Nonlinear Dynamical Mean-Field Theory

J. K. Freericks

Department of Physics

Georgetown University

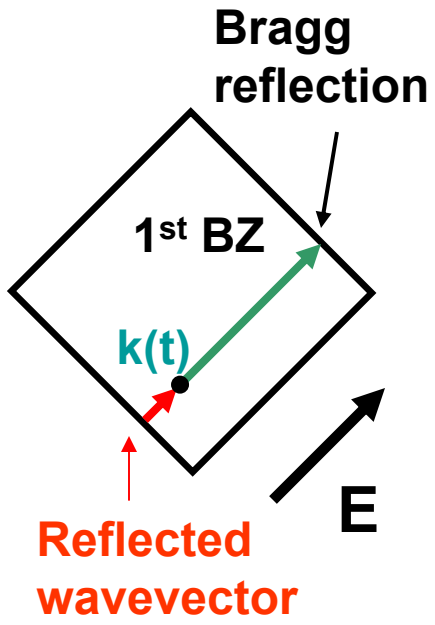
Funding from ONR and NSF

Supercomputer time from a DOD CAP and a NASA NLCS allocation

Thanks to Volodmyr Turkowski and Veljko Zlatic' for collaborating on this work.

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.

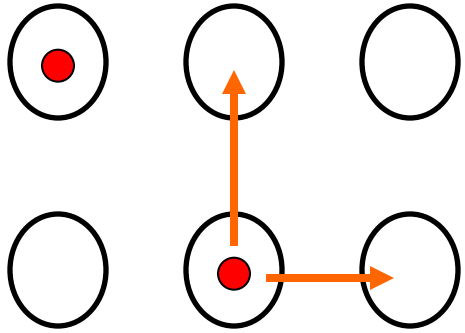
Quenching Bloch oscillations

- **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*.**

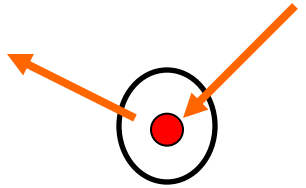
Many-body physics and the dynamical mean-field theory approach to nonequilibrium problems

Dynamical mean field theory
(Vollhardt, Metzner, Brandt, Georges, Kotliar)

- Models of strongly correlated materials are difficult to solve.
- Nevertheless, 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**.

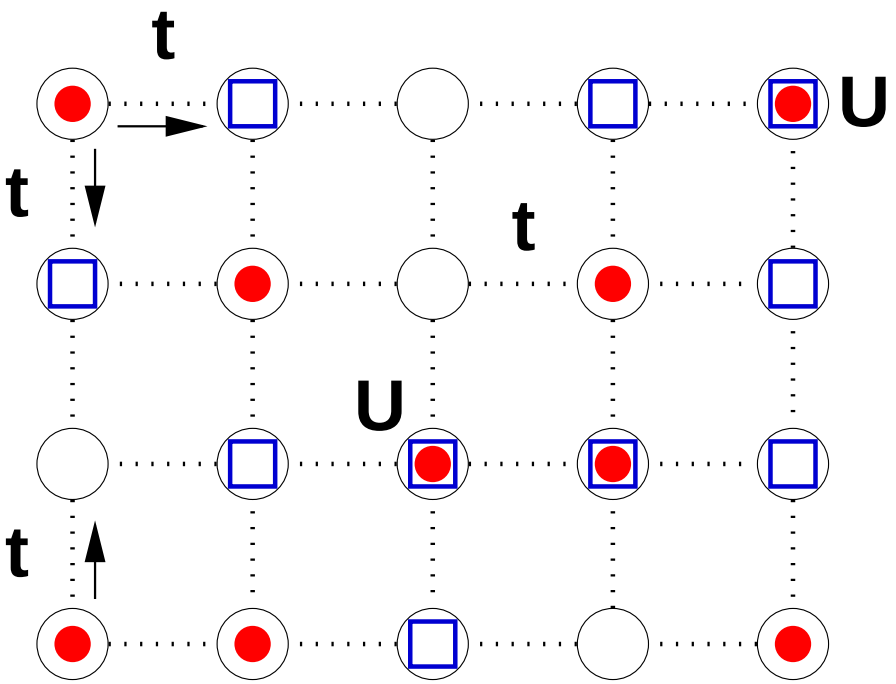


Lattice



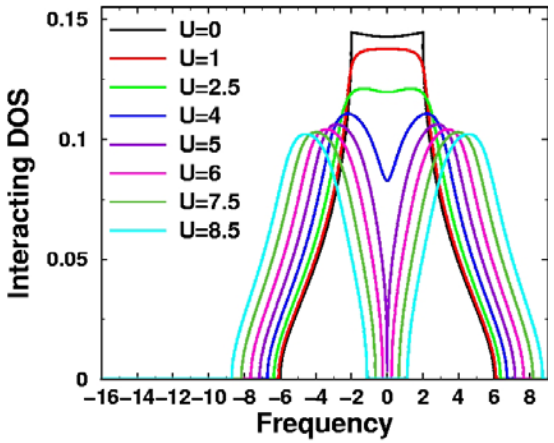
Impurity site

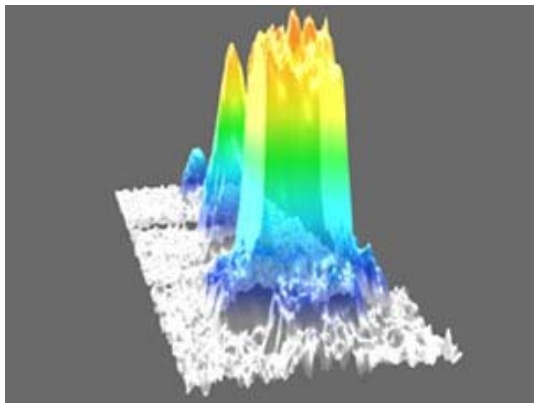
Falicov-Kimball Model



- 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**.

