Extensions of Dynamical Mean Field Theory: Nonequilibrium and Spatial Correlations

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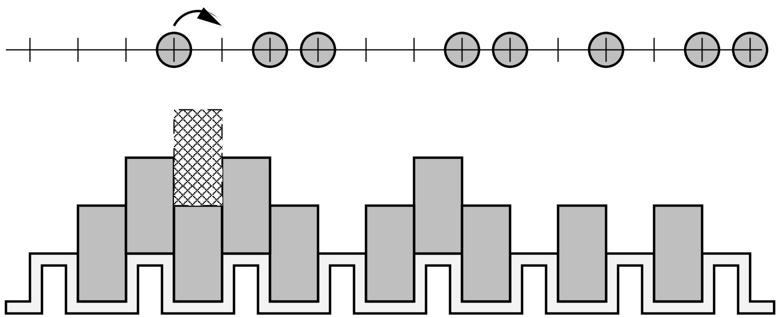
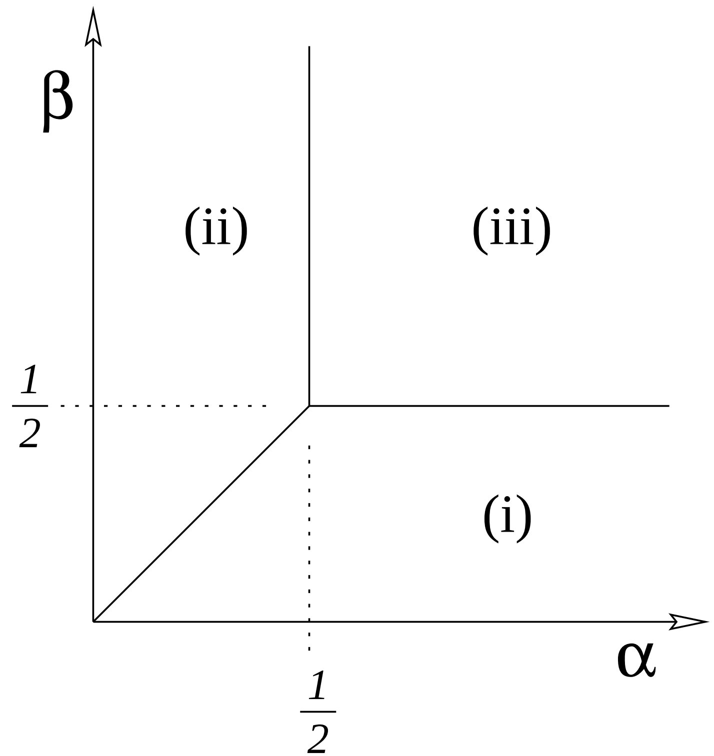
Nonequilibrium Physics: Simple Classical Systems

Even simple classical systems can lead to quite complicated physics:

linear chain:

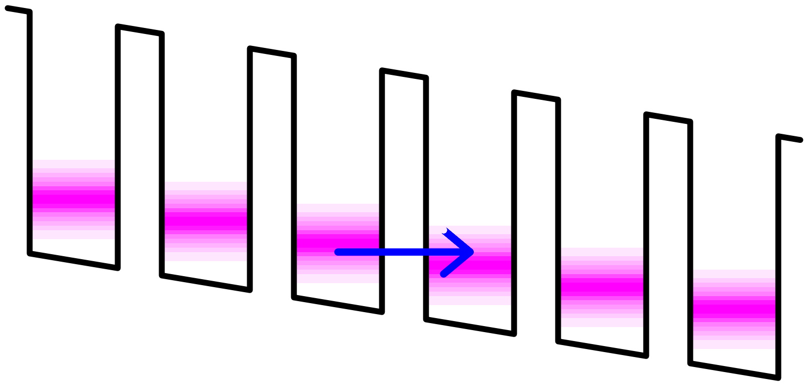




Derrida, Bouchaud, Domany ...

Nonequilibrium Physics: Quantum Systems

Strong electric field:

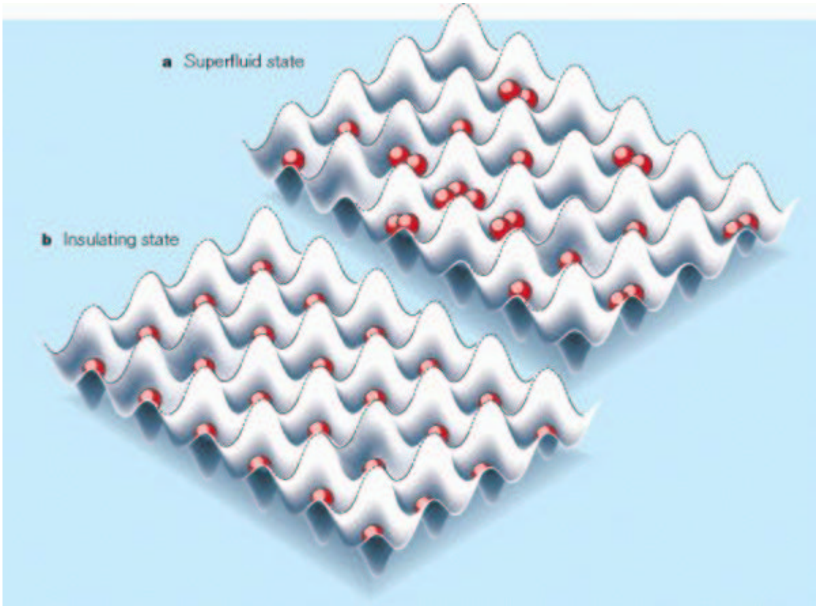


- Arrays of quantum dots
- Atoms in an optical lattice
- Correlated electrons in a solid
- Quantum wells
- . . .

