Transient response of strongly correlated electrons to large electric fields

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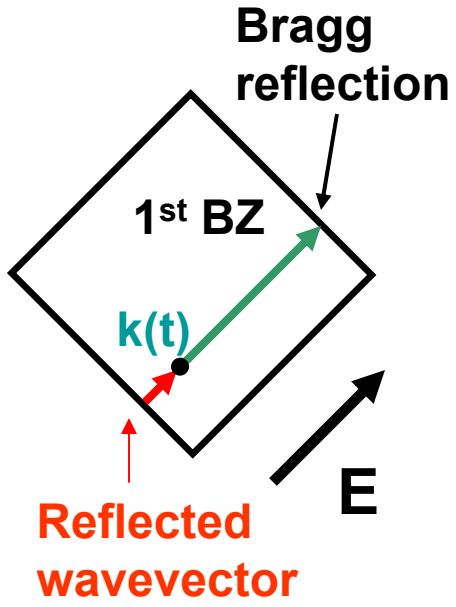
Electrons driven by a constant electric field

- 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*.**

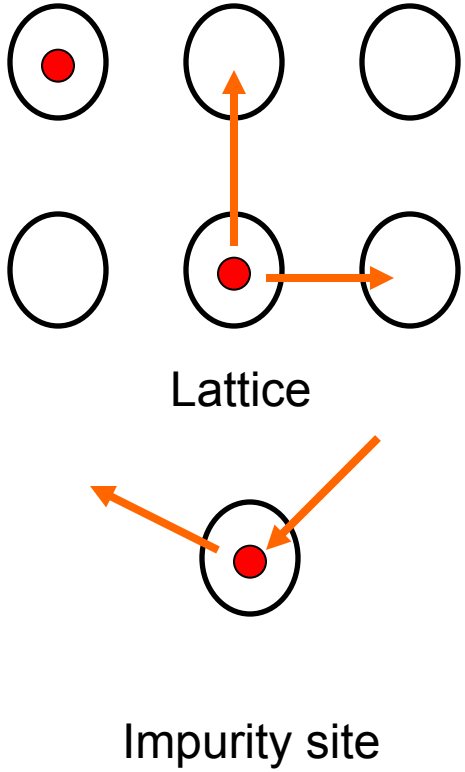
Military Relevance

- Strongly correlated electron materials have properties (conductivity, magnetism, superconductivity) that can be **tuned** by varying pressure, temperature, or doping.
- They have potential for use in so-called **smart materials technologies**.
- Many military applications involve subjecting materials and devices to extreme conditions with **strong electromagnetic fields**, where **nonequilibrium** and **nonlinear** effects are important (*examples include lightning strikes or electronic warfare attacks on devices, or high-power applications*)

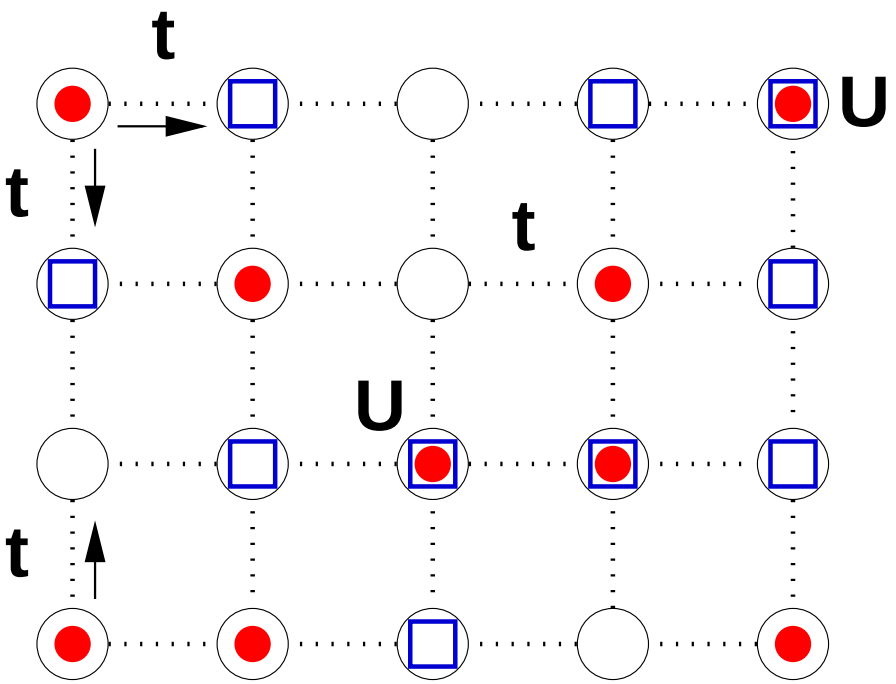
Many-body physics and the dynamical mean-field theory approach to nonequilibrium problems

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**.

