Nonequilibrium Dynamical Mean-Field Theory: from strongly correlated electrons to ultracold atoms

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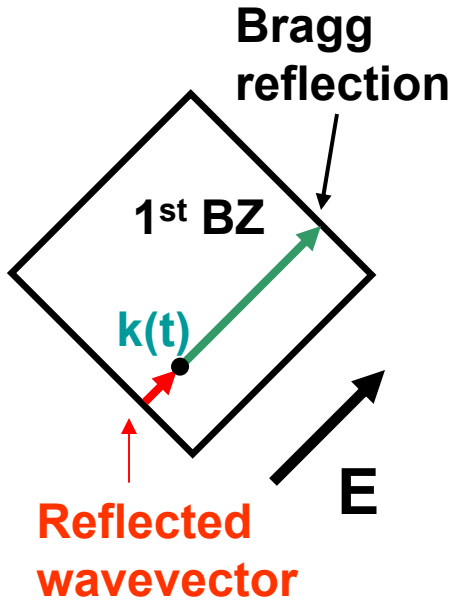
Electrons driven by a constant electric field

- In a **semiclassical** picture, the electron momentum, written as **ħk=P**, evolves with a linear time-dependence corresponding to the **acceleration** due to the field: **k(t)=eEt/ħ**.
- **Periodicity** modifies this picture: since the electrons are in a periodic lattice, the wavevector cannot increase **outside** of the first Brillouin zone; as it tries to move beyond the 1BZ it is **Bragg reflected** to the opposite side of the zone.
- Defects, impurities, lattice vibrations, and other electrons are sources of **scattering**, which also interrupt the evolution of the wavevector in the BZ.



Bloch Oscillations (Bloch 1928, Zener 1932)

Constant potential difference (constant E field)

Oscillating current

- When on a periodic lattice, the electrons' motion is governed by their electronic bandstructure **ε(k).** In metals the last band is partially filled, so electrons can easily move. In insulators, the bands are completely filled, with a band-gap to the first unoccupied band.
- The electrons move with an effective velocity **v(k)=dε(k)/dħk**. So they carry a current equal to **ev(k)** summed over all wavevectors **k**.
- As the **wavevector** evolves over the 1BZ, it changes **periodically**, and so does **v(k).**
- Hence, **Bragg reflection makes the current periodic in time!** ***A dc electric field creates a periodic ac current in a perfect metal with electrons moving in a crystalline lattice*.**

But this is **never** seen in any conventional metal no matter how clean it is.

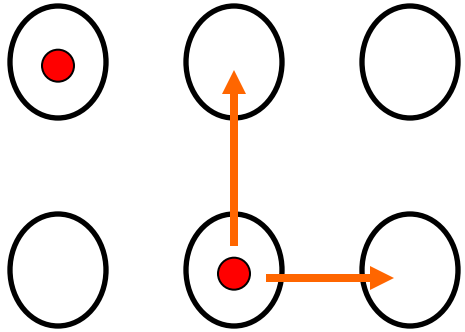
Quenching Bloch oscillations

- **Tunneling between bands** makes the electrons move as if the lattice was not there. They continue to accelerate and do not undergo periodic motion. In this case there are no Bloch oscillations. It only occurs if the energy stored in the field is large enough to induce a tunneling between bands. ***This will not be considered in this work*.**
- If the scattering due to defects, impurities, lattice vibrations, or other electrons is **frequent enough**, the electrons won't have enough time to undergo the Bloch oscillation, as their wavevector becomes randomly changed with each scattering event, and they must start their acceleration in the field again. ***This is why Bloch oscillations are not commonly seen in metals*.**

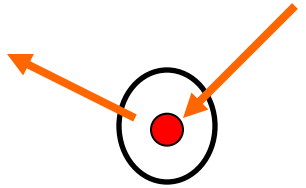
Many-body physics and the dynamical mean-field theory approach to nonequilibrium problems

Dynamical mean field theory

- Models of strongly correlated materials are difficult to solve.
- Significant progress has been made over the past 18 years by examining the limit of **large spatial dimensions**.
- In this case, the lattice problem can be mapped onto a self-consistent impurity (single-site) problem, in a time-dependent field that **mimics the hopping of electrons onto and off of the lattice sites**.

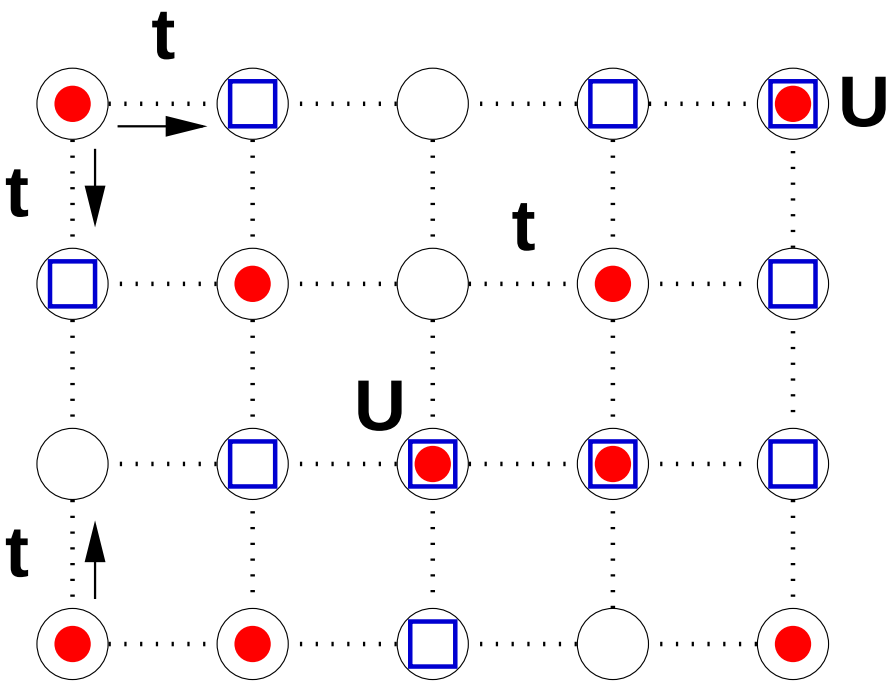


Lattice



Impurity site

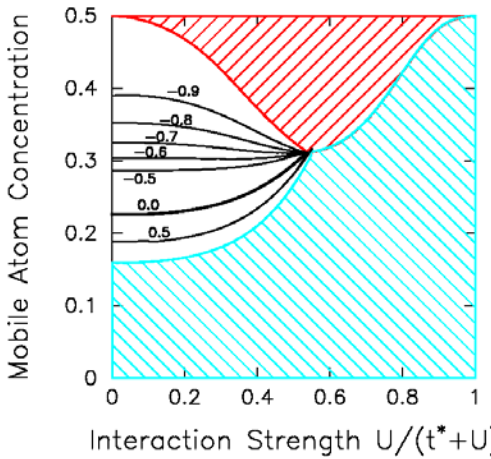
Falicov-Kimball Model

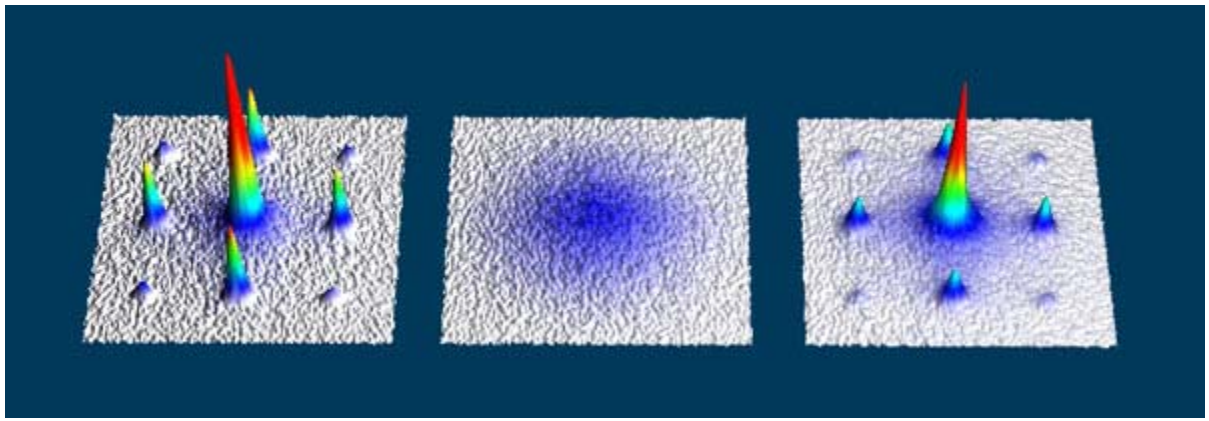


- Two kinds of particles: (i) **mobile electrons** and (ii) **localized electrons**.
- When both electrons are on **the same site** they interact with a correlation energy U.
- Many-body physics enters from an **annealed average over all localized electron configurations**.

Physical importance of the Falicov-Kimball Model

- Simplest many-body problem that has a Mott-like metal-insulator transition (but it has no Fermi-liquid behavior).
- Possible solid-state systems include NiI_2 and Ta_xN
- Possible cold atom systems include mixtures of light alkali atoms (Li or K), with heavy alkali atoms (Rb or Cs) in optical lattices.