In mesoscopic systems mostly Keldysh formalism, also recent attempts with RG

Quantum phase transition from a Mott phase to a superfluid phase:

N. Elstner and HM, PRB '99, T. D. Kühner, S. R. White, and HM, PRB '00



M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch and I. Bloch

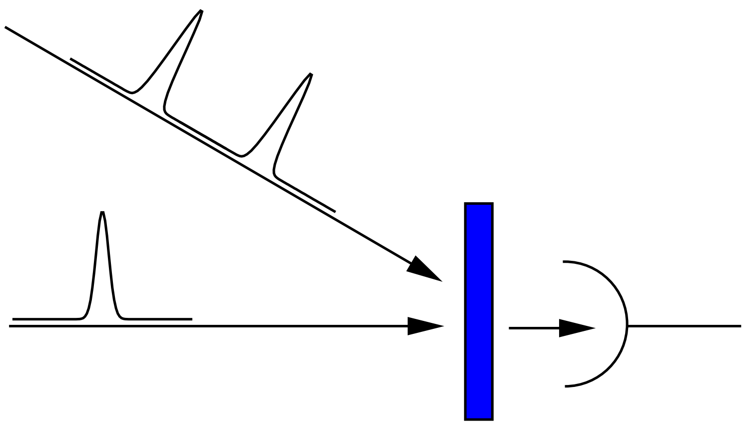
Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms

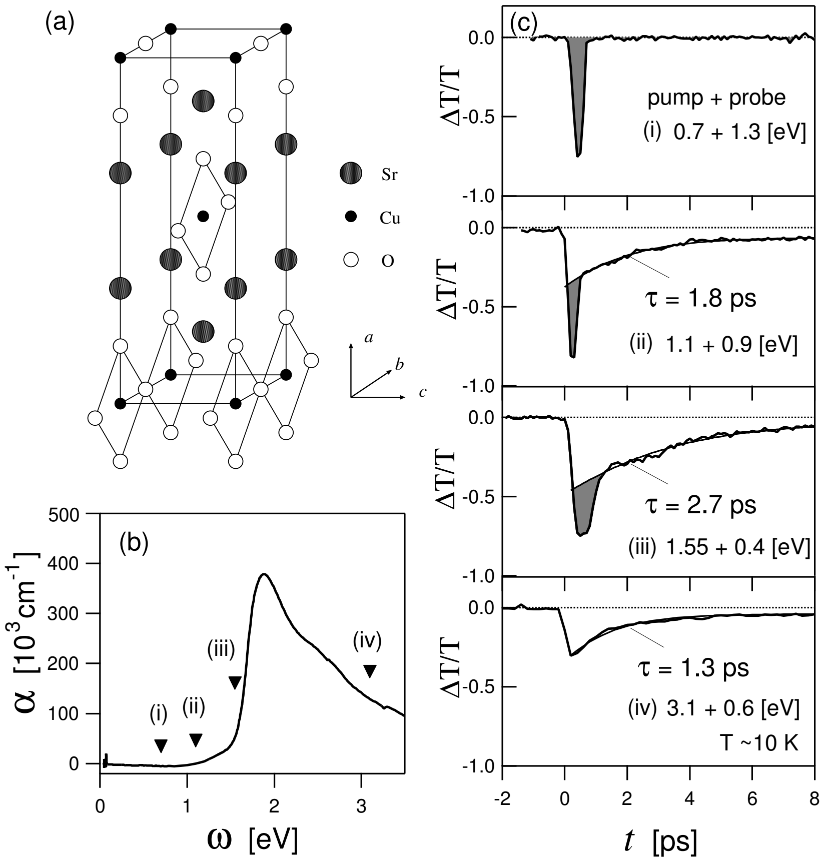
Nature 415, 39-44 (3 January 2002)

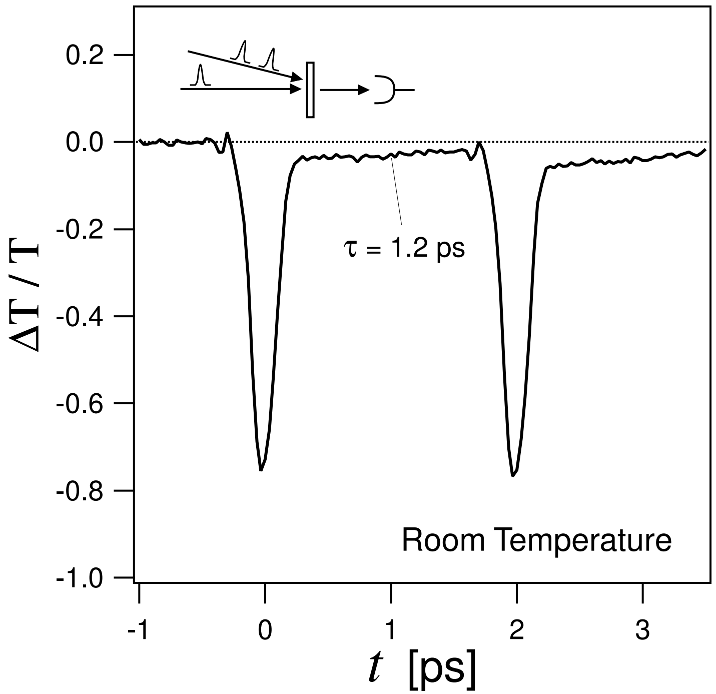
Experimental Motivation

Ogasawara et al. PRL 85, 2204 (2000)

