Green's function based approaches to the nonequilibrium problem on a lattice
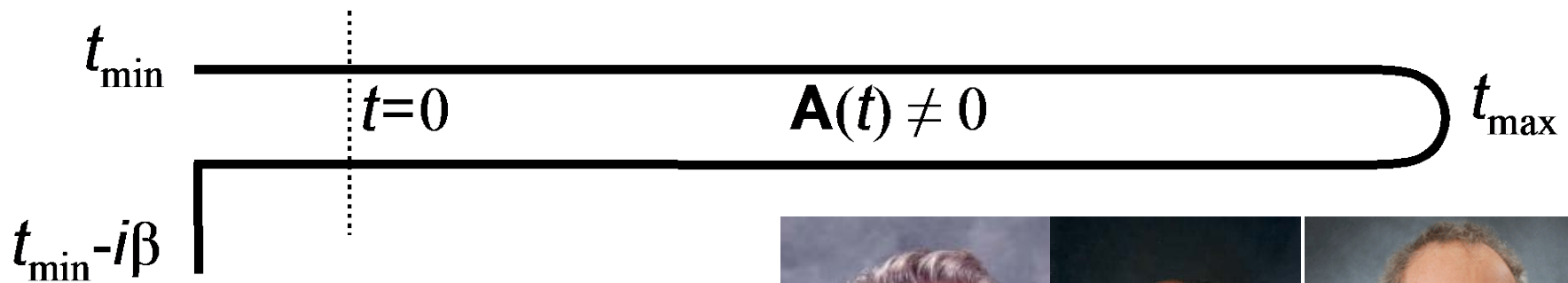
Jim Freericks
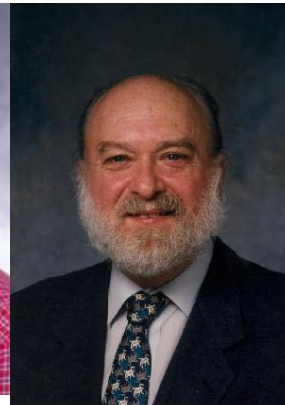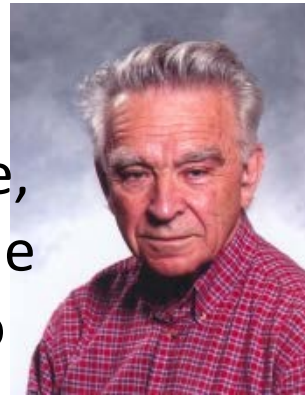
Georgetown University

Early days of nonequilibrium many-body physics (1960s)

Work with quantities on the Keldysh-Kadanoff-Baym contour

Analytic calculations are impossible, numerical calculations too big at the time, but field is handled exactly to all orders in perturbation theory!

Exact solution for the noninteracting contour-ordered Green's function on a lattice with a single band

$$G_{ij}^c(t,t') = -iTrT_c e^{-\beta H(t_{\min})} c_{i\sigma}(t)c_{j\sigma}^+(t')$$

$$G_{ij}^c(t,t') = -i[f(\varepsilon_k - \mu) - \Theta_c(t,t')]e^{-i\int_{t'}^t dt''[\varepsilon_{k-A(t'')} - \mu]}$$

$t_{\min}$

$t=0$ $\mathbf{A}(t) \neq 0$ $t_{\max}$

$t_{\min}\text{-}i\beta$
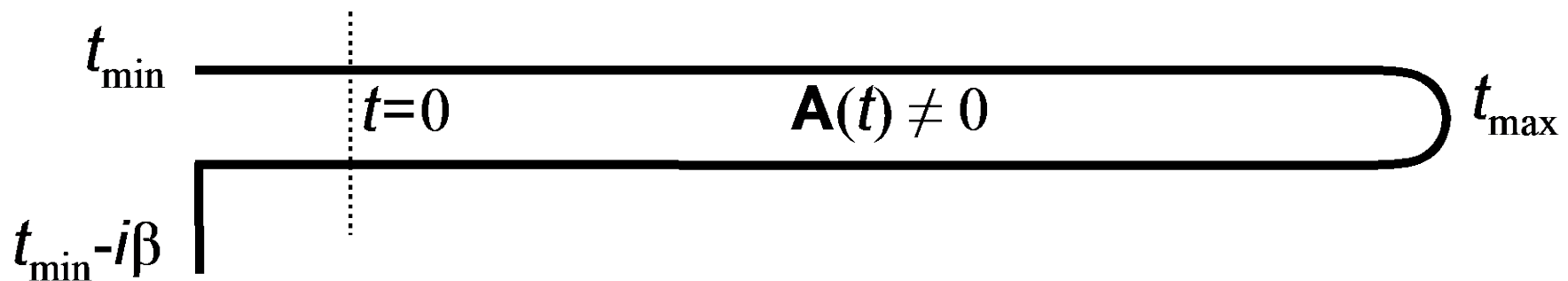
Peierl's substitution and the Hilbert transform

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

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

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 (in infinite dimensions).

Multiband models can also be solved

If the bands have opposite parity, they can be connected by a dipole matrix element. This has not been used in too many calculations.

If the bands have the same symmetry due to a lattice with a basis, Peierls substitution only will solve the problem, which is formally like Landau-Zener for each k.

But the Hamiltonian no longer commutes with itself at different times.
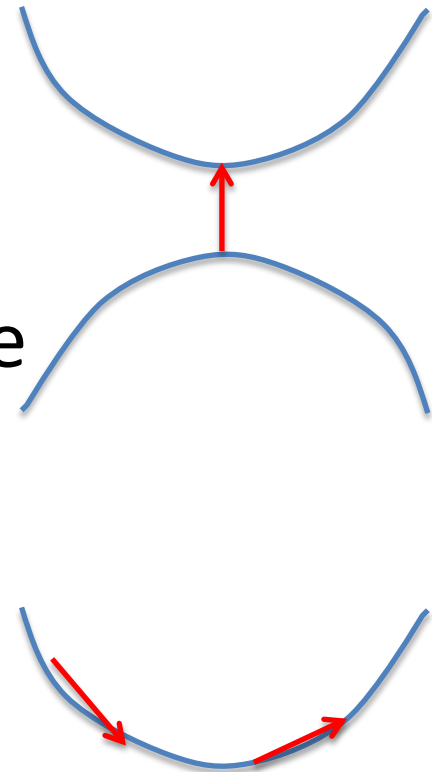
Exact solution for evolution operator for a simple CDW insulator

$$U(t, t'; \boldsymbol{k}) = U(t, t - \delta t; \boldsymbol{k}) U(t - \delta t, t - 2\delta t; \boldsymbol{k}) \cdots U(t' + \delta t, t'; \boldsymbol{k})$$

Trotter formula

$$U(t, t - \delta t; \boldsymbol{k}) =$$

$$\begin{pmatrix} \cos[\delta t \gamma(\bar{t}; \boldsymbol{k})] - i \dfrac{\left|\epsilon\left(k - \frac{eA(\bar{t})}{\hbar c}\right)\right|}{\gamma(\bar{t}; k)} \sin[\delta t \gamma(\bar{t}; \boldsymbol{k})] & i\dfrac{U}{2}\dfrac{\sin[\delta t \gamma(\bar{t}; k)]}{\gamma(\bar{t}; k)} \\[3em] i\dfrac{U}{2}\dfrac{\sin[\delta t \gamma(\bar{t}; k)]}{\gamma(\bar{t}; k)} & \cos[\delta t \gamma(\bar{t}; \boldsymbol{k})] - i\dfrac{\left|\epsilon\left(k - \frac{eA(\bar{t})}{\hbar c}\right)\right|}{\gamma(\bar{t}; k)} \sin[\delta t \gamma(\bar{t}; \boldsymbol{k})] \end{pmatrix}$$

$$\gamma(\bar{t}; \boldsymbol{k}) = \sqrt{\epsilon^2\left(k - \frac{eA(\bar{t})}{\hbar c}\right) + \frac{U^2}{4}}$$