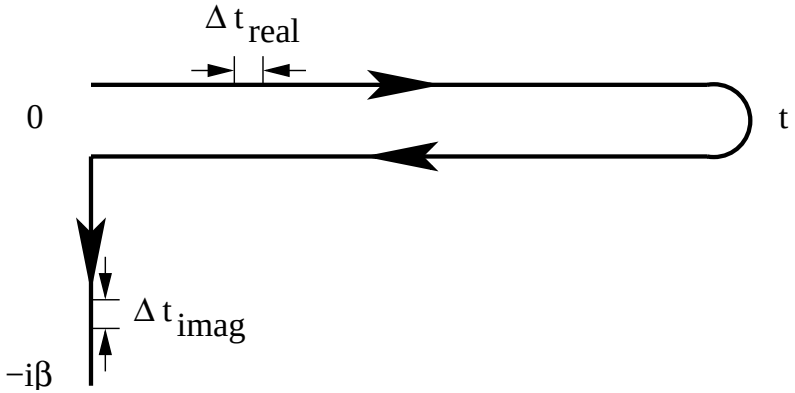




Dissipation in nonequilibrium systems

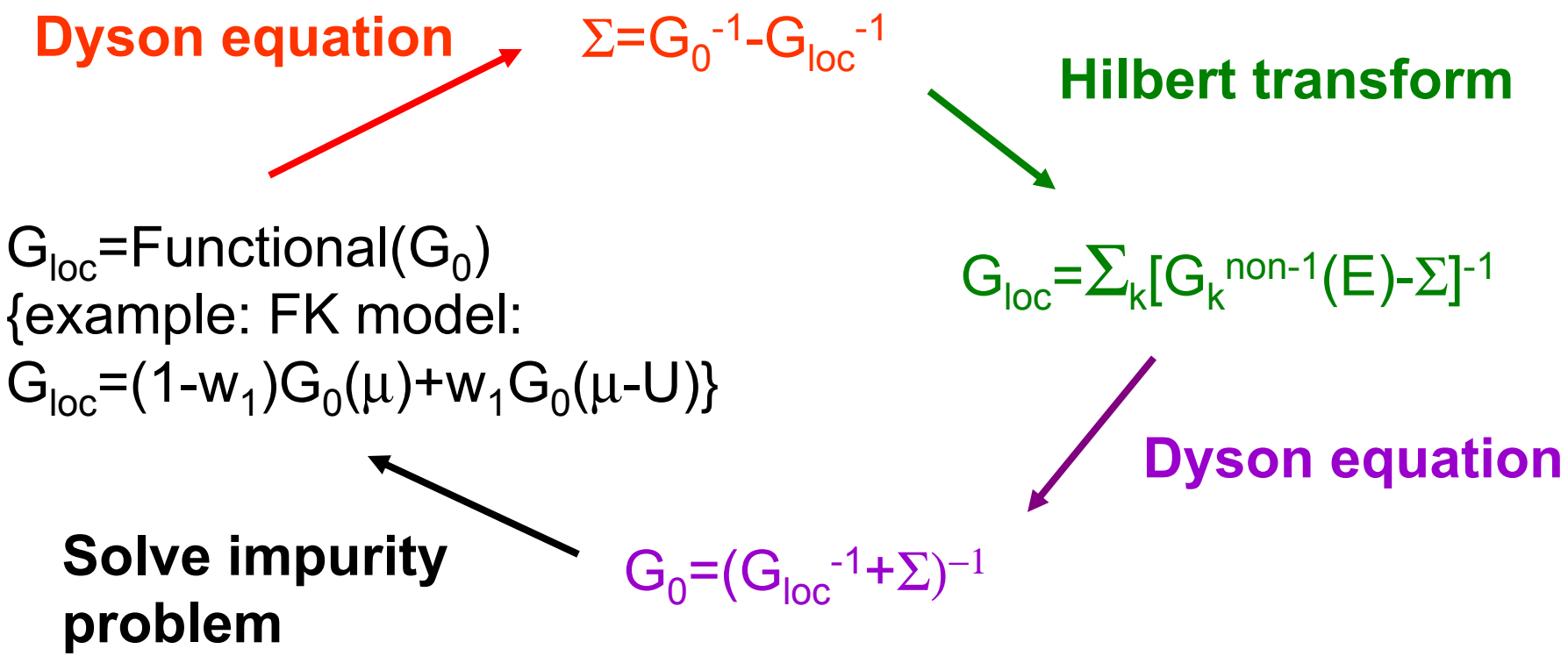
- Our many-body models have no explicit dissipation in the Hamiltonian, i.e. no phonons.
- But dissipation occurs and steady states can be reached, because we have an open system attached to infinite reservoirs which exchange particles and energy with the system, and allow for the Joule heat created by the driving electric field ($J \cdot E$) to be transported to and deposited into the attached reservoirs.

Kadanoff-Baym-Keldysh formalism



- Problems without time-translation invariance can be solved with a so-called **Keldysh formalism**.
- Green's functions are defined with time arguments that run over the **Kadanoff-Baym-Keldysh contour**.
- The electrons evolve in the fields **forwards** in time, then de-evolve in the fields **backwards** in time (we use the **Hamiltonian gauge, where the scalar potential vanishes**).
- **Functional derivatives** are then used to determine the Green's functions and other correlation functions of interest.

Dynamical mean-field theory algorithm



All objects (G and Σ) are **matrices** with each time argument lying on the contour.

Peierl's substitution and the Hilbert transform

The band structure is a sum of cosines on a hypercubic lattice:

$$\varepsilon(k) = -\frac{t^*}{2\sqrt{d}} \sum_{i=1} \cos k_i \Rightarrow -\frac{t^*}{2\sqrt{d}} \sum_{i=1} \cos[k_i - eA_i(t)] = \varepsilon \cos[eA(t)] + \bar{\varepsilon} \sin[eA(t)]$$

which becomes the sum of two "band energies" when the field lies in the diagonal direction after the Peierl's substitution.

These band energies have a joint Gaussian density of states, so a summation over the Brillouin zone can be replaced by a two-dimensional Gaussian-weighted integral.

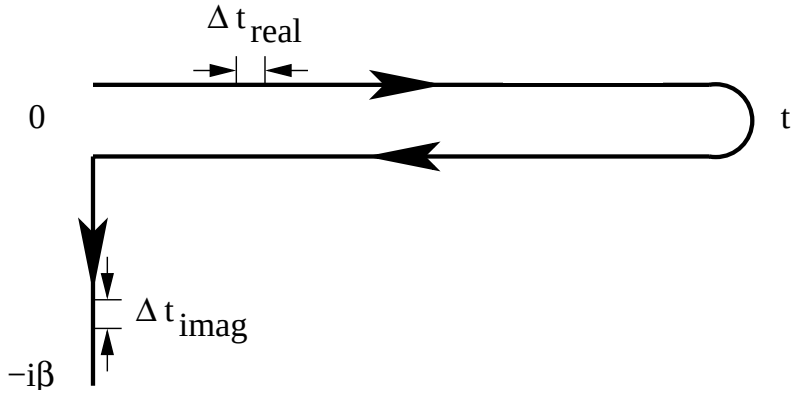
We use about 100 Gaussian quadrature points *in each dimension* to perform the integration.

Steady state formalism

- When we have a uniform field turned on at a given time, then one can change variables in the retarded Green's function and find a representation that depends solely on the relative time. This allows the retarded Green's function of a nonequilibrium system to be solved with an equilibrium-like formalism.
- We have not yet determined whether such a simplification is also possible for the lesser Green's function and are working on that problem currently

Computational elements for a massively parallel solution of the many-body problem

Computational elements



The key issue in calculating the real-time Green's function is to evaluate the **Dyson equation of a continuous integral operator** defined on the Kadanoff-Baym-Keldysh contour.

This operator is first **discretized** on a grid to be represented by **finite-dimensional** matrices.

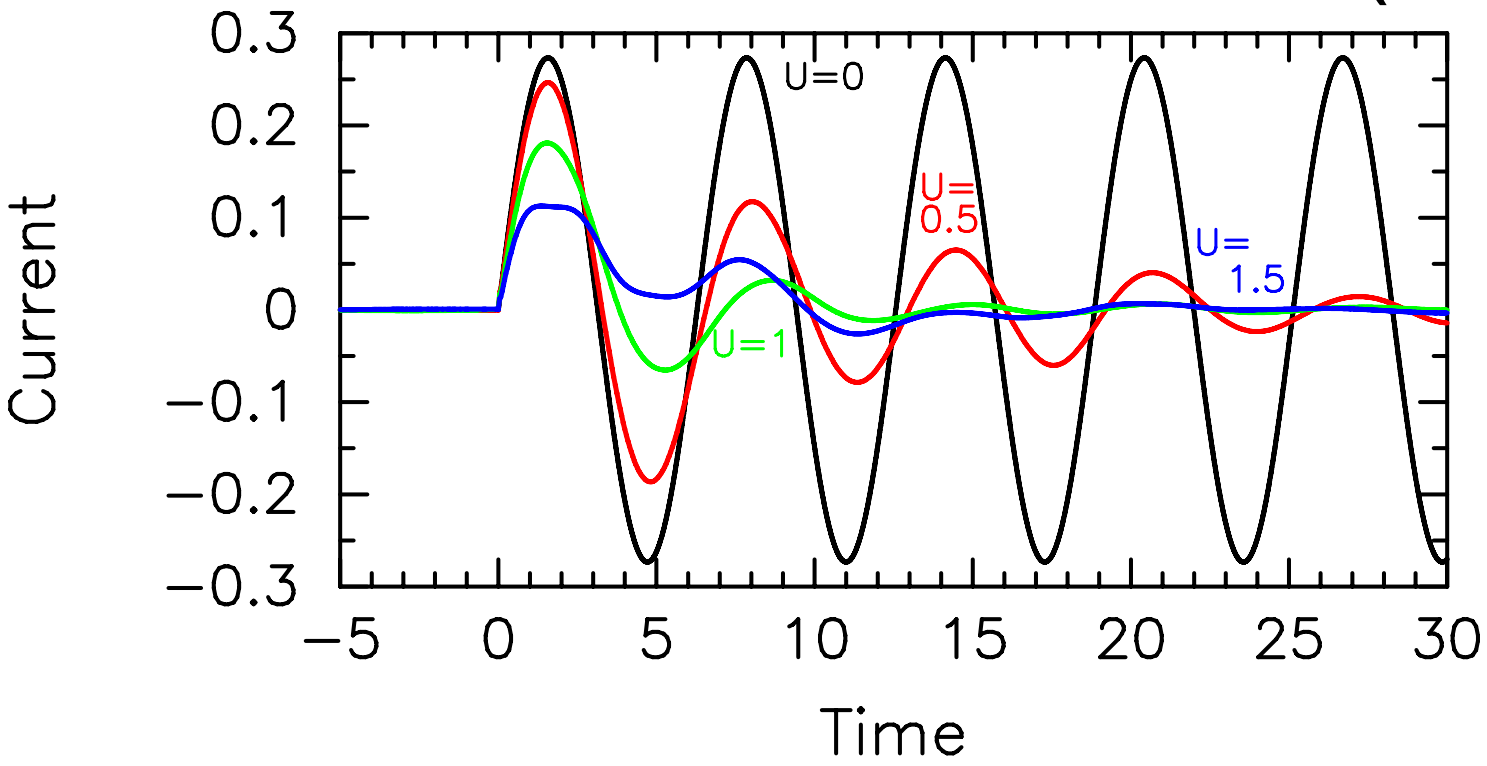
Next, we need to integrate the dependence of the **matrix elements** over a **two-dimensional** energy space.