Pump + probe experiment:

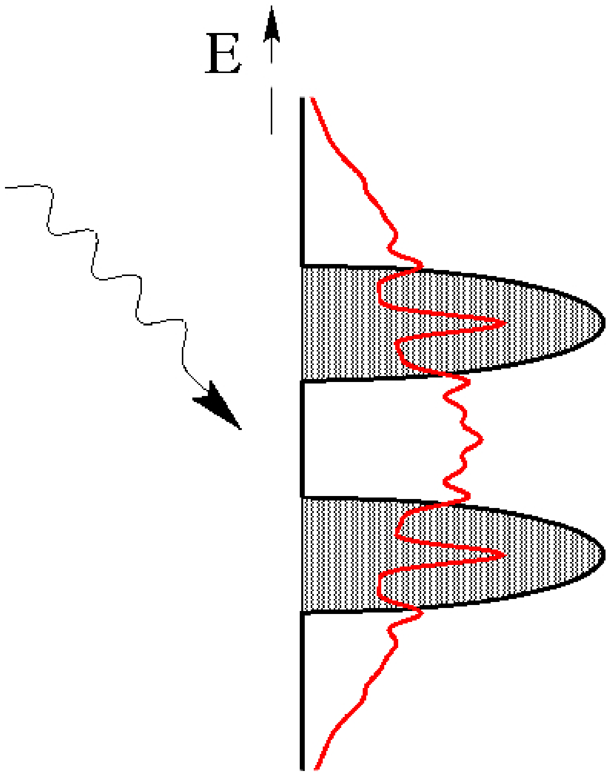






- One-photon and two-photon processes nearly degenerate in the special 1D material, different from semiconductors!
  - large dipole moment
  - large nonlinearity
- Spin excitations allow for non-radiative decay channel (large bandwidth $\sim$ 1eV)
  - ultrafast recovery rate
- Question:
  - limited to 1D compounds?
  - coupling to spin excitations?

Strongly correlated systems out of equilibrium:



- nature of states very different from noninteracting system
- strong external perturbation can create real states in the gap
- photo-doping should be strongly nonlinear
- other possible relaxation channels (spin)

Model:

Hubbard model in a time-dependent external potential:

$$\hat{H} = -t \sum_{ij\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \Gamma \cos\left(\Omega t\right) \hat{A}$$

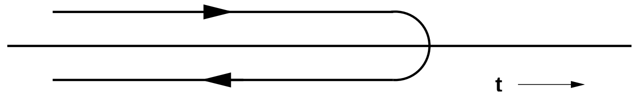
A "trivial" example is $\hat{A} = \sum_i A_i n_i$. In this case the $q = 0$ component acts like a time dependent chemical potential. For light we are mostly interested in the limit $q \rightarrow 0$ since $v_F/c \ll 0$.

- Since the Hamiltonian is explicitly time dependent the energy is not conserved. However there "quasi-energy" $E_n = E + n\Omega$ is still conserved up to integer multiples of Ω.
- The average energy, $\Omega \int_t^{t+1/\Omega} dt' E(t')$, is constant with time. This fact allows steady state solutions.

Schwinger-Keldysh formalism:

We assume that the time evolution can still be described by a density matrix! ("small deviations" from equilibrium)

We do not know the future: Keldysh-Schwinger contour . . . .



Green's functions with arguments on different can be related to the standard retarded and advanced Green's function - with an additional Green's function the Keldysh component.

$$
\begin{aligned}
G^{ret} &= G^{++} - G^{+-} \\
G^{av} &= G^{+-} - G^{--} \\
G^{keld} &= G^{++} + G^{--}.
\end{aligned}
$$

The sign, $\pm$, refers to the upper and lower branch of the Keldysh contour.

Noninteracting case:

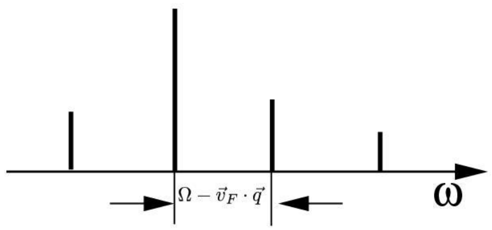
equation of motion:

$$i\hbar\partial_t c_{k\sigma}(t) = \left[c_{k\sigma}(t), \hat{H}_{kinetic} + \hat{H}_t\right]$$

which has the solution:

$$c_{k\sigma}(t) = e^{-\frac{i}{\hbar}\left(\epsilon_k t + \int^t dt_1 A cos\Omega t_1\right)} c_{k\sigma} = \sum_{n=-\infty}^{+\infty} J_n\left(\frac{A}{\hbar\Omega}\right) e^{-\frac{i}{\hbar}(\epsilon_k + n\hbar\Omega)t} c_{k\sigma}$$

where J_n are the Bessel functions. Note the appearance of sidebands, $E = \epsilon_k + n\Omega$, which are decaying with increasing n. The energy is not conserved. Similar to the Bloch problem there is still a conservation of "quasi-energy", $E = E' + n\Omega$.



