Nonequilibrium dynamical mean-field theory

J. K. Freericks

Department of Physics

Georgetown University

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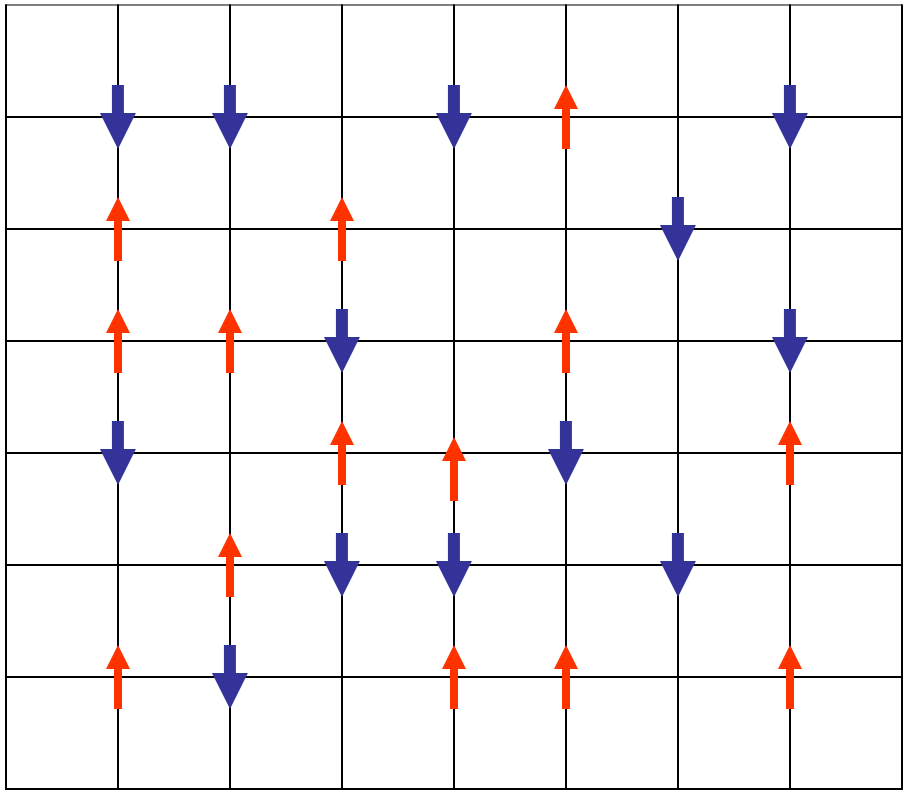
Dynamical mean-field theory

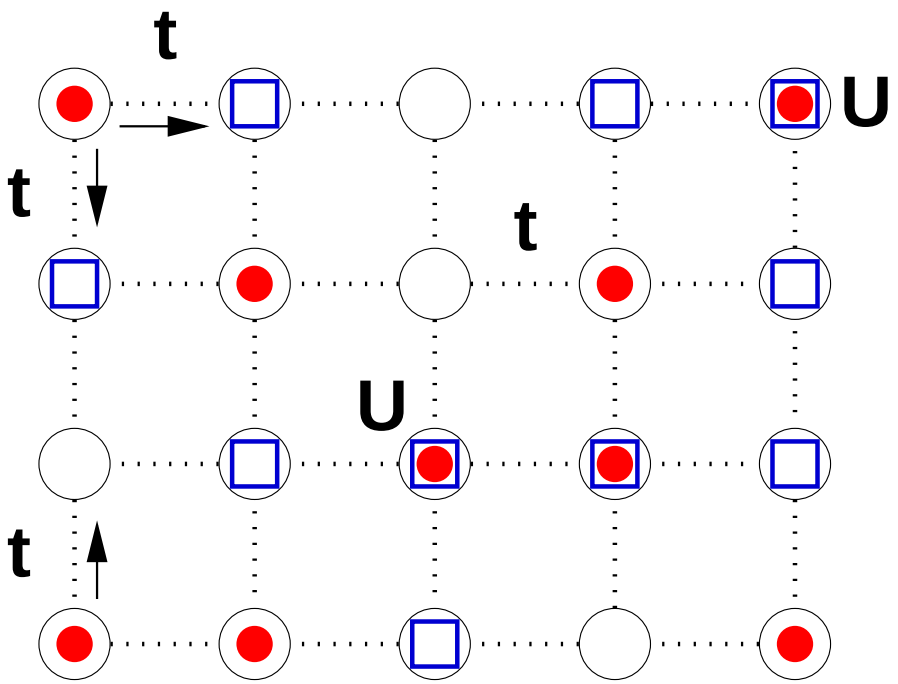
- Invented in 1989 by Brandt and Mielsch after Metzner and Vollhardt motivated looking at the large dimensional limit to simplify the many-body problem
- Has solved nearly all many-body models of solid state physics in equilibrium and is currently being applied to “real materials”
- Here we show how to generalize to nonequilibrium situations

Our model involves the mixture of mobile electrons and localized electrons

- Localized f or d electrons
- Delocalized conduction electrons
- A metal-insulator transition can occur when the occupancies of the different types of electrons change



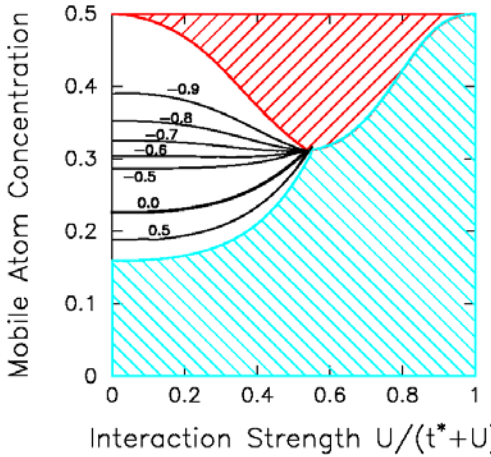
Falicov-Kimball Model

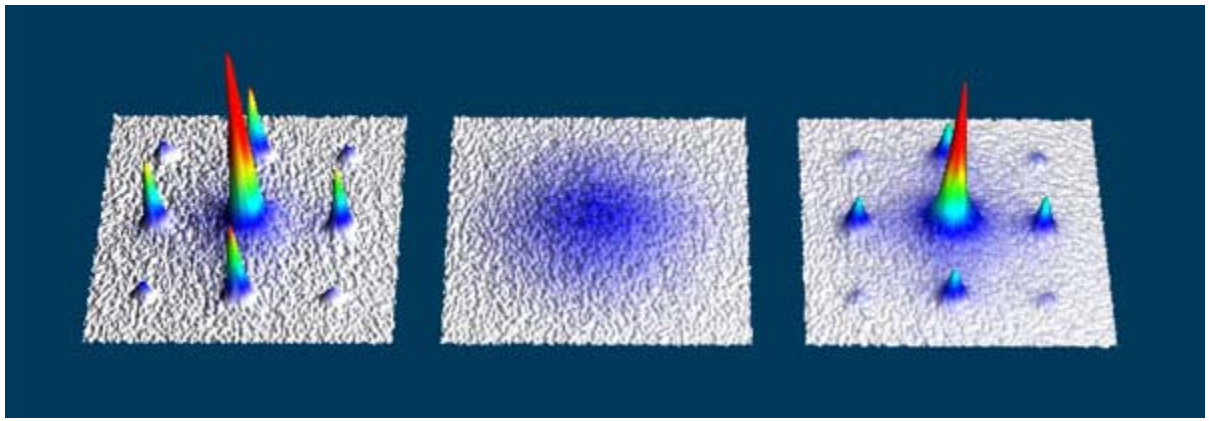


- Two kinds of particles: (i) **mobile electrons** and (ii) **localized electrons**.
- When both electrons are on **the same site** they interact with a correlation energy U.
- Metal-insulator transition occurs when the total number of electrons equals the number of lattice sites and U is large enough.