Each matrix element is constructed from **one matrix inverse** and **two matrix multiplications**. We typically work with (approximately 10,000) **general complex matrices** of size up to 5700X5700.

Since the only information needed to generate the matrices is the local self-energy matrix Σ, the electric field **E**, and the temperature T, **this procedure is easily parallelized**.

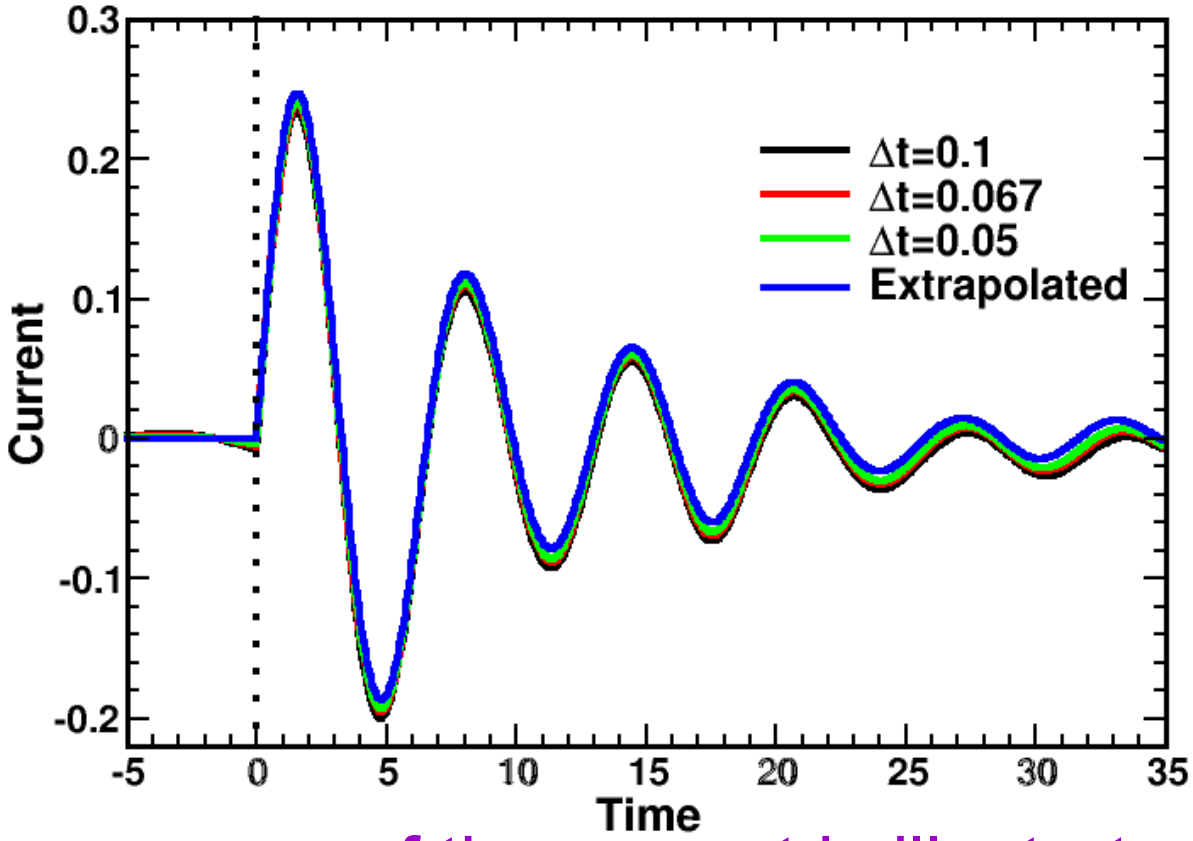
Computational Results

Bloch oscillations in metals (E=1)



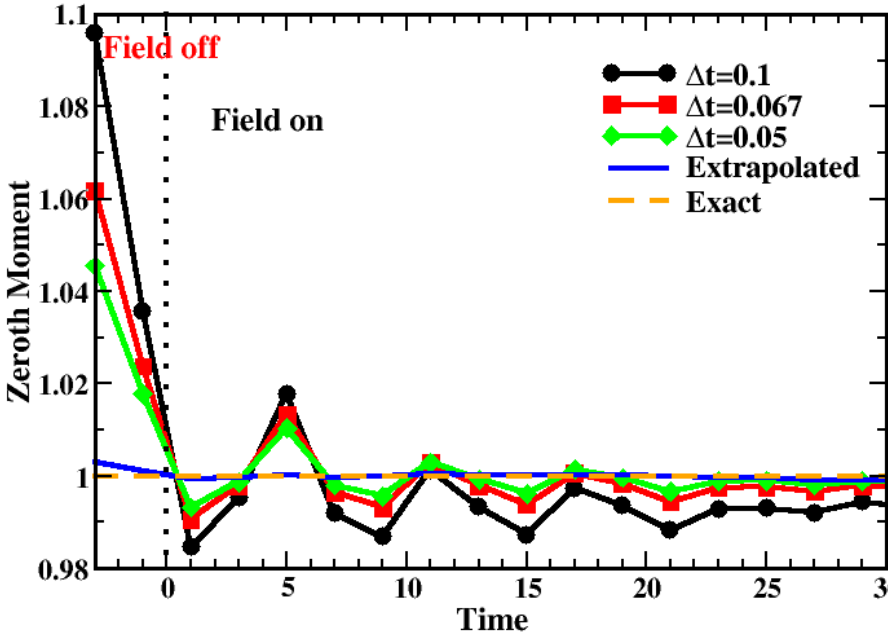
As the scattering increases, the amplitude of the current decays faster, but we cannot tell whether the oscillations survive at long time, or are completely damped.

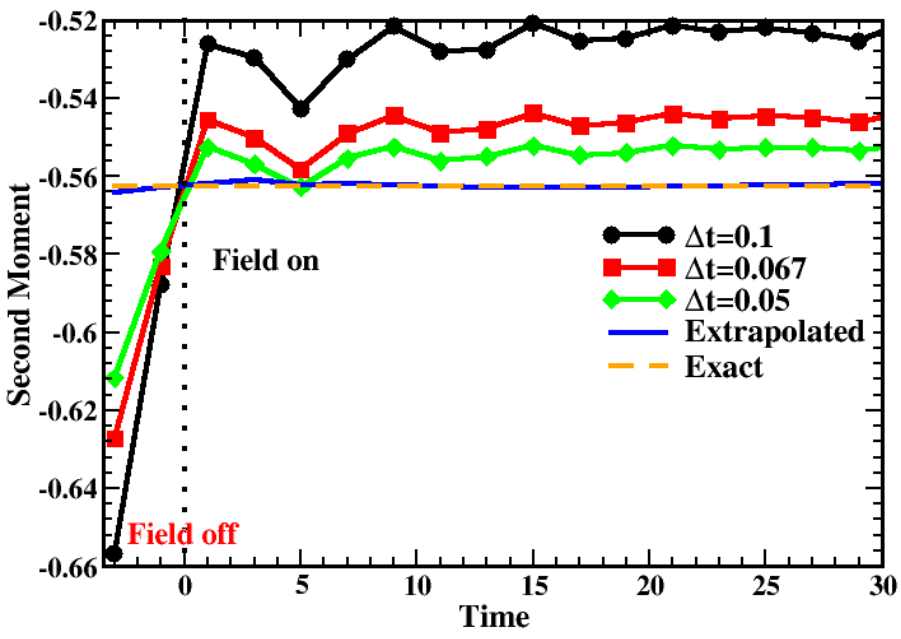
Accuracy of results—scaling of the current (E=1, U=0.5)



The accuracy of the current is illustrated here with a plot showing results for different discretizations and the extrapolated current.

