Correlated electrons in nonequilibrium

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Outline

1. Equilibrium
   - Definition
   - Statistical mechanics

2. Nonequilibrium
   - Time evolution of quantum systems
   - Relaxation to new equilibrium
   - Thermalization

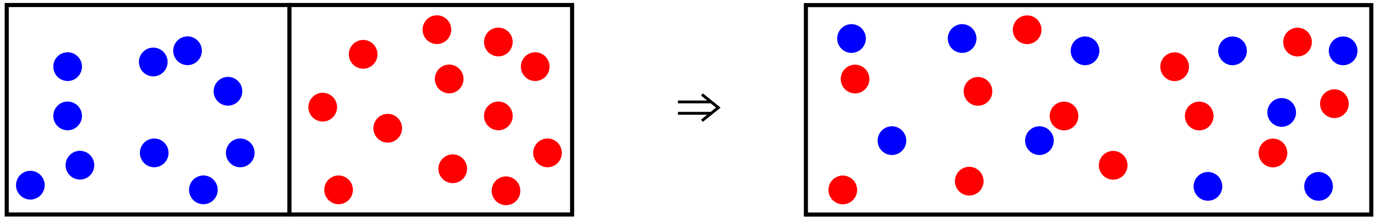
3. Correlated electrons
   - Hubbard model
   - Sudden interaction quench
   - Pump-probe spectroscopy

1. Equilibrium

- Definition
- Statistical mechanics

Equilibrium: a state of balance

When is a many-body system in equilibrium?



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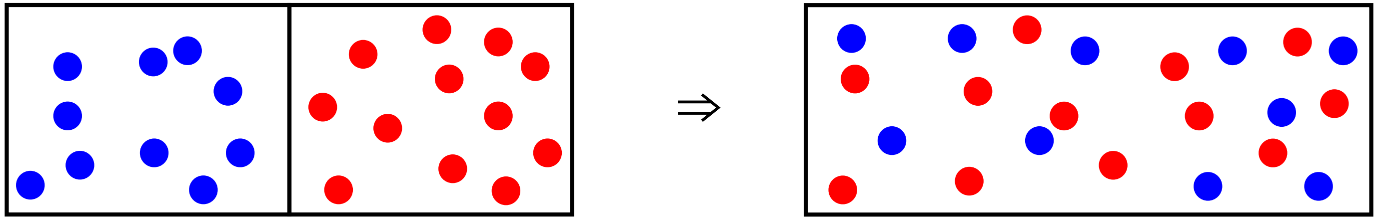

Thermodynamic equilibrium: no net flow of energy

- thermal equilibrium
- mechanical equilibrium
- chemical equilibrium
- radiative equilibrium
- ...

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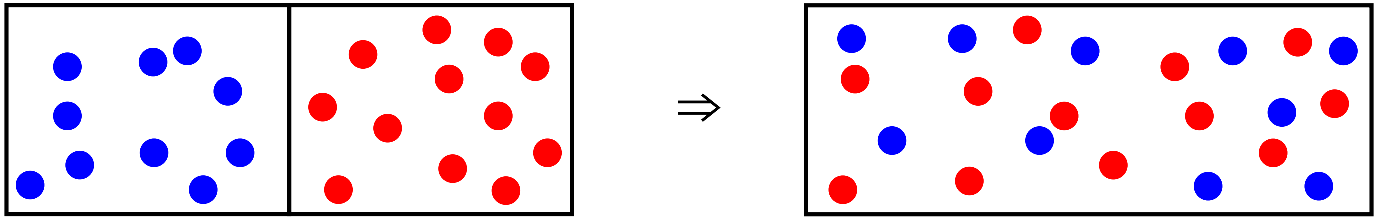

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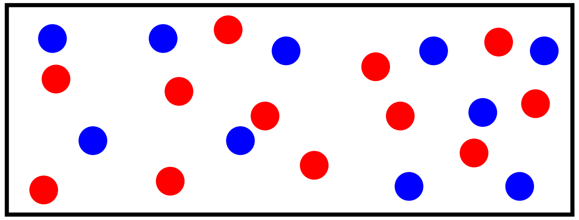
Isolated system in equilibrium

$\Leftrightarrow$

Properties described by statistical mechanics

Equilibrium statistical mechanics

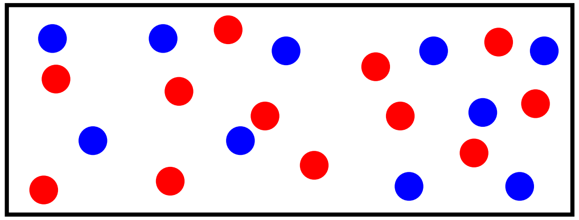
Prediction for equilibrium state:



- *Fundamental postulate*:

All accessible states are equally probable to be observed

Equilibrium statistical mechanics



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$$\langle \hat{A} \rangle = \frac{1}{Z} \sum_{\substack{n \\ E-\delta E \le E_n \le E}} \langle n | \hat{A} | n \rangle$$

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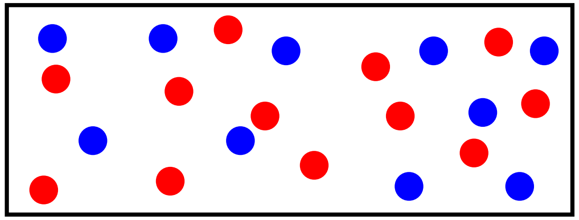
energy $= E = \langle \hat{H} \rangle$

Equilibrium statistical mechanics



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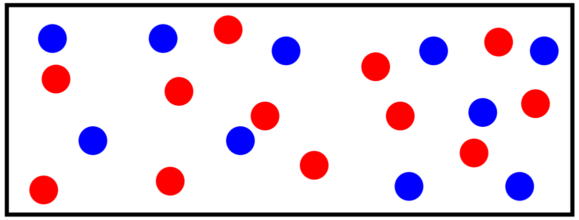
- Microcanonical ensemble:

$$\hat{\rho}_{\text{mic}} = \frac{1}{Z} \sum_{\substack{n \\ E-\delta E \le E_n \le E}} |n\rangle\langle n| \qquad \Rightarrow \qquad \langle \hat{A} \rangle = \text{Tr}[\hat{\rho}_{\text{mic}} \hat{A}]$$

Equilibrium statistical mechanics



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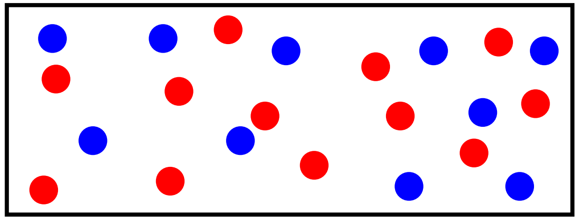
- $\hat{\rho} = \hat{\rho}_{\text{mic}}$ maximizes entropy: $S = -k_B \text{Tr}[\hat{\rho} \ln \hat{\rho}]$

Equilibrium statistical mechanics



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Equilibrium statistical mechanics

Generalization:

- Maximize $S = -k_B \mathrm{Tr}[\hat{\rho} \ln \hat{\rho}]$ with constraints
- $[\hat{A}_i, \hat{H}] = 0 \;\Rightarrow\; \hat{A}_i$ conserved $\Rightarrow$ fix $\mathrm{Tr}[\hat{\rho}\hat{A}_i] \overset{!}{=} \langle \hat{A}_i \rangle_{t=0}$

$$\Rightarrow \; \hat{\rho} \propto \exp(-\sum_i \lambda_i \hat{A}_i)$$

Boltzmann-Gibbs ensemble

Maxwell 1866, Boltzmann 1872, Gibbs 1878
von Neumann 1927, Jaynes 1957, ..., Balian 1991