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 cold atom systems include mixtures of light alkali atoms (Li or K), with heavy atoms (Sr or Yb) in optical lattices.
- Possible solid-state systems include NiI_2 and Ta_xN

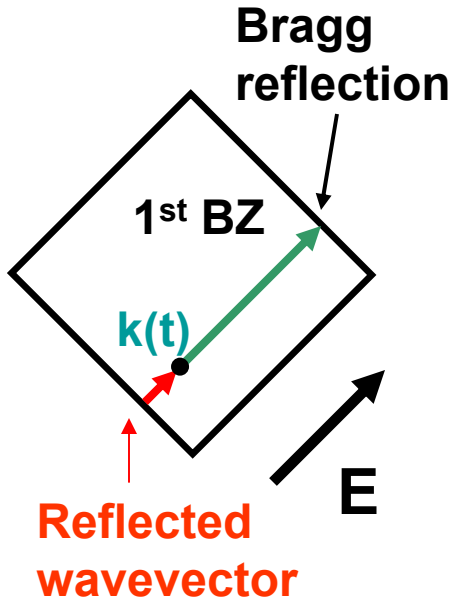




Bulk materials in large electric fields---quenching of Bloch oscillations

Uniform electric field drives current

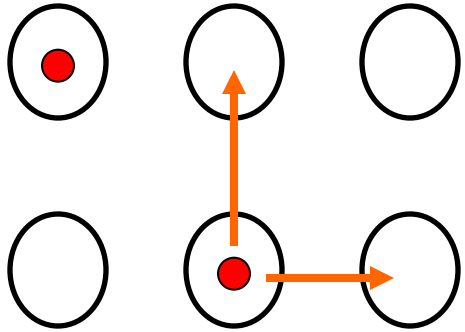
- In a **semiclassical** picture, the electronic momentum, written as **ħk=P**, evolves with a linear time-dependence corresponding to the **acceleration** due to the "field": **k(t)=Et**.
- **Periodicity** modifies this picture: since the electrons are in a periodic lattice, the wavevector cannot increase **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 (so-called Bloch oscillations).
- Other electrons are sources of **scattering**, which also interrupt the evolution of the wavevector in the BZ.



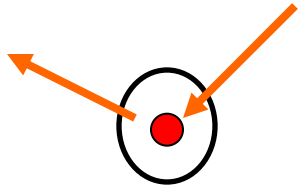
Many-body physics and the dynamical mean-field theory approach to nonequilibrium problems

Dynamical mean field theory

- Models of strongly correlated electrons are difficult to solve.
- Significant progress has been made over the past 19 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**.

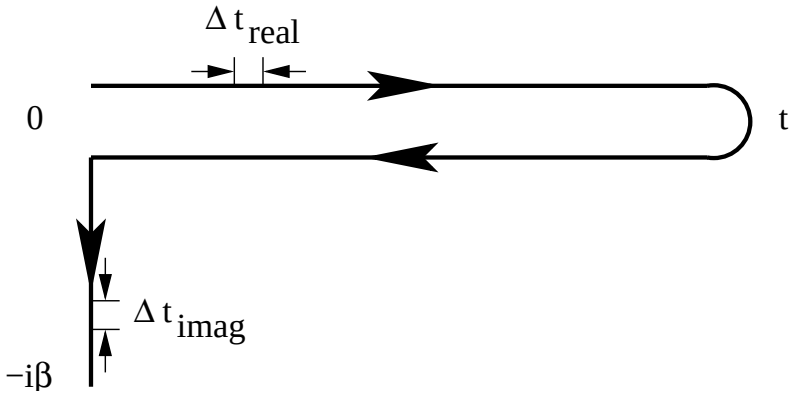


Lattice



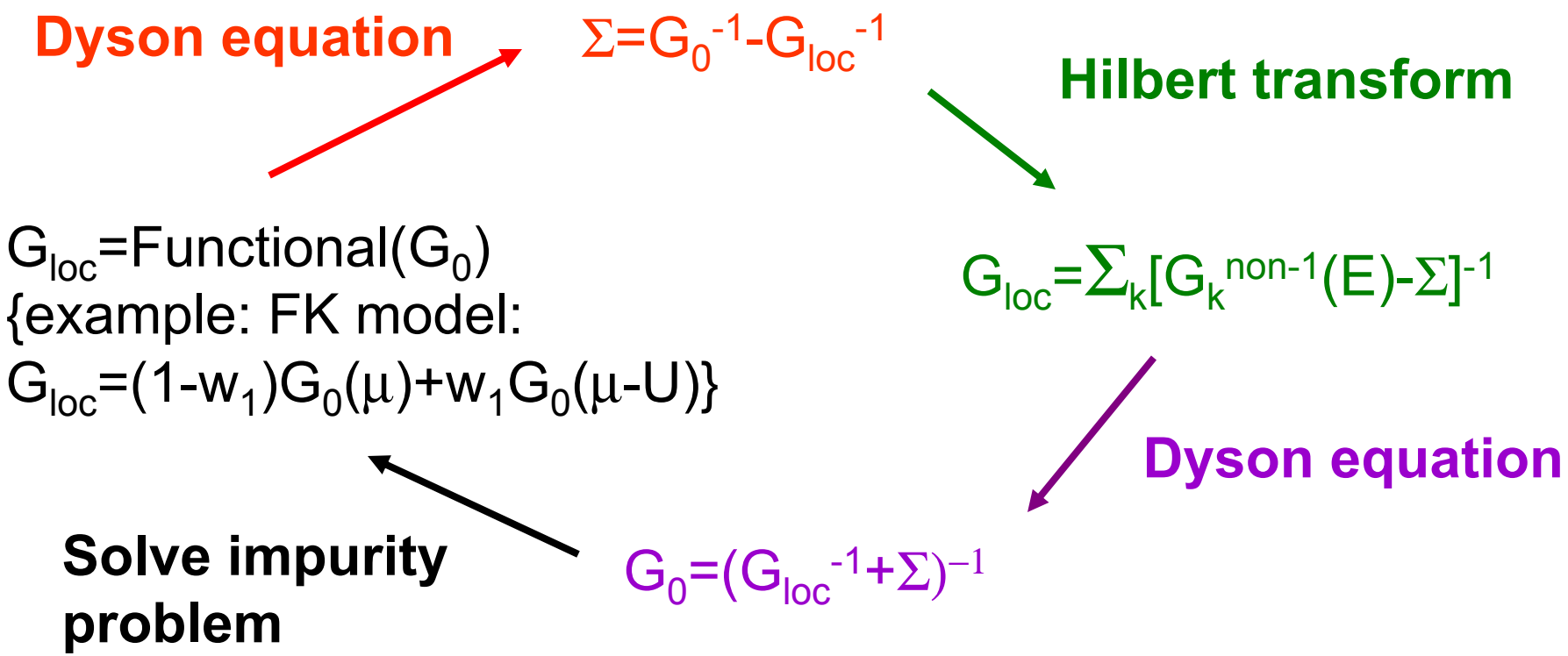
Impurity site

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.
- **Functional derivatives** are then used to determine the Green's functions.