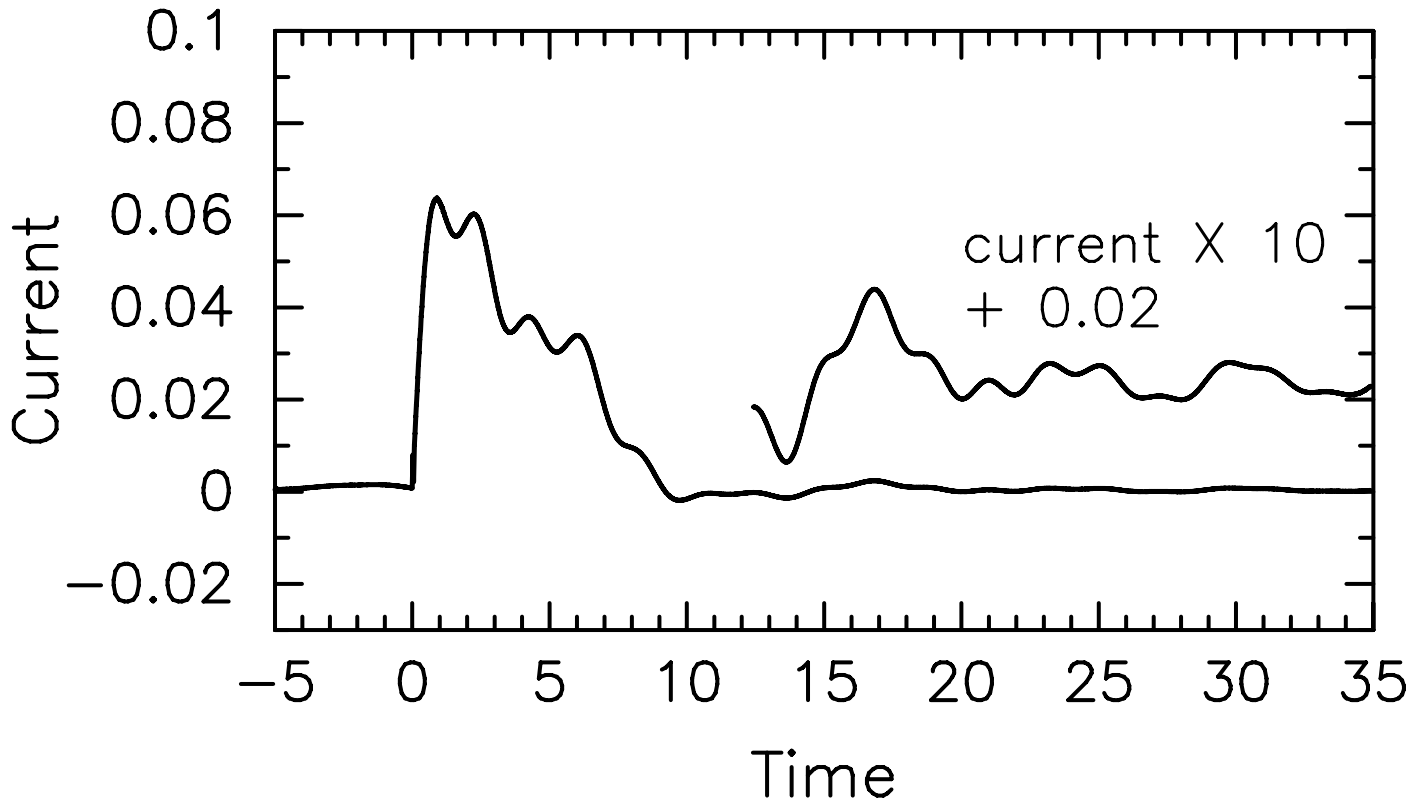
Accuracy of the results---scaling of moments (E=1, U=0.5)





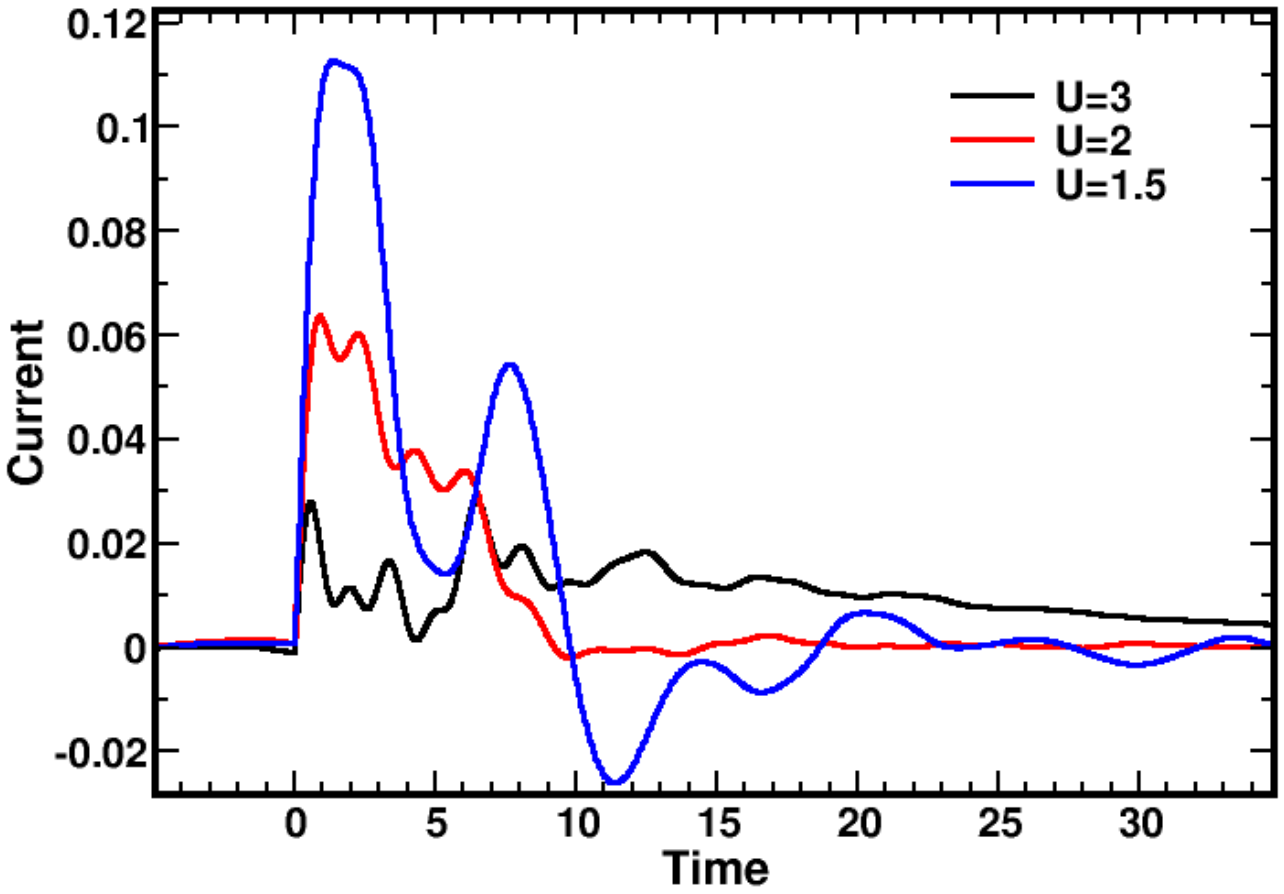
Exact results are known for the equal time Green's functions and their first two derivatives.
Extrapolating the results to zero discretization size yields **excellent agreement** with the exact results.

Current in the Mott Insulator (E=1, U=2)



In the Mott insulator, The regular Bloch oscillations are replaced by irregular oscillations. Note that they survive out to long times.

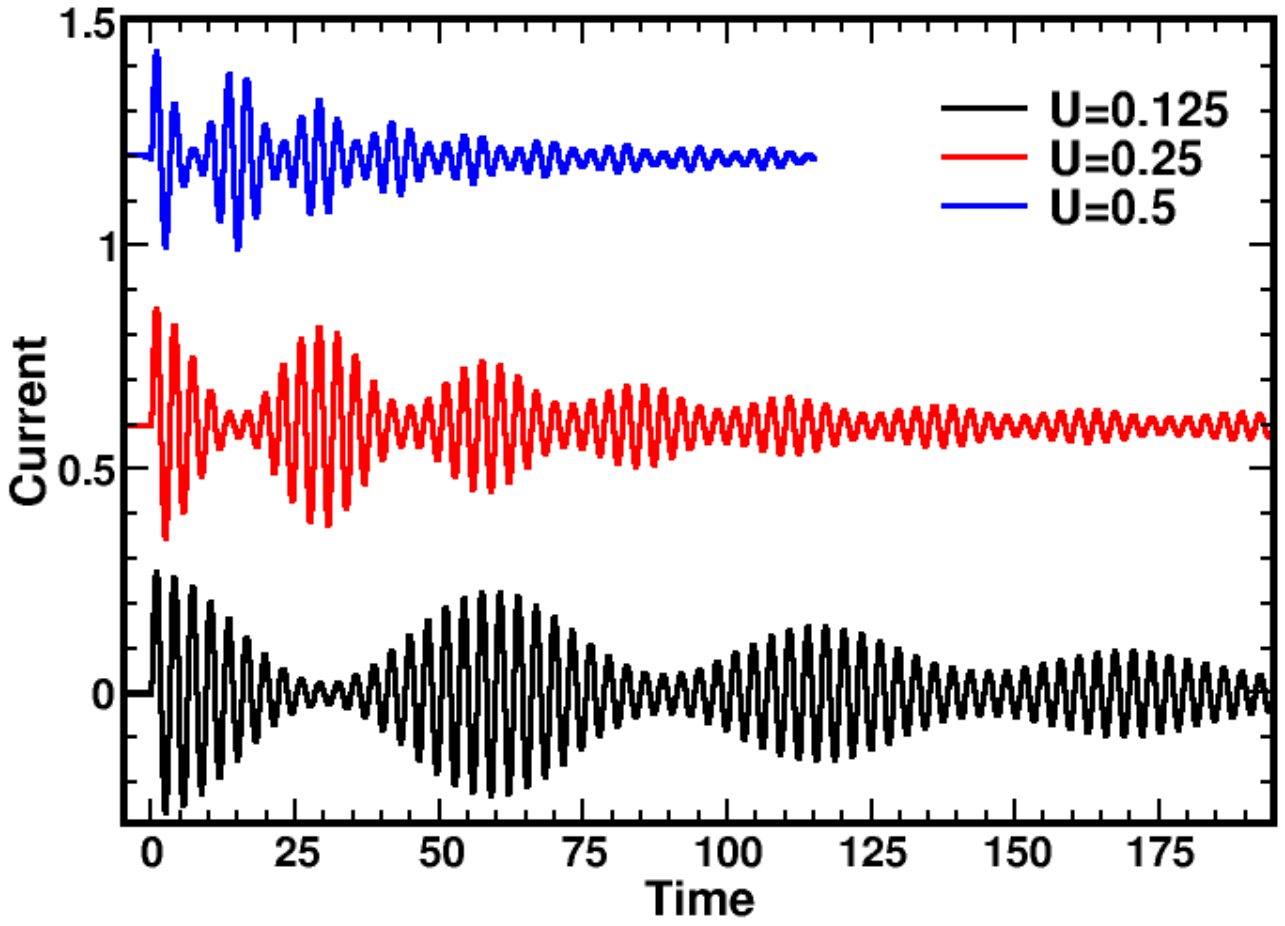
Current in the Mott Insulator ctd.



