### Correlated Electron Dynamics and Nonequilibrium Dynamical Mean-Field Theory

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#### Outline

- 1. Quantum many-body systems in nonequilibrium
- 2. Nonequilibrium Green functions
- 3. Nonequilibrium Dynamical Mean-Field Theory
- 4. Interaction quench in the Hubbard model

Review on Nonequilibrium DMFT:

H. Aoki, N. Tsuji, M. Eckstein, M. Kollar, T. Oka, and P. Werner, Rev. Mod. Phys. **86**, 779 (2014)

## 1. Quantum many-body systems in nonequilibrium

How to put a quantum many-body system out of equilibrium and observe its relaxation

#### **Time-resolved pump-probe spectroscopy**

- > Pump-probe setup:
  - Pump laser pulse: puts system into nonequilibrium
  - Probe laser pulse: looks at system after delay time
- > Various time-resolved probes:
  - t.-r. ARPES: photoemitted electrons
  - t.-r. optical spectroscopy: transmitted/reflected light
  - t.-r. X-ray or electron **diffraction**: snapshots of atomic positions



#### Melting of a Charge Density Wave in TbTe<sub>3</sub>

Schmitt, Kirchmann, Bovensiepen, Moore, Rettig, Krenz, Chu, Ru, Perfetti, Lu, Wolf, Fisher, Shen, Science '08

#### > trARPES on TbTe<sub>3</sub>: 1.5-eV 50-fs pump pulse, 6-eV 90-fs probe pulse

## > photodoping → closing of CDW gap → electron thermalization → vibrational excitation

Fig. 3. (A) Detail of the FS plot in Fig. 1A' with indicated positions (white circles) of time-resolved data shown in (B) to (D) for fixed k as a function of time delay. Indicated cut position (red line) of photoelectron intensity is shown as a function of energy, and position [(E) to (I)] for a momentum scan is shown as a function of time delays. All data were collected at 100 K and  $F = 2 \text{ m}/\text{cm}^2$ .  $k_{\rm E}$  is marked in (E) to (I) (red dot). Error bars indicate the distance to the neighboring sample points, which is a good estimate for the error of kE.



#### **Quenched Bose condensate**

Abrupt increase of interaction of <sup>87</sup>Rb atoms:

Greiner, Mandel, Hänsch, Bloch '02

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

Relaxation

2,000

t (us)

3,000



#### Time scales in nonequilibrium dynamics

- Time scales in pump-probe experiments
  - Excitation due to pump pulse
  - Relaxation due to electron scattering
  - Energy transfer to ion lattice
- > Time scales in cold-atom experiments
  - Switching times
  - Relaxation times



- ~ 10...100 fs
  - ~ 0...1000 fs
    - ~ 1...10 ps

- ~ 1...1000 ms
- ~ 1...1000 ms

→ study relaxation of **isolated** quantum systems first

How can an isolated system relax to an equilibrium state?

#### Time evolution of isolated systems

- > Schrödinger equation:  $i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle$
- > Quantum quench: Prepare  $|\psi_0\rangle$  and switch to H at t = 0
  - Time evolution for  $t \ge 0$ :  $|\psi(t)\rangle = e^{-iHt} |\psi_0\rangle$
  - Energy after quench:  $E = \langle \psi(t) | H | \psi(t) \rangle = \langle \psi_0 | H | \psi_0 \rangle$
  - Expectation values:  $\langle A \rangle_t = \langle \psi(t) | A | \psi(t) \rangle$
- Thermalization:

$$\langle A \rangle_t \xrightarrow{t \to \infty} \langle A \rangle_{\text{therm}} = \frac{\text{Tr} A e^{-\beta H}}{\text{Tr} e^{-\beta H}}$$
?  
with effective  $\beta$  from  $\langle H \rangle_{\text{therm}} = E$ 

#### The thermal state:

## Putting a system into equilibrium by coupling it to a *heat bath*

#### Gibbs ensemble for system + bath

Maxwell 1866, Boltzmann 1872, Gibbs 1878

> System + heat bath: 
$$E_{tot} = E_s + E_b = const$$
  
> Boltzmann relation:  $S = \ln \Omega$ ,  $\beta = \frac{1}{T} = \frac{\partial S}{\partial E}$   
> Obtain # of system states from bath:  
 $\ln \Omega_b (E_{tot} - E_s) = \ln \Omega_b (E_{tot}) + \beta (E_{tot} - E_s) + ...$  bath  $(E_b)$ 

$$P(E_s) \propto \Omega_b(E_{\text{tot}} - E_s) \propto \exp(-\beta E_s)$$

- > System in thermal state when in equilibrium with bath
- Microcanonical ensemble gives same results (in thermodyn. limit)