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 generalized Hilbert transform

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

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

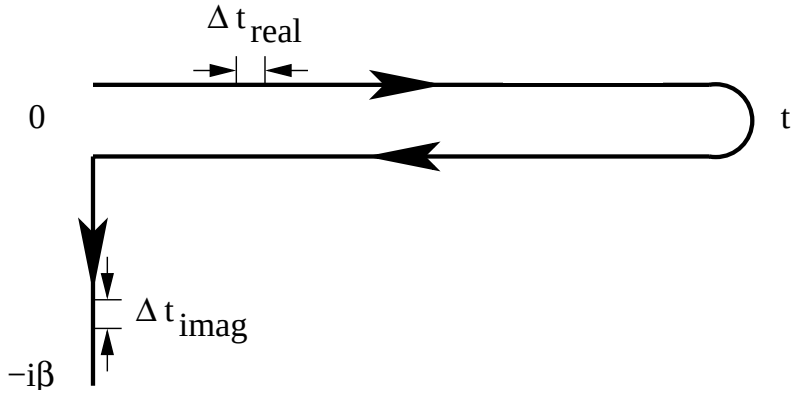
which becomes the sum of two "band energies" when the electric field lies in the diagonal direction.

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 integral.

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

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.

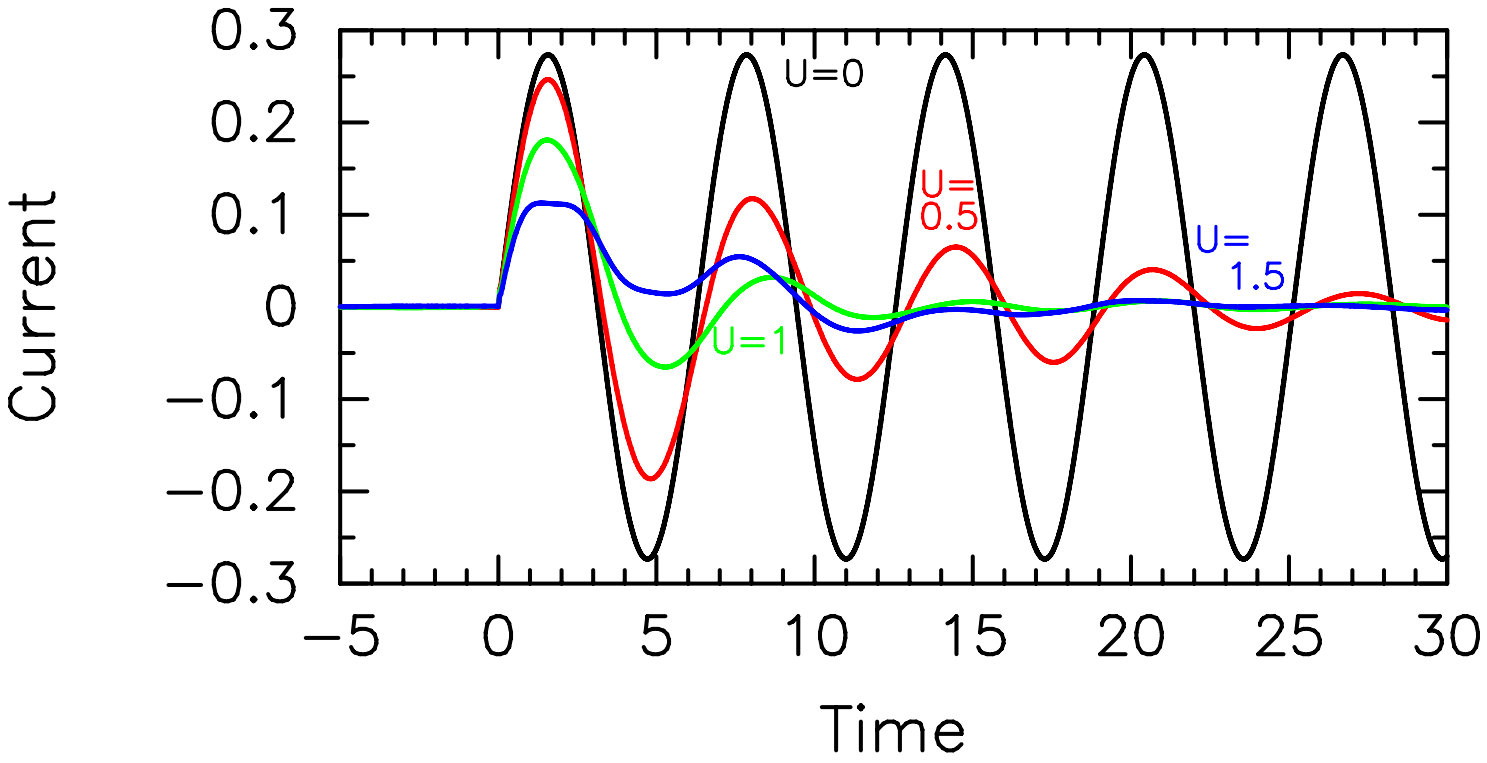
Next, we need to integrate the dependence of the **matrix elements** over a **two-dimensional** energy space.

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**.

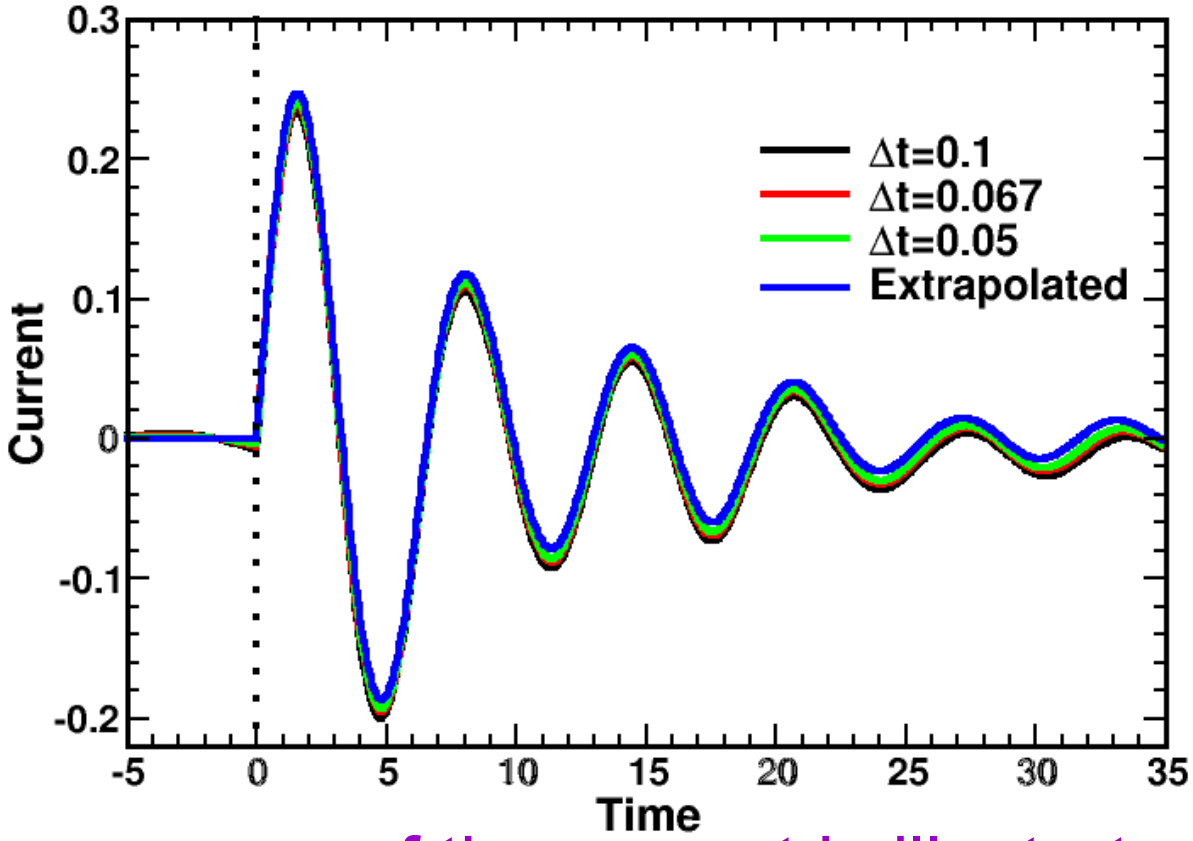
Computational Results

Bloch oscillations in conductors (E=1)