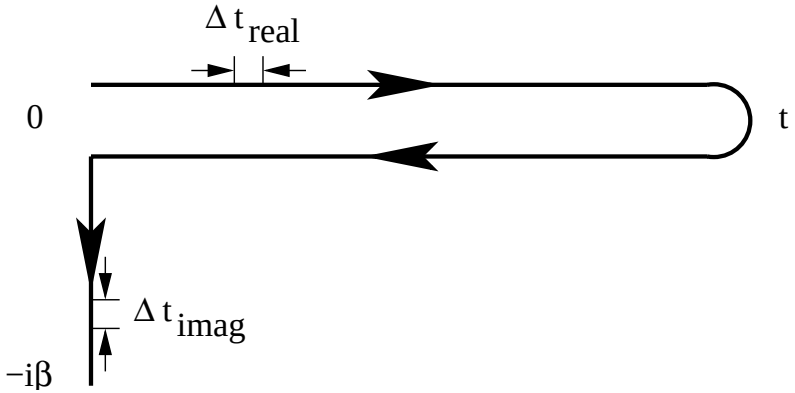
Physical importance of the Falicov-Kimball Model





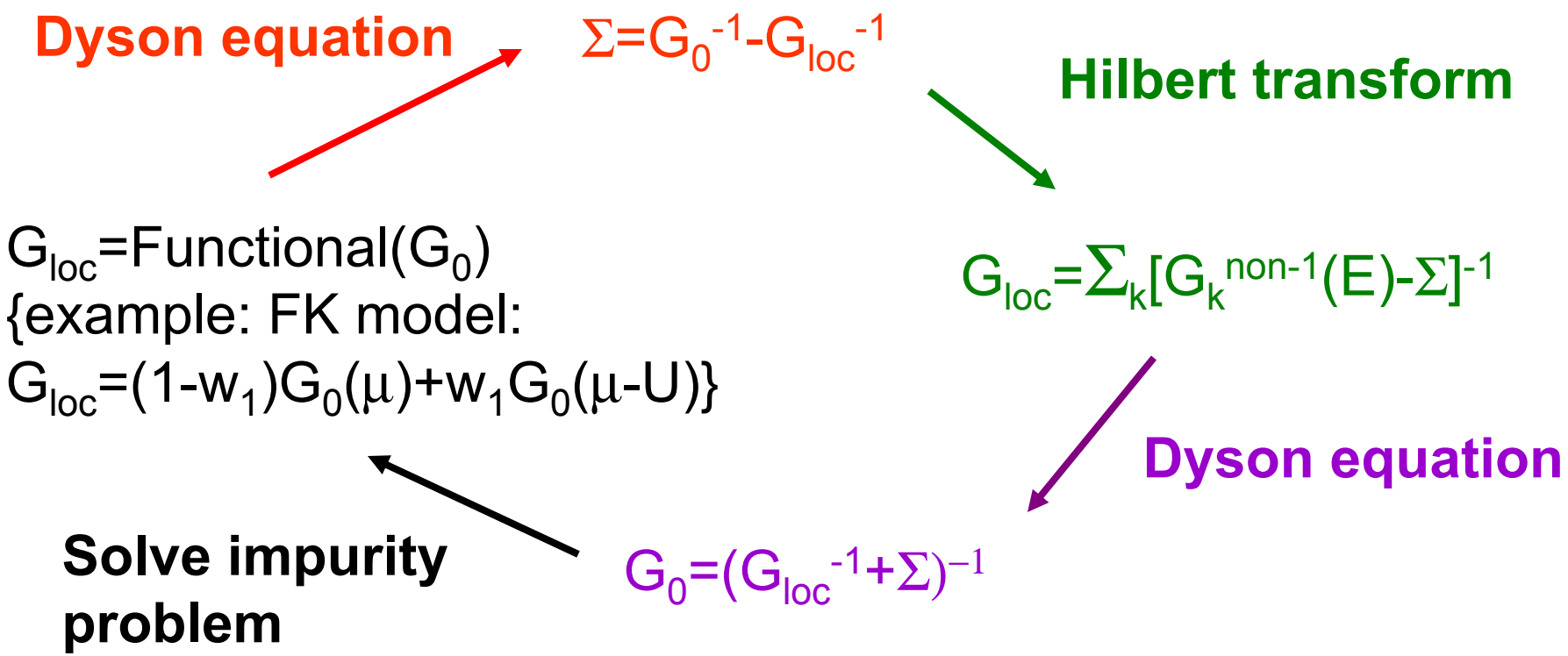
- Simplest many-body problem that has a **Mott-like metal-insulator transition** (but it has no Fermi-liquid behavior).
- Possible solid-state systems include NiI_2 and Ta_xN
- Possible cold atom systems include mixtures of light alkali atoms (Li or K), with heavy alkali atoms (Rb or Cs) in optical lattices.

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:

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

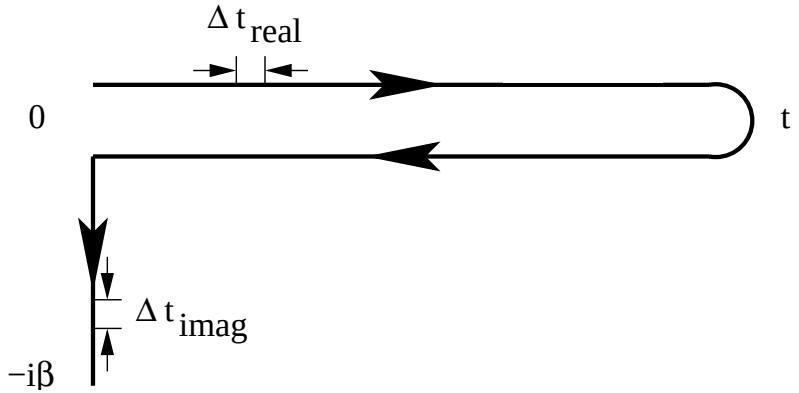
which becomes the sum of two **"band energies"** when the field lies in the diagonal direction after the Peierl's substitution.

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 integration points for each dimension to perform the two-dimensional quadrature.