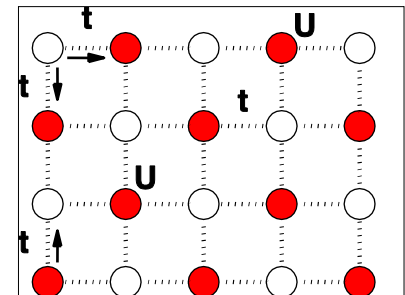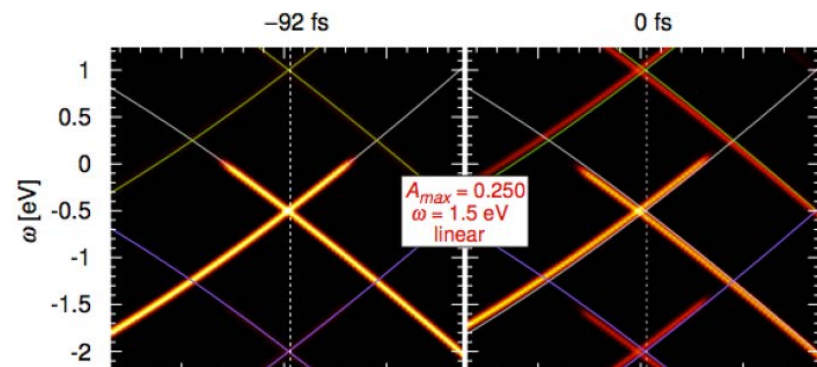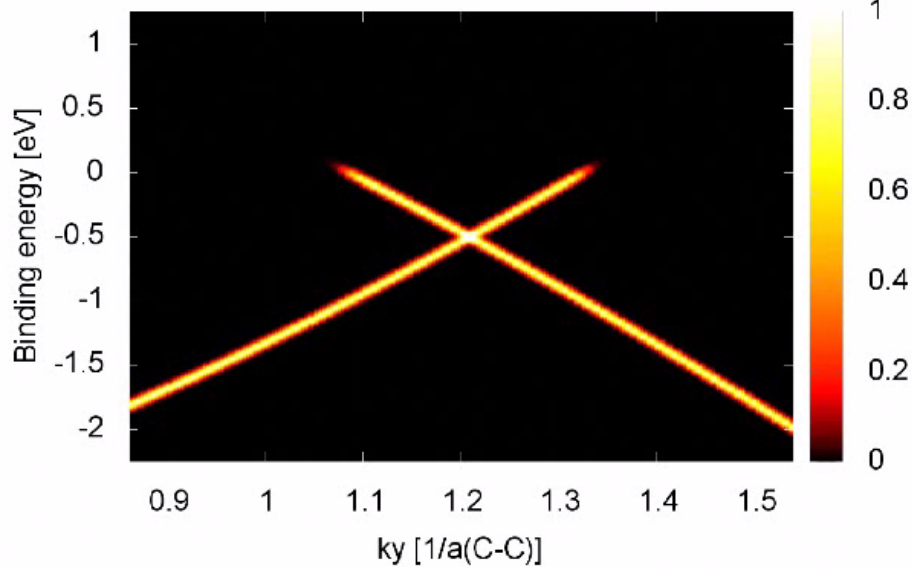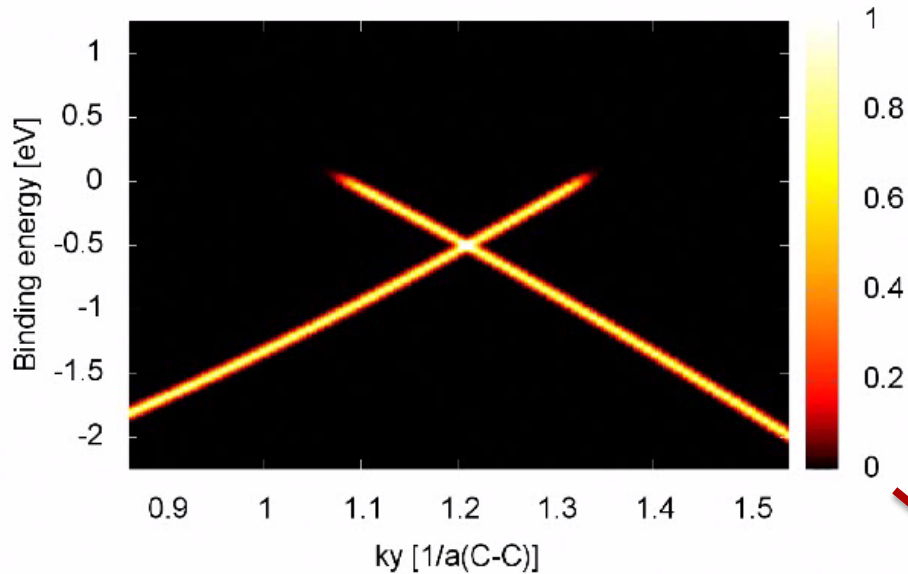# TR-PES for different field amplitudes
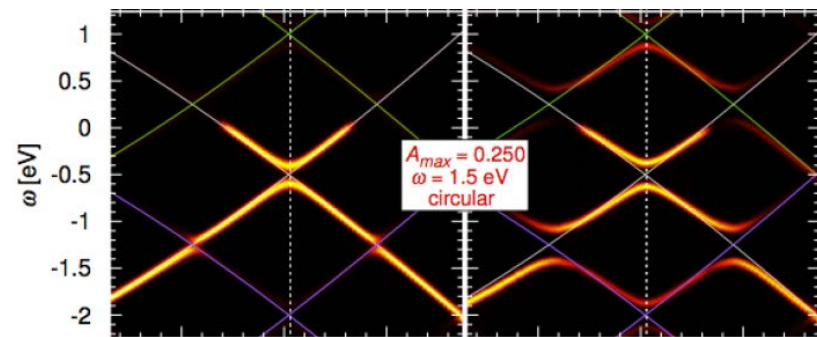
$E_0=0.75$ $E_0=5$
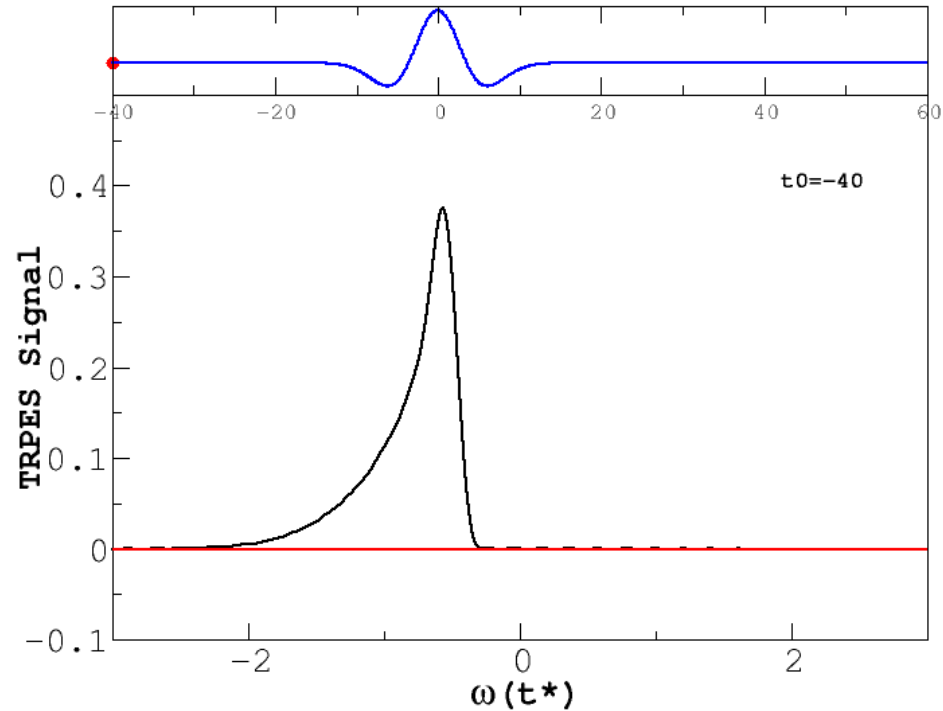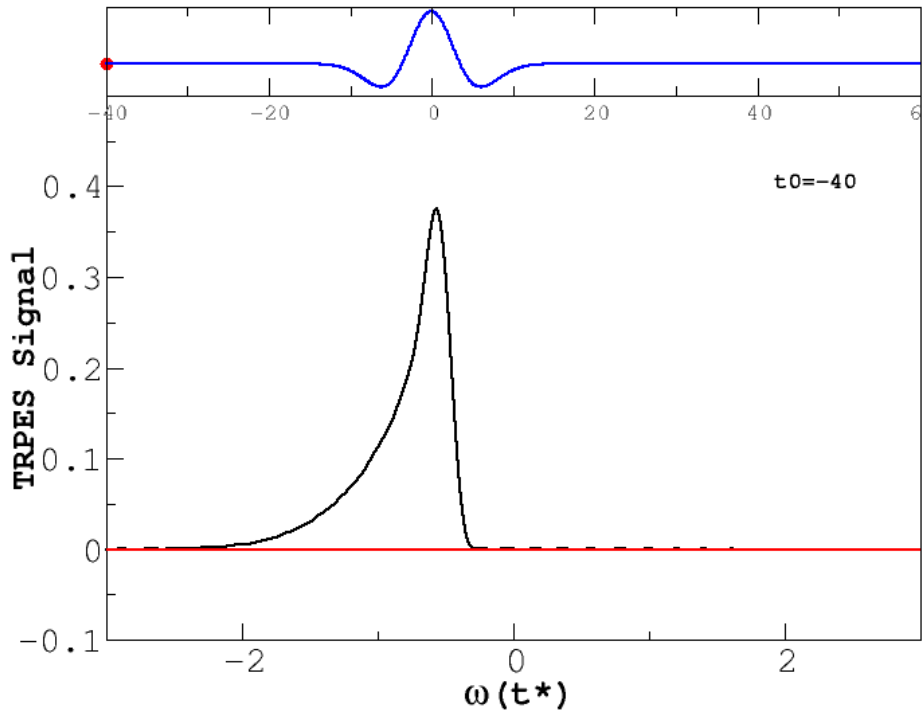
Time resolved photoemission signal for
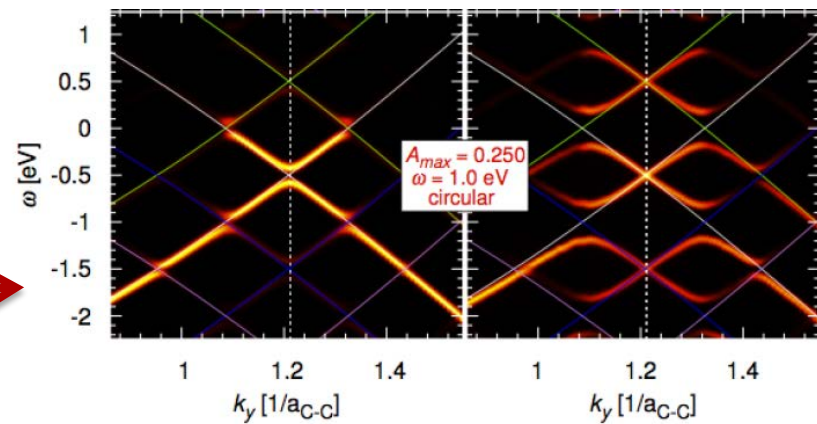$A(t)=-E_0\exp(-t^2/25)t$ with probe width $=14$