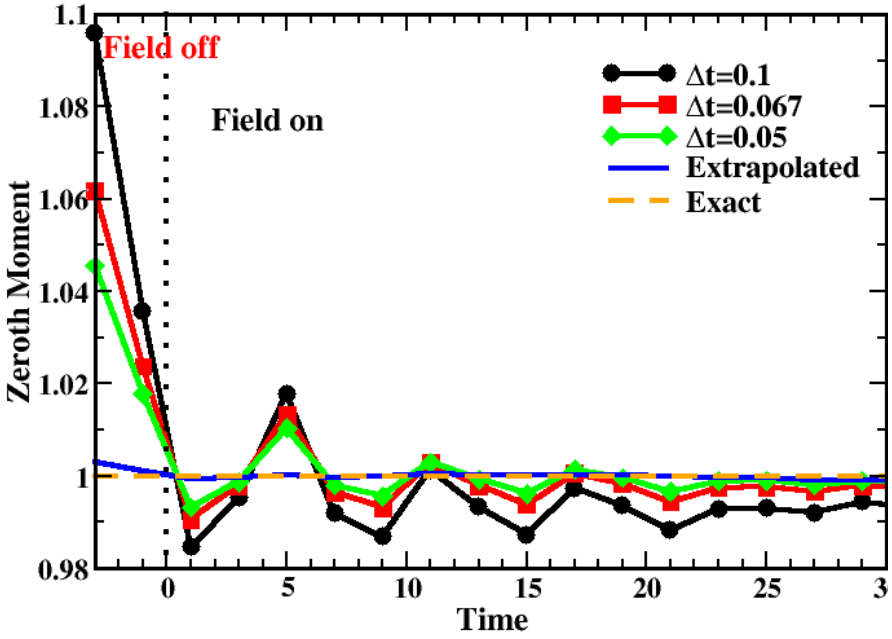
As the scattering increases, the amplitude of the current decays faster, but we cannot tell whether the oscillations survive at long time, or are completely damped.

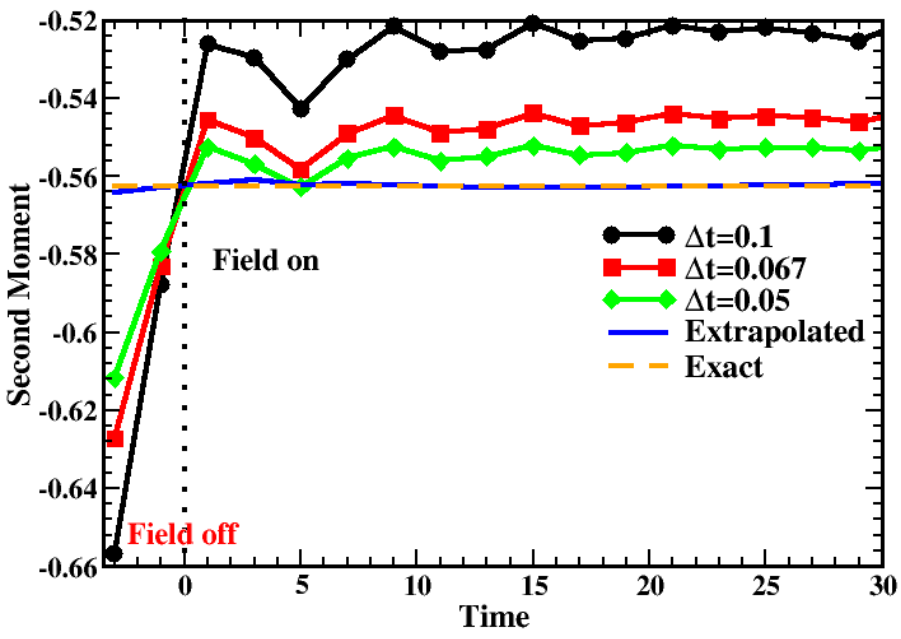
Accuracy of results—scaling of the current (E=1, U=0.5)



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

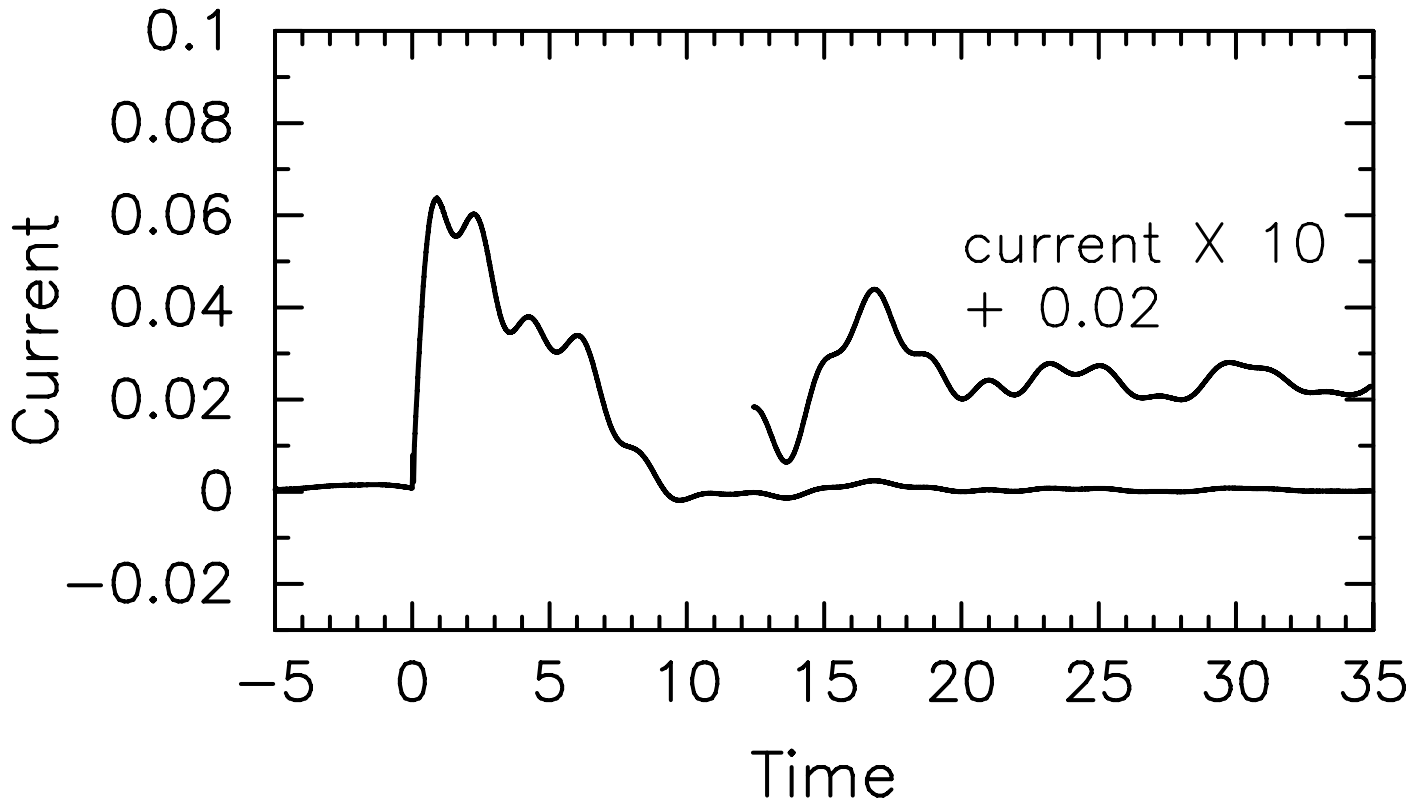
Accuracy of the results---scaling of moments (E=1, U=0.5)