Computational algorithm 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 4900X4900.

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**.

Parallel implementation

(1) **Solve** for the local self-energy using Dyson's equation on the master node.

(2) **Broadcast** the self-energy $\Sigma(t,t')$, the field **E**, and the temperature T to **all slave nodes**.

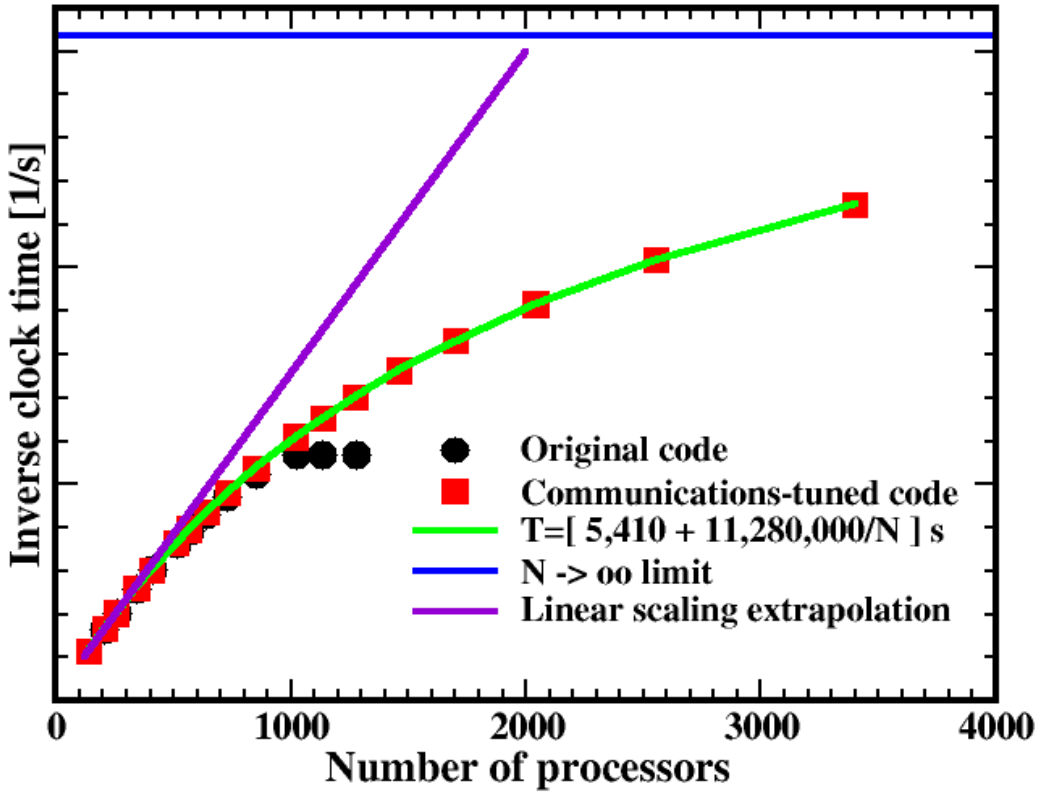
(3) **Send** each **slave node** a value of energies for the momentum dependence of the Green's function and compute the **matrix** that enters the two-dimensional quadrature. LAPACK routines are used for efficiency.

(4) **Store** data on the **slave nodes** for accumulation; use **recursive binary gather** to accumulate for the **master**.

(5) **Solve** the impurity problem on the **master** node to determine the new self energy.

(6) **Repeat until converged**. Then extract the interesting time-dependent quantities like the current as a function of time, or the distribution of the electrons.

Scaling



The algorithm has a natural parallelizable piece and a serial piece, so it can never achieve pure linear scaling for strong scaling. The green curve is the strong scaling prediction, red squares the actual data.

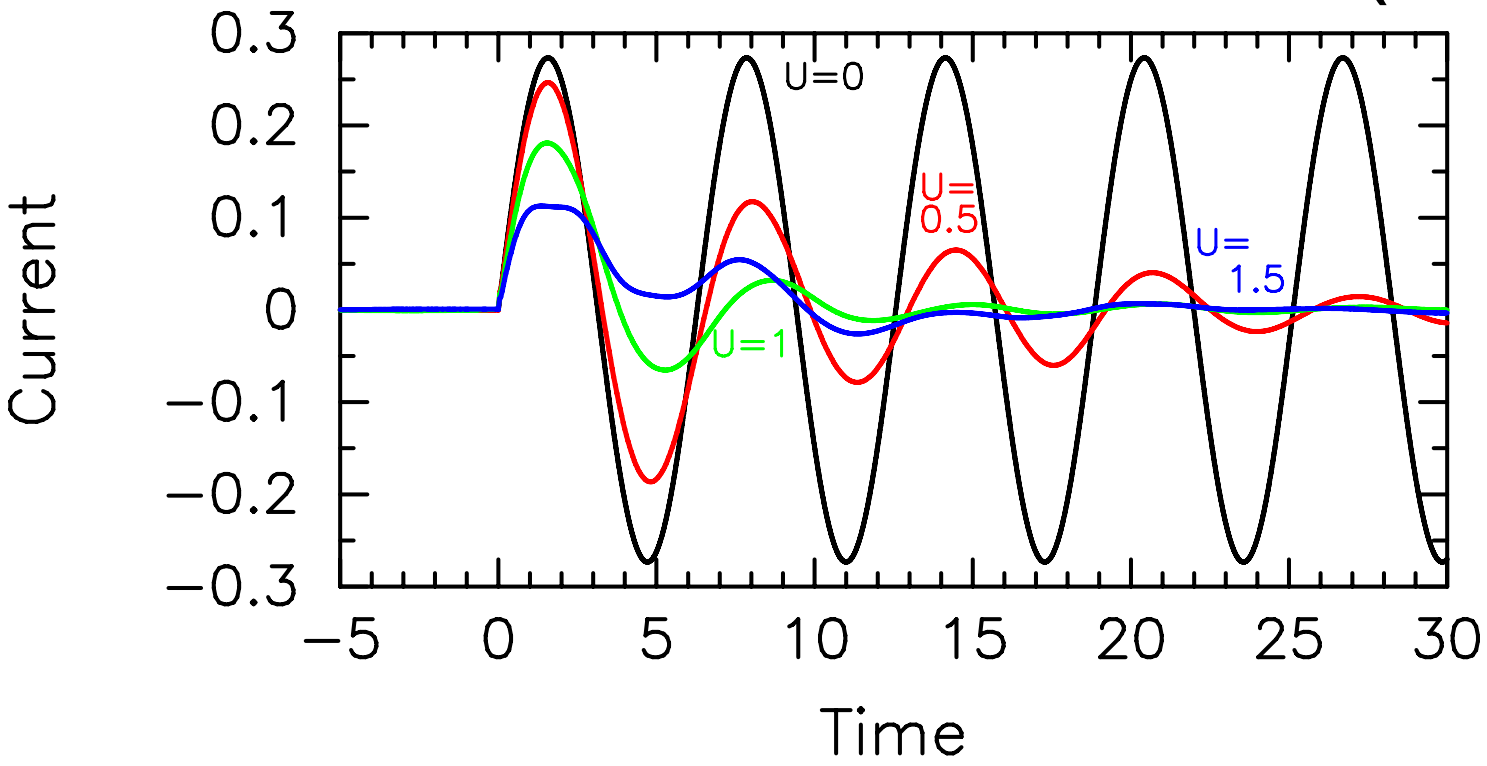
When originally scaled, the data showed a bottleneck when increased beyond about 900 processors. This was a communications issue, resolved by using a recursive binary gather operation. Strong scaling is sublinear, but achieves about 70% of scale up on 1500 procs.