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- Canonical and grand-canonical ensembles:

  $\hat{\rho}_{\mathrm{can}} \propto \exp(-\hat{H}/(k_B T))$ with T fixed by $\langle \hat{H} \rangle$

  $\hat{\rho}_{\mathrm{gcan}} \propto \exp(-(\hat{H} - \mu \hat{N})/(k_B T))$ with T, μ fixed by $\langle \hat{H} \rangle$, $\langle \hat{N} \rangle$

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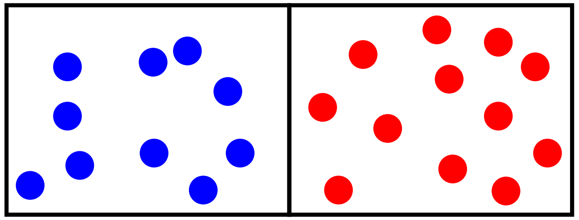
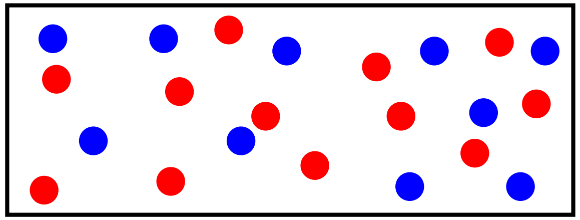
System in *thermal state*
$\Leftrightarrow$
Properties described by $\hat\rho_{\mathrm{mic}}$, $\hat\rho_{\mathrm{can}}$, or $\hat\rho_{\mathrm{gcan}}$

2. Nonequilibrium

- Time evolution of quantum systems
- Relaxation to new equilibrium
- Thermalization

Time evolution of isolated quantum systems

Schrödinger equation: $i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$

$|\psi(0)\rangle =$  $\Rightarrow$ $|\psi(t)\rangle =$ 

q.m. expectation values:

$$\langle \hat{A} \rangle_t = \langle \psi(t)|\hat{A}|\psi(t)\rangle$$

Quantum quench:

- Start with $|\psi_0\rangle$ and switch suddenly to Hamiltonian $\hat{H}$ at $t = 0$
- Time evolution for $t \geq 0$:

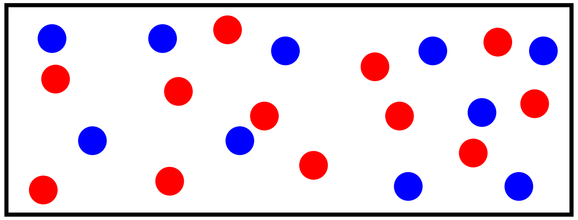
$$|\psi(t)\rangle = e^{-i\hat{H}t}|\psi_0\rangle = \sum_n \langle n|\psi_0\rangle \; e^{-iE_n t}|n\rangle$$

components of wave function oscillate forever

Relaxation to equilibrium state

Relaxation to stationary state? $\langle \hat{A} \rangle_{t \to \infty} \stackrel{?}{=} \text{const}$

$\Rightarrow$ possible only for large systems



Expectation values:

- Observable $\hat{A}$:

$$\langle \hat{A} \rangle_t = \langle \psi(t) | \hat{A} | \psi(t) \rangle = \sum_{n,m} c_n c_m^* e^{-i(E_n - E_m)t} \langle m | \hat{A} | n \rangle$$

- Time averaging:

$$\overline{\langle \hat{A} \rangle} = \lim_{t \to \infty} \frac{1}{t} \int_0^t \langle \hat{A} \rangle_{t'} \, dt' = \sum_n |c_n|^2 \langle n | \hat{A} | n \rangle$$

$=$ long-time limit of $\langle \hat{A} \rangle_t$ (if any)

Quenched Bose condensate

Abrupt increase of interaction of ^{87}Rb atoms:

Greiner, Mandel, Hänsch, Bloch '02

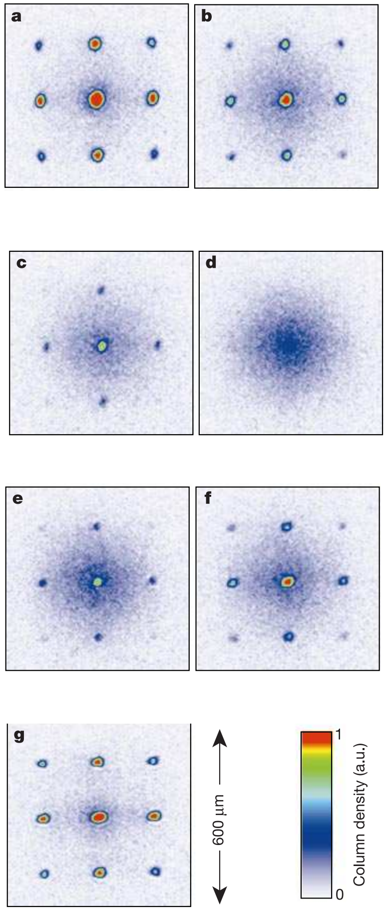
$\langle \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} \rangle$

$t=0\mu s$ $t=100\mu s$

$t=150\mu s$ $t=250\mu s$

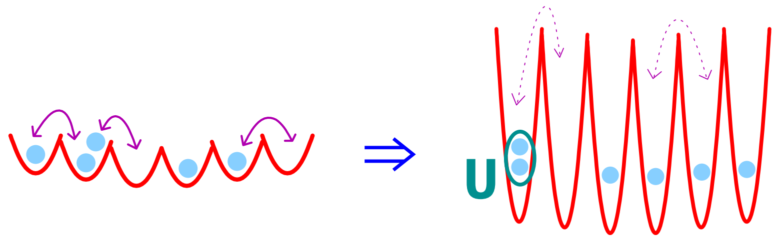
$t=350\mu s$ $t=400\mu s$

$t=550\mu s$



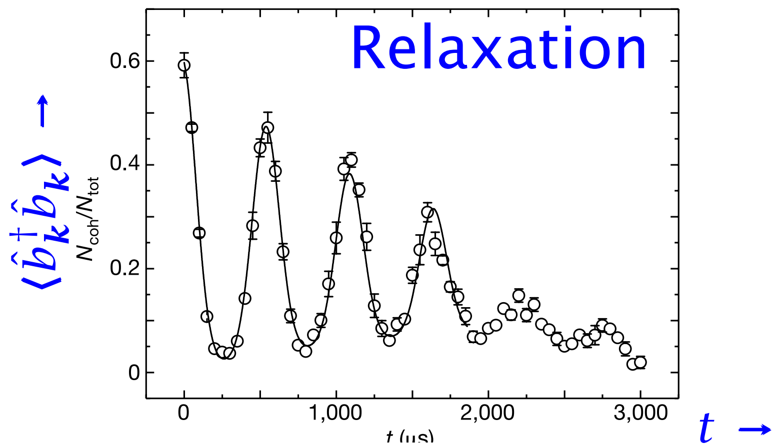
collapse and revival

$|\psi(0)\rangle$ = Bose condensate



$$H \approx U \sum_i \hat{n}_i^2$$

$|\psi(t)\rangle = e^{-i\hat{H}t}\,|\psi(0)\rangle$ oscillates



Thermalization

Equilibration to thermal state = 'thermalization'

- Thermal state = prediction of statistical mechanics:

$$\langle \hat{A} \rangle_{t\to\infty} = \sum_n |c_n|^2 \langle n|\hat{A}|n\rangle \stackrel{?}{=} \langle \hat{A} \rangle_{\text{mic/can/gcan}}$$

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- Thermalization is possible:
  - if only $\langle \hat{H} \rangle$ and $\langle \hat{N} \rangle$ are relevant, not all details of $|\psi(0)\rangle$
  - for sufficiently complicated $\hat{H}$
  - for not too correlated $\hat{A}$

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- Thermalization apparently depends:
  - on interaction strength
  - on integrability (# of constants of motion)

Kollath, Läuchli, Altman '07
Manmana et al.'07
Cramer et al.'08
Rigol, Dunjko, Olshanii '08
Moeckel & Kehrein '08, '09
Barmettler et al. '08
Rossini et al. '08
Eckstein, Kollar, Werner '09
...