Linear pump: no gap at *K*

Circular pump breaks trs: gap at *K*

Graphene

Gap breakdown for strong field!

Dynamical mean-field theory

Uwe Brandt pioneered many of the important methods used including the first example of an exact DMFT solution in equilibrium and the first use of contour-ordered Green's functions.

Basic idea is that self-energy is local so the lattice problem can be mapped to a self-consistent impurity problem in a time-dependent field.

Lattice
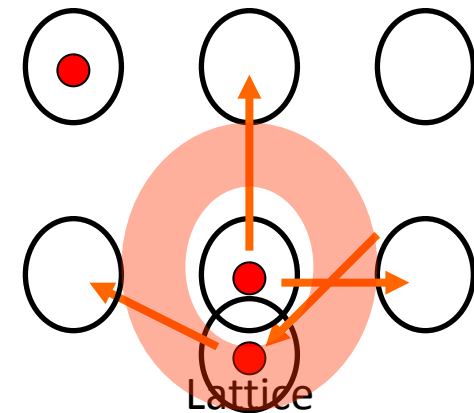
Impurity site

Dynamical mean-field theory algorithm

Dyson equation

$$\Sigma = G_0^{-1} - G_{loc}^{-1}$$

Hilbert transform

$$G_{loc} = \Sigma_k [G_k^{non-1}(E) - \Sigma]^{-1}$$

G_{loc}=Functional(G_0)
{example: FK model:
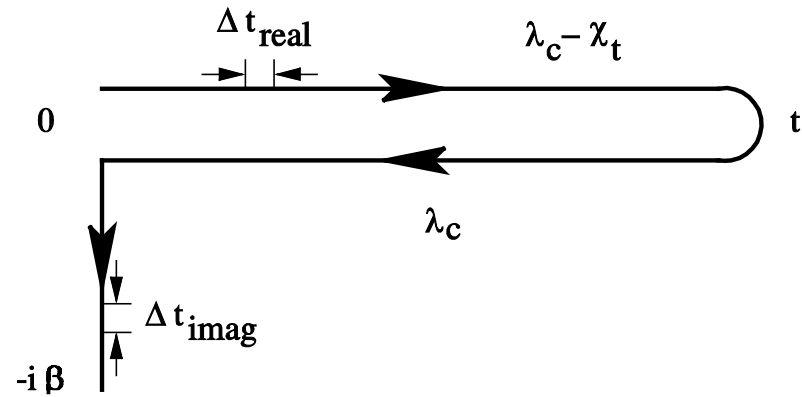$G_{loc} = (1-w_1)G_0(\mu) + w_1 G_0(\mu - U)$}

Dyson equation

Solve impurity problem

$$G_0 = (G_{loc}^{-1} + \Sigma)^{-1}$$

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

Dyson equations

Brute-force approach

The diagram shows a contour in the complex time plane. Labels include Δt_{real}, $\lambda_c - \chi_t$, 0, t, λ_c, Δt_{imag}, and $-i\beta$.
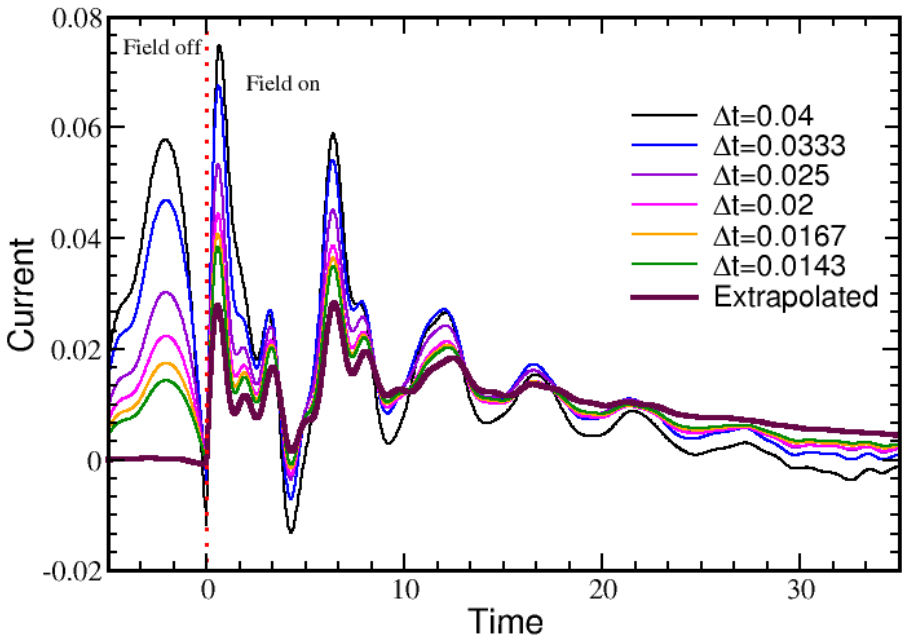
- Discretize contour to make all objects finite matrices