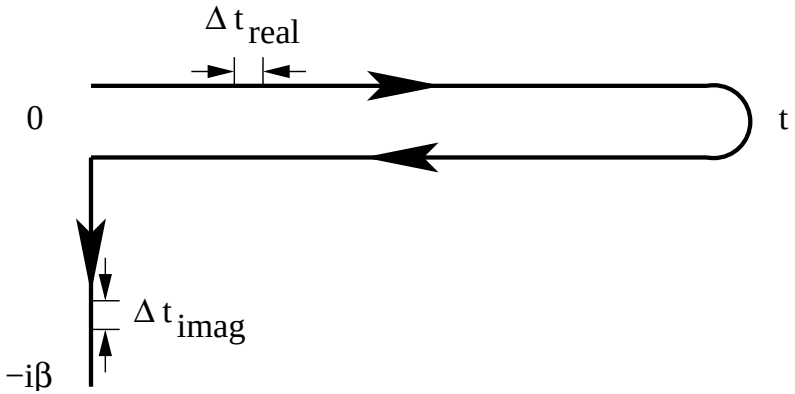


Falicov-Kimball Model



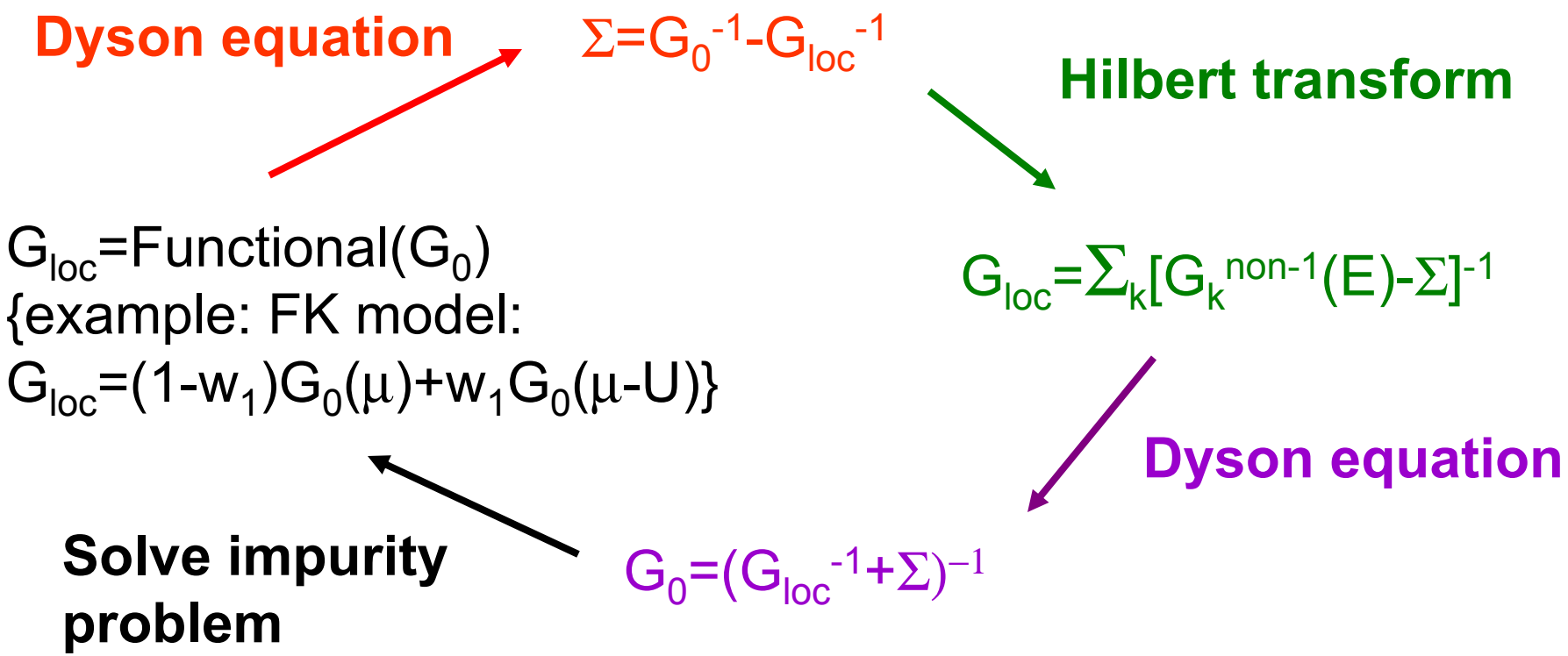
- Two kinds of particles: (i) **mobile electrons** and (ii) **localized electrons**.
- When both electrons are on **the same site** they interact with a correlation energy U.
- Many-body physics enters from an **annealed average over all localized electron configurations**.