Quantum Newton's cradle

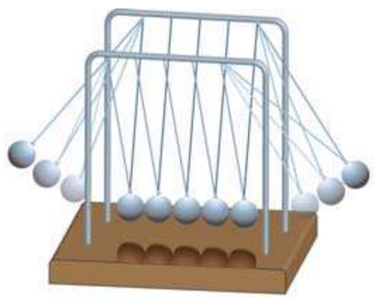
Oscillations of trapped ^{87}Rb atoms:

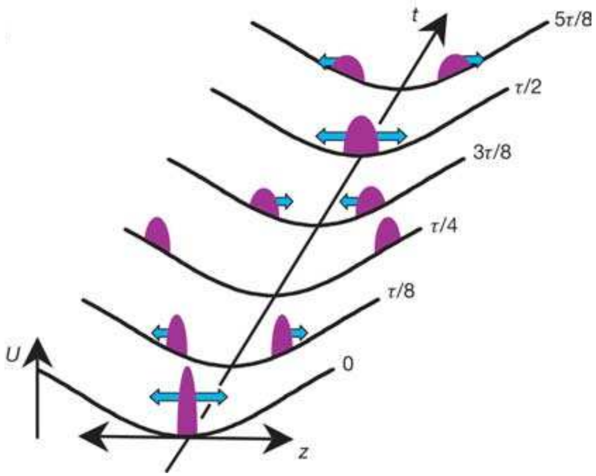
Kinoshita, Wenger, Weiss '06

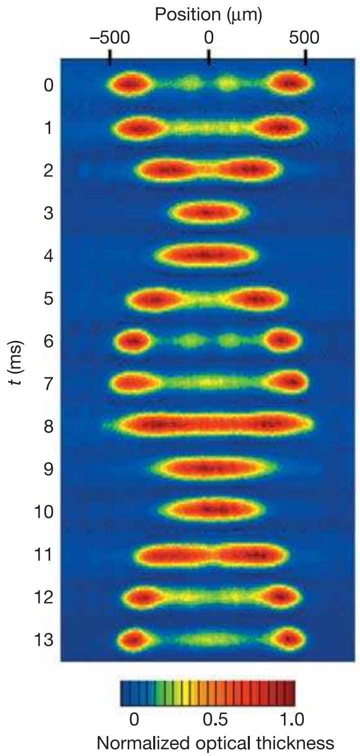
$\langle \hat{b}_k^\dagger \hat{b}_k \rangle$ reaches stationary, but not thermal state

momentum distribution

for $t \leq 13\ ms$

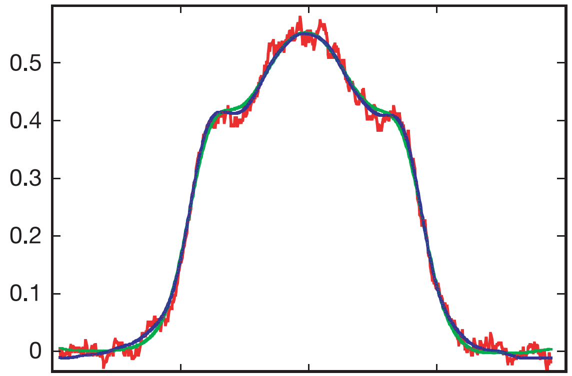






stationary momentum distribution

for $t \gtrsim 200\ ms$



(thermal state: Gaussian)

lack of thermalization
due to (near-)integrability

Integrable vs. nonintegrable systems

Integrable systems: $\hat{H}_{\text{eff}} = \sum_{\alpha=1}^{L} \epsilon_\alpha \hat{n}_\alpha \;\Rightarrow$ many constants of motion

- much fewer accessible states!
- *Generalized Gibbs ensembles*: $\hat{\rho}_{\text{GGE}} \propto \exp(-\sum_\alpha \lambda_\alpha \hat{n}_\alpha)$
- $\langle \hat{A} \rangle_{t\to\infty} = \langle \hat{A} \rangle_{\text{GGE}}$ for certain $\hat{A}$ and $|\psi(0)\rangle$

Girardeau '69
Rigol et al. '06
Cazalilla '06
Rigol et al.'07
Barthel & Schollwöck '08
Kollar & Eckstein '08
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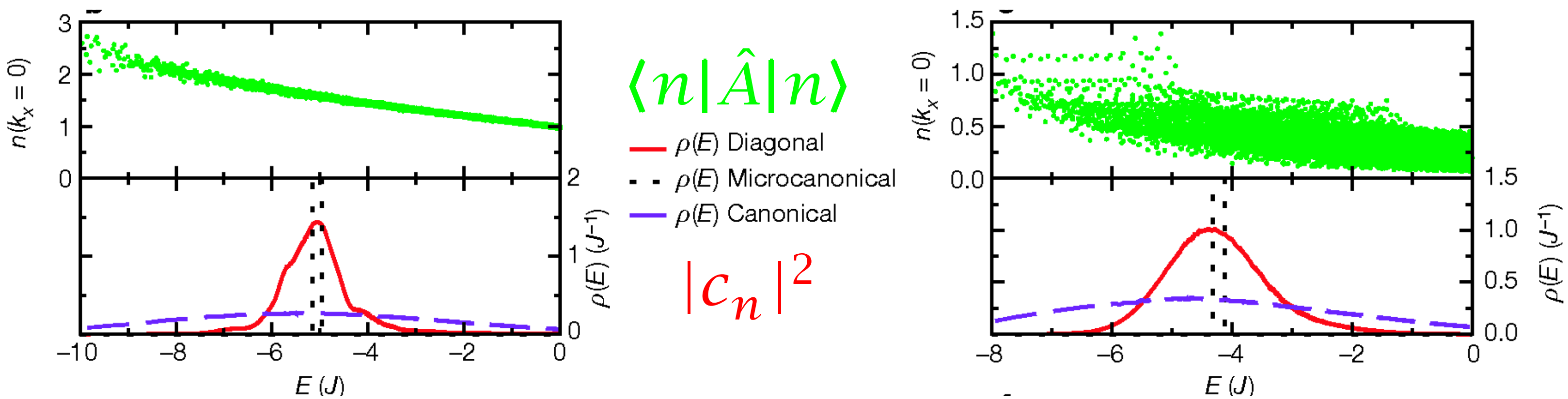
Contributions to long-time average: $\overline{\langle \hat{A} \rangle} = \sum_n |c_n|^2 \langle n|\hat{A}|n\rangle$

Nonintegrable Integrable



$\langle n|\hat{A}|n\rangle \approx \mathcal{A}(E_n)$ $\langle n|\hat{A}|n\rangle \neq \mathcal{A}(E_n)$

Rigol, Dunjko, Olshanii '08

Thermalization in nonintegrable systems

Eigenstate thermalization hypothesis:

Srednicki '95,'99
Rigol, Dunjko, Olshanii '08

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- $|c_n|^2$ is peaked at $E_n = E = \langle \hat{H} \rangle$
- Hypothesis: $\langle n|\hat{A}|n\rangle \approx \mathcal{A}(E_n)$ depends only on E_n

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$$\Rightarrow \quad \langle \hat{A} \rangle_{\text{mic}} = \frac{\sum\limits_{\substack{n \\ E-\delta E \le E_n \le E}} \langle n|\hat{A}|n\rangle}{\sum\limits_{\substack{n \\ E-\delta E \le E_n \le E}} 1} = \mathcal{A}(E) + \mathcal{O}(\delta E) \simeq \overline{\langle \hat{A} \rangle} \quad ✔$$

$\langle \hat{A} \rangle$ thermalizes!