Recursive Binary Gather

- In computing the two-dimensional matrix-valued integration, we originally used a **many-to-one** communication, sending results to the master node immediately after being completed.
- But all nodes finished at **about the same time**, creating a data bottleneck with the master node.
- The **recursive binary gather** operation has each node store their results until all computation is finished, then the slave nodes are divided in two, and one half sends their data to the other half.
- The sending of data and "collapsing" of the nodes is **repeated** until all data is on one node, which is then sent to the master node.

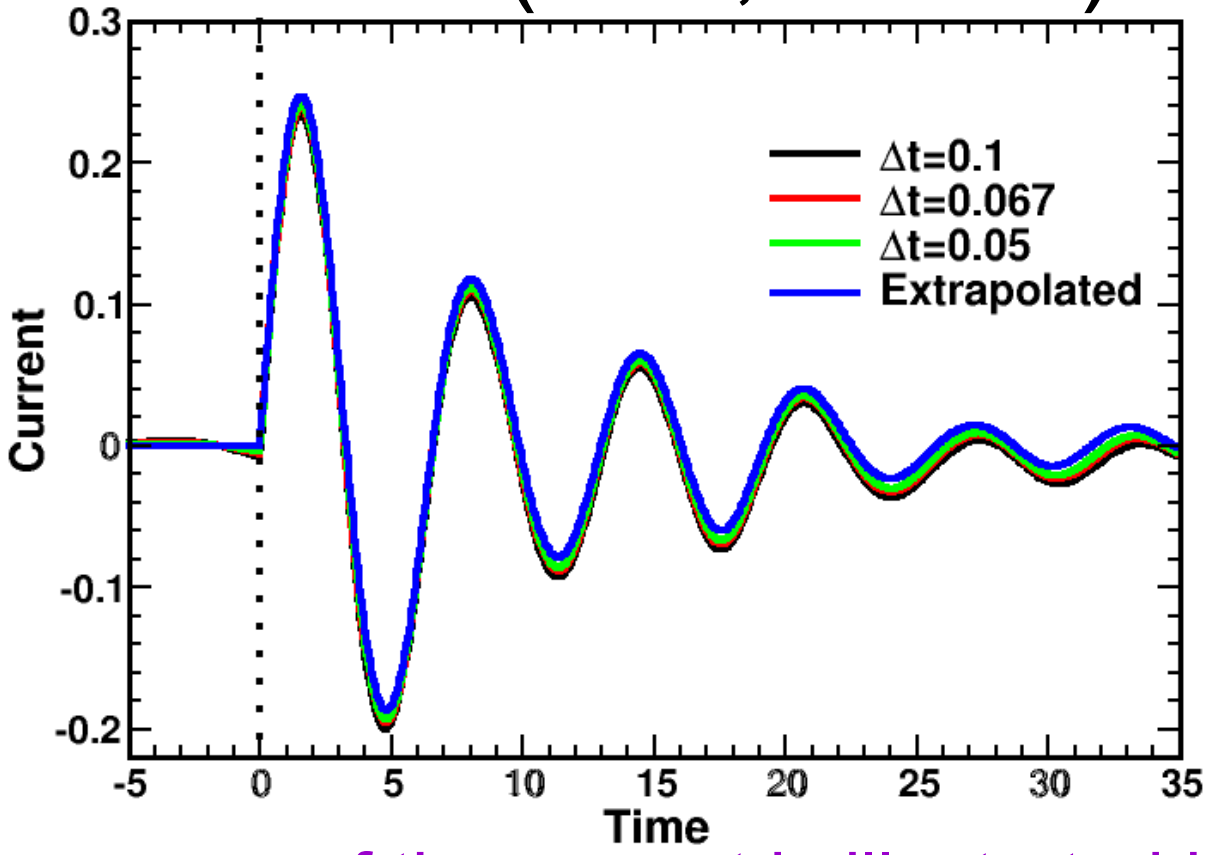
Computational Results

Bloch oscillations in metals (E=1)