In general the Green's function of the system depends on two time arguments. In the case of a single driving frequency the time dependence is simpler:

$$G_k(t,t') = \tilde{G}_k(t-t', t+t')$$

$\tilde{G}$ is periodic in $t+t'$ with period so $1/\Omega$ a new Green's function can be defined:

$$G_{k,n,m}(\omega) = G_k(\omega - n\Omega, \omega - m\Omega)$$

In a more compact notation: $(\hat{G}_k(\omega))_{n,m} = G_{k,n,m}(\omega)$.

Propagators ($R = A/(\Omega - \vec{v}\cdot\vec{q})$):

$$\begin{aligned} g^R_{k,k-nq}(\omega, \omega - m\Omega) &= \delta_{mn} \sum_l \frac{J_l(R) J_{l-n}(R)}{\omega - \epsilon_k - l(\Omega - \vec{v}\cdot\vec{q}) + i\eta} \\ g^K_{k,k-nq}(\omega, \omega - m\Omega) &= -2\pi i \sum_l \left[1 - 2f(\epsilon_{k-lq})\right] J_l(R) J_{l-n}(R) \end{aligned}$$

Dyson equation for the nonequilibrium problem

The Dyson equation

$$\hat{G}(k,\omega) = \left[\hat{G}_0{}^{-1}(\omega) - \hat{\Sigma}(\omega)\right]^{-1}$$

can be written as ($\hat{D}^{R/A} = \left[\left(\hat{G}_0^{R/A}\right)^{-1} - \hat{\Sigma}^{R/A}\right]^{-1}$):

$$\hat{G}(k,\omega) = \begin{bmatrix} 0 & \hat{D}_k^A \\ \hat{D}_k^R & \hat{D}_k^R \left\{ (\hat{G}_0^R)^{-1} \hat{G}_0^{\text{keld}} (\hat{G}_0^A)^{-1} + \hat{\Sigma}^{\text{keld}} \right\} \hat{D}^A \end{bmatrix}$$

with The selfenergy will be calculated using IPT which is complicated by the matrix form of the propagator.

$$\hat{G}^{\text{new}}(\omega) = \int_{-\infty}^{+\infty} d\epsilon \rho(\epsilon) \left(\hat{G}_{0_\epsilon}{}^{-1}(\omega) - \hat{\Sigma}(\omega) \right)^{-1}$$

Derivation of the DMFT equations:

Action:

$$
\begin{aligned}
S &= \int_C dt (\sum_{i\sigma} \left[\overline{\psi}_{i\sigma}(t) \left(i\partial_t + \mu \right) \psi_{i\sigma}(t) + \sum_{\delta} t_\delta \overline{\psi}_{i\sigma}(t) \psi_{i+\delta\sigma}(t) \right] \\
&- U \sum_i \hat{n}_{i\uparrow}(t) \hat{n}_{i\downarrow}(t) - \sum_{i\sigma} V_i(t) \hat{n}_{i\sigma}(t))
\end{aligned}
$$

with

$$
V_i(t) = \frac{A}{2} \left(\exp(-i\vec{q} \cdot \vec{r}_i + i\Omega t) + \exp(+i\vec{q} \cdot \vec{r}_i - i\Omega t) \right)
$$

This problem has to be mapped to an effective impurity model.

Integrating out one site:

$$\mathcal{G}(\omega, \omega - n\Omega)^{-1} = (\omega + \mu)\delta_{n0} - \frac{A}{2}(\delta_{n1} + \delta_{n-1}) - \sum_{i,j} t_{i0}t_{j0}G^{(0)}_{ij}(\omega, \omega - n\Omega)$$

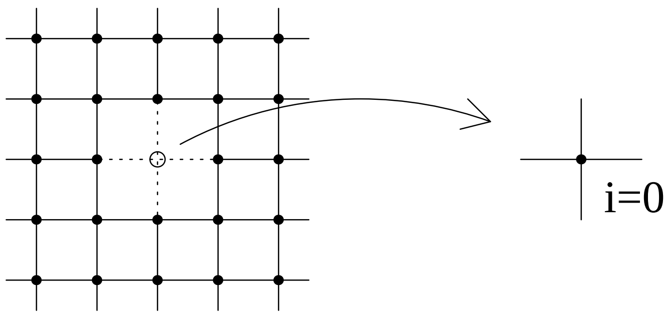
$G^{(0)}_{ij}$ is the Green's function with one site removed ($G^{(0)}_{ij} = G_{ij} - G_{i0}G^{-1}_{00}G_{0,j}$).
$\mathcal{G}$ is the Weiss field.

