.

# Fit of the resistivity at T=25K requires **U to change** as a function of doping due to changes in the screening.



# Temperature dependence for fixed x values is **not insulating enough**. Thermopower has some similarities, but **does not pick up all of the trends**.





# Future work

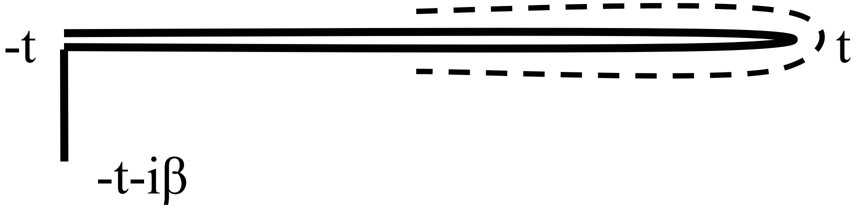
- Model JJ's using the **low temperature fit** to the resistivity and the FK model.
- Develop the **typical medium theory** of DMFT which allows for an Anderson transition, and should **restore the stronger T dependence** in the data.
- Generalize the typical medium theory to the **superconducting state** to calculate the figure of merit.

# Nonlinear response

- Often the **nonlinearities** of a device determine it's ultimate performance.
- So-called "smart" materials usually involve **strongly correlated systems** because their materials parameters can be tuned by doping, pressure, or temperature variations.
- Many devices of interest to the Navy will be subject to **large electromagnetic fields** or **field pulses**, which can affect their performance.

# Nonequilibrium formalism

- In a nonequilibrium situation, the quantum-mechanical operators must be evolved **forward in time**, and then de-evolved **backward in time**, in order to determine operator averages with respect to the original equilibrium distribution.
- A Keldysh-like formalism is used to calculate the so-called **contour ordered Green's function**. In our case, the field is turned on at **t=0**, as indicated by the dashed line.