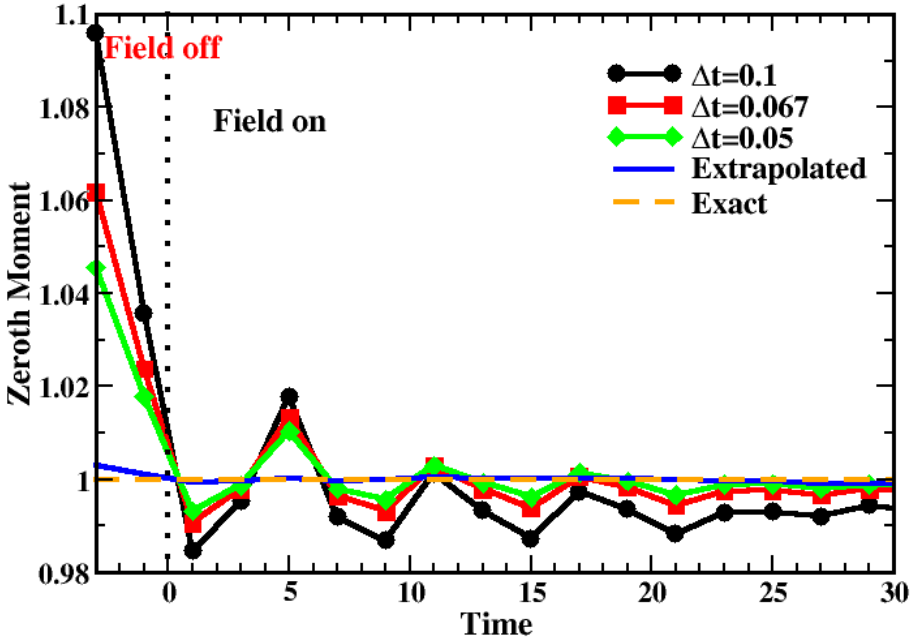
As the scattering increases, the amplitude of the current decays faster, but we cannot tell whether the oscillations survive at long time, or are completely damped.

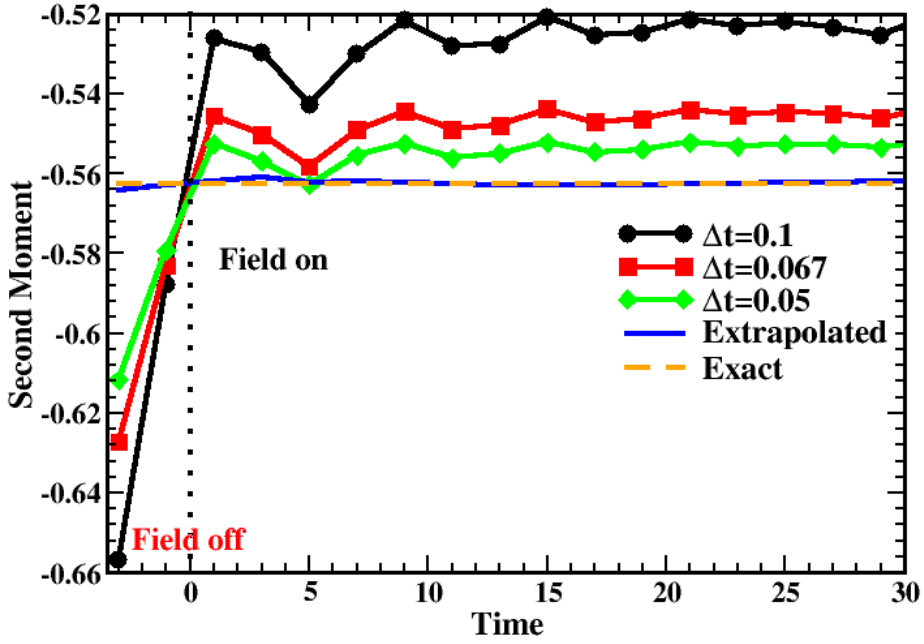
Accuracy of results—scaling of the current (E=1, U=0.5)



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

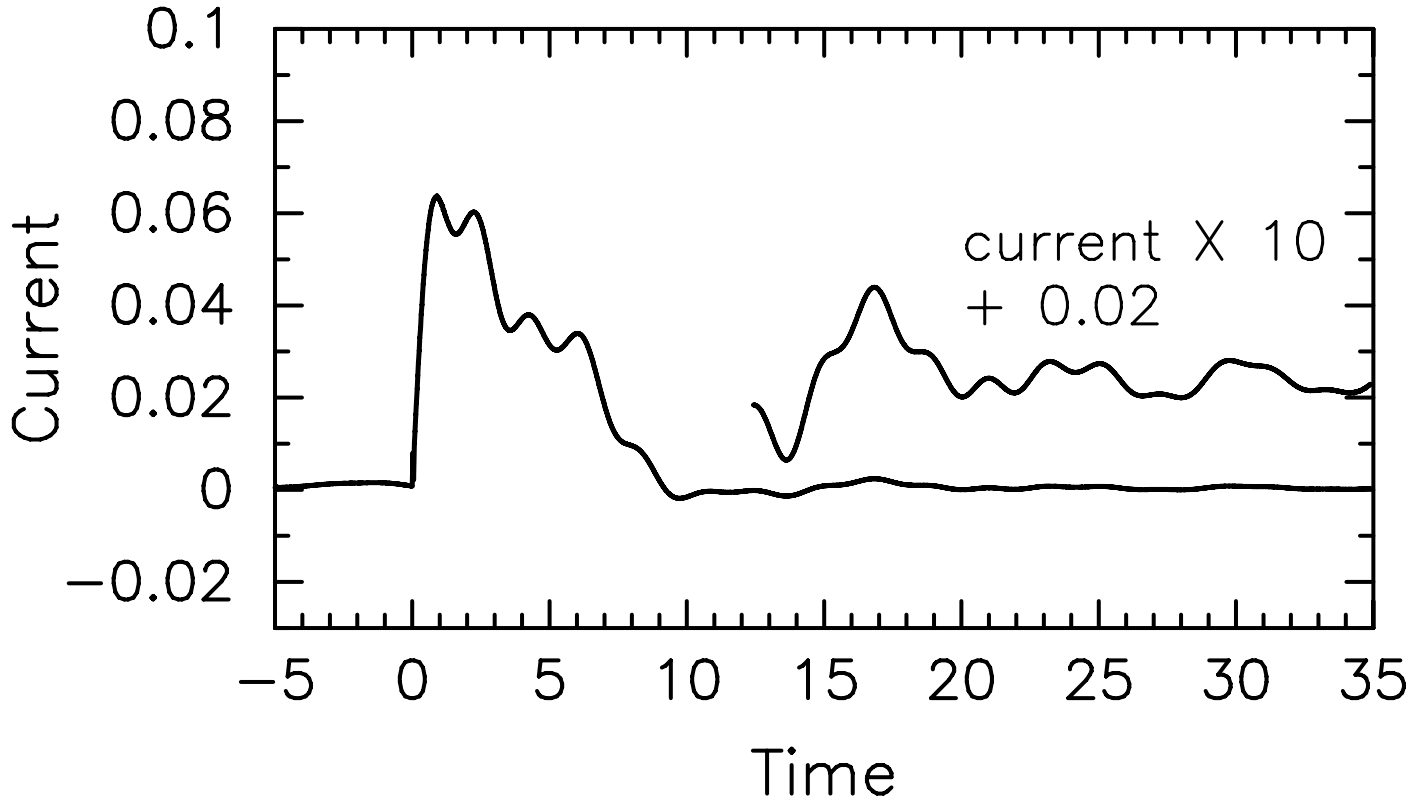
Accuracy of the results---scaling of moments (E=1, U=0.5)