Fourier transform of the second term yields

$$\longrightarrow \sum_k \epsilon_k \epsilon_{k-nq} \left[\hat{G}^{(0)}_q(k, \omega)\right]_{0n}$$

In the limit $q \longrightarrow 0$ this can be done:

$$\int d\epsilon N(\epsilon)\epsilon^2 \left(\hat{g}^{-1} - \hat{\Sigma}\right)^{-1}$$



Self consistency equations $(q = 0)$

The self energy matrix can be computed using IPT.

$$
\begin{aligned}
\hat{G}(\omega) &:= \int d\epsilon N(\epsilon) \left[\hat{g}^{-1}(\epsilon,\omega) - \hat{\Sigma}(\omega)\right]^{-1} \\
\tilde{D}(\epsilon) &:= -\frac{1}{\pi} Im G^R_{00}(\epsilon, A = 0) \\
D_{n_1 n_2}(\epsilon) &:= -\frac{1}{\pi} Im G^R_{n_1 n_2}(\epsilon) \\
D^l_{n_1 n_2}(\epsilon) &:= J_{l-n_1}(A/\Omega) J_{l-n_2}(A/\Omega) \tilde{D}(\epsilon - l\Omega)
\end{aligned}
$$

Please note: $\hat{G}$ is the Hilbert transform of a non-symmetric matrix. The Hilbert transform has to be calculated relatively efficiently.

With these functions the spectral functions for the Weiss field can be constructed:

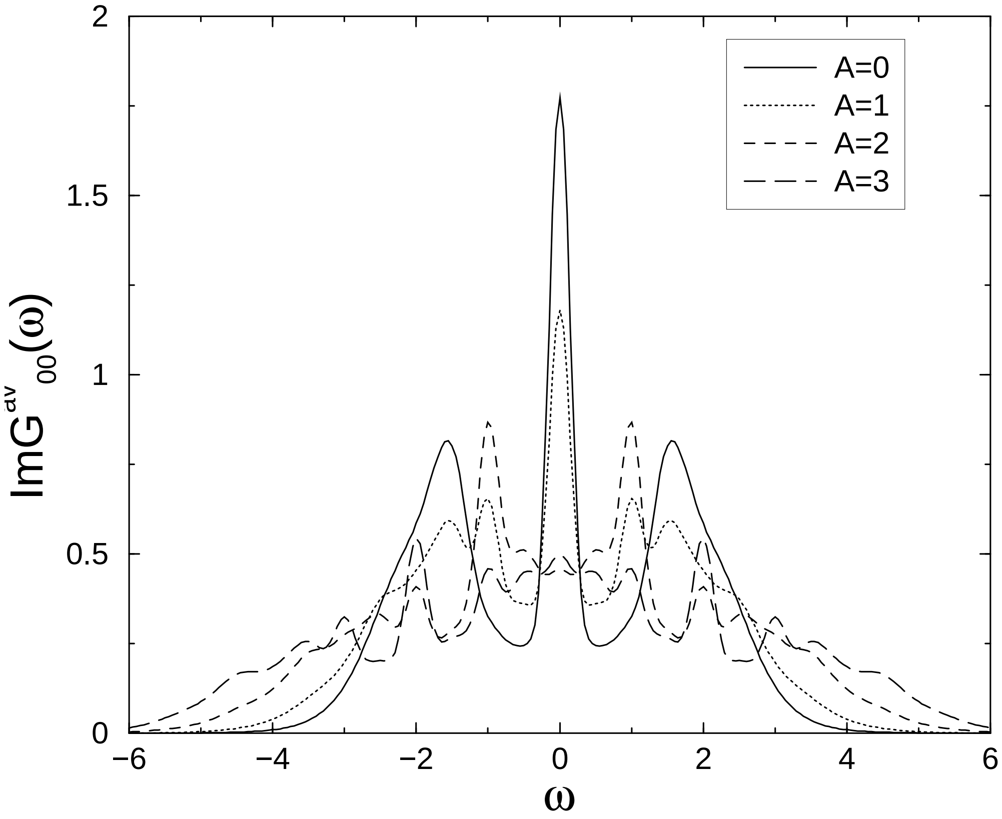
$$\begin{aligned}\mathcal{G}^{R/A}(\omega) &= \int d\epsilon \frac{D_{n_1 n_2}(\epsilon)}{\omega - \epsilon \pm i\eta} \\ \mathcal{G}^{K}(\omega) &= -2\pi i \sum_l (1 - f((\omega - l\Omega) + \mu) D^l_{n_1 n_2}(\omega)\end{aligned}$$

These Weiss fields have then to be put back in the effective impurity model.

Note: The impurity model which has to be solved is now a set of impurity models coupled by the various Weiss fields. For practical purposes it is sufficient to keep a relatively small number of Weiss fields (up to 15).