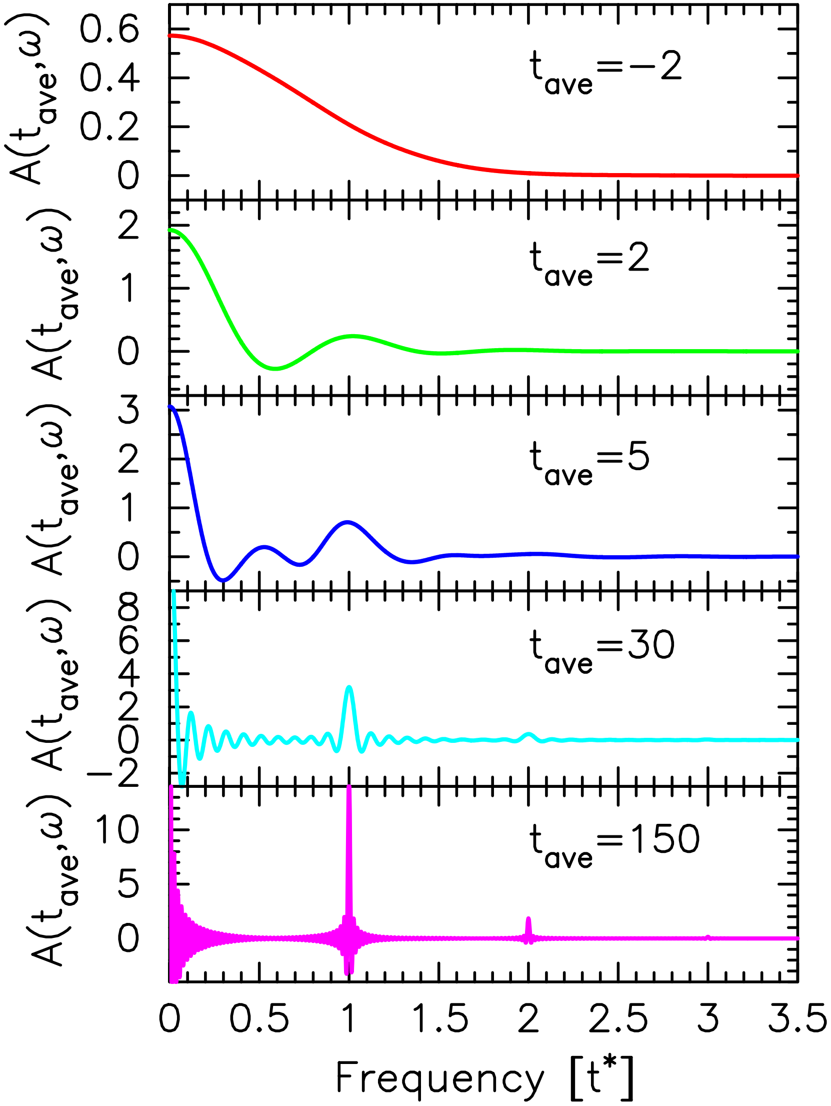


# Nonlinear effects in perfect conductors

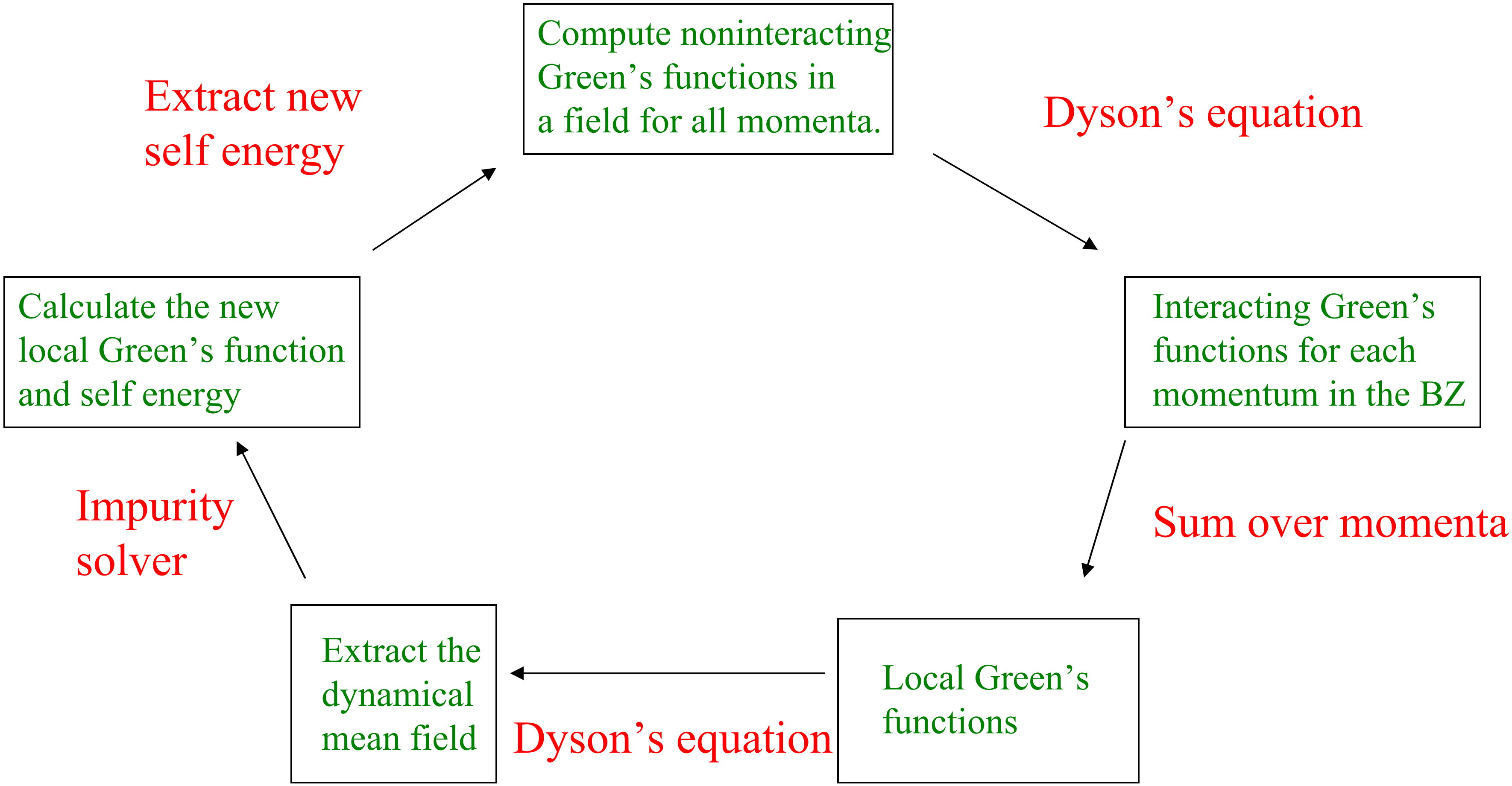
- In a metal with no scattering, applying a voltage initially produces a linear-response current, but nonlinear effects rapidly take over creating a nonlinear sinusoidal current called a **Bloch oscillation** (because the wavevector of the electrons must remain within the first Brillouin zone).
- The DOS evolves into what is called a **Wannier-Stark ladder**, consisting of delta function peaks spaced evenly by the Bloch oscillating frequency.
- There are numerous analogs with JJ's here---**applying a dc voltage yields an ac current**, and the **currents never decay in time** because there is no scattering.