Notice how the oscillations change character from damped Bloch oscillations to irregular damped oscillations as the size of the gap in the Mott insulator increases.

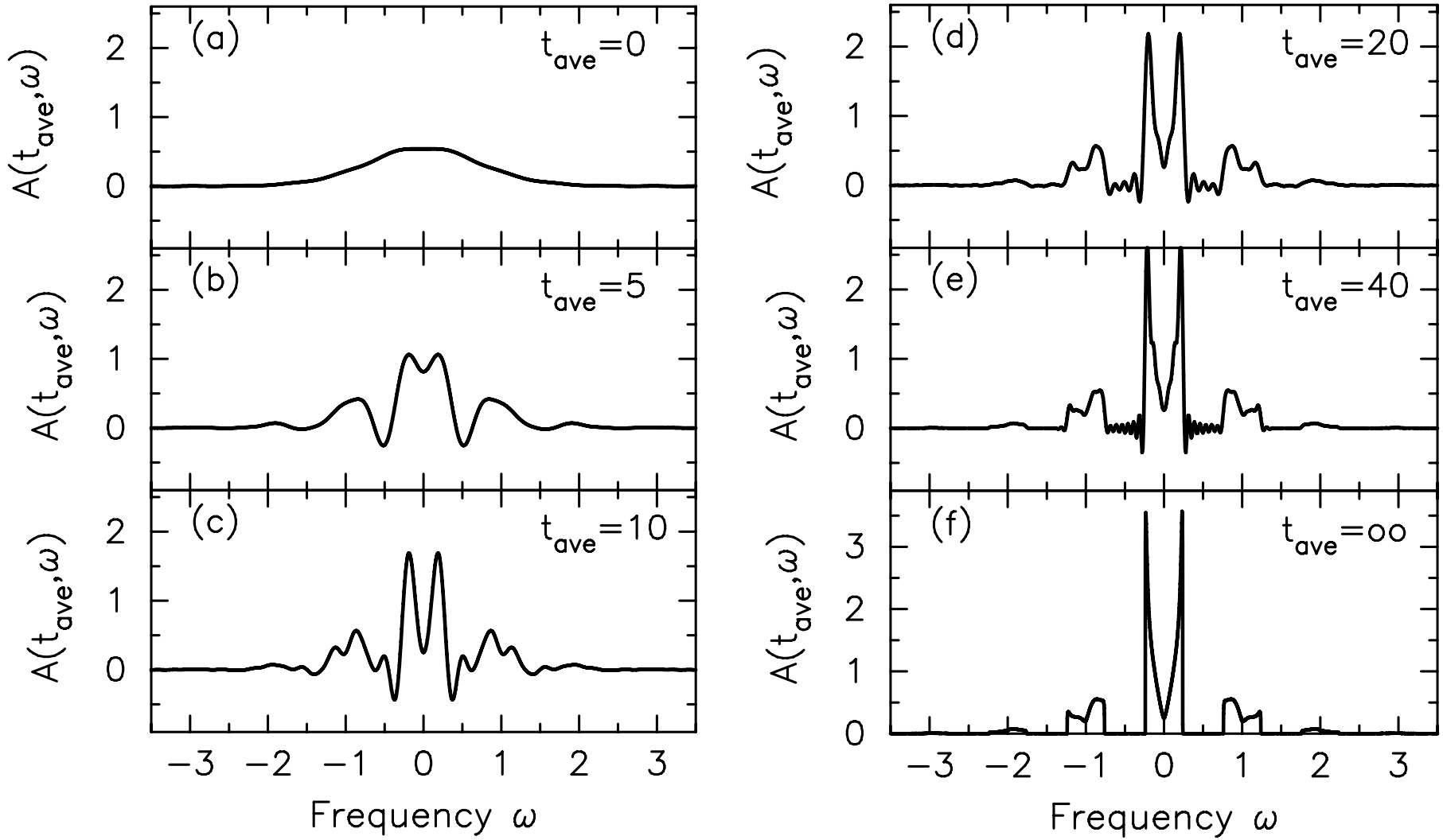
J. K. Freericks, Georgetown University, APCTP SCE Workshop talk, 2007

Beats in the current at large field

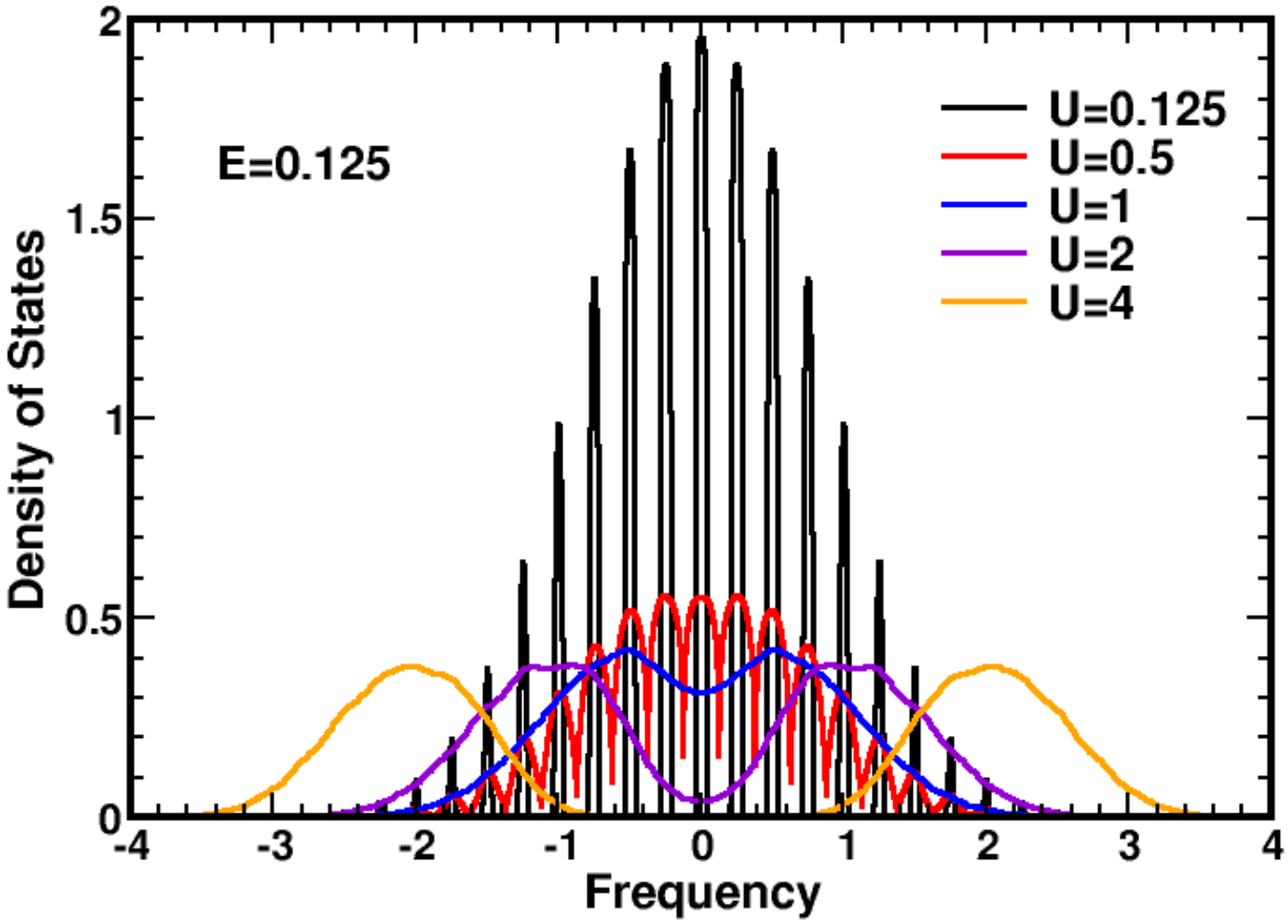


When the field is large (E=2 here), near beats develop with a beat period proportional to 1/U. The origin of the beats is a splitting in the DOS peaks by U.