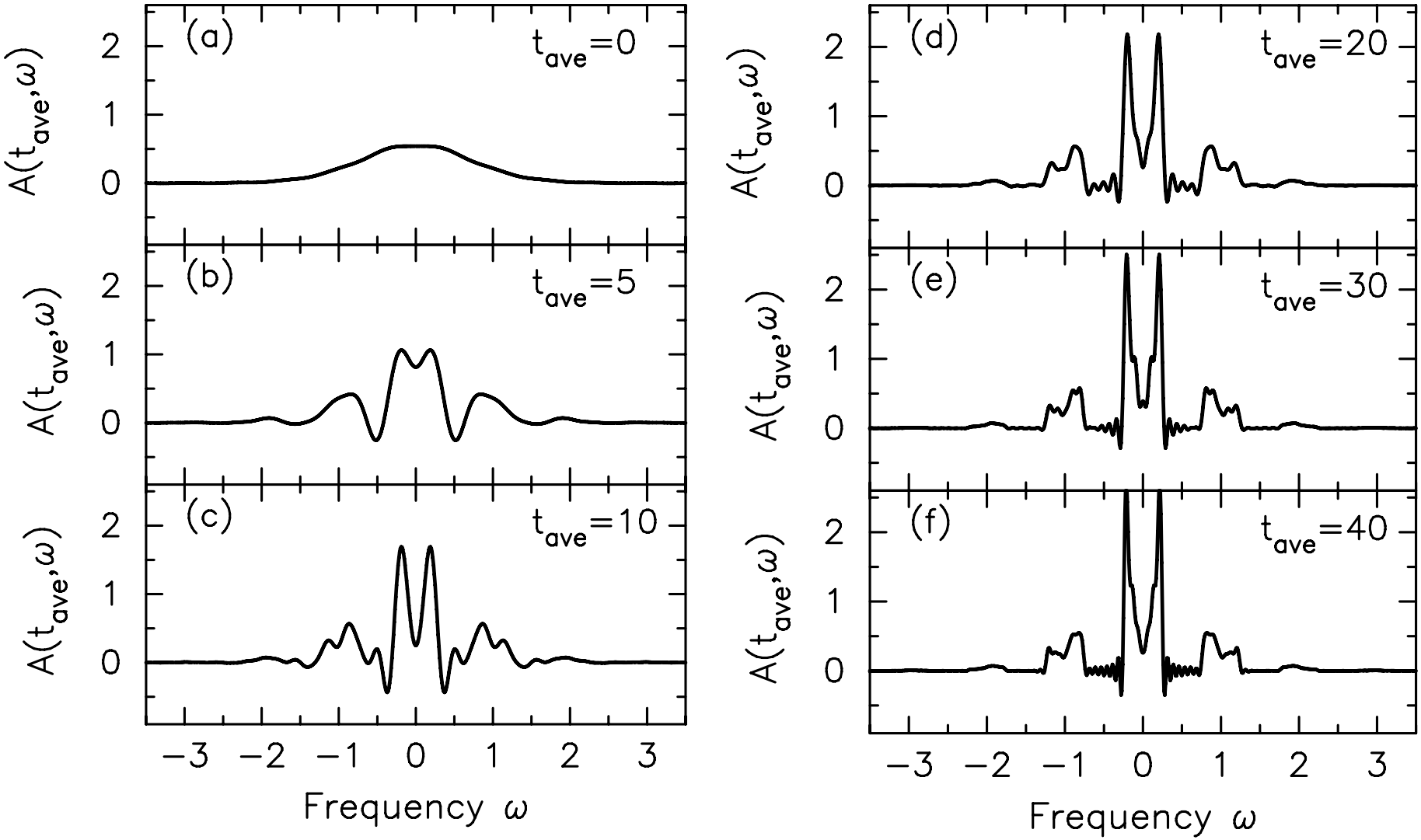
Exact results are known for the equal time Green's functions and their first two derivatives.
Extrapolating the results to zero discretization size yields **excellent agreement** with the exact results.