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:

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

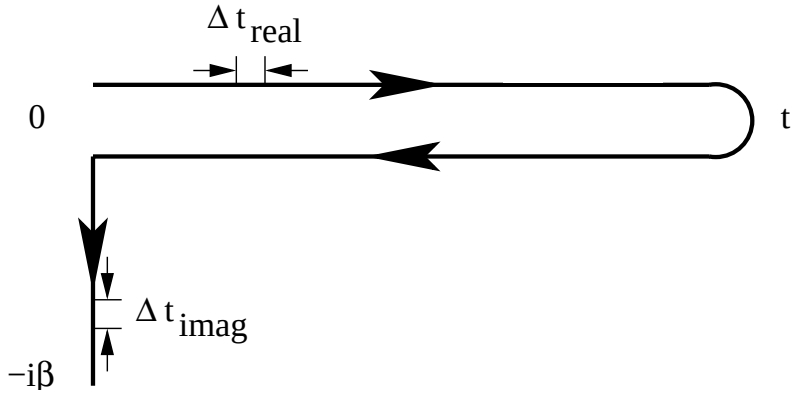
which becomes the sum of two "band energies" when the field lies in the diagonal direction after the Peierl's substitution.

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.

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**.

Parallel implementation

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

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

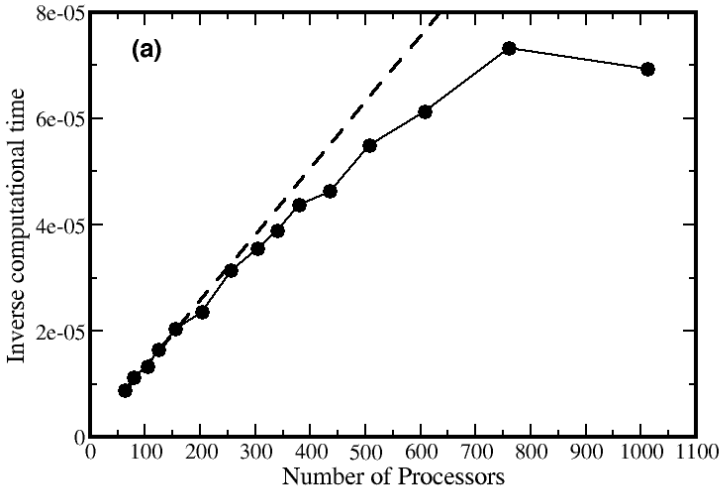
(3) **Send** each **slave node** a value of energies for the momentum dependence of the Green's function and compute the **matrix** that enters the two-dimensional quadrature. LAPACK routines are used for efficiency.

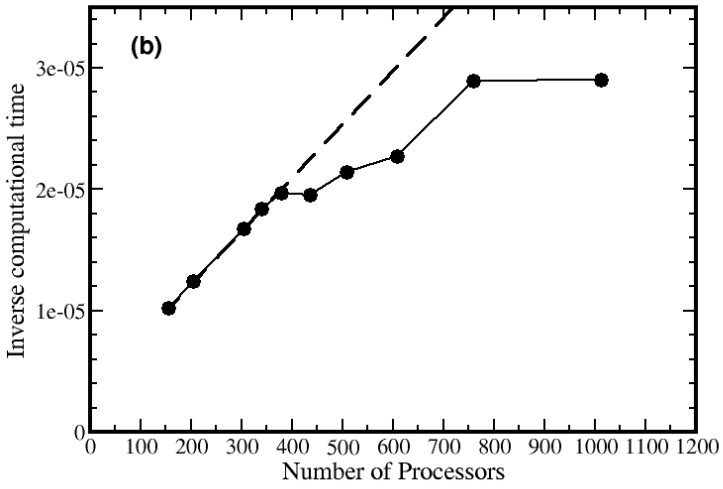
(4) **Store** data on the **slave nodes** for accumulation; use **recursive binary gather** to accumulate for the **master**.