# Formation of the Wannier-Stark ladder

- The Wigner DOS corresponds to the **Fourier transform of the relative time coordinate** of the two-time Green's function.
- Note how we clearly see the **formation of the Wannier-Stark ladder** as the average time increases.



# Exact algorithm to include interactions



Compute noninteracting Green's functions in a field for all momenta.

Dyson's equation

Interacting Green's functions for each momentum in the BZ

Sum over momenta

Local Green's functions

Dyson's equation

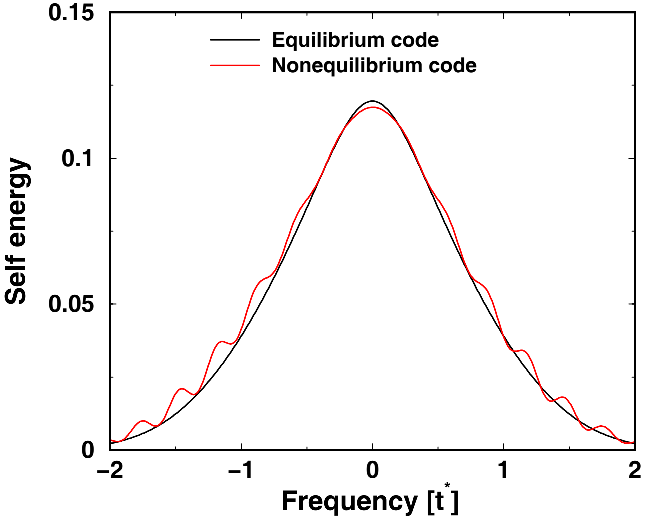
Extract the dynamical mean field

Impurity solver

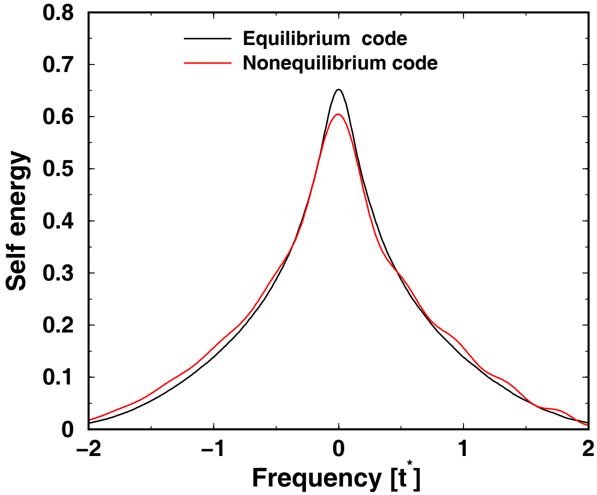
Calculate the new local Green's function and self energy