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

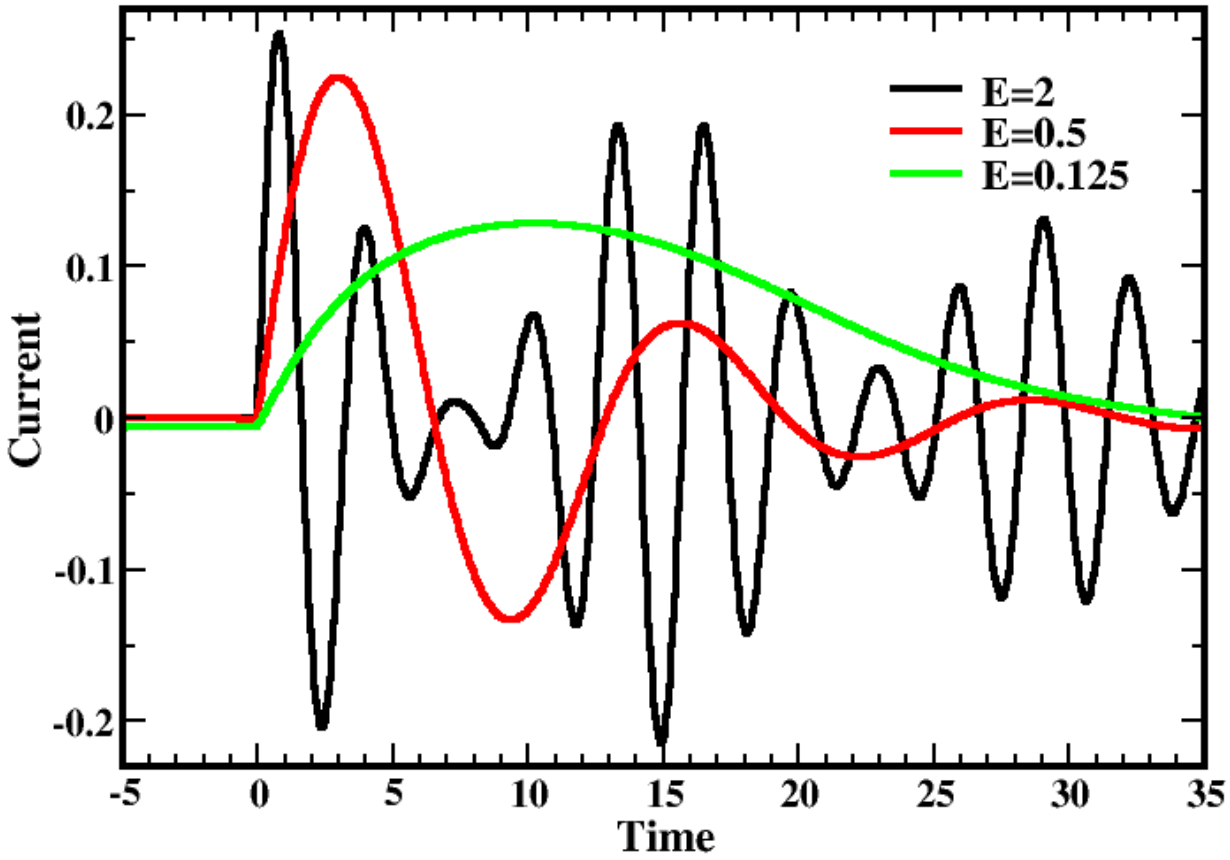


In the Mott insulator, the regular Bloch oscillations are replaced by **irregular oscillations**. Note that they survive out to long times as shown in the blow-up.

Transient density of states in a metal (E=1, U=0.5)



Current in a metal with different field strengths

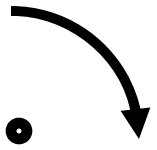


Beats appear to develop as the field gets large! It isn't clear what the origin is, but the beat frequency is inversely proportional to U (here U=0.5).

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 field.