An equivalent *equilibrium* formulation:

## **Ensembles** containing microstates with same a priori probabilities

#### **Reformulation with fundamental postulate**

#### Prediction for equilibrium state:

• Fundamental postulate:

All accessible states equally probable  $\Leftrightarrow S = -\text{Tr}[\rho \ln \rho] = \max$ 

- $A_i$  conserved  $\Rightarrow$  fix  $\text{Tr}[\rho_{\text{ensemble}}A_i] = \langle A_i \rangle_{t=0}$ 
  - $\Rightarrow \rho_{\text{ensemble}} \propto \exp(-\sum_i \lambda_i A_i)$

Boltzmann-Gibbs ensemble

von Neumann 1927, Jaynes 1957, ... Balian 1991

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Integrable systems:  $H_{\text{eff}} = \sum_{\alpha=1}^{L} \epsilon_{\alpha} n_{\alpha} \Rightarrow \text{ many constants of motion}_{\text{Jaynes '57}}$ 

• Generalized Gibbs ensembles:  $\rho_{GGE} \propto \exp(-\sum_{\alpha} \lambda_{\alpha} n_{\alpha})$ 

Jaynes '57 Girardeau '69 Rigol et al. '06 Cazalilla '06 Rigol et al.'07

•  $\langle A \rangle_{t \to \infty} = \langle A \rangle_{GGE}$  for simple observables and initial states Kollar & Eckstein '08 Barthel & Schollwöck '08 Why does a many-body system relax to the *thermal* state?

#### **Eigenstate Thermalization Hypothesis (ETH)**

 $\langle n|A|n \rangle \approx \mathcal{A}(E_n) + \text{smaller}, n\text{-dep. terms}$ 

Deutsch PRA '91, Srednicki PRE '94 Rigol, Dunjko, Olshanii, Nature '08

#### Nonintegrable

Integrable



### **Eigenstate Thermalization Hypothesis (ETH)**

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Deutsch PRA '91, Srednicki PRE '94 Rigol, Dunjko, Olshanii, Nature '08

> Energy dependence is that of microcanonical ensemble:

 $A_{\min}(E) = \mathsf{Tr}[\rho_{\min}(E_n) A]$ 

 $= \frac{1}{Z_{\text{mic}}} \sum_{E - \delta E < E_n < E} \langle n | A | n \rangle = \mathcal{A}(E) + \text{smaller terms}$ 

> Long-time average tends to thermal value:

 $\overline{A(t)} = \overline{\langle \psi(t) | A | \psi(t) \rangle}$  $= \sum_{n} \underbrace{\langle n | A | n \rangle}_{\approx A_{\text{mic}}(E_n)} \underbrace{|\langle \psi(0) | n \rangle|^2}_{\text{peaked at } E} \approx A_{\text{mic}}(E)$ 

ETH sufficient for thermalization!

• <u>Nonequilibrium:</u>

Thermalization is due to dependence of expectation values *only on energy* 

• Equilibrium:

Thermal Gibbs state is due to immersion in *structureless heat bath* 

### 2. Nonequilibrium Green functions

#### **Quantum time evolution**

➤ Hamiltonian:  $\mathcal{H}(t) = H(t) - \mu N(t)$ > Density matrix:  $\rho(0) = \frac{1}{Z}e^{-\beta \mathcal{H}(0)} = \frac{1}{Z}\sum_{n} e^{-\beta E_n} |n\rangle \langle n|$ > Propagator:  $\rho(t) = U(t,0) \rho(0) U(0,t)$  $\frac{d}{dt}U(t,t') = -i\mathcal{H}(t)U(t,t')$  $U(t,t') = \begin{cases} \operatorname{Texp}\left(-i\int_{t'}^{t} d\bar{t} \,\mathcal{H}(\bar{t})\right) & \text{for } t > t' \\ \bar{\operatorname{Texp}}\left(-i\int_{t'}^{t} d\bar{t} \,\mathcal{H}(\bar{t})\right) & \text{for } t < t' \end{cases}$ 

> Expectation value of observable A:

$$\langle A \rangle_t = \operatorname{Tr} \Big[ \rho(t) A \Big] = \frac{1}{Z} \operatorname{Tr} \Big[ U(-i\beta, 0) U(0, t) A U(t, 0) \Big]$$

#### Kadanoff-Baym formalism with time contour

> Expectation value of observable *A*:

 $\langle A \rangle_t = \frac{1}{Z} \operatorname{Tr}[U(-i\beta, 0)U(0, t) A U(t, 0)]$ 