- Use linear-algebra packages for efficient coding

- Extrapolate to continuum limit

- Simple and fast to code and parallelize the DMFT algorithm

- Does not take advantage of causality or extrapolation methods

Discretization errors are under good control
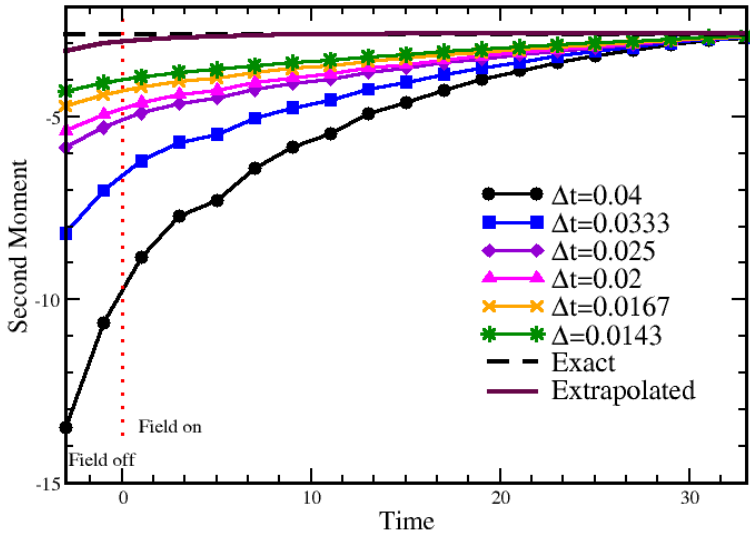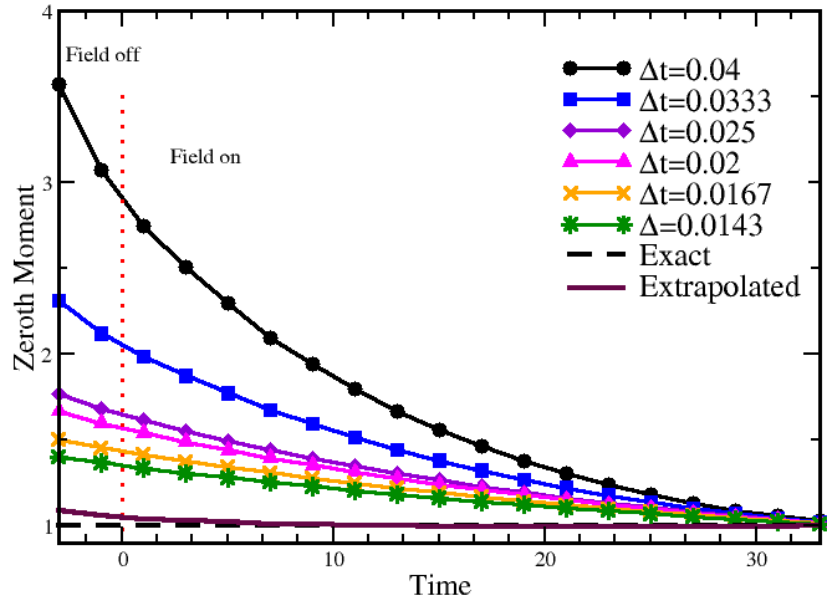
Scaling is needed to get accurate results.

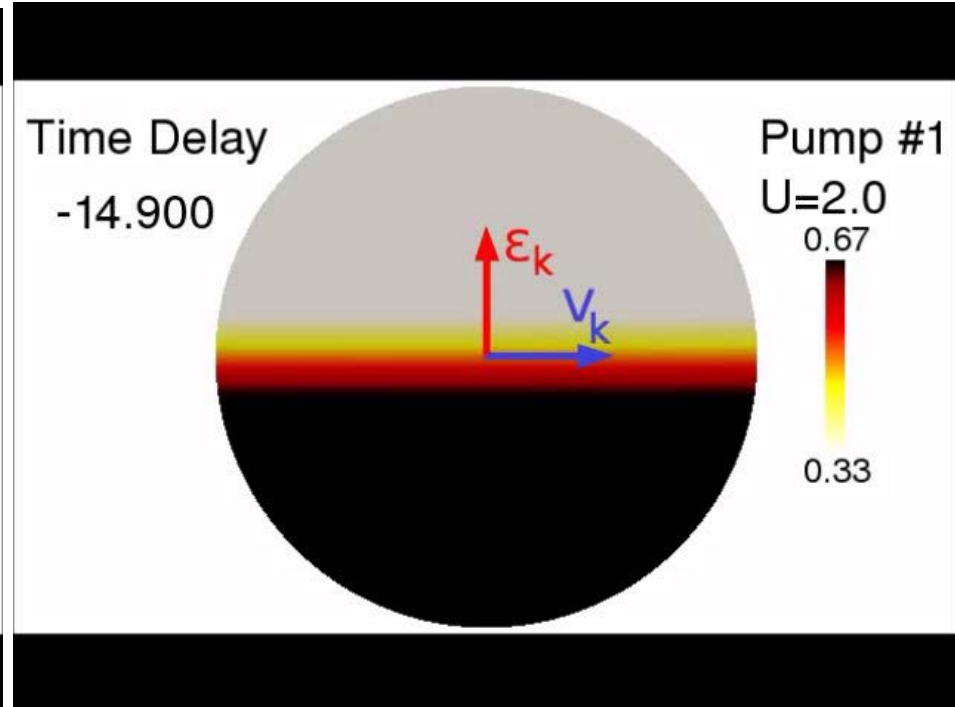# TR-PES for a metal vs a Mott insulator
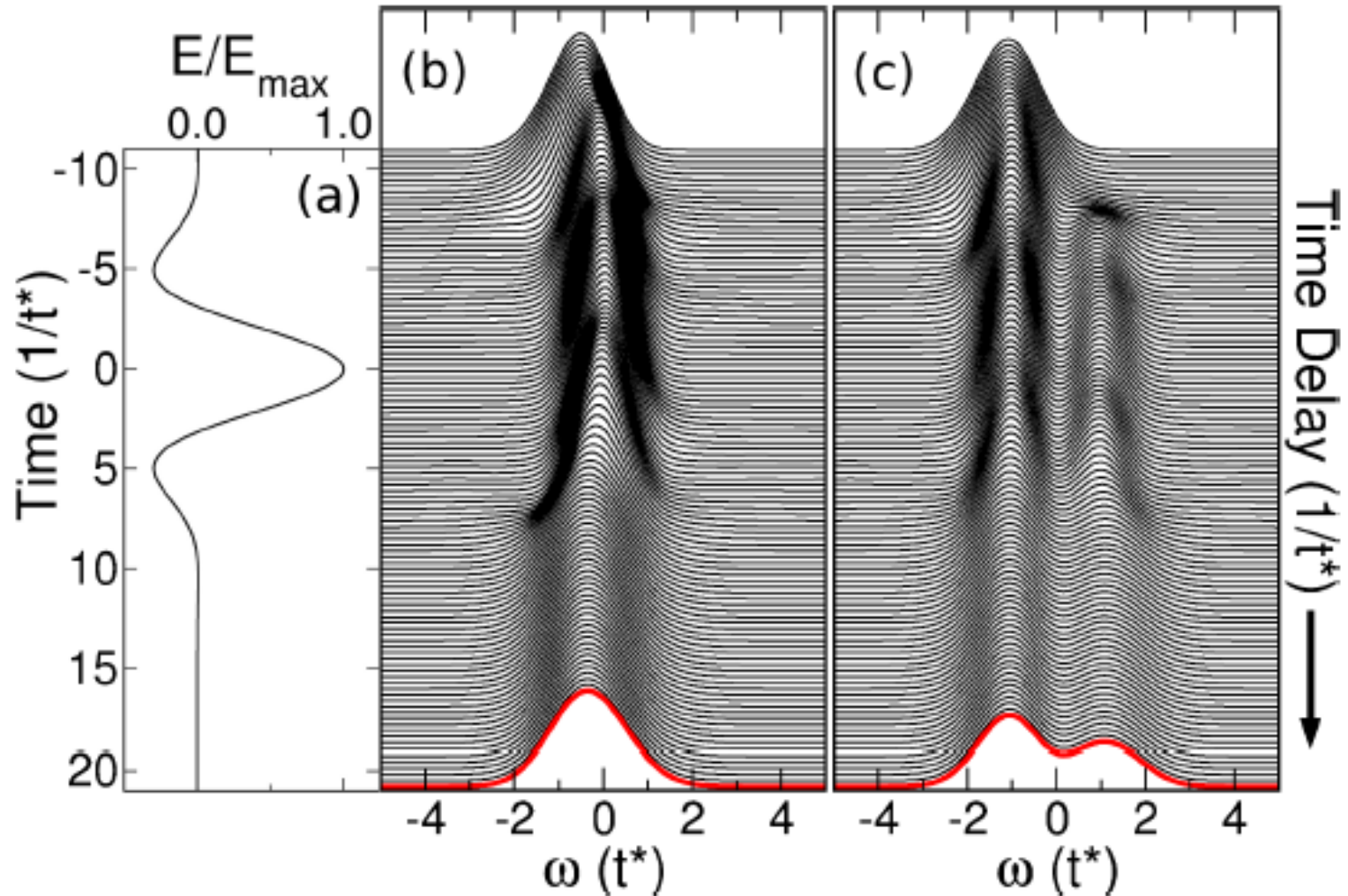
Momentum distributions
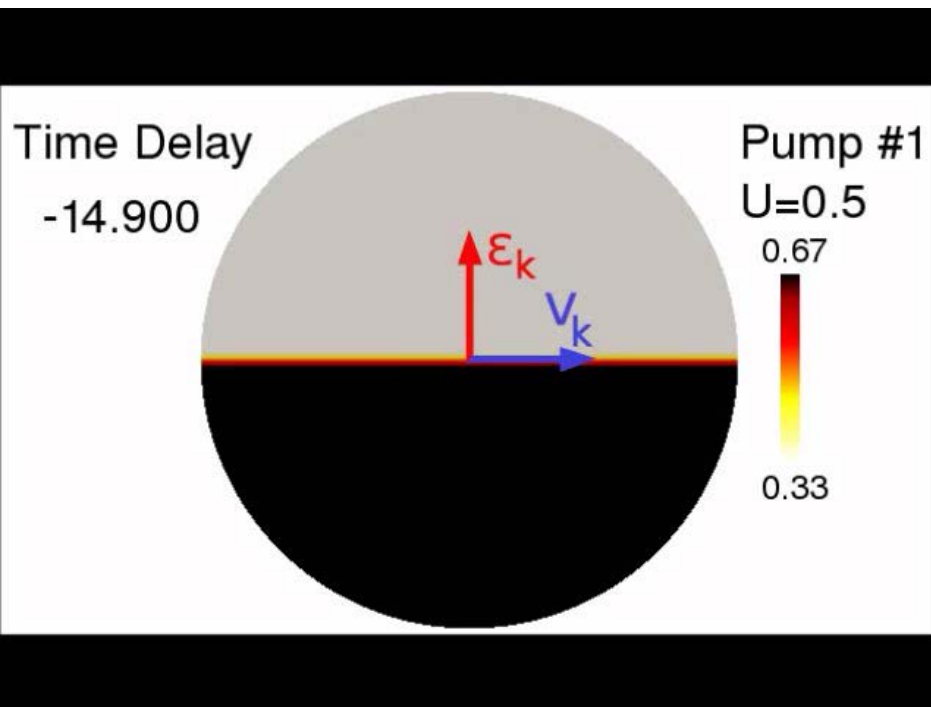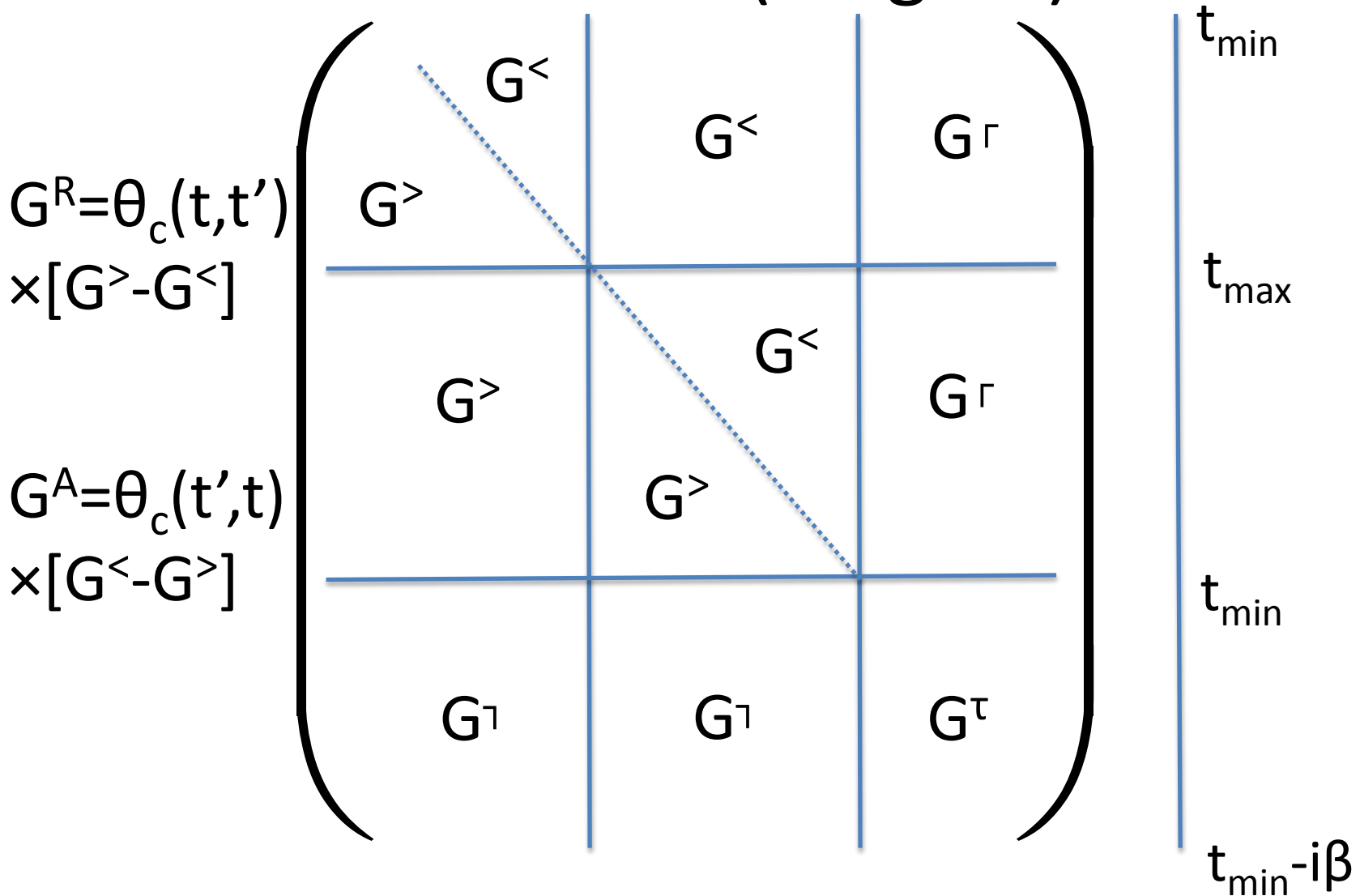