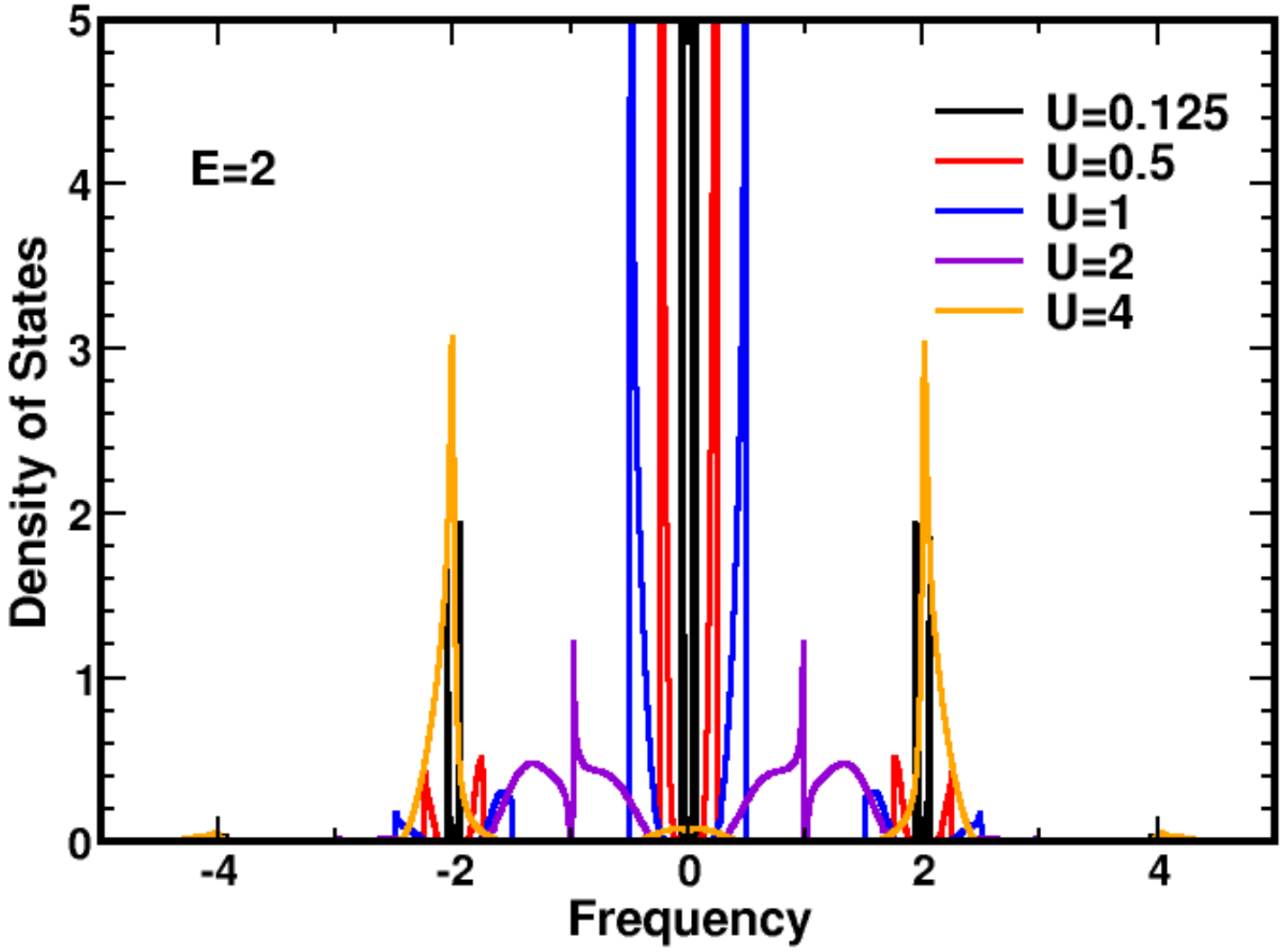
Density of states (E=1, U=0.5)



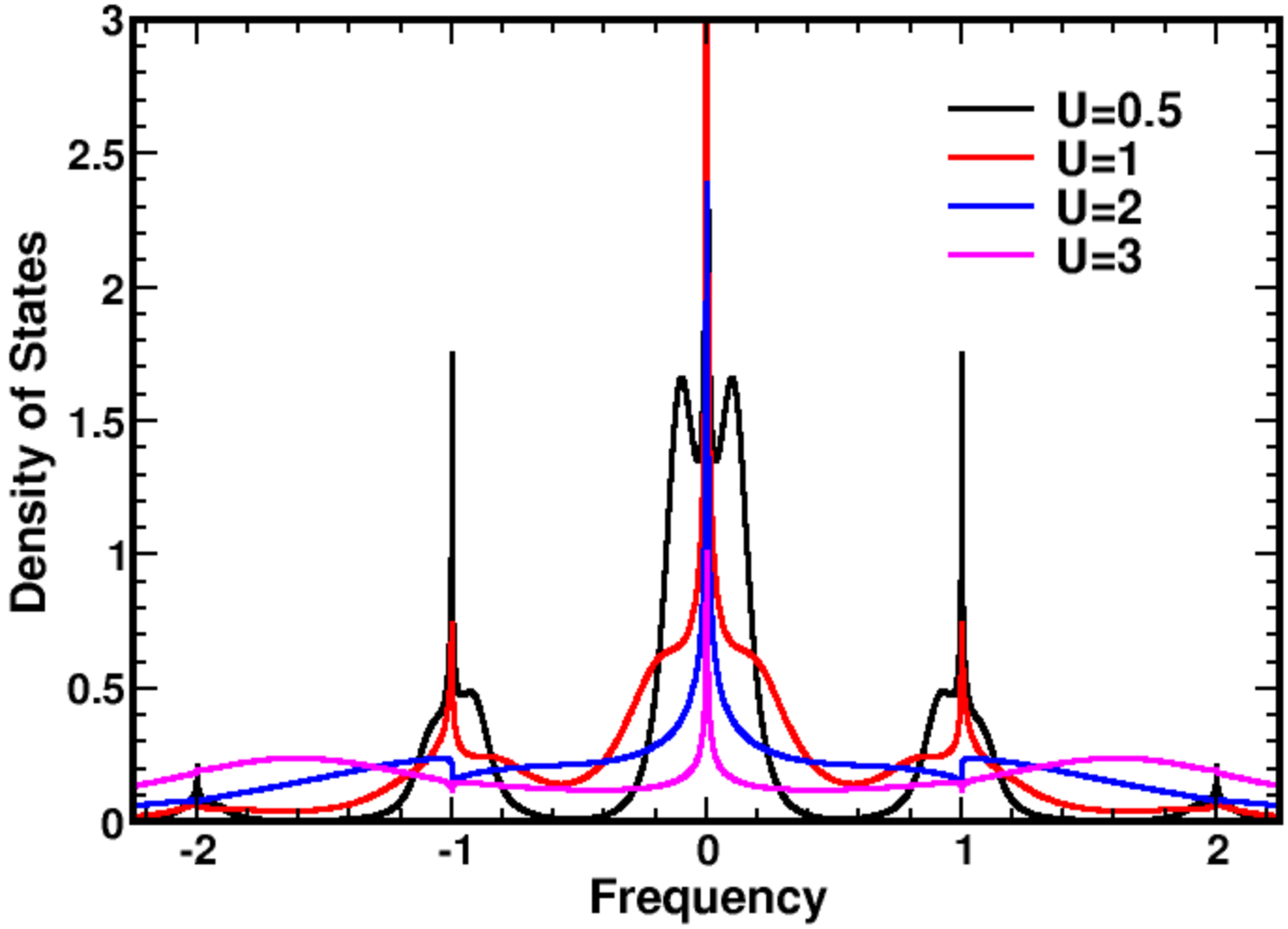
Density of states (E=0.125)



Density of states (E=2)



Density of states (Hubbard, E=1)



Distribution function of the electrons

In a cold atom system, one can detune the optical lattice, so it acts like it is being pulled in a particular direction. If we "pull" in the diagonal direction, this is equivalent to applying an electric field in the diagonal direction. The distribution of the light atoms through the Brillouin zone can be measured via a time-of-flight experiment. Theoretically, it is given by the equal-time lesser Green's function.

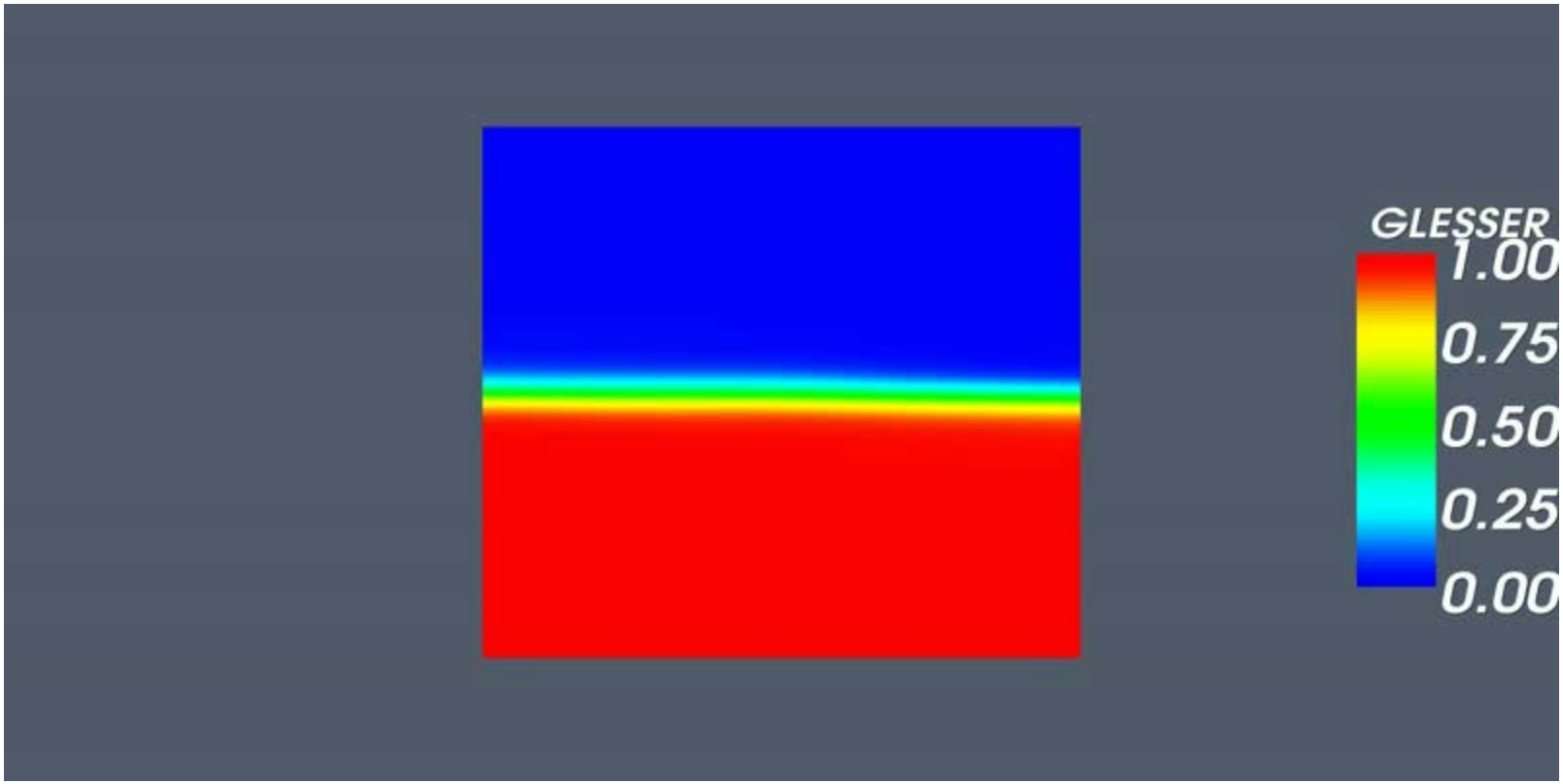
Gauge invariant vs. in a gauge

The measurable distribution function is the so-called **gauge-invariant Green's function**. This is related to the Hamiltonian-gauge Green's function by a **transformation to a rotating frame** with the rate of rotation set by the electric field strength.