Extract new self energy

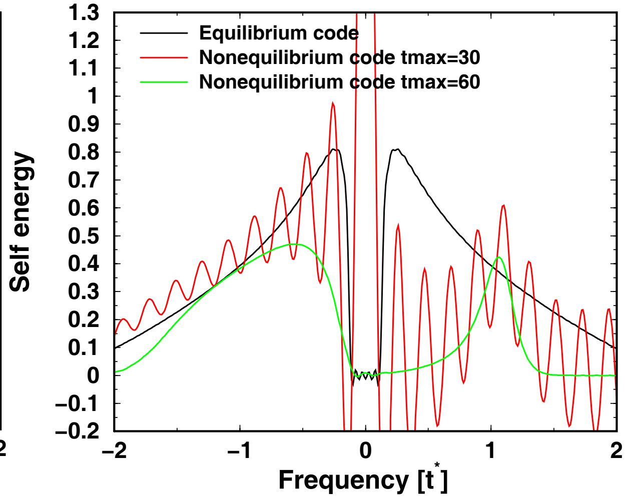
# Test case: equilibrium self-energy with the nonequilibrium formalism



U=0.5

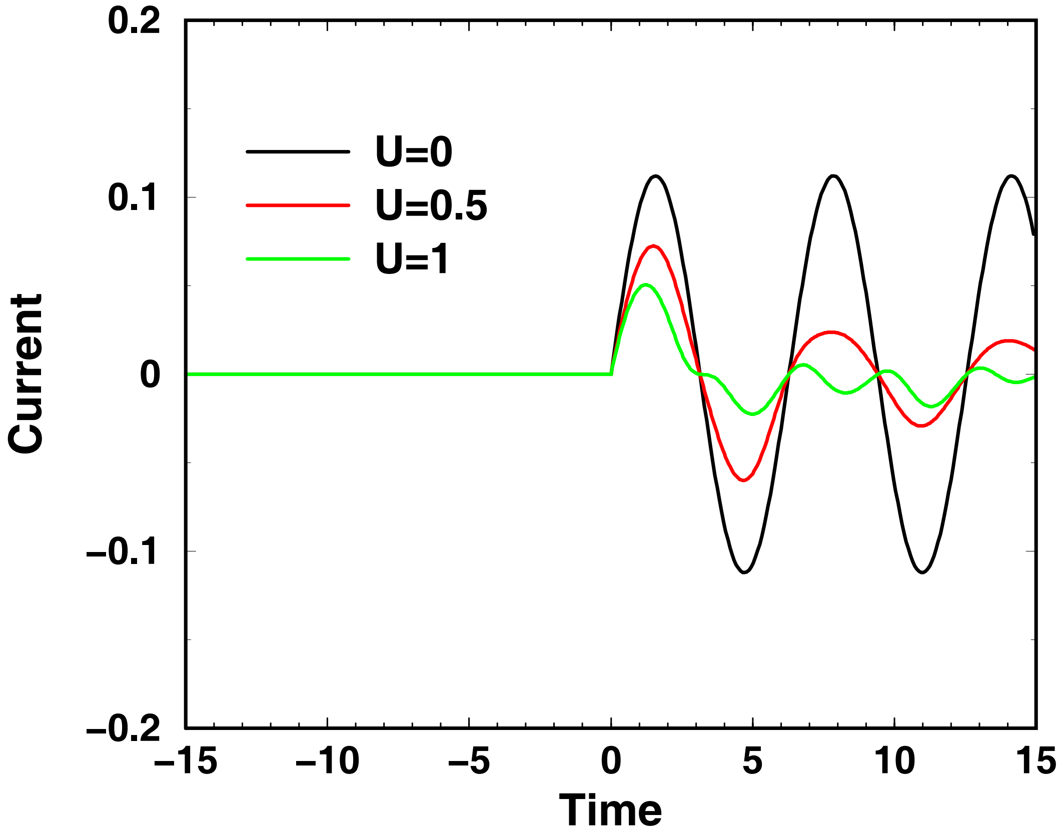


U=1



U=2

# Preliminary results: nonlinear and transient current response of a strongly scattering metal



Note how the Bloch oscillations remain for a large electric field, but the amplitude is attenuated at longer times due to the scattering.

# Future work

- Compute the **nonlinear response of a Mott insulator**. Generalize the code to work with nanostructures in addition to the bulk.
- Determine **figure of merit** and systematics of $Ta_xN$ junctions.
- Generalize to **multiband models** derived from band-structure and tight-binding to model c-axis $MgB_2$ junctions.