(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.

We achieved good scaling up to 760 single-core processors, but we noticed much more severe run-to-run variations than on other machines. These runs used the four-way X2200 nodes on midnight. We achieve about 70% of linear scaling at 760 procs.

Large memory jobs

Total computational time for one iter

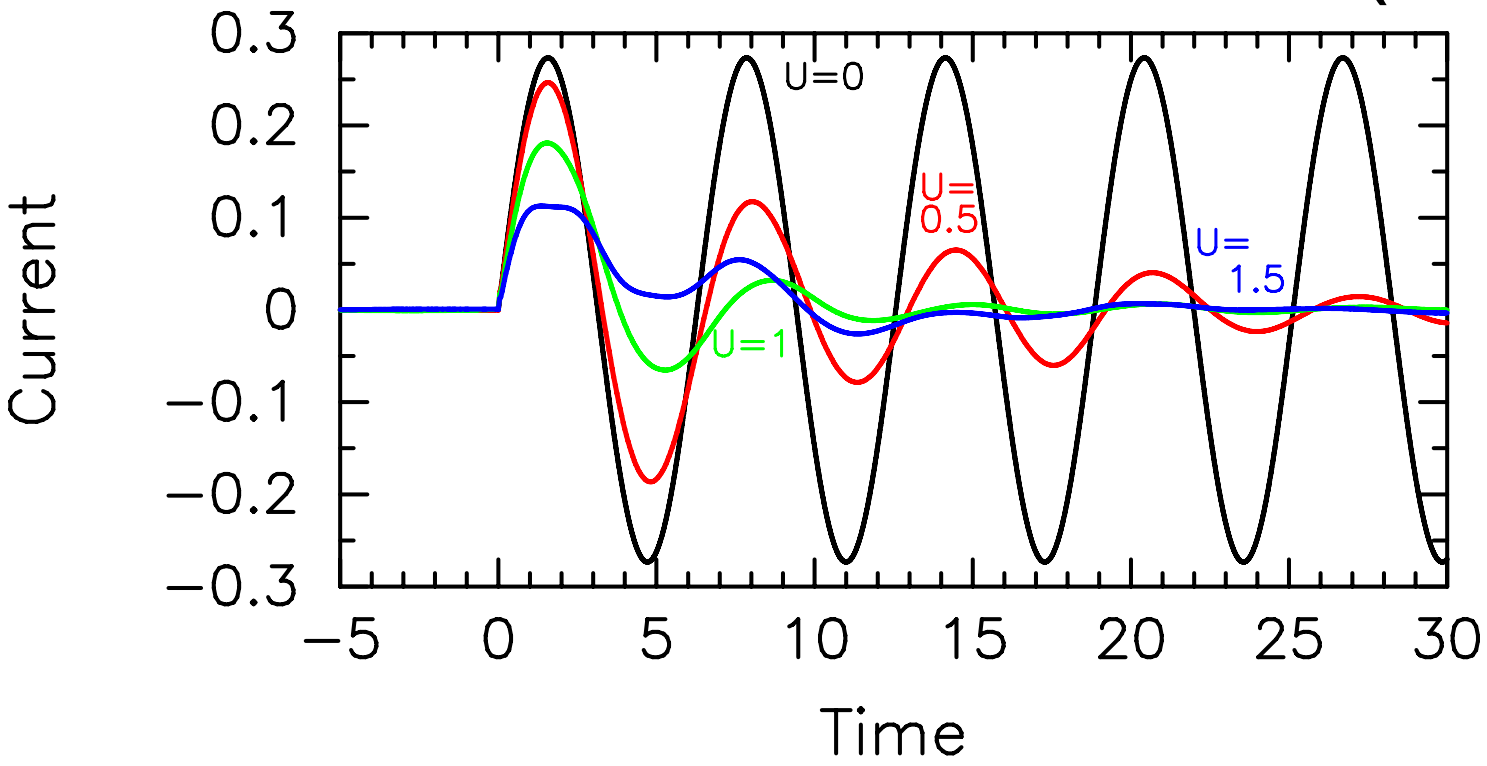
job size	midnight opteron	columbia altix	sapphire XT3
900x900	12.5	6	10
4100x4100	1200	1925	--
4900x4900	2250	10500	--
5700x5700	4200	--	--