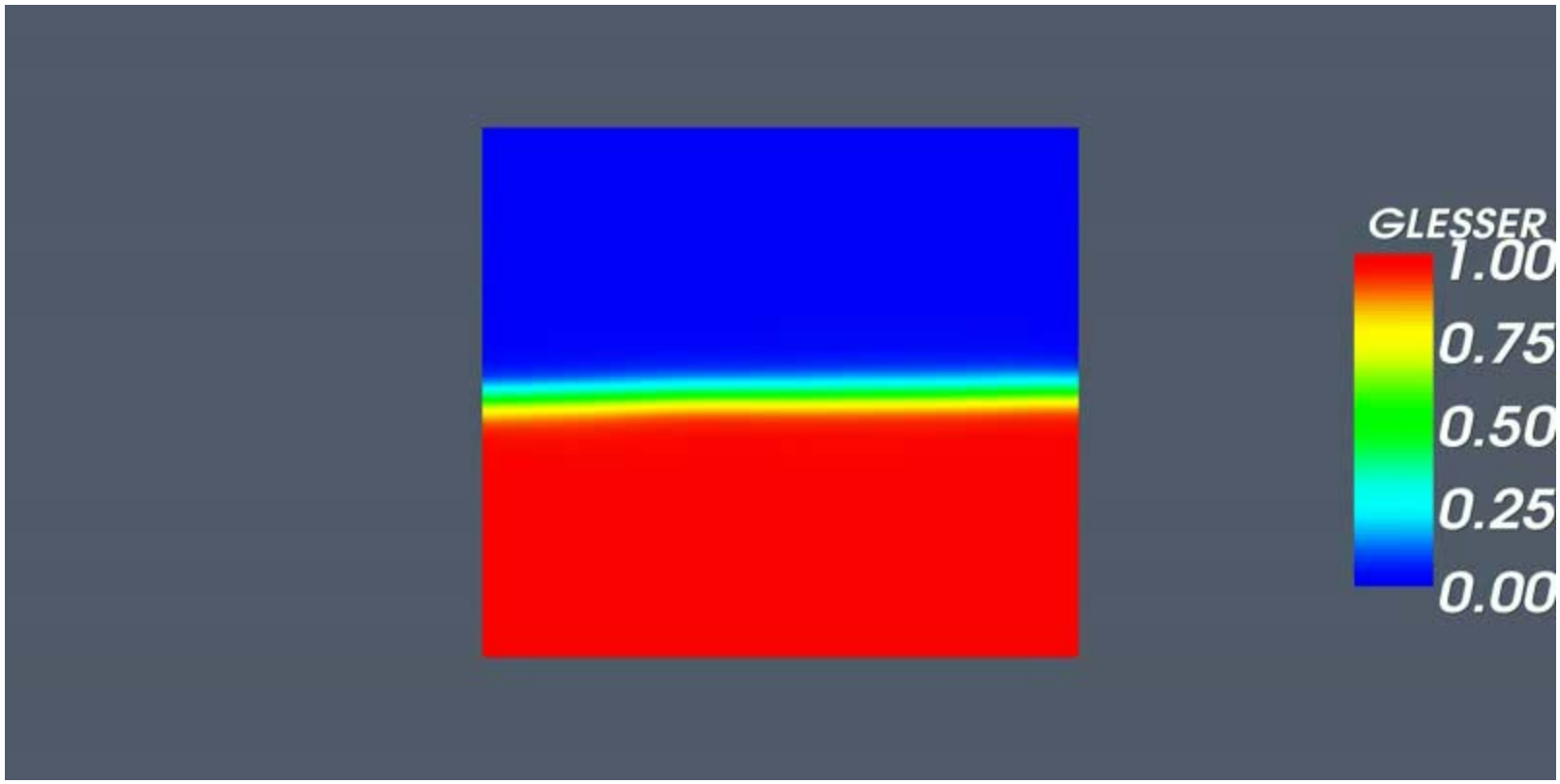
For example, in the noninteracting system, the distribution function is a **Fermi-Dirac distribution** in the Hamiltonian gauge $f(\varepsilon)$ and a **rotating Fermi-Dirac distribution** $f(\varepsilon\cos[Et]+\bar{\varepsilon}\sin[Et])$ in the gauge-invariant case.

When interactions are included, the distribution is **smoothed out due to scattering** and can **change its character** as the field strength increases.

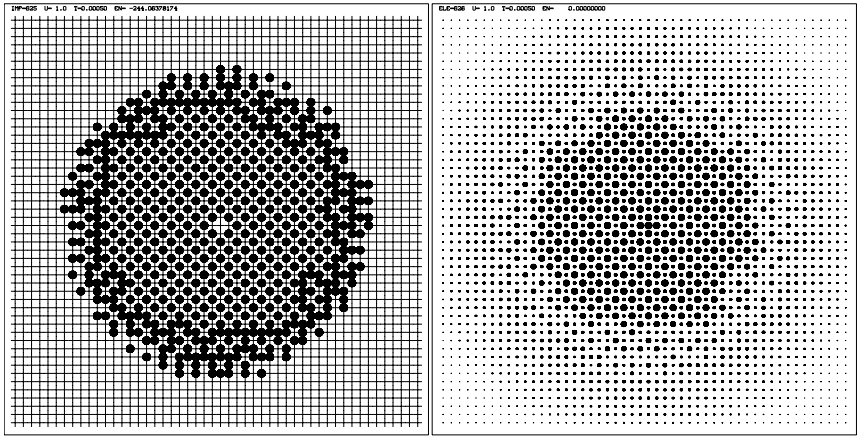
Strongly scattering metal (small field)

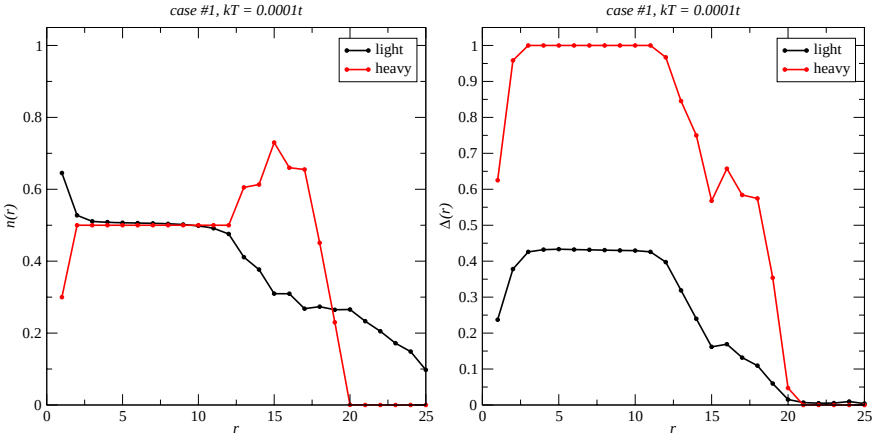


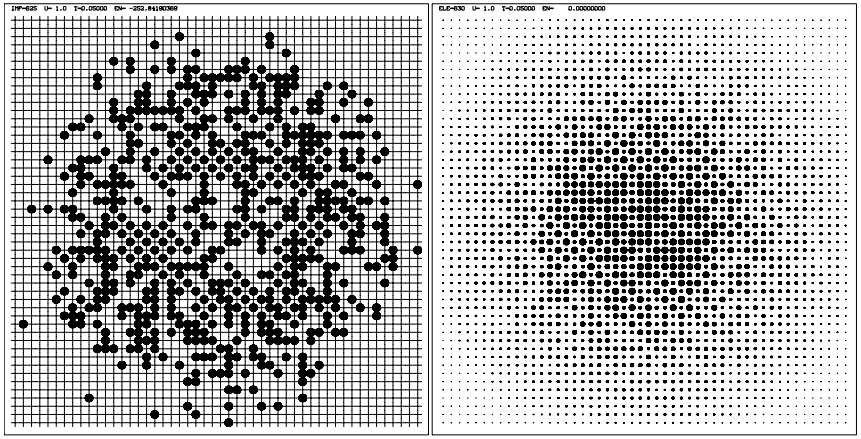
Strongly scattering metal (large field)

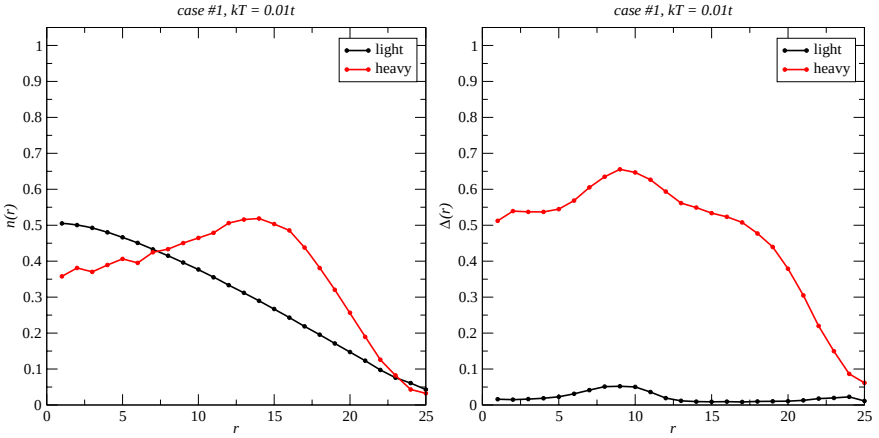


Two-d simulation results (R=12.9)