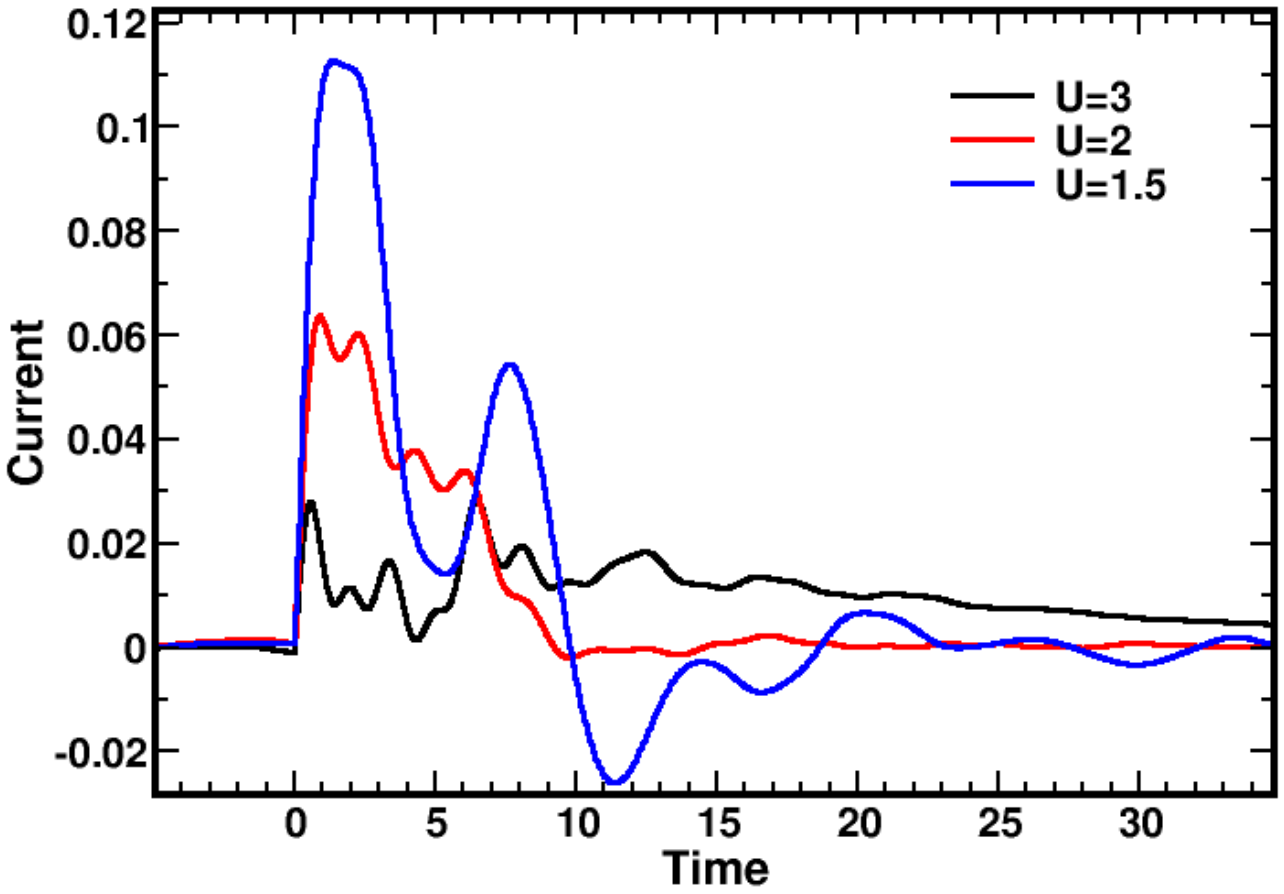
Exact results are known for the equal time Green's functions and their first two derivatives.
Extrapolating the results to zero discretization size yields **excellent agreement** with the exact results.

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



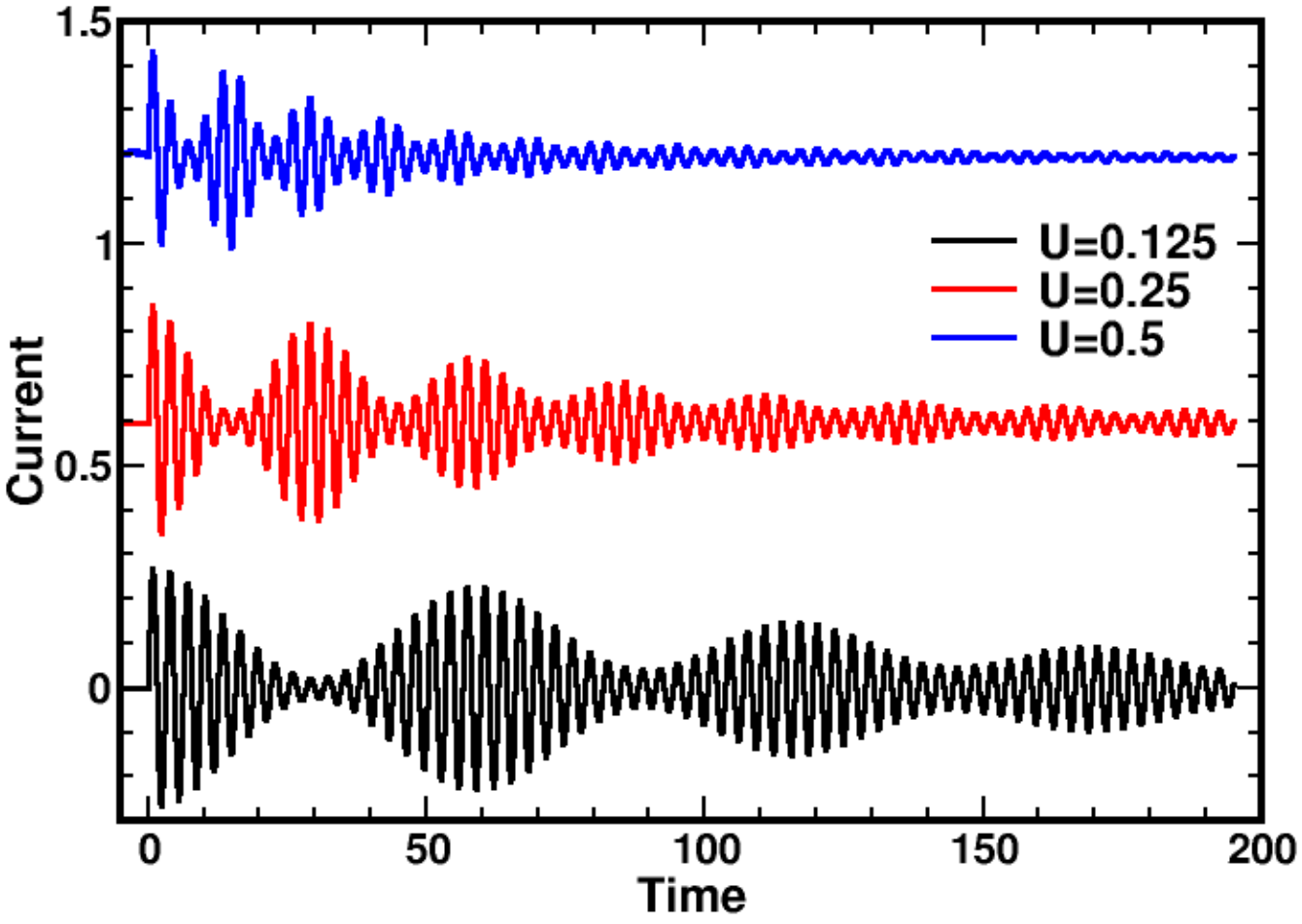
In the Mott insulator, the regular Bloch oscillations are replaced by irregular oscillations. Note that they survive out to long times (albeit with low amplitude).