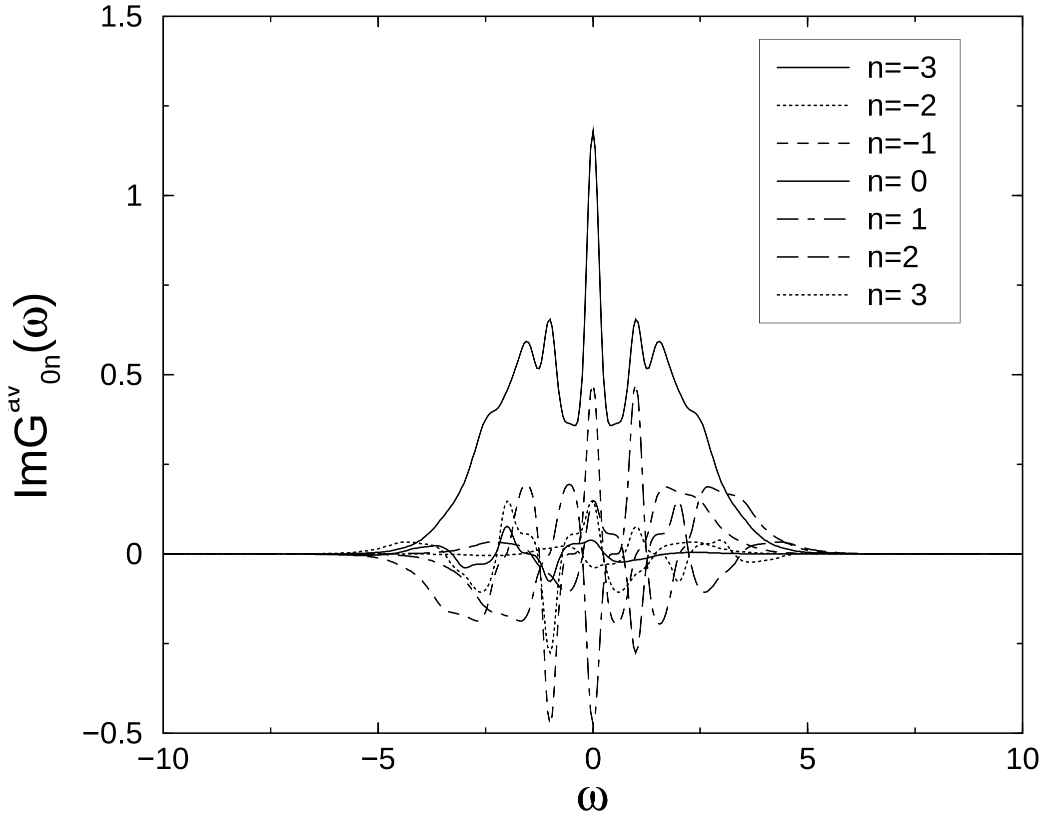
Spectral function in the steady state

varying the amplitude



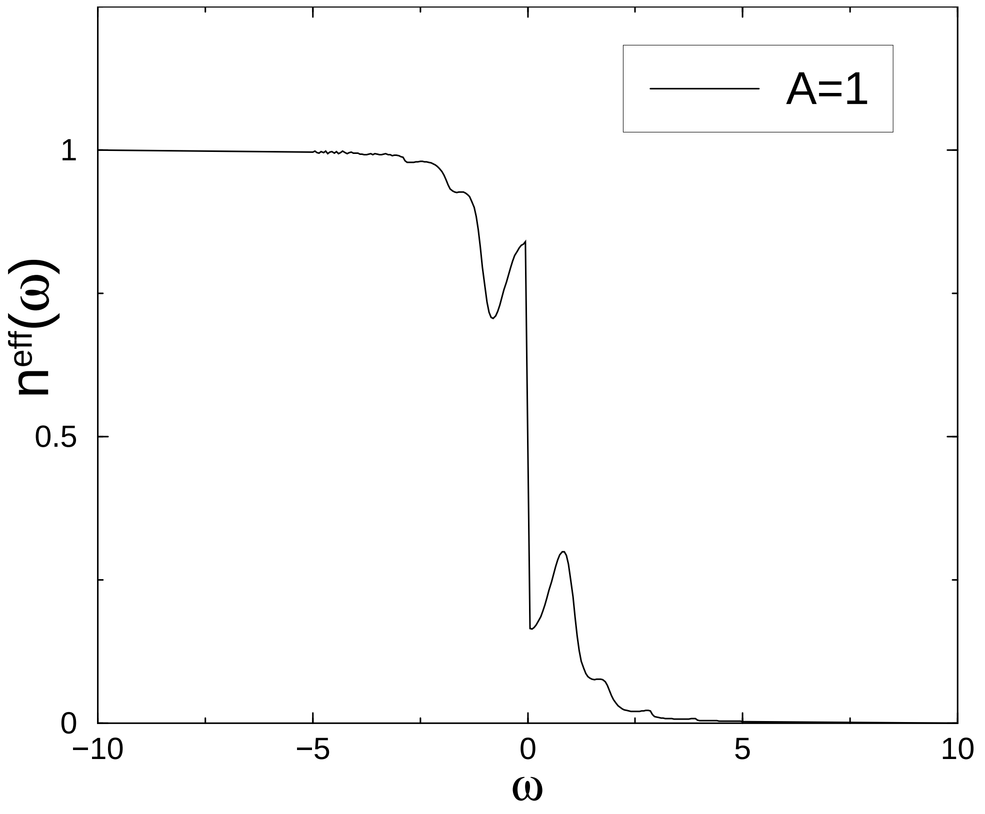
Spectral function in the steady state

decomposition in sidebands



Distribution function in the steady state

Amplitude = 1



Excitonic Insulator under Time-Dependent External Field

$$
\begin{aligned}
H &= \sum_i \left(E_a a_i^\dagger a_i + E_b b_i^\dagger b_i \right) - \sum_{<ij>} \left(t_{ij}^a a_i^\dagger a_j + t_{ij}^b b_i^\dagger b_j \right) \\
&- V \sum_i a_i^\dagger b_i b_i^\dagger a_i + A(t) \sum_i \left(a_i^\dagger b_i b \dagger_i a_i \right)
\end{aligned}
$$

- Excitonic insulator:
  - 2 orbitals per lattice site
  - local attractive exchange interaction between carriers on different orbitals
- Time-dependent field:
  - transitions between on-site orbitals
  - A(t) $=$ pump pulse (Gaussian, δ-function ...)