> Represent as integral over time contour  $C_1 + C_2 + C_3$ :



Insert formal time dependence into Schrödinger operator A:

$$\langle A \rangle_t = \frac{\operatorname{Tr} \operatorname{T}_C A(t) \, \exp[-i \int_C d\bar{t} \, \mathcal{H}(\bar{t})]}{\operatorname{Tr} \operatorname{T}_C \, \exp[-i \int_C d\bar{t} \, \mathcal{H}(\bar{t})]}$$

## **Contour calculus**

С

#### **Contour Green functions**



> Green function with 2 time arguments on branches  $C_1$  or  $C_2$  or  $C_3$ :  $G(t,t') = -i\langle c(t)c^{\dagger}(t') \rangle = -\frac{i}{Z} \operatorname{Tr} \left[ \operatorname{T}_C \left\{ \exp(S)c(t)c^{\dagger}(t') \right\} \right]$ 

> Let  $G_{ab}(t, t')$  have time arguments on branches a, b = 1, 2, 3

> Symmetries:  $G_{11}(t,t') = G_{12}(t,t')$  for  $t \le t'$  etc.

 $G_{13}(t,\tau') = G_{23}(t,\tau'),$ 

#### **Keldysh Green functions**



#### Noninteracting case and Self-energy

- Free electrons:  $\mathcal{H}_{0}(t) = \sum_{k} [\epsilon_{k}(t) \mu] c_{k}^{\dagger} c_{k}$   $\mathcal{H}_{0}(t) = -i \langle c_{k}(t) c_{k}^{\dagger}(t') \rangle$   $\mathcal{H}_{0}(t) = -i \langle c_{k}(t) c_{k}^{\dagger}(t') \rangle$
- > EOM:  $[i\partial_t + \mu \epsilon_k(t)]G_{0,k}(t,t') = \delta_C(t,t')$
- > Def. of inverse GF:  $G_{0,k}^{-1}(t,t') = [i\partial_t + \mu \epsilon_k(t)]\delta_C(t,t')$
- > Solution:  $G_{0,k}(t,t') = -i \Big[ \theta_C(t,t') f(\epsilon_k(0) \mu) \Big] e^{-i \int_{t'}^t d\bar{t} \left[ \epsilon_k(\bar{t}) \mu \right]}$

- > Self-energy  $\Sigma$ : 1-particle irreducible amputated Feynman diagrams
- > Dyson equation for full GF:  $G = G_0 + G_0 * \Sigma * G$
- > Def. of inverse of full GF:  $G^{-1} = G_0^{-1} \Sigma$

# **3.** Nonequilibrium Dynamical Mean-Field Theory

### The DMFT philosophy

> Start from limit of infinite lattice dimension  $d \rightarrow \infty$ 

> Scale the kinetic energy, i.e., NN hopping amplitude  $t_{ij} \propto \frac{1}{\sqrt{d}}$ 

Map lattice problem onto

*dynamic single-site problem* with *self-consistency condition* 

[e.g. single-impurity Anderson model (SIAM)]

and solve numerically

- Extend to e.g.
  - finite *d* using clusters, dual fermions, dyn. vertex approx., ...
  - magnetic phases, phonons, ...
  - input from density functional theory, ...

#### The cavity method I

 $S = S_0 + \Delta S + S^{(0)},$ 

- > Time-dep. Hubbard model:  $H(t) = \sum_{ij\sigma} t_{ij}(t) c_{i\sigma}^{\dagger} c_{j\sigma} + U(t) \sum_{i} n_{i\uparrow} n_{i\downarrow}$
- > Pick out single site i=0 from lattice action:

Equil.: Georges et al. RMP 1996 Noneq.: Gramsch et al PRB 2014

$$S_{0} = -i \int_{C} dt \left[ U(t) n_{0\uparrow}(t) n_{0\downarrow}(t) - \mu \sum_{\sigma} n_{0\sigma}(t) \right],$$
  
$$\Delta S = -i \int_{C} dt \left[ \sum_{i \neq 0, \sigma} t_{i0}^{\sigma}(t) c_{i\sigma}^{\dagger}(t) c_{0\sigma}(t) + \text{h.c.} \right],$$

$$S^{(0)} = -i \int_C dt \,\mathcal{H}^{(0)}(t)$$

> Integrate out rest of lattice:  $S_{\text{eff}} = S_0 + \tilde{S}$ 

$$Z = \operatorname{Tr} \left[ \operatorname{T}_{C} \left\{ \exp(S_{0} + \Delta S + S^{(0)}) \right\} \right]$$
$$= \operatorname{Tr}_{0} \left[ \operatorname{T}_{C} \left\{ \exp(S_{0}) \operatorname{Tr}_{rest} \left( \exp(\Delta S + S^{(0)}) \right) \right\} \right]$$
$$= \operatorname{Tr}_{0} \left[ \operatorname{T}_{C} \left\{ \exp(S_{0} + \tilde{S}) \right\} \right] Z_{S^{(0)}}$$