Current in the Mott Insulator ctd.



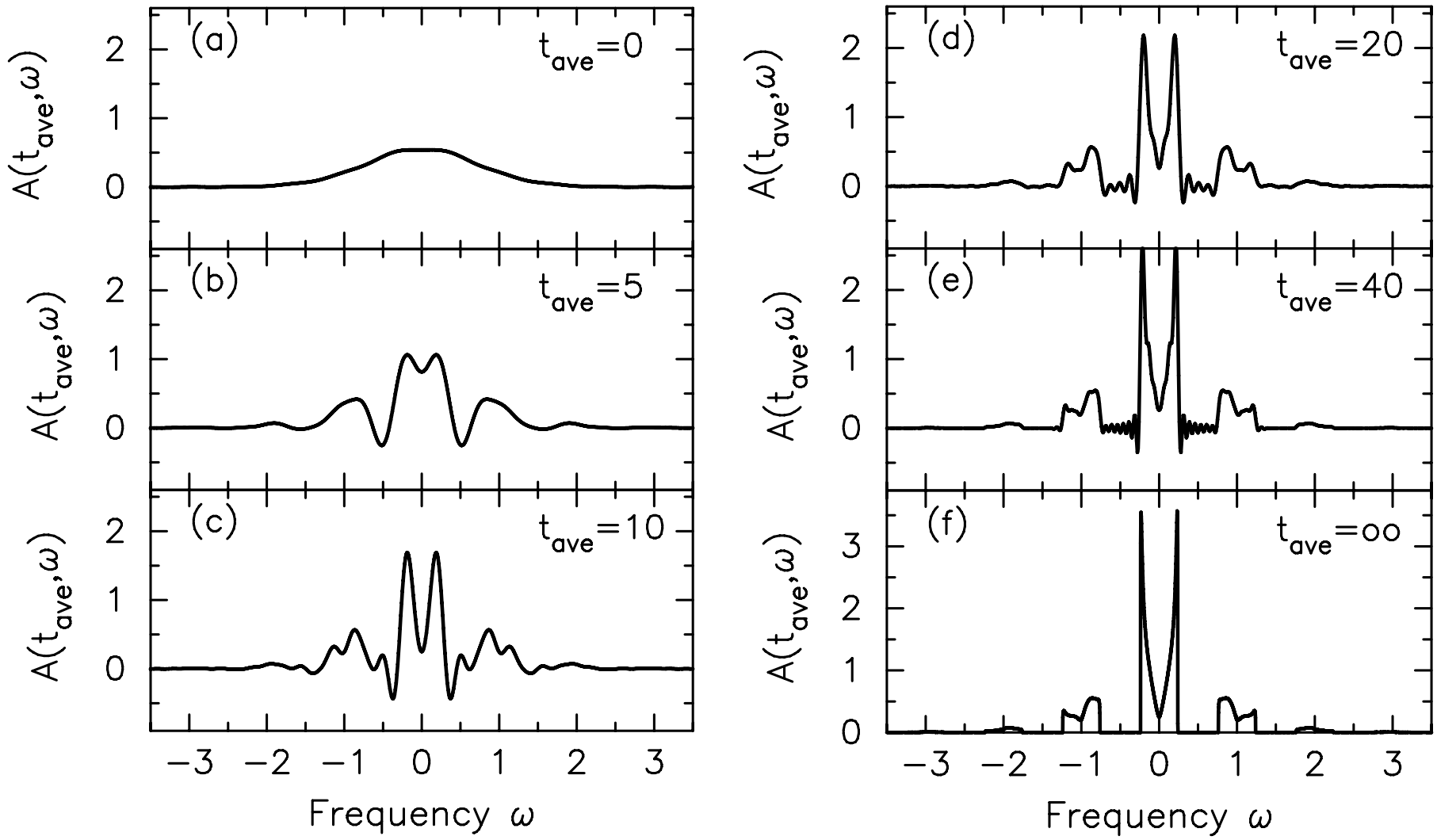
Notice how the oscillations change character from damped Bloch oscillations to irregular damped oscillations as the size of the gap in the Mott insulator increases.

Beats in the current at large field

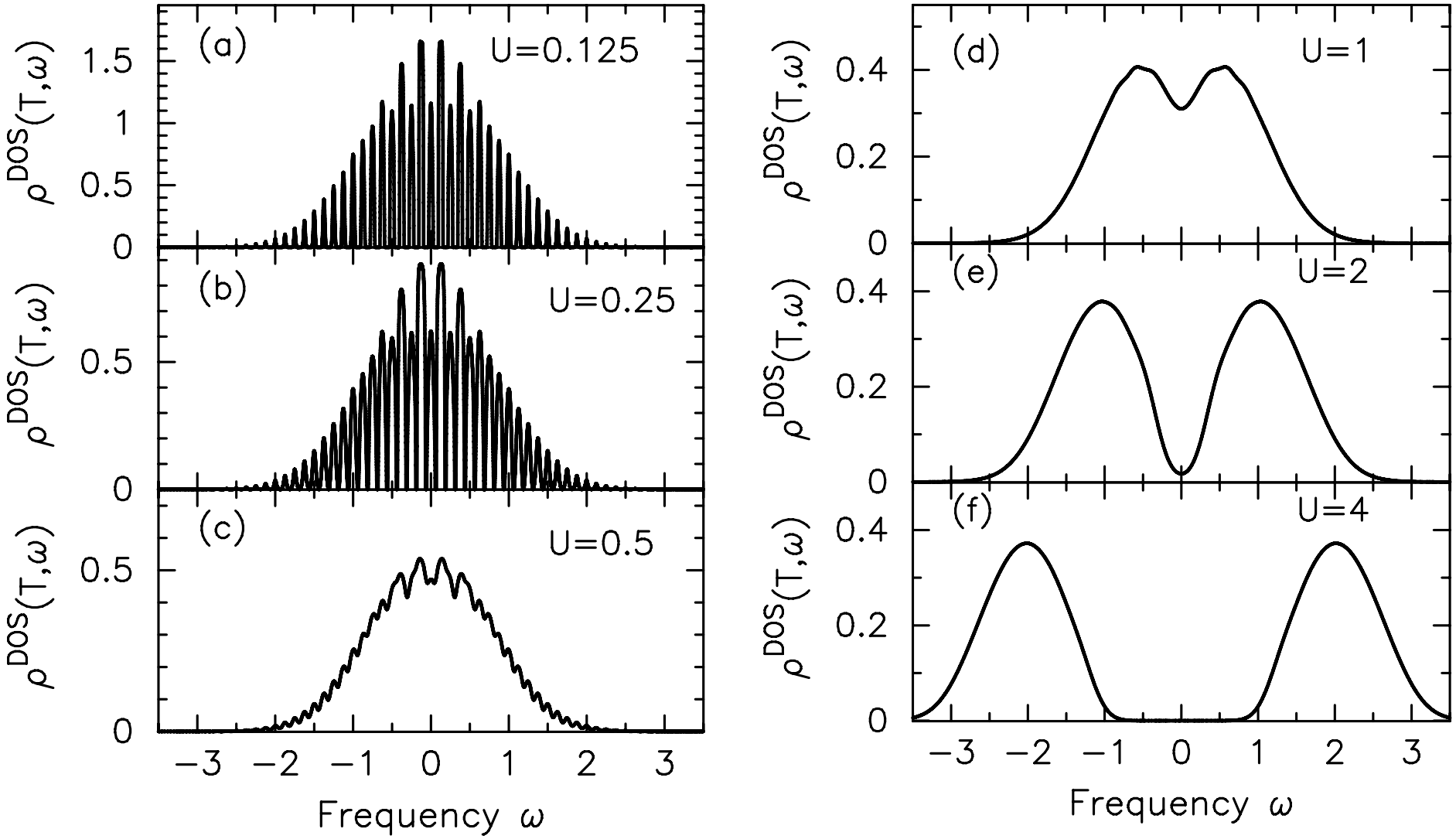


When the field is large (E=2 here), near beats develop with a beat period proportional to 1/U. The origin of the beats is a splitting in the DOS peaks by U.