Metal   Mott

Integral equation approach

- Uses causality and extrapolation to predict next data points

- Uses efficient algorithms to numerically integrate Volterra integral equations.

- Very difficult to code.

- Most useful when coupled to impurity solvers that share the causality and extrapolation conditions.

Five (plus two) different Green's functions (Wagner)

$G^R = \theta_c(t,t') \times [G^> - G^<]$

$G^A = \theta_c(t',t) \times [G^< - G^>]$

Matrix contents:

Row 1: $G^>$, $G^<$, $G^\ulcorner$ (with $G^<$ along diagonal top)

Row 2: $G^>$, $G^<$, $G^\ulcorner$

Row 3: $G^\urcorner$, $G^\urcorner$, G^τ

Right axis labels: t_{min}, t_{max}, t_{min}, $t_{min} - i\beta$

Theory background: Evolution operators and ensemble average

$$G_{\mathbf{k}}(t, t') = -\frac{i}{Z} \mathrm{Tr} \left\langle \mathcal{T} \, U(-i\beta, t_0) U(t_0, t) \, \psi_{\mathbf{k}} \, U(t, t') \, \psi_{\mathbf{k}}^{\dagger} \, U(t', t_0) \right\rangle$$
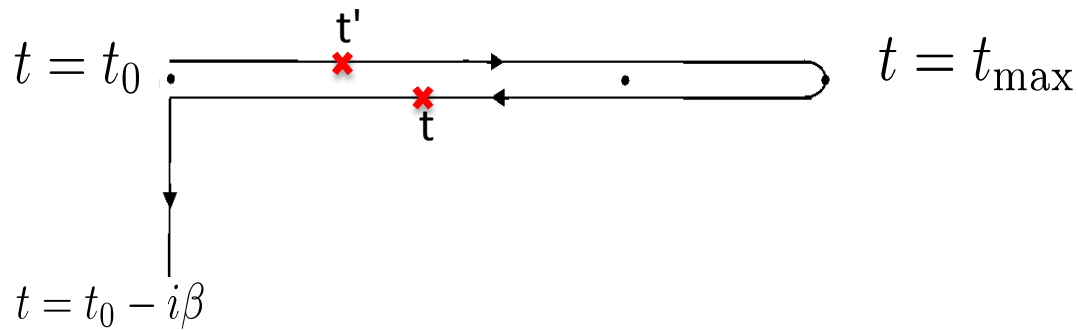
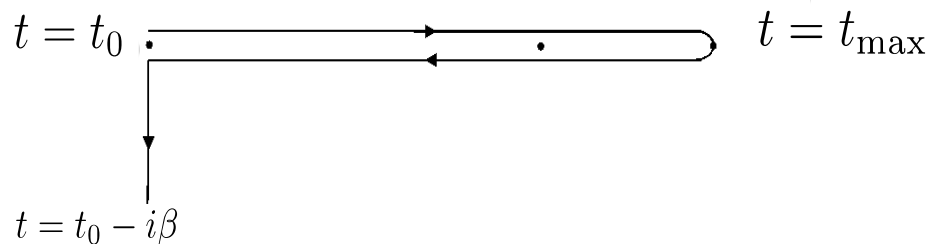There are now 7 Green's functions, depending on where their arguments lie

$$G^< \quad G^> \quad G^R \quad G^A \quad \middle| \quad G^\rceil \quad G^\lceil \quad \middle| \quad G^M$$