- Hypothesis verified numerically, related to typicality/ergodicity

3. Correlated electrons

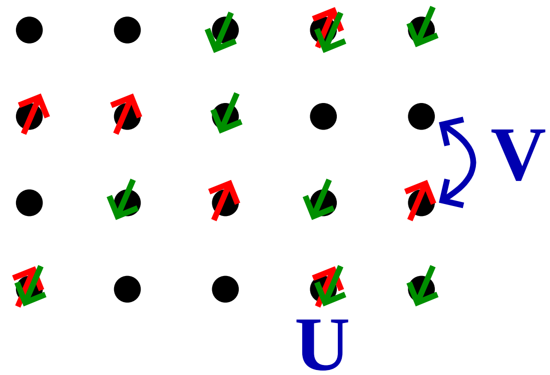
- Hubbard model
- Sudden interaction quench
- Pump-probe spectroscopy

Hubbard model

Single-band Hubbard model:

Gutzwiller '63; Kanamori '63; Hubbard '63

$$H = \underbrace{\sum_{ij\sigma} V_{ij}\, \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}}_{= \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}}\, \hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma} \text{ band structure}} + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$



$\Rightarrow$ Mott metal-insulator transition at $U = U_c \sim \mathcal{O}(\text{bandwidth})$

Mott '49

Hubbard model

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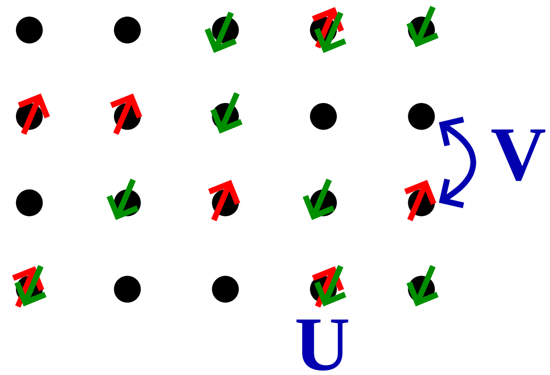

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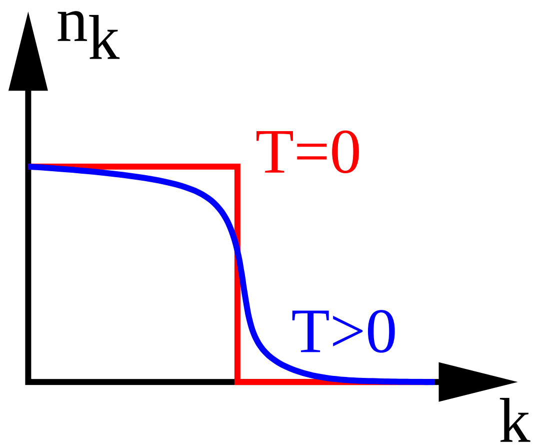
Mott ’49

Fermi liquid: quasiparticle excitations

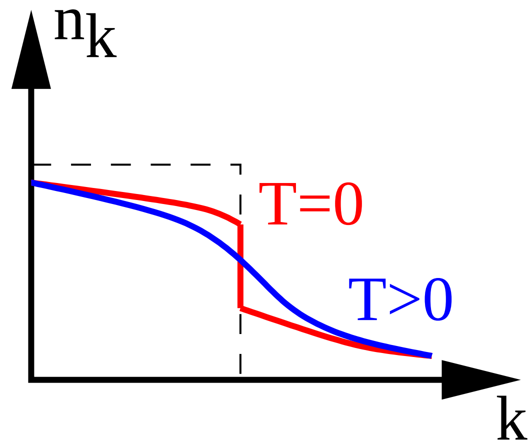
Landau ’56

$U = 0$



Fermi gas

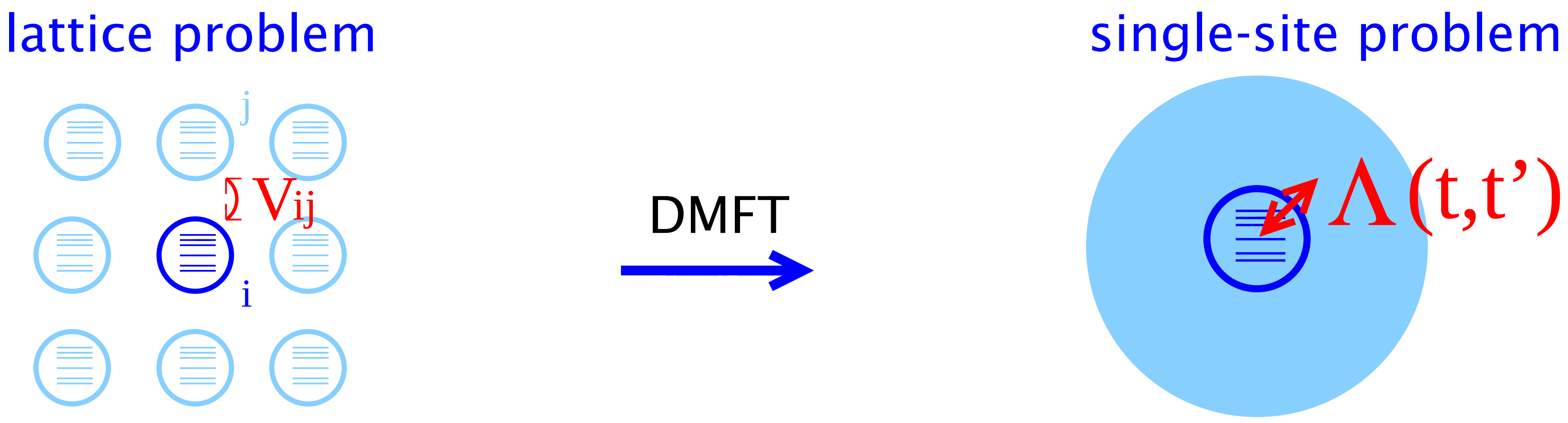
$0 < U < U_c$



Fermi liquid

Dynamical mean-field theory for nonequilibrium

DMFT in equilibrium: "integrate out the lattice"



- Exact for dimension $d = \infty$ — Metzner & Vollhardt '89, Georges et al. RMP '96
- Mapped onto single-site problem + self-consistency — Brandt & Mielsch '89, Georges & Kotliar '92
- Conserving approximation; no lattice finite-size effects

DMFT for nonequilibrium:

Schmidt & Monien '02
Turkowski & Freericks '05
Freericks, Turkowski & Zlatić '06
Eckstein & Kollar '08
Tsuji, Oka & Aoki '08
...