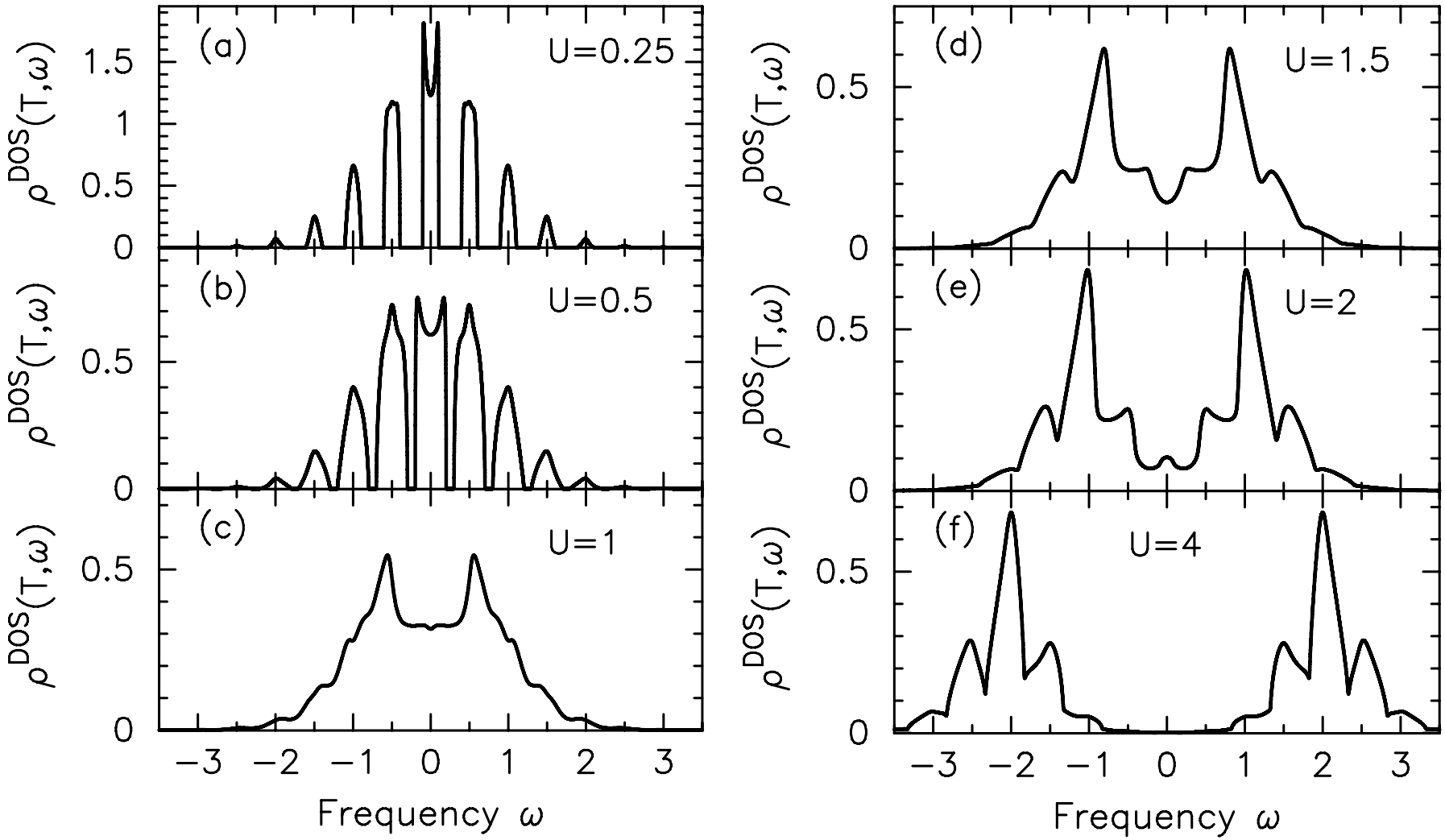
Transient density of states (E=1, U=0.5)



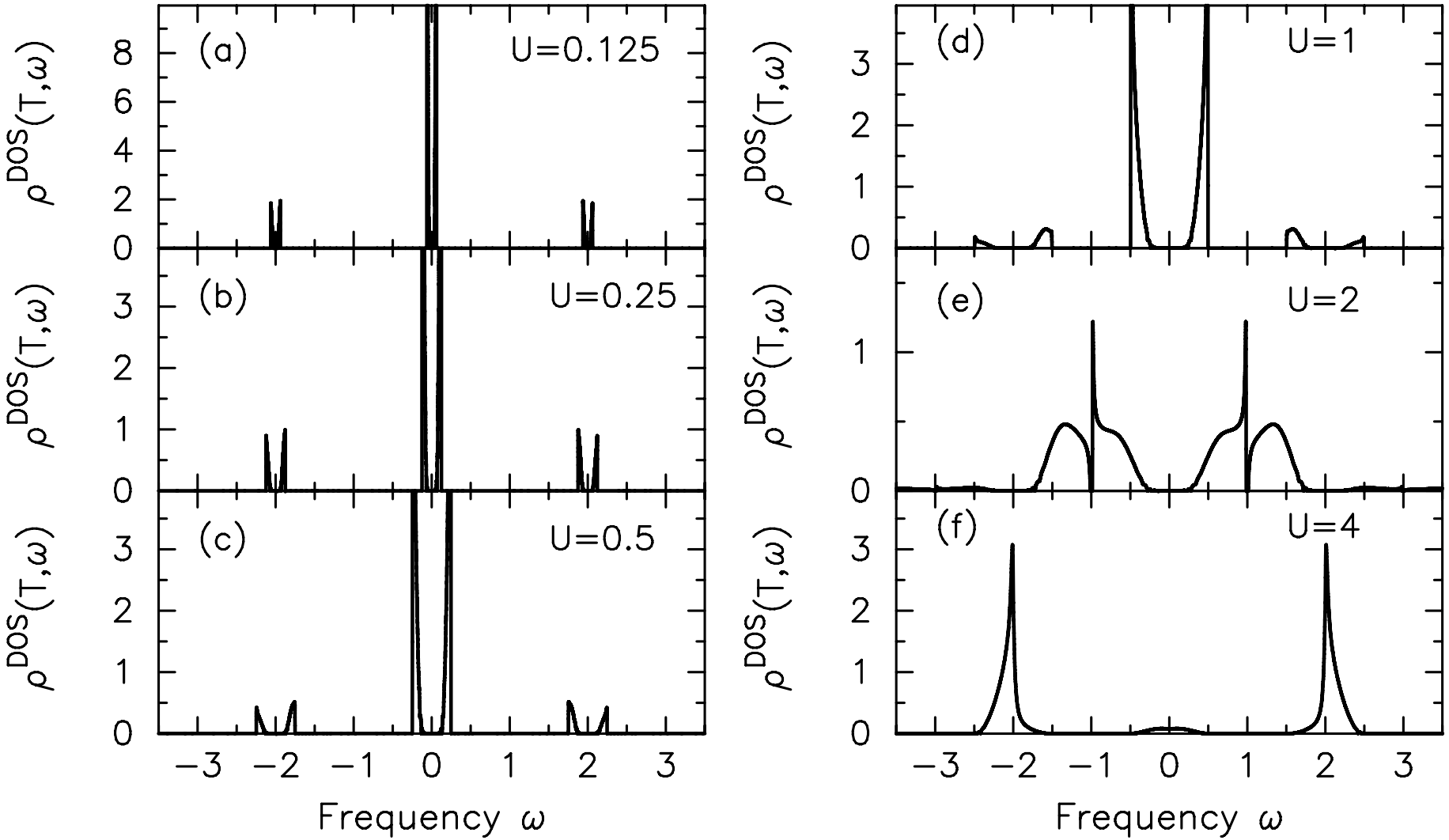
Steady-state DOS (E=0.125)