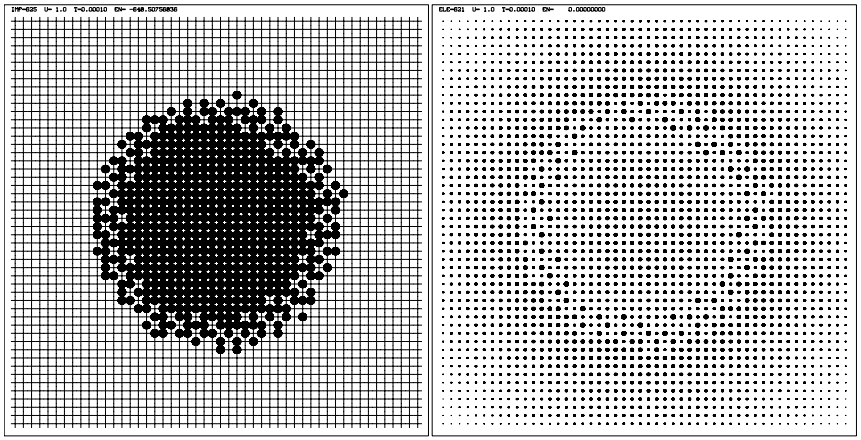


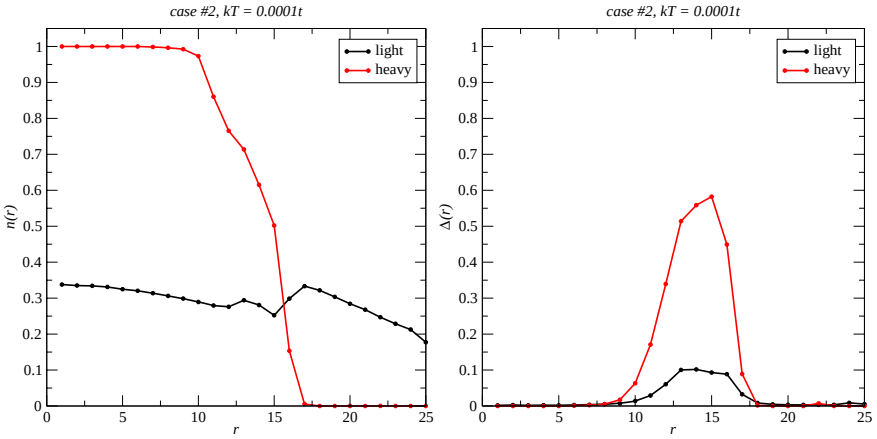


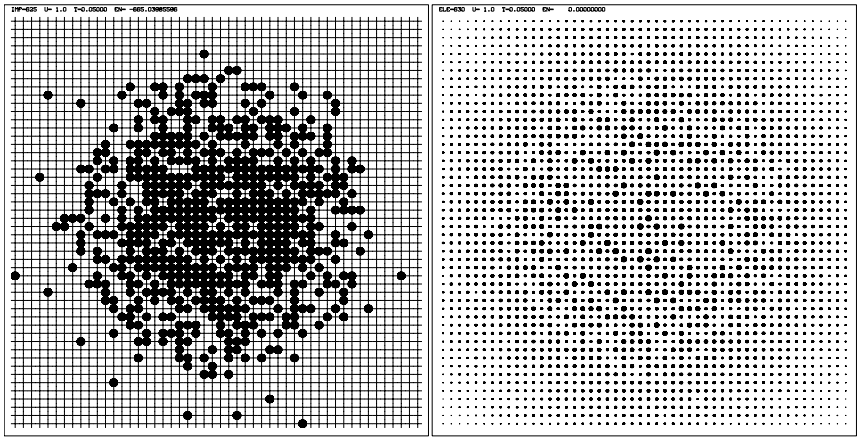


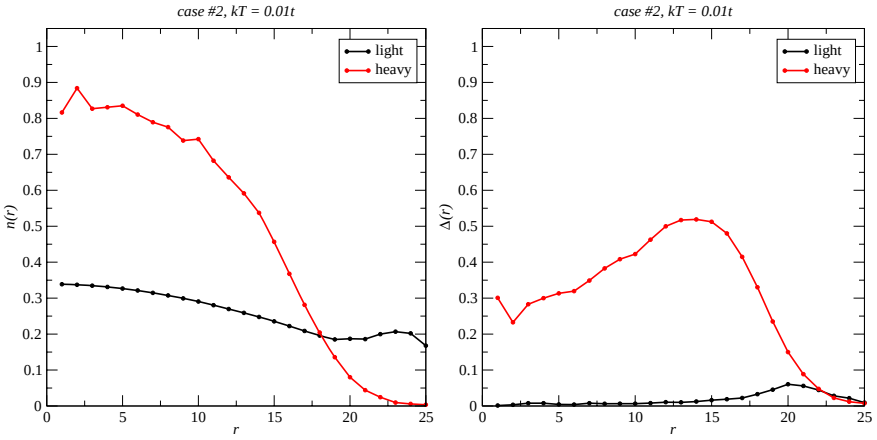


Two-d simulation results (R=17)

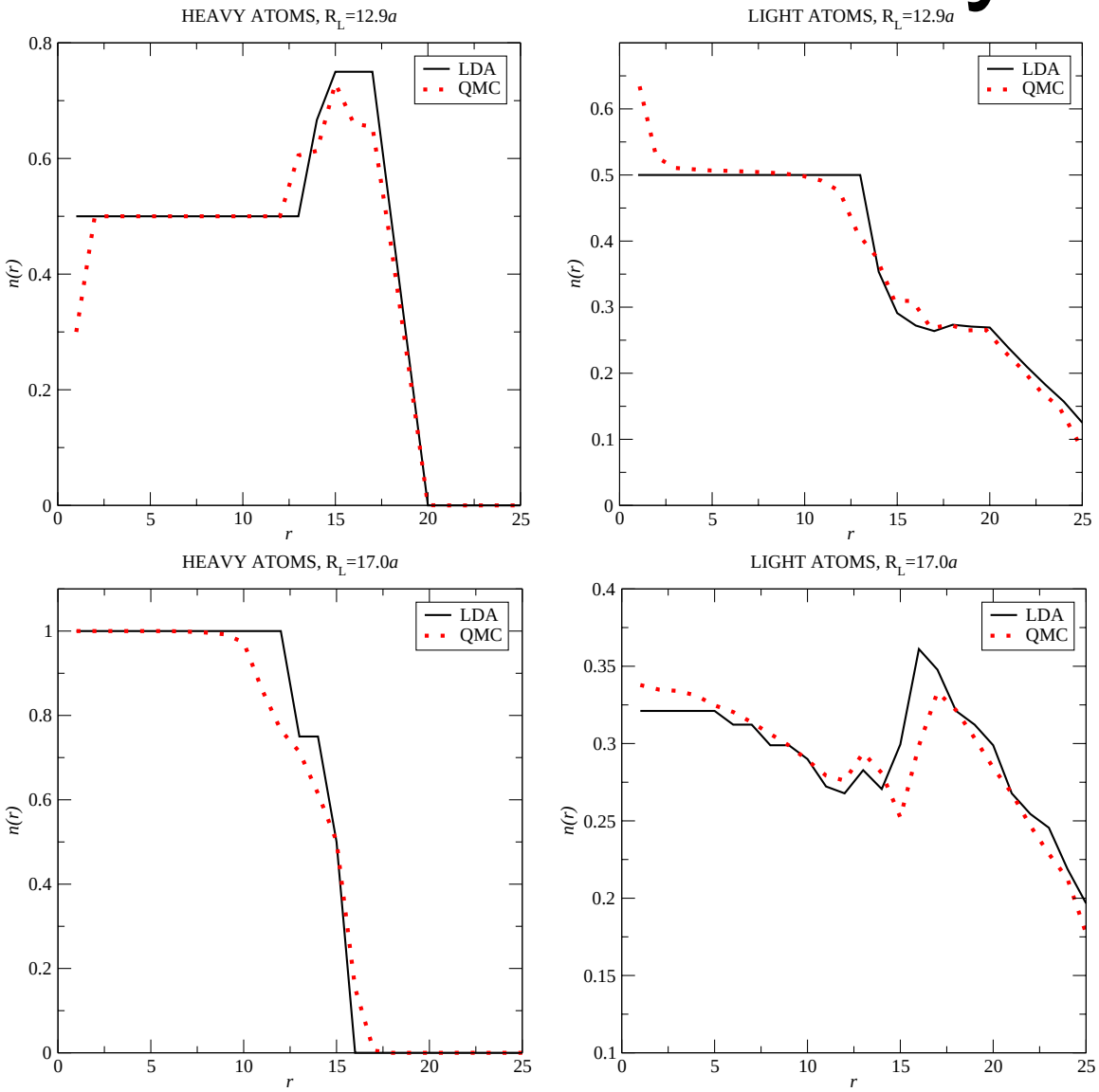








Two-d local density approximation



Comparison of the T=0 lda to the finite-T qmc for the two cases: R=12.9 (top) and R=17 (bottom). Note the remarkable agreement.

Conclusions

- Showed how to implement an **efficient parallel algorithm** to solve the **Keldysh problem** for strongly correlated electrons described by the Falicov-Kimball model.
- The procedure was applied to the **question of Bloch oscillations** and **how they disappear** as scattering is increased**.**
- Our algorithm showed **efficient usage and good scaling** to thousands of processors on a **Cray-XT3, an SGI Altix, and a Sun Opteron** (we used a total of about **2,500,000 cpu-hours** on the project and sustained over 60% peak speed on the Altix).