Self-Consistency Equation

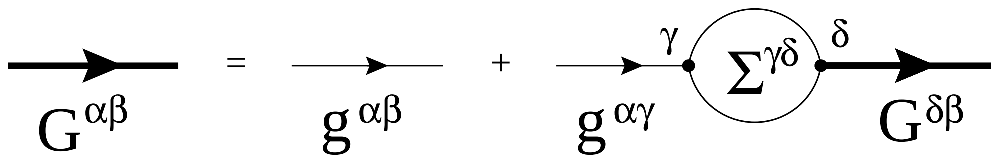
$$E_a = -E_b = E, t_a = -t_b = t$$

$$\boxed{\begin{aligned} \left[\mathcal{G}^{-\infty}\right]^{\alpha,\beta}(\omega,\ \omega') &= \alpha\delta_{\alpha\beta}\{[\omega + \mu - E\tau_3]\,\delta_{\omega,\ \omega'} - A(\omega - \omega')\tau_1\} \\ &- \alpha\beta t^2 \tau_3 G^{\alpha\beta}(\omega,\ \omega')\tau_3 \end{aligned}}$$

$\mathcal{G}$, G are matrices in (a, b), Keldysh and frequency space

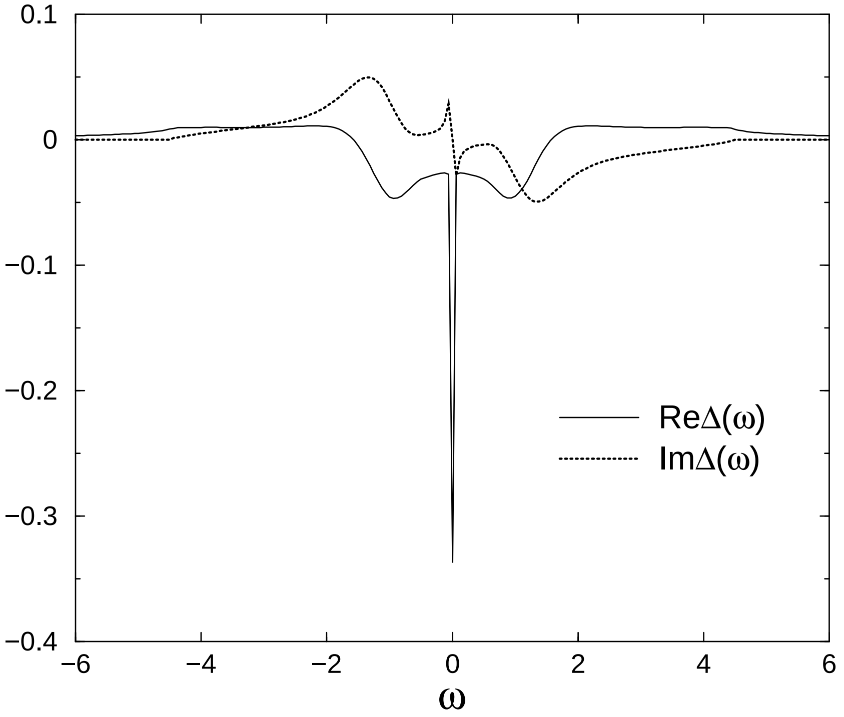
DMFT: local self energy: $\Sigma(k,\ \omega,\ \omega') = \Sigma_{local}(\omega,\ \omega')$

Identify local self energy with the impurity self energy

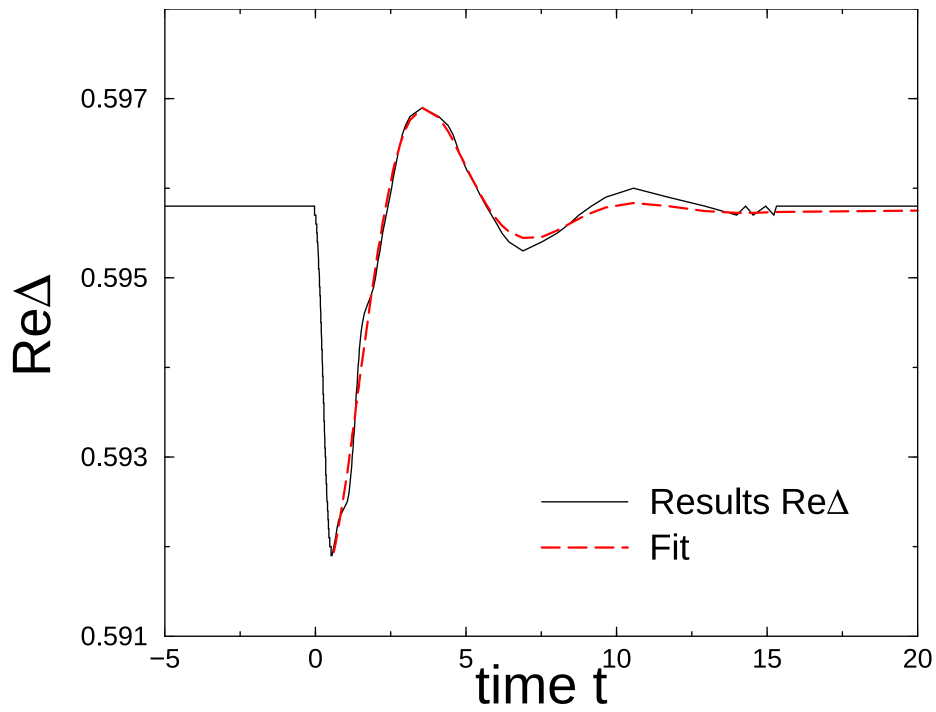


Response to Ultrashort Pulse: $A(t) = A\delta(t)$

frequency response:

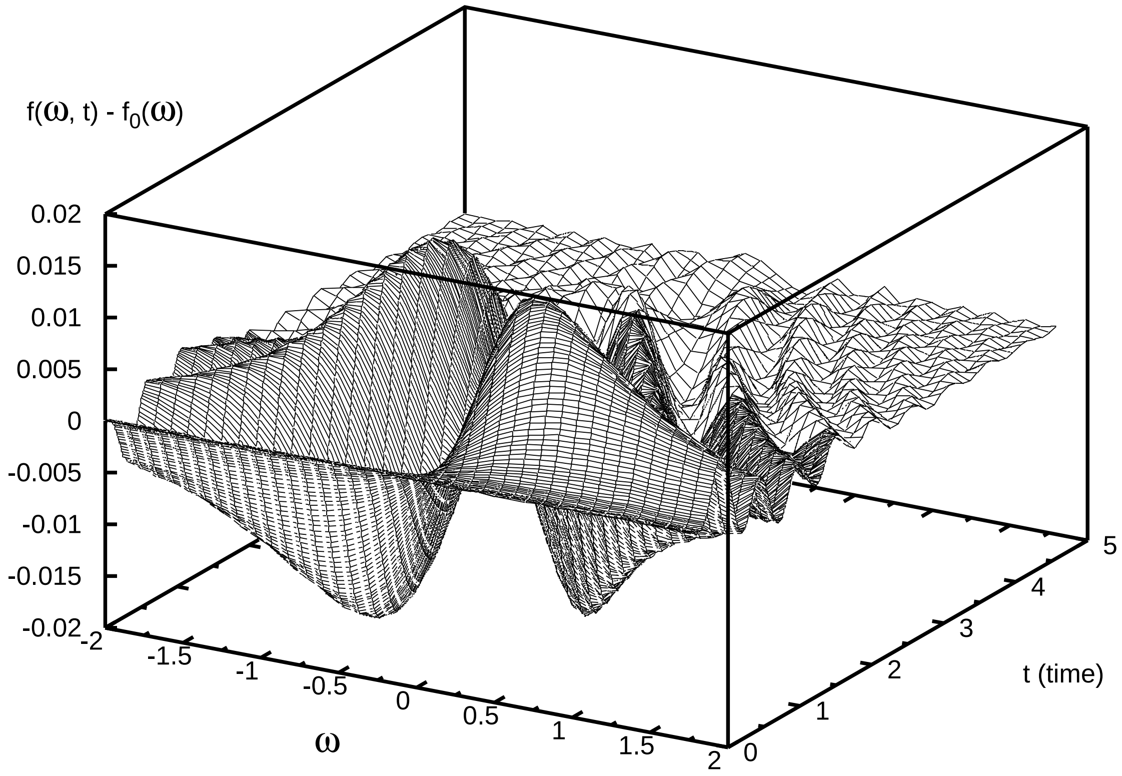


time response:



Fit: $C\cos(\omega t)e^{-t/\tau} + \Delta_0$

Change in the Distribution Function



Nonequilibrium with DMRG

M. Cazalilla and J. B. Marston, Phys. Rev. Lett. (2002)

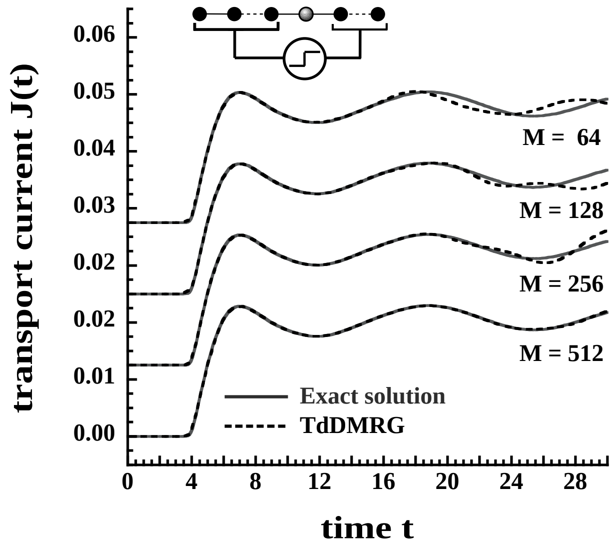
Recipe:

- Use DMRG to truncate Hilbert space
- Do time development with truncated Hamiltonian

$$i\hbar\partial_t \left|\Phi(t)\right\rangle = \left[(H_{trunc} - E_0) + H'(t)\right] \left|\Phi(t)\right\rangle$$

BUT: Only comparison to noninteracting exact results

Comparison with exact results:



Conclusions

- Extension of the DMFT to nonequilibrium models
- Two Problems:
  - Periodically Driven Problem
  - Short Pulse
- Future Problems:
  - More realistic coupling to the external field
  - Better understanding of the impurity problem in nonequilibrium
  - Experimental realizations