Steady state DOS (E=0.5)



Steady state DOS (E=2)



Steady-state approach and the Hubbard model

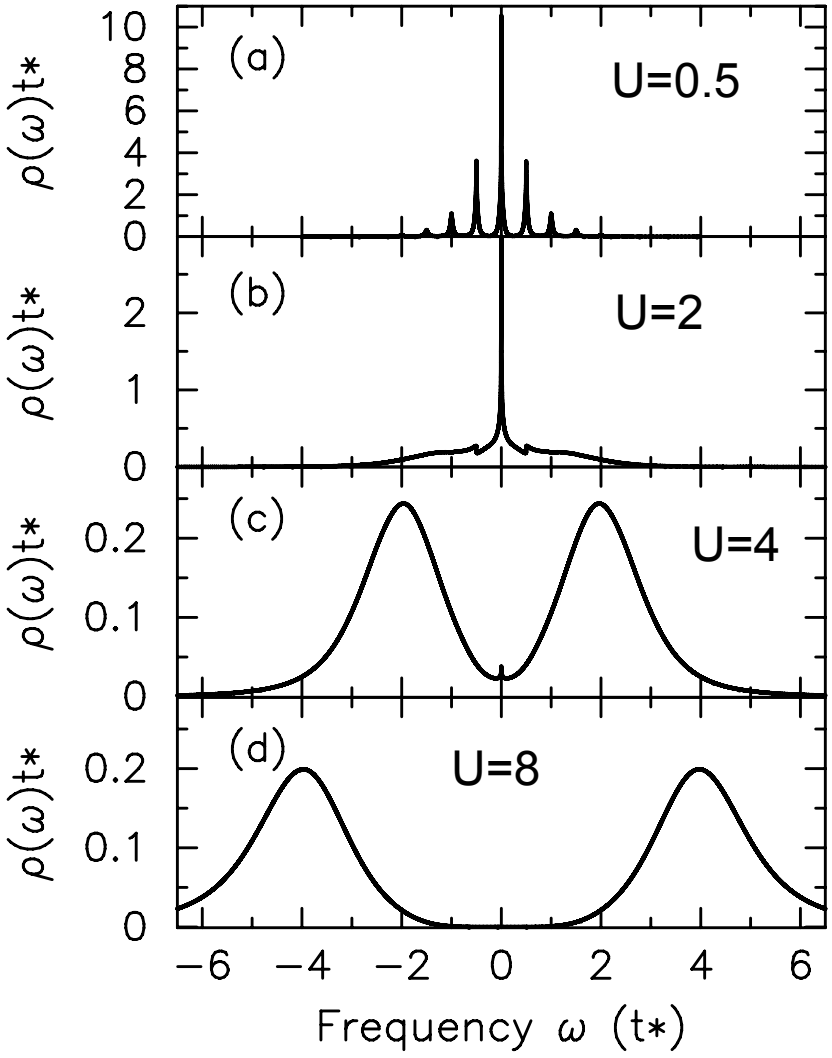
Steady-state formalism

Make the ansatz that the self-energy is independent of average time.

Dyson equation on the lattice now couples frequencies that differ by the Bloch frequency---it can be solved via matrix algebra

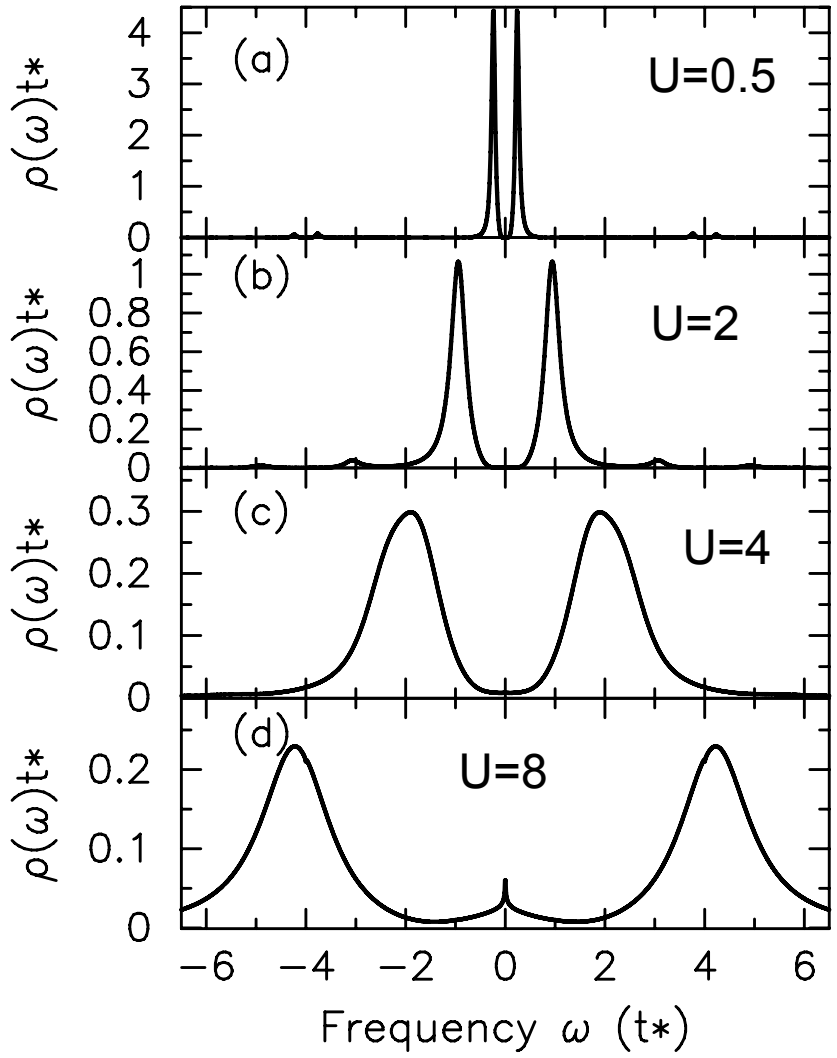
Use the NRG impurity solver to solve the impurity problem---result is approximate for the DOS because it maps to an effective equilibrium problem

Small field (E=0.5)



The system evolves from broadened Wannier-Stark ladder states to a Mott-insulator-like band with a quasiparticle-like peak in the center, but the self-energy never looks like that of a Fermi liquid.

Large field (E=2)



Now the Wannier-Stark states are initially split by U and broadened. The splitting continues until they merge to create a Mott-like DOS. Commensuration effects give a zero-frequency peak in the bottom panel.

Conclusions

- Illustrated how one can generalize dynamical mean-field theory to solve a number of nonequilibrium problems
- Worked with a transient-response formalism and a steady-state formalism.
- A full steady-state formalism is not possible yet, due to the issue of needing to find the appropriate boundary condition for the Keldysh/lesser/greater Green's functions, which is known only at $t=-\infty$.