Note how the altix machine performs best for small size jobs because it has a larger cache, but that once the job becomes very large, midnight's performance improves dramatically. For the largest case we used the medium memory model with 3 running processors for every 4-way node.

Midnight has 4Gb per processor and one can share memory up to 16Gb on one motherboard for the X2200 nodes. Since jobs on shared memory machines run much slower once the memory lies outside of a single motherboard, midnight has a significant speed advantage over many other machines for large memory jobs.

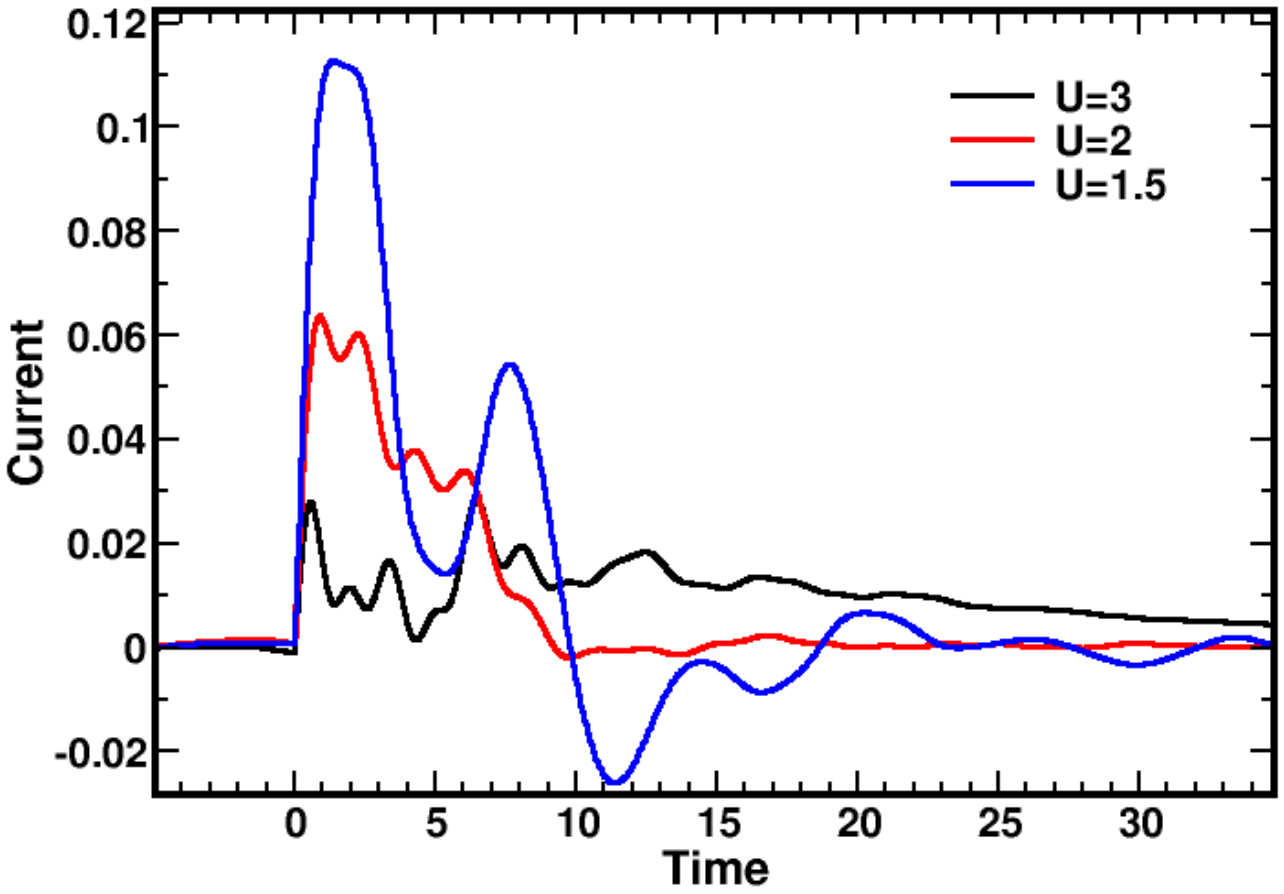
Computational Results

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.