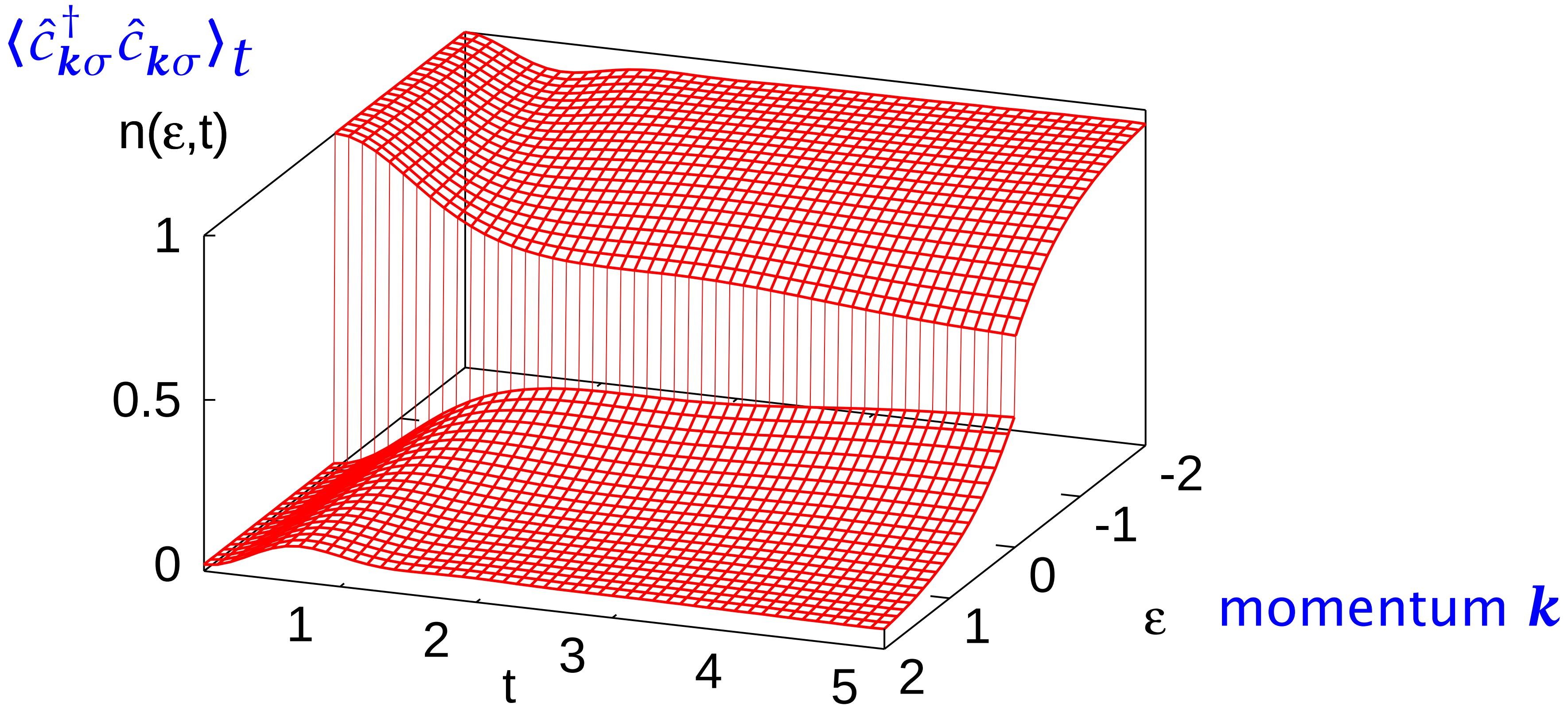
- Similar, but $G(t,t')$ instead of $G(t-t')$

Interaction quench in the Hubbard model

Hubbard model: Bandwidth = 4V, density $n = 1$, U_c=4.8V, T_c=0.05V

Quench from $U = 0$ to $U = 2V$:

Eckstein, Kollar, Werner '09, '10



Slow relaxation: *Prethermalization plateaus*
due to vicinity of free system ($U = 0$)

Moeckel & Kehrein '08
Uhrig '09

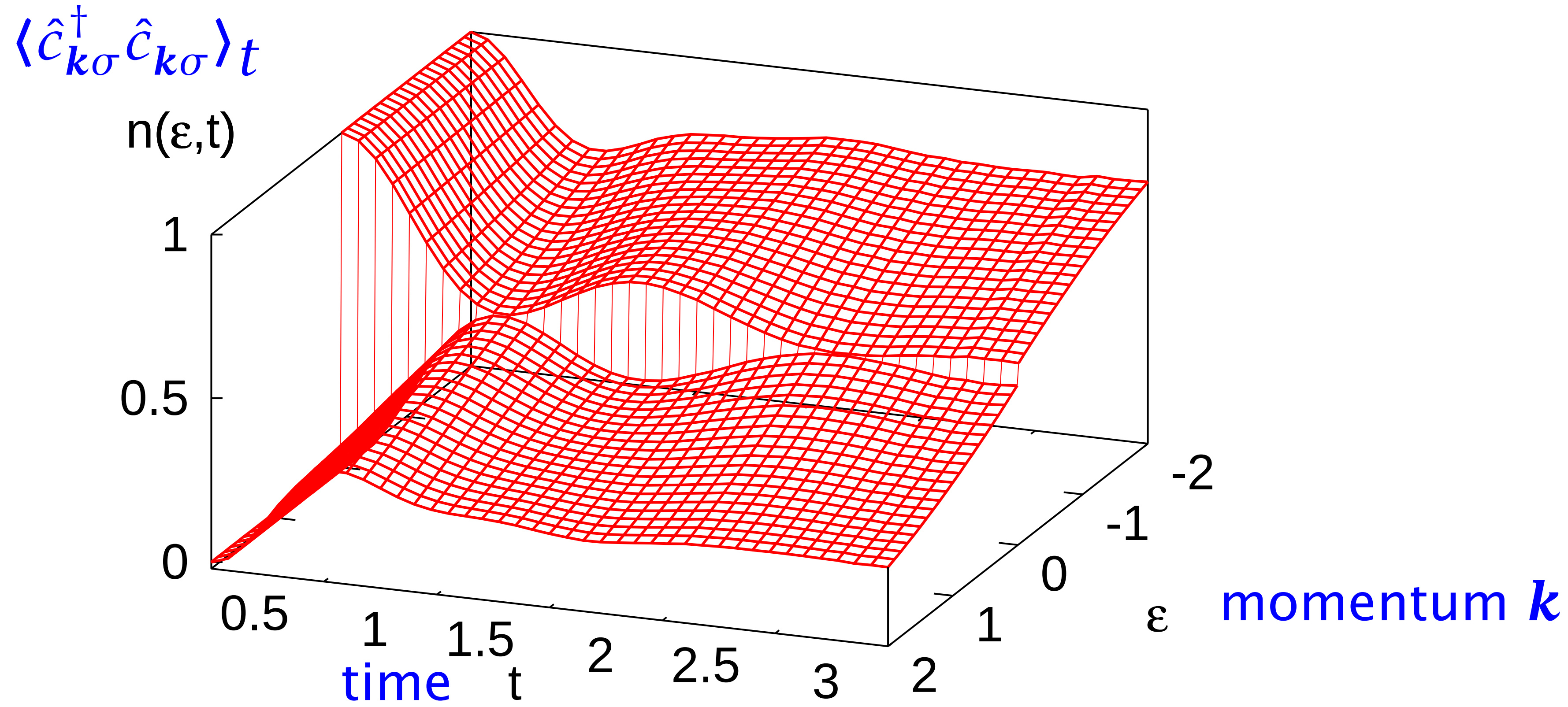
⇒ plateaus are also predicted by perturbed GGEs Kollar, Wolf, Eckstein '11

Interaction quench in the Hubbard model

Hubbard model: Bandwidth = 4V, density $n = 1$, U_c=4.8V, T_c=0.05V

Quench from $U = 0$ to $U = 5V$:

Eckstein, Kollar, Werner '09, '10



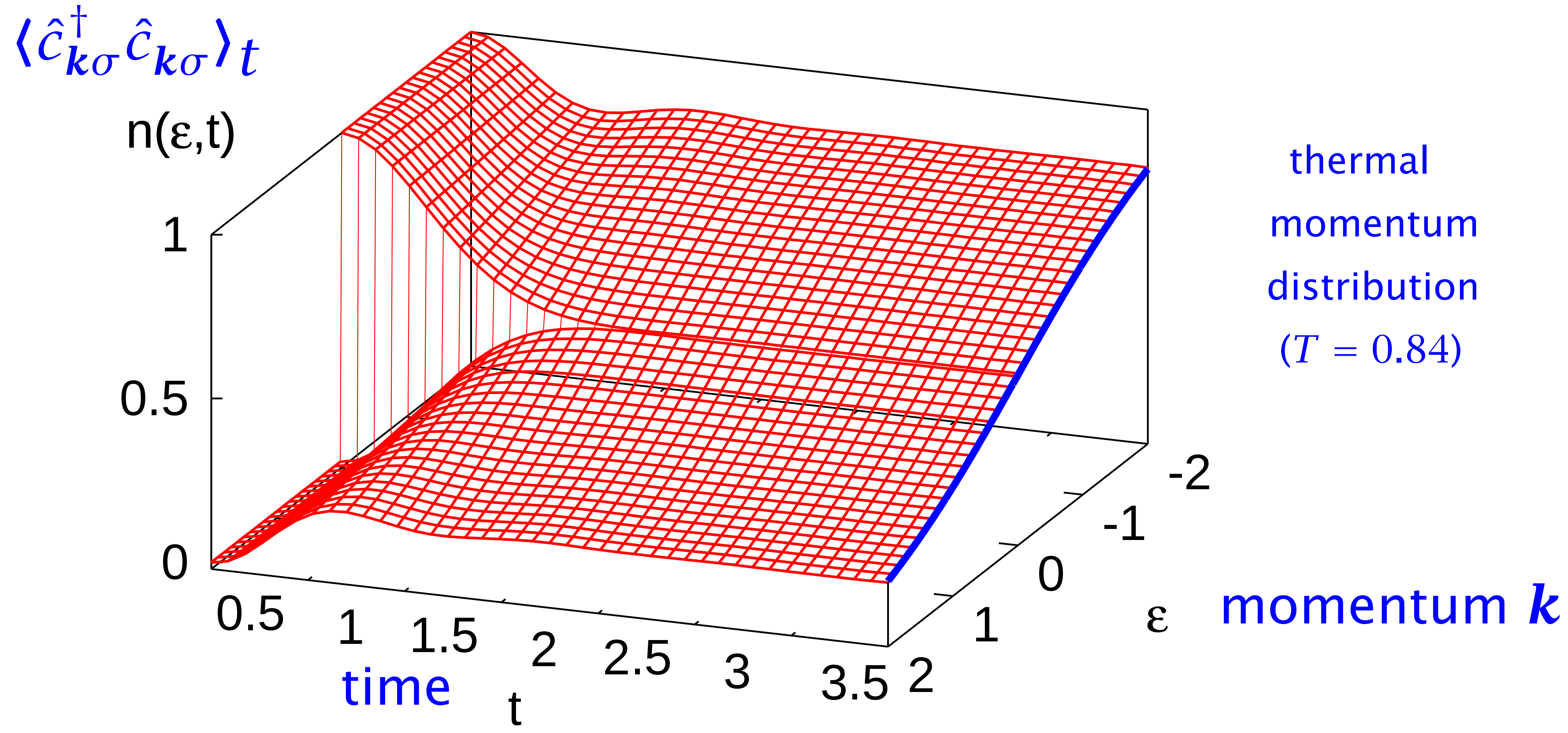
Persisting *collapse-and-revival* oscillations
due to vicinity of atomic limit ($U = \infty$)

Interaction quench in the Hubbard model

Hubbard model: Bandwidth = 4V, density $n = 1$, U_c=4.8V, T_c=0.05V

Quench from $U = 0$ to $U = 3.3V$:

Eckstein, Kollar, Werner '09, '10



Fast thermalization at intermediate U:

both prethermalization and oscillations disappear at $U_c^{\text{dyn}} \approx 3.2V$

Different regimes of interaction strength

$U = 0$
free particles
no thermalization

intermediate U
rapid thermalization
'dynamic criticality'

$U = \infty$
atomic limit
no thermalization

Rigol et al '07
Cazalilla '06
...

Barmettler et al '09
Schiró, Fabrizio '10
Gambassi & Calabrese '10

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Sensarma et al '10
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Thermalization delayed near integrable points
due to approximate constants of motion

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Thermalization delayed near integrable points
due to approximate constants of motion

Possible explanations of dynamical critical points:

- Variational wave functions: — Schiró, Fabrizio '11

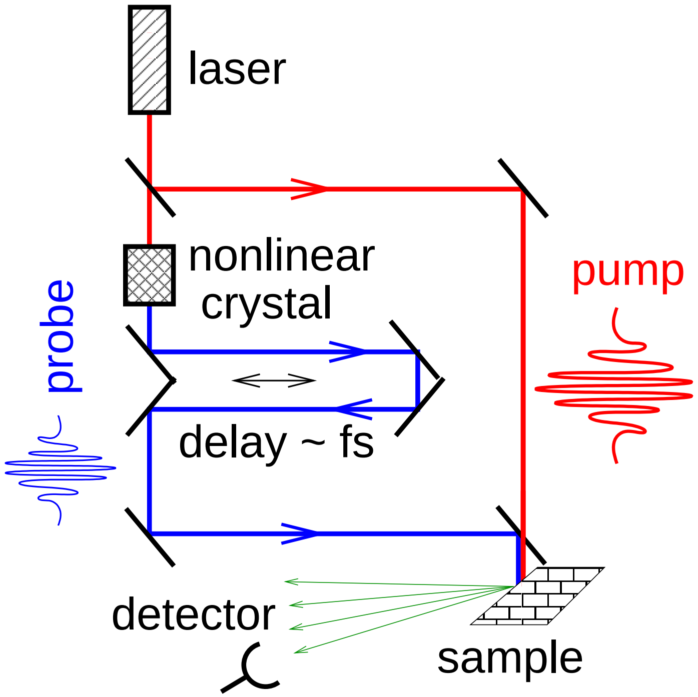
  dynamics change qualitatively at U_c (here $U_c \approx$ 3.4V)

- Dynamical phase transitions: — Heyl, Polkovnikov, Kehrein '12

  cusps develop in $\langle\psi(0)|e^{-i\hat{H}t}|\psi(0)\rangle$ for quench across QCP

Pump-probe spectroscopy

The pump-probe setup:



- pump laser pulse:

  puts system into
  a nonequilibrium state

- probe laser pulse:

  looks at response of system
  after delay time t_d

- Time-resolved photoemission spectroscopy / optical spectroscopy

  analyze emitted electrons / transmitted light

- Time-resolved x-ray diffraction / electron diffraction

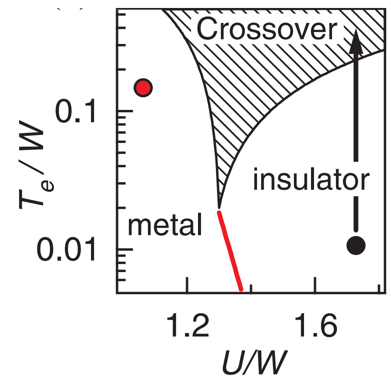
  determine structural dynamics

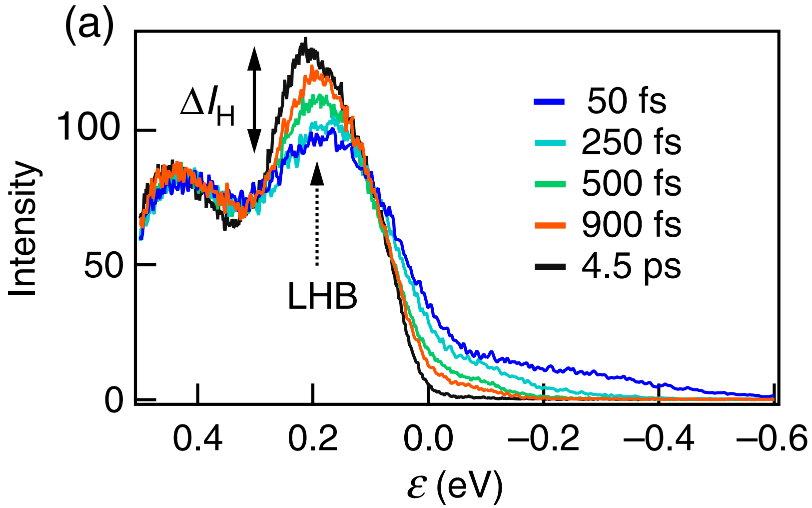
Ex.: Photoemission spectroscopy on $1T$-TaS_2