Theory background 2: Final ingredients

$$\left(i\partial_t - \varepsilon_{\mathbf{k}}\right) G_{\mathbf{k}}(t,t') = \delta(t-t') + \int d\bar{t}\, \Sigma(t,\bar{t}) G_{\mathbf{k}}(\bar{t},t')$$

*Green's function for quantum state **k***

Interaction kernel, depends on $\sum_k G_{\mathbf{k}}$

$t = t_0$ $t = t_{\mathrm{max}}$

$t = t_0 - i\beta$

<u>Causality implies that there cannot be any dependence on later times</u>

(1) Solve ensemble average on the imaginary spur
    (Many methods available for this)

(2) Make contour successively longer
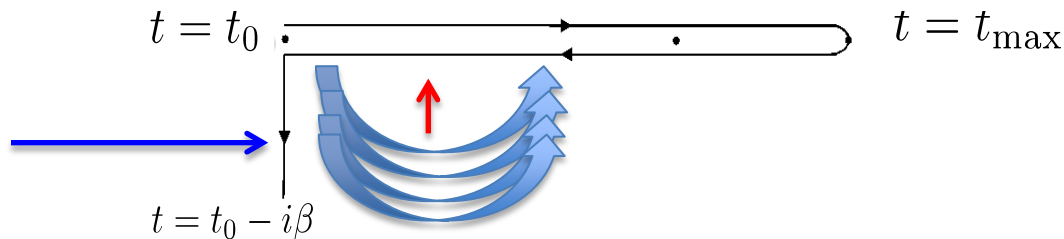
Solving the real-time portion of the contour

(1) $t=t_0$ is known from ensemble average

(2) For each **k** evaluate the RHS for Green's function equations of motion

$$i\partial_t G^{\lessgtr}(t,t') = \int_0^t d\bar{t}\,\Sigma^R(t,\bar{t})G^{\lessgtr}(\bar{t},t') + \int_0^{t'} d\bar{t}\,\Sigma^{\lessgtr}(t,\bar{t})G^A(\bar{t},t') + \frac{1}{i}\int_0^\beta d\bar{\tau}\,\Sigma^{\rceil}(t,-i\bar{\tau})G^{\lceil}(-i\bar{\tau},t'),$$

$$i\partial_t G^{\rceil}(t,-i\tau) = \int_0^t d\bar{t}\,\Sigma^R(t,\bar{t})G^{\rceil}(\bar{t},-i\tau) + \int_0^\beta d\bar{\tau}\,\Sigma^{\rceil}(t,-i\bar{\tau})G^M(\bar{\tau}-\tau),$$

$$t = t_0 \qquad\qquad\qquad t = t_{\max}$$

$$t = t_0 - i\beta$$

(3) Using Euler (or something more complicated), step forward in time

    i.   Form the interaction kernel Σ at the new time. [Σ depends on all G_k]
    ii.   Step forward in time again using new Σ
   iii. Repeat until converged

(1) Go back to (2) for the next time step

(Some) computational details

- 6,400 quantum k states are needed (somewhat reducible by symmetry)

- For each k, the G matrix must be stored and one copy of Σ
  - Roughly 20 million unique entries
  - Entries are complex double 1x1 or 2x2 matrices (0.5 Gb or 2 Gb)

- Hybrid parallelism
  - MPI used to distribute set of G_k among MPI tasks
  - OpenMP used to parallelize integrations and other time loops

Techniques used to solve electron-phonon coupled states both in the normal and ordered phases.

Momentum distribution for electron-phonon coupled systems
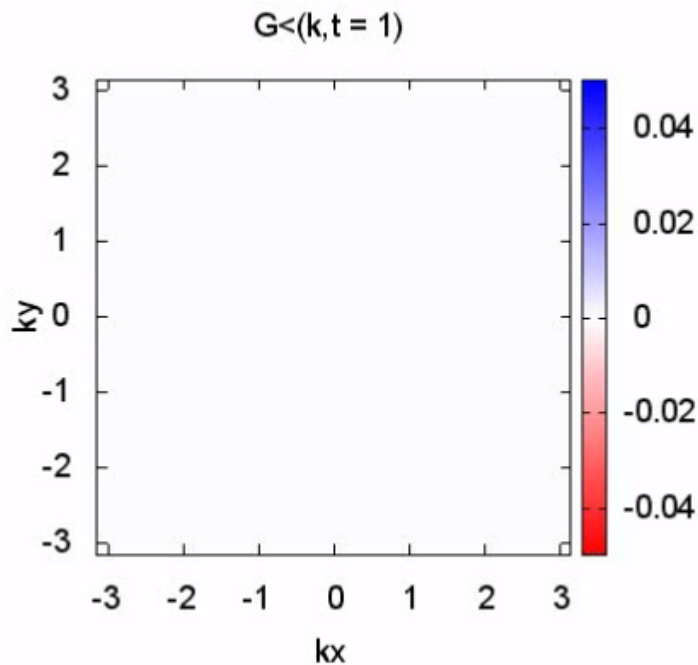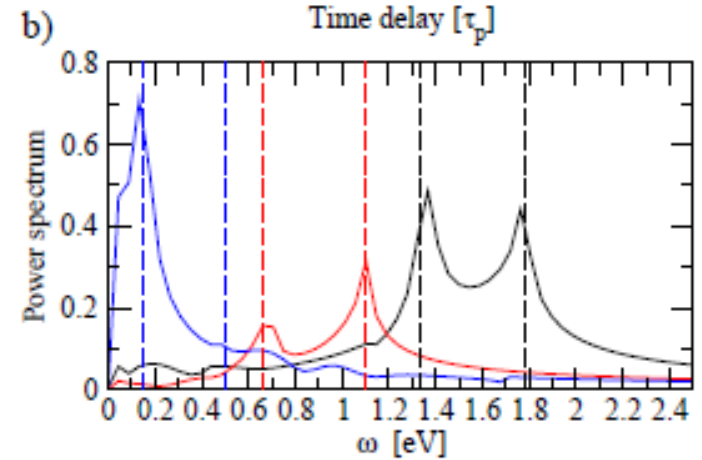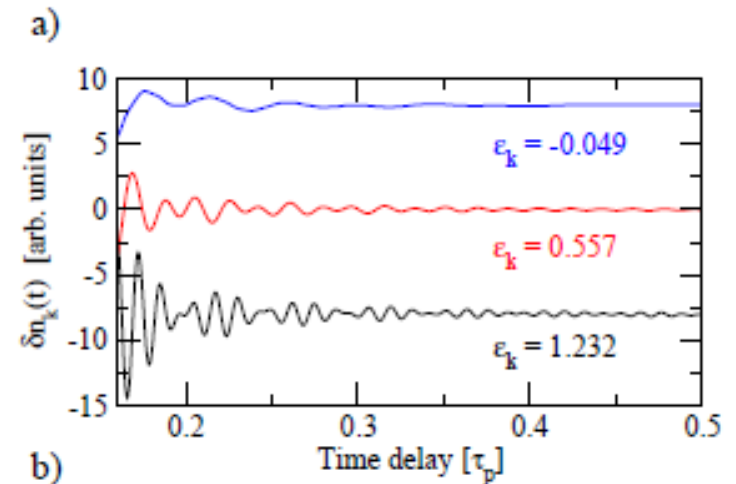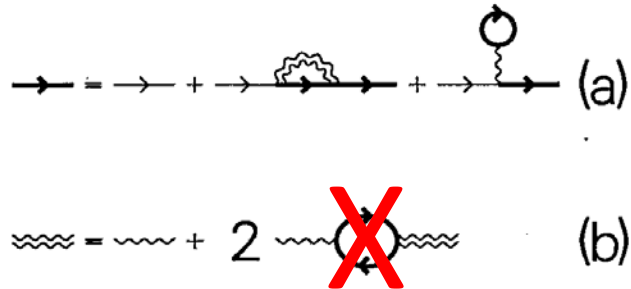
Phonon window effect
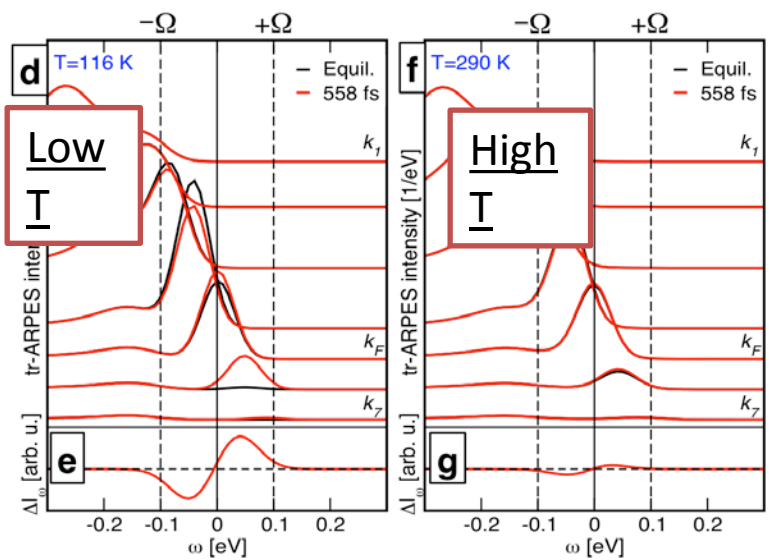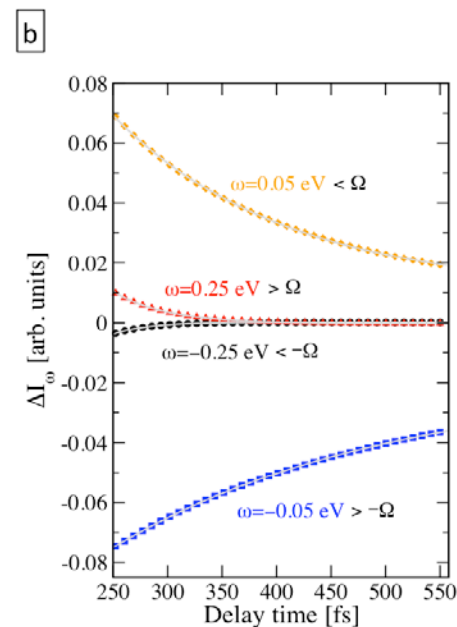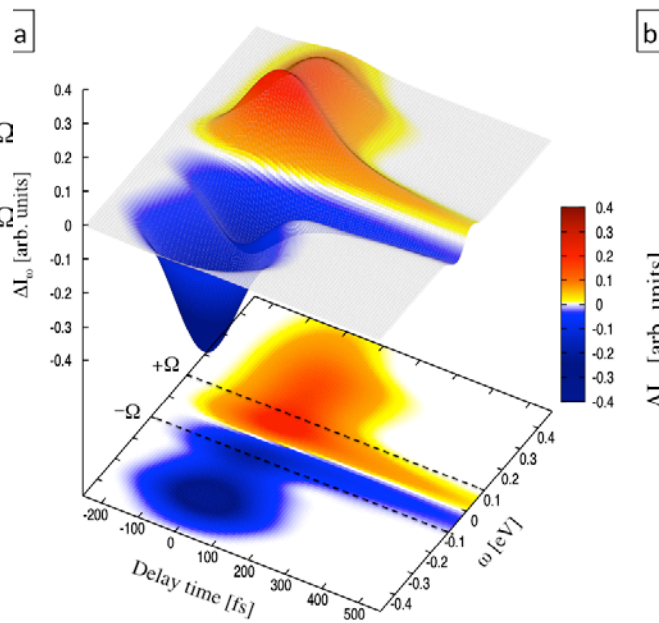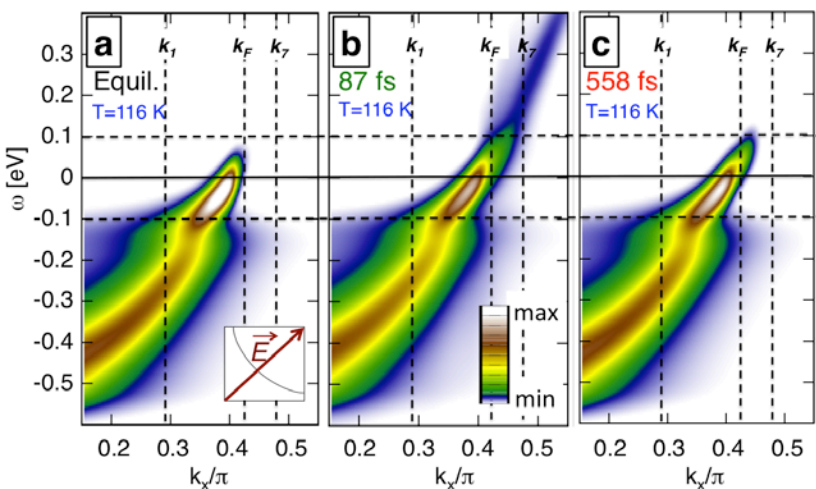
"slow" versus "fast" relaxation:
phonon window effect