Current in the Mott Insulator



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.

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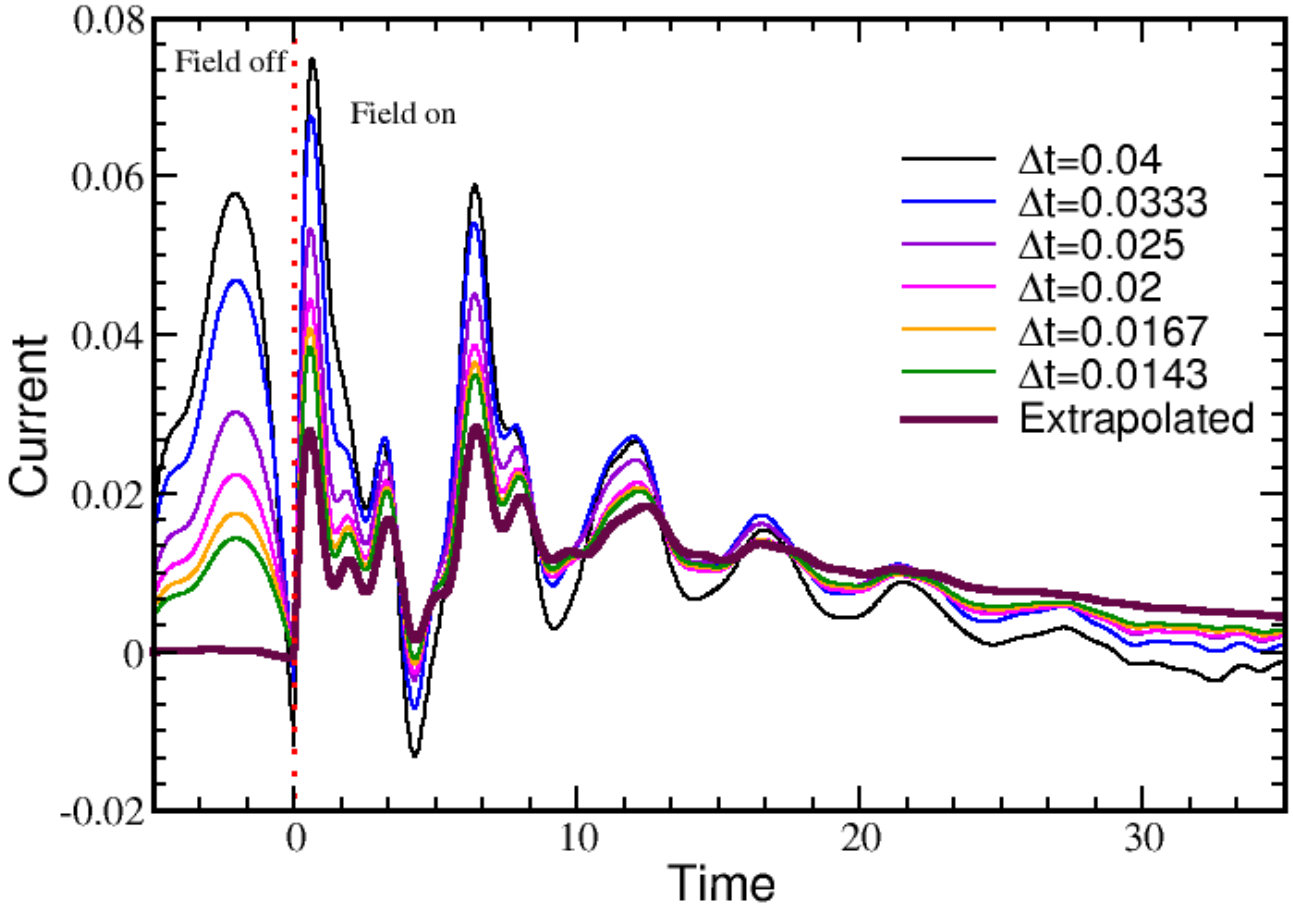
Scaling shows need for large jobs



The data would not scale to zero discretization until the three smallest discretizations were calculated. Note how the scaling changes the overall shape of the current.