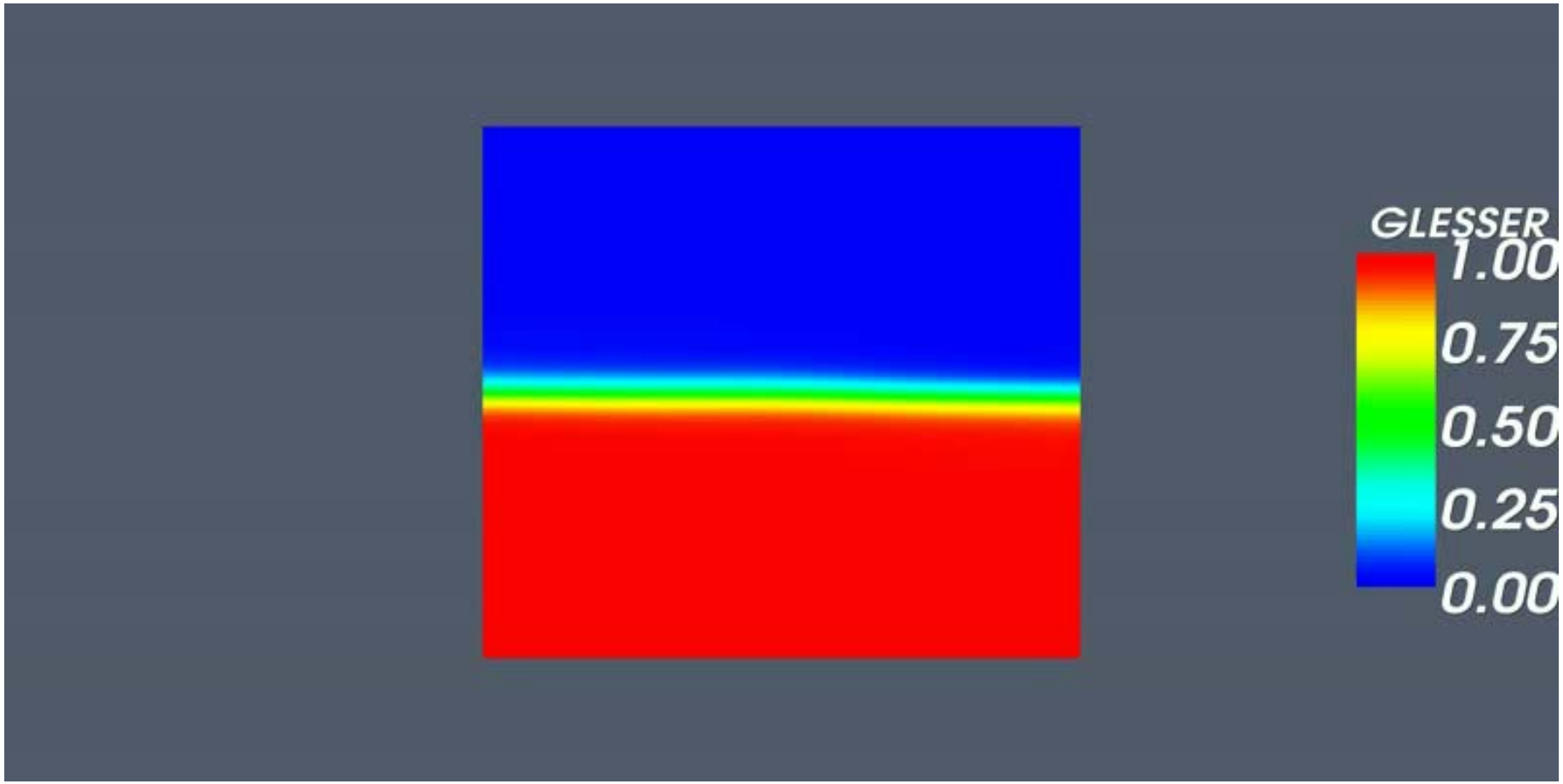
$f(\varepsilon)$

$f[\varepsilon\cos(Et) + \varepsilon\sin(Et)]$

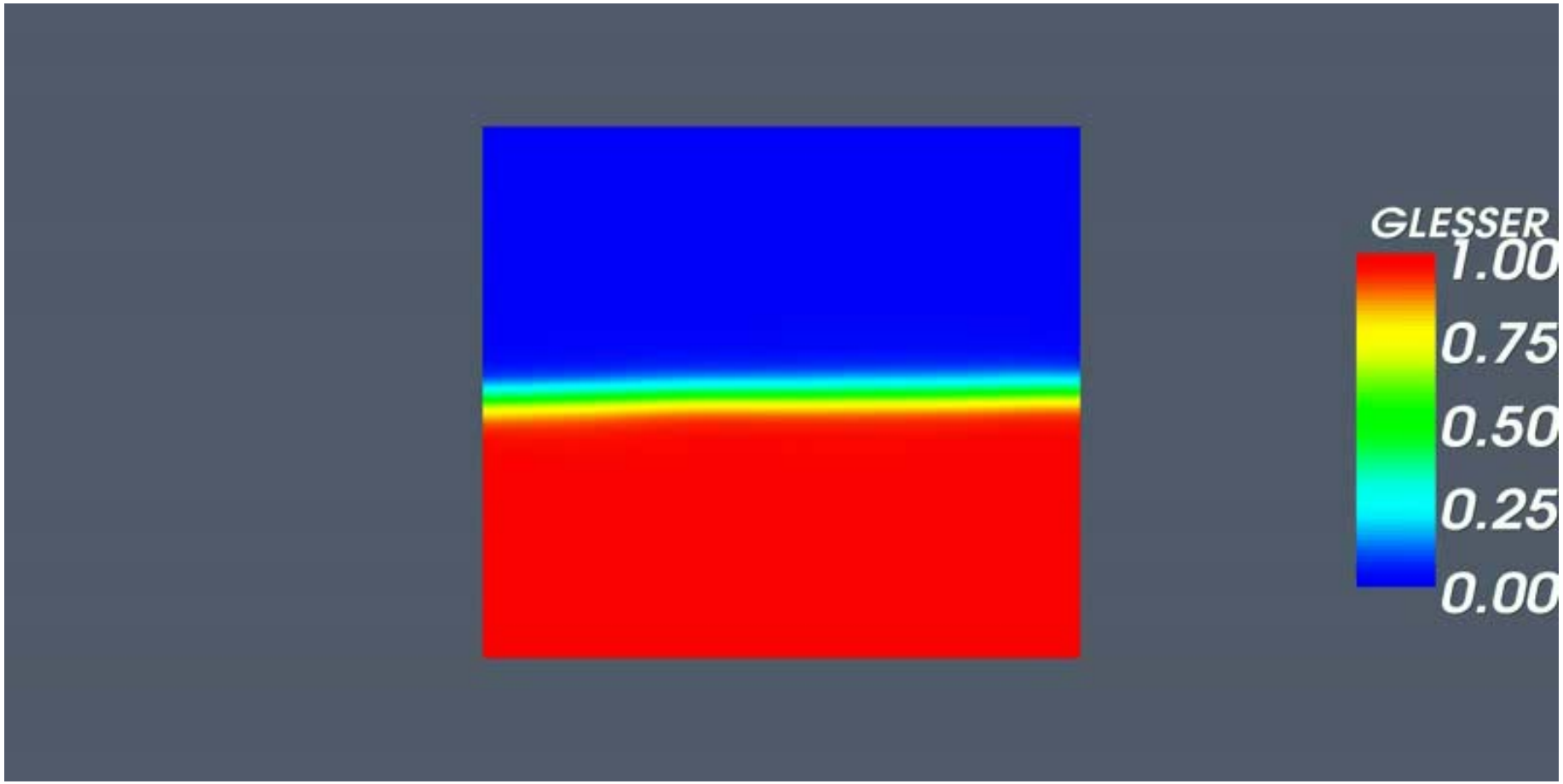
For example, the noninteracting system is just a **FD distribution** in the Hamiltonian gauge case and a **rotating FD distribution** in the gauge-invariant case.

When interactions are included, the distribution is **smoothed out** due to correlations, and can develop **new structure** in the field.

Strongly scattering metal (small field E=0.25; U=0.5)



Strongly scattering metal (large field E=2; U=0.5)



Conclusions

- Showed how to implement an **efficient parallel algorithm** to solve the **Keldysh problem** for strongly correlated electrons described by dynamical mean-field theory.
- The procedure was applied to the **question of Bloch oscillations** and **how they disappear** as scattering is increased**.**
- We presented a wide range of different numerical results on the **current**, the **density of states** and the **distribution functions**. Our numerical algorithms scale efficiently to thousands of processors.