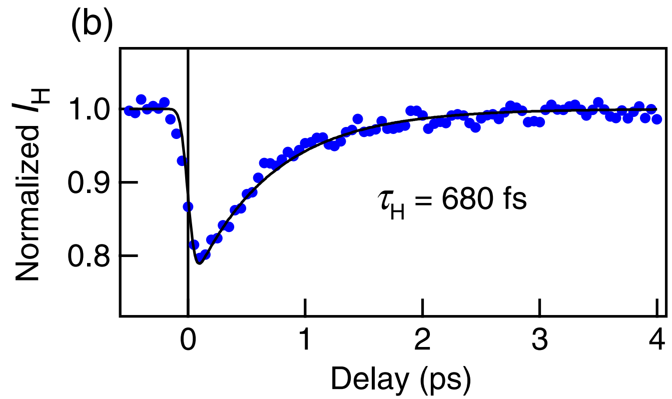
Photoexcitation of a Mott/CDW insulator:

Perfetti, Loukakos, Lisowski, Bovensiepen, Berger, Biermann, Cornaglia, Georges, Wolf '06; '08

50-fs pump pulse (1.5 eV), 80-fs probe pulse (6 eV)







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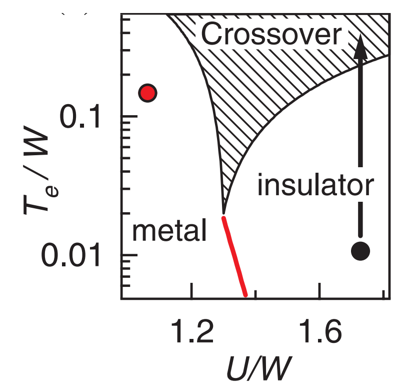
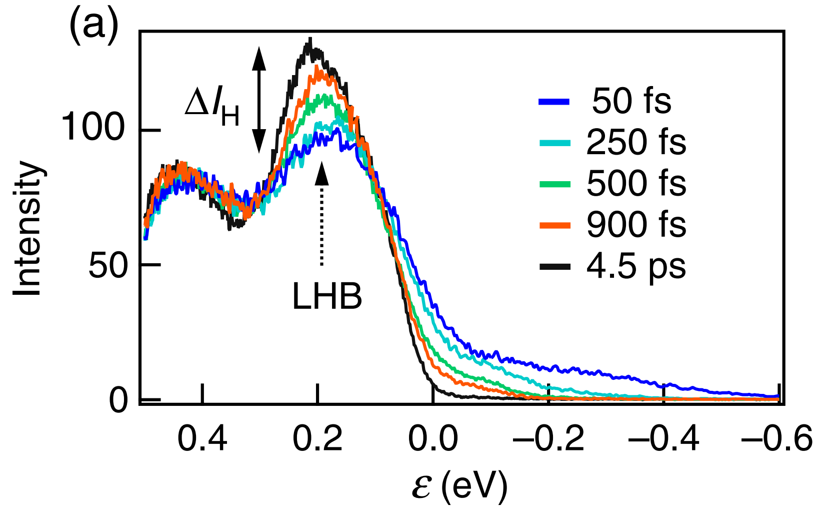
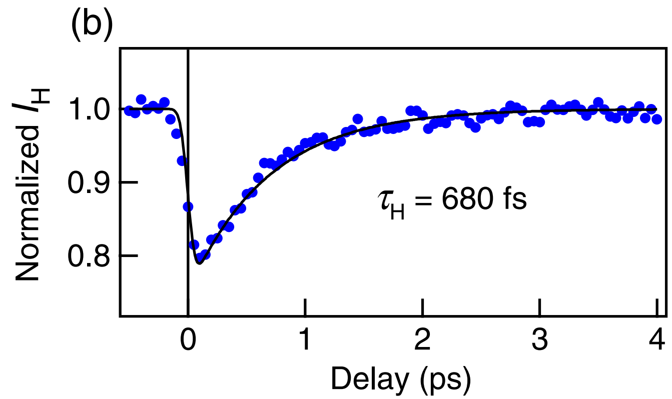


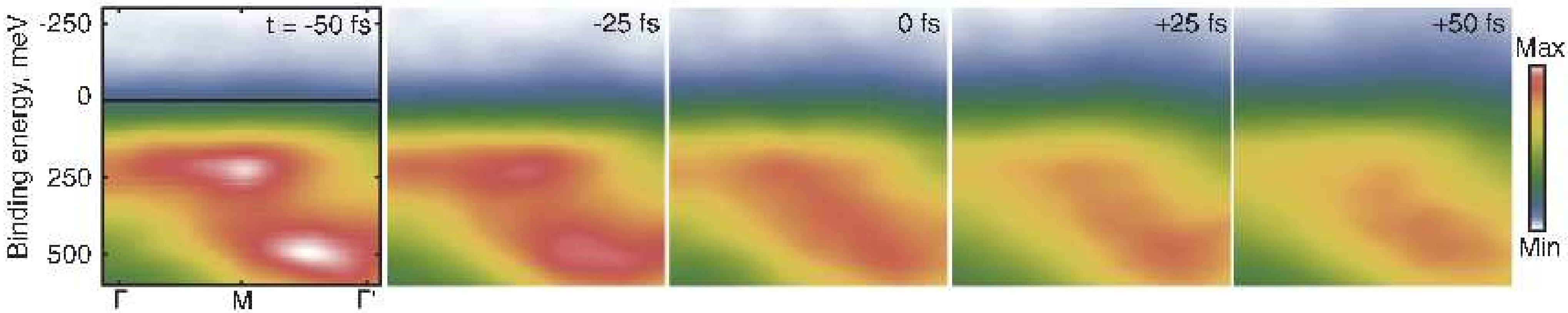




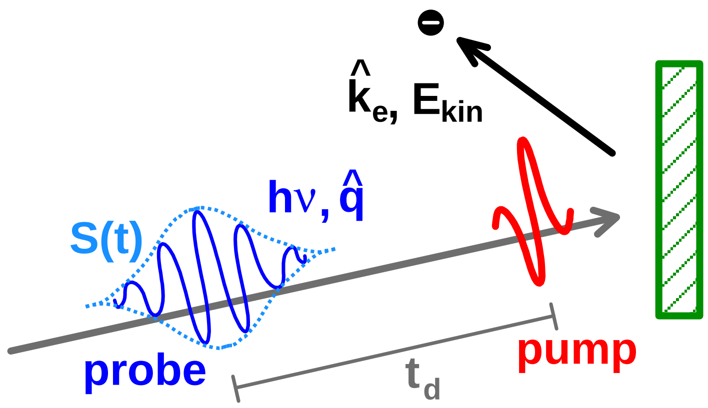
Closing of CDW gaps below Fermi energy:

Petersen, Kaiser, Dean, Simoncig, Liu, Cavalieri, Cacho, Turcu, Springate, Frassetto, Poletto, Dhesi, Berger, Cavalleri '11

30-fs pump pulse (1.2 eV), 30-fs probe pule (20.4 eV)



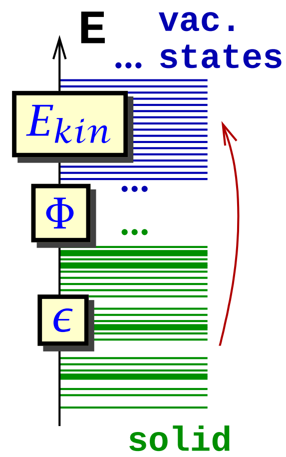
Photoemission: "Sudden Approximation"



Intensity of photoelectrons:

$$I(\hat{\boldsymbol{k}}_e, E_{\text{kin}}; \boldsymbol{q}, t_d) = \frac{dN(\hat{\boldsymbol{k}}_e, E_{\text{kin}}; \boldsymbol{q}, t_d)}{d\Omega_{\hat{\boldsymbol{k}}_e} dE_{\text{kin}}}$$

Sudden approximation: Coherent transfer to vacuum state



Neglect matrix element effects:

$$I(\hat{\boldsymbol{k}}_e, E_{\text{kin}}; \boldsymbol{q}, t_d) \propto \sum_{\boldsymbol{k}\sigma} \delta_{\boldsymbol{k}_{||}+\boldsymbol{q}_{||}, \boldsymbol{k}_{e||}} \, \mathrm{I}_{\boldsymbol{k}\sigma}(E_{\text{kin}} - E_{\text{photon}} - \Phi; t_d)$$

$$\mathrm{I}_{\boldsymbol{k}\sigma}(\omega; t_d) = -i \int dt \int dt' \underbrace{S(t)}_{\text{pulse envelope}} S(t') \, e^{i\omega(t'-t)} \, G^{<}_{\boldsymbol{k}\sigma}(t+t_d, t'+t_d)$$

Freericks, Krishnamurthy, Pruschke '08

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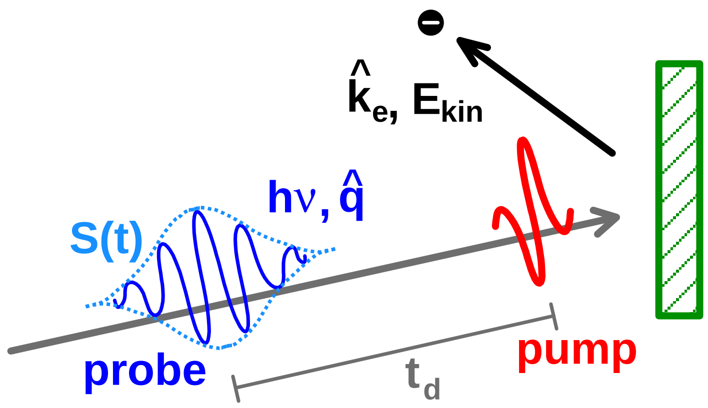

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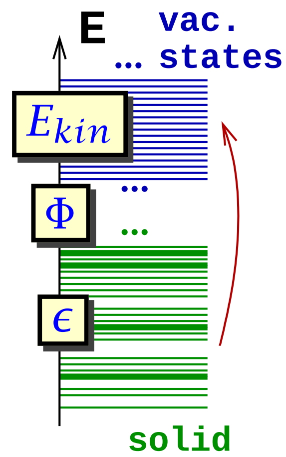

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Freericks, Krishnamurthy, Pruschke ’08

Limited resolution:

energy uncertainty $\delta E \approx \hbar/\delta$ $\Leftrightarrow$ pulse duration δ

Spectrum of an excited Mott insulator

Mott-Isolator (Falicov-Kimball model, $V_{ij\downarrow} = 0$, $U = 10V$)

pumped into metallic state ($U = 1V$):

Eckstein & Kollar '08

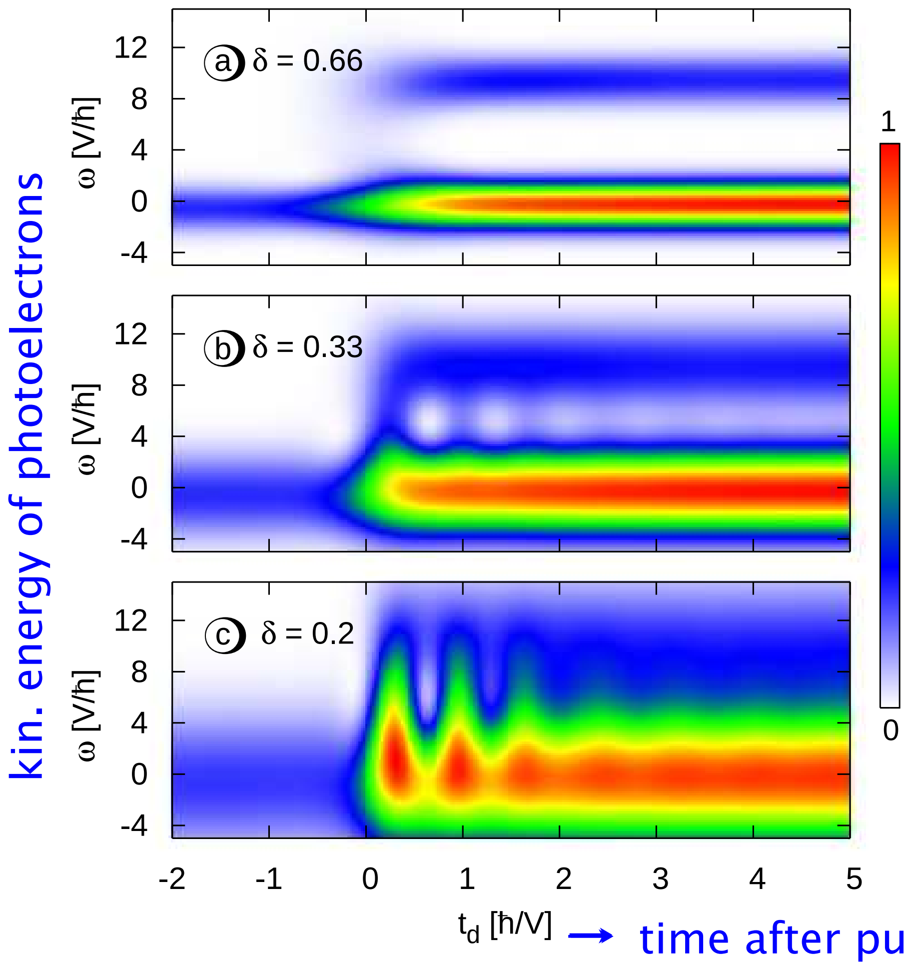
long pulse

poor time resolution

medium pulse

short pulse

good time resolution



upper Hubbard band

good energy resolution

lower Hubbard band

good time and

energy resolution

poor energy resolution

→ time after pump pulse, $\frac{\hbar}{V} \approx \mathcal{O}(10\ \text{fs})$

⇒ collapse and revival oscillations in Mott gap

Summary

Thermalization in isolated many-body systems

- Thermalization delayed for very small/large interaction
- Fast thermalization for intermediate interaction possible

Pump-probe spectroscopy on correlated systems:

- Photodoping: spectral weight transfer
- Photoemission: energy-time limitations

More on nonequilibrium:

- Exp.: C.Giannetti, D.Fausti, F.Novelli, M.Mitrano, R.Singla, . . .
- Theory: M.Schiró, A.Amaricci, M.Nuss, . . .