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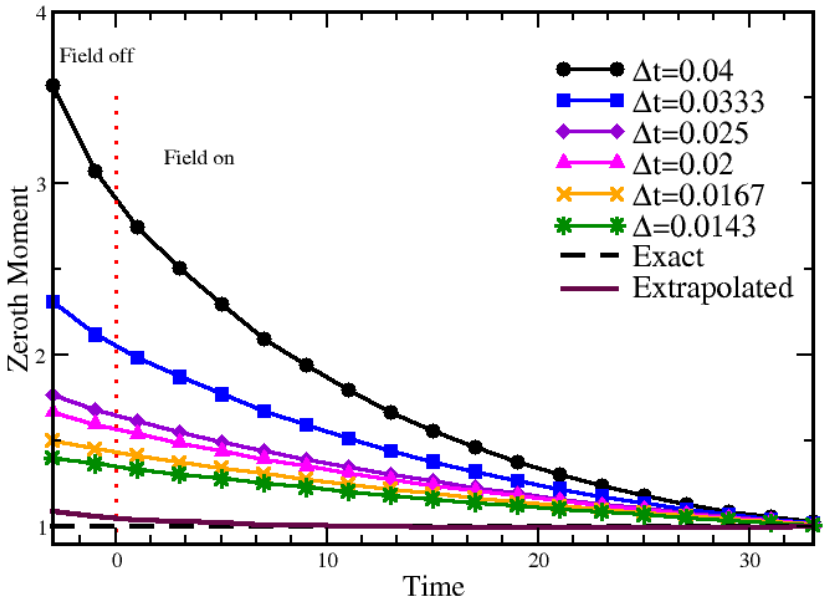
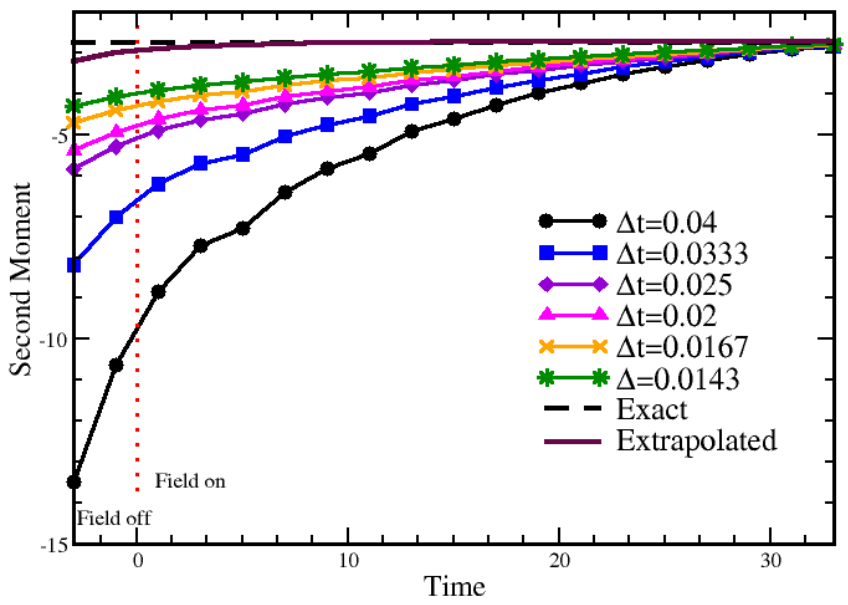
Exact moments show accuracy when data is scaled





Exact results are known for the zeroth and second moments of the retarded Green's function as a function of the average time. The errors are large for the raw data, but once scaled, the errors are less than about 5%!

Conclusions

- Showed how to implement an **efficient parallel algorithm** to solve the **Keldysh problem** for strongly correlated electrons described by the Falicov-Kimball model.
- We illustrated **good scaling** for a strong scaling problem and we showed the advantage midnight has for **running large memory jobs** over some other machines.
- We illustrated the accuracy of the calculations by showing the current and the moments of a Mott insulator. These calculations would only scale to the continuous limit **when the large memory results were available**.