Impurity problems

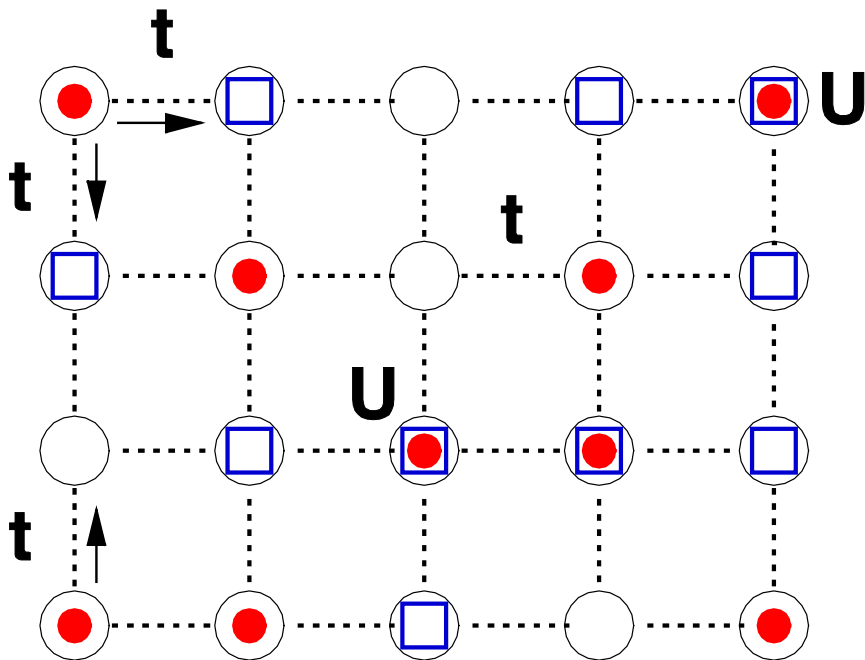# Single atomic field (FK model)
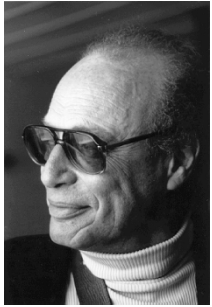
Light particles mobile, Heavy particles static. Take annealed average over all configurations. In trace over states, heavy particle is present or not for all times.

Partition function and Green's function

$$Z = \sum_{n_c} \sum_{n_f} T_c e^{-i \int_c dt H_{imp}(t)} e^{-\int_c dt \int_c dt' c^+(t) \Lambda_c(t,t') c(t')}$$

$$G_c(t,t') = i \frac{\delta}{\delta \Lambda_c(t',t)} \ln Z$$

Since each n_f sector looks like a noninteracting problem it can be solved exactly.

FK model solution

$$G_{ij}^c(t, t') = (1 - w_1) G_{0ij}^c(t, t') + w_1 [{G_{0ij}^c}^{-1} - UI]^{-1}(t, t')$$

W_1 represents the probability to find a heavy particle at the given site. G_0^c is the noninteracting Green's function in the dynamical mean-field and it can be calculated exactly.

Hence one can solve for G using simple linear algebra methods.

Two atomic fields (Hubbard model)
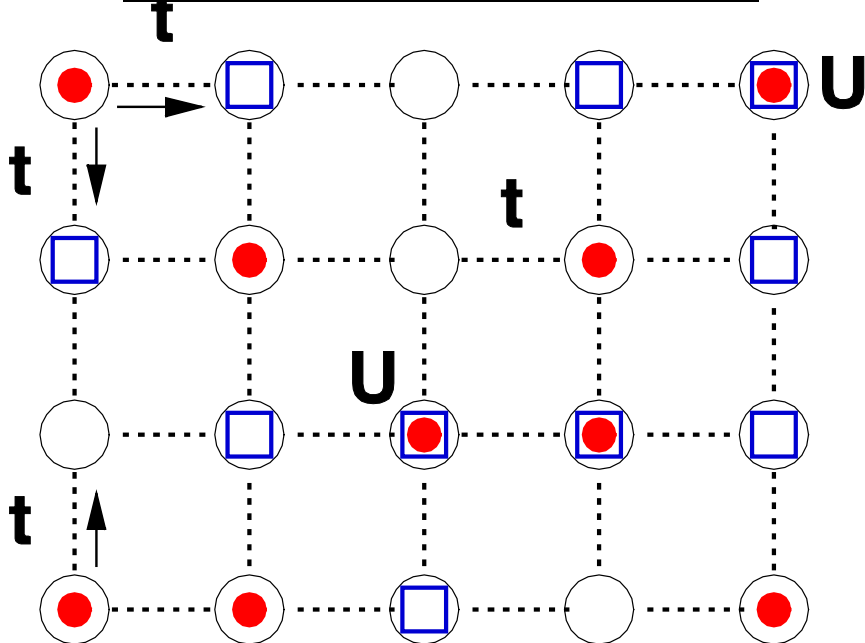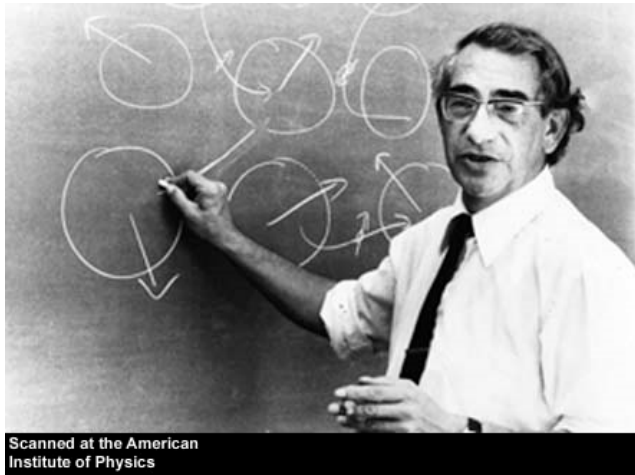
Now both particles hop, so up spin number can change as time evolves when examining the down spin objects and *vice versa.*

Partition function and Green's function

$$Z = \sum_{0\uparrow\downarrow d} T_c e^{-i\int_c dt H_{imp}(t)} e^{-\sum_\sigma \int_c dt \int_c dt' c_\sigma^+(t)\Lambda_{c\sigma}(t,t')c_\sigma(t')}$$

$$G_{c\sigma}(t,t') = i\frac{\delta}{\delta\Lambda_{c\sigma}(t',t)}\ln Z$$

Because the Heisenberg representation of spin up depends on the number of spin down particles, and they can change with time, we cannot write down the solution.

Numerical methods

Perturbation theory

- Introduce a small parameter, be it, U, Λ, or a hybridization (which is introduced later), and expand in a power series.

- Self-consistent expansions usually perform better than truncated expansions, but usually when a truncated expansion fails, this indicates when a self-consistent calculation will also lose accuracy.

Benefits

- Usually easy to code and not too numerically intensive for low orders.

- Causal features and extrapolations can be incorporated into the analysis.

- In many cases, solutions can be extended for longer times than with other techniques.

# Second-order perturbation theory for the Hubbard model
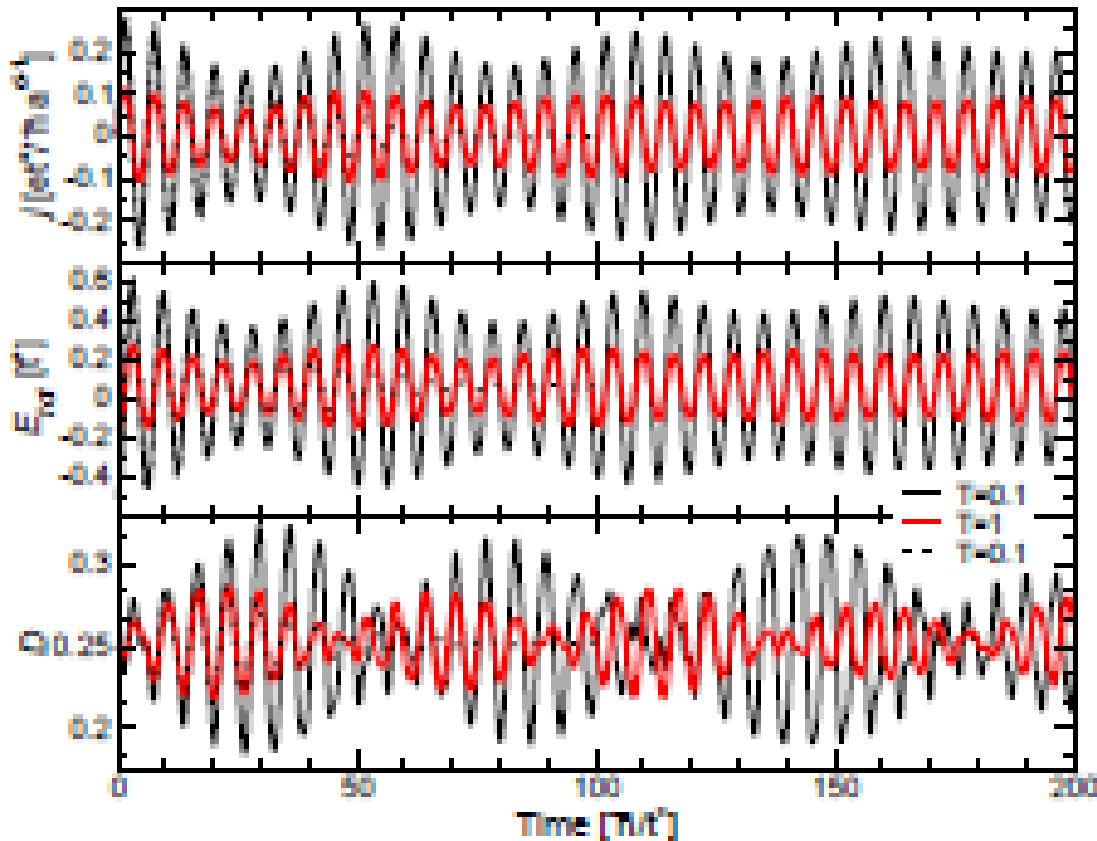
Truncated calculations are shown in black (low T) and red (high T). Self-consistent IPT in dotted line. One can see truncated calculations show little to no damping.

Quantum Monte Carlo

- Continuous time approach uses Monte Carlo approach to sample high order diagrams---Monte Carlo can increase the order, reduce the order, or change the location of time indices.

- Numerically exact, but suffers from super "sign" problem called phase problem, so can only extend a small distance down the real time axis.

Numerical renormalization group-based approaches
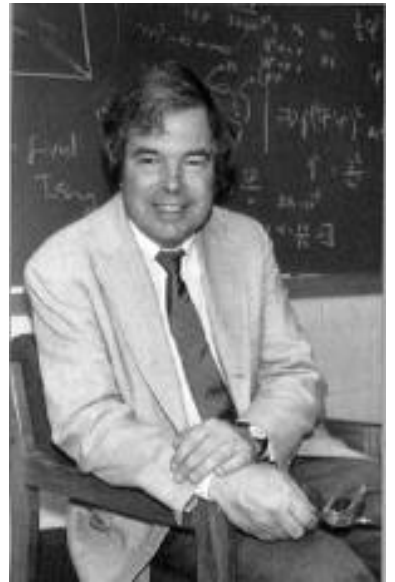
- Map the dynamical mean-field Λ_c to a set of bath states that have energies E_α and hybridizations $V_{t\alpha}$ that can change with time.

- Then we can construct the bath Hamiltonian

$$H(t) = H_{imp}(t) + \sum_{\alpha\sigma}(V_{t\alpha}c_\sigma^+ c_{\alpha\sigma} + h.c) + \sum_{\alpha\sigma}E_\alpha c_{\alpha\sigma}^+ c_{\alpha\sigma}$$

$$\Lambda_c(t,t') = \sum_\alpha V_{t\alpha}G_{c\alpha}^0(t,t')V_{\alpha t'}^+$$

Method has great potential

- But has not been tried for the general case yet, and preliminary results show it may end up yielding shorter evolution times than the QMC approach does.

- More work needs to be done on this, as it has not yet been fully explored.

The community needs a stable nonequilibrium impurity solver that can extend to long times.

New ideas welcome!

Acknowledgements

Thanks to

Michael Senthef

Tom Devereaux,   Hulikal Krishnamurthy,   Amy Liu   Lex Kemper,   Brian Moritz   Wen Shen