#### The cavity method II

> Result of integration over lattice sites  $i \neq 0$ :

$$\tilde{S} = -i \sum_{n=1}^{\infty} \sum_{\sigma_1 \dots \sigma'_n} \int_C dt_1 \dots \int_C dt'_n \Lambda_{\sigma_1 \dots \sigma'_n}(t_1, \dots, t'_n) c^{\dagger}_{0\sigma_1}(t_1) \dots c_{0\sigma'_n}(t'_n)$$

> Hybridization functions:

$$\Lambda_{\sigma_1...\sigma'_n}(t_1,...,t'_n) = \frac{(-i)^{n-1}}{n!^2} \sum_{i_1,...,j_n} t_{0i_1}(t_1) \cdots t_{j_n0}(t'_n) \ G^{(0),c}_{i_1\sigma_1,...,j_n\sigma'_n}(t_1,...,t'_n)$$
cavity Green function

> Power counting for  $d \rightarrow \infty$ :

cavity Green function (site *i=0* removed)

$$\begin{split} \Lambda_{\sigma_1\dots\sigma'_n}(t_1,\dots,t'_n) &\propto \sum_{\substack{i_1,\dots,j_n\\ \propto d^{2n}}} \underbrace{t_{0i_1}(t_1)\dots t_{j_n0}(t'_n)}_{\propto(\sqrt{d})^{-2n}} \underbrace{\mathcal{G}_{(i_1\sigma_1),\dots,(j_n\sigma'_n)}^{(0),\mathsf{c}}(t_1,\dots,t'_n)}_{\propto(\sqrt{d})^{-2(2n-1)}} \end{split}$$

> Only one-particle Green functions (n=1) remain in hybridization!

#### The DMFT action

Action for the cavity site *i=0*:

$$S_{\text{eff}} = -i \int_{C} dt \left[ U(t) n_{\uparrow}(t) n_{\downarrow}(t) - \mu \sum_{\sigma} n_{\sigma}(t) \right]$$
$$- i \int_{C} dt_{1} \int_{C} dt_{2} \sum_{\sigma} \Lambda_{\sigma}(t_{1}, t_{2}) c_{\sigma}^{\dagger}(t_{1}) c_{\sigma}(t_{2})$$

> Hybridization function:

$$\Lambda_{\sigma}(t,t') = \sum_{i,j} t_{0i}(t) G_{ij\sigma}^{(0),c}(t,t') t_{j0}(t')$$

> Self-consistency for NN hopping on the Bethe lattice  $t_{ij} = \frac{v}{\sqrt{z}}$ 

 $\Lambda_{\sigma}(t,t') = v(t)G_{\sigma}(t,t')v(t')$ 

#### Local self-energy and self-consistency

> Lattice and impurity Green function:

 $G_{ij}(t,t') = -i \langle c_i(t) c_j^{\dagger}(t') \rangle_S$   $G(t,t') = G_{00}(t,t')$ 

> Lattice and impurity self-energies:

$$\begin{aligned} (G_{\text{lat}}^{-1})_{ij}(t,t') &= [\delta_{ij}(i\partial_t + \mu) - t_{ij}(t)]\delta_C(t,t') - (\Sigma_{\text{lat}})_{ij}(t,t') \\ G^{-1}(t,t') &= (i\partial_t + \mu)\delta_C(t,t') - \Lambda(t,t') - \Sigma(t,t') \end{aligned}$$

> For DMFT action:  $(\Sigma_{\text{lat}})_{ij}(t,t') = \delta_{ij}\Sigma(t,t')$  local self-energy!

► Self-consistency conditions: lattice and impurity Dyson equation  $\int_{C} dt_{1} \sum_{l} \left[ \left[ \delta_{il}(i\partial_{t} + \mu) - t_{il}(t) \right] \delta_{C}(t, t_{1}) - \Sigma(t, t_{1}) \right] G_{lj}(t_{1}, t') = \delta_{ij} \delta_{C}(t, t')$   $\int_{C} dt_{1} \left[ (i\partial_{t} + \mu) \delta_{C}(t, t_{1}) - \Lambda(t, t_{1}) - \Sigma(t, t_{1}) \right] G(t_{1}, t') = \delta_{C}(t, t')$ 

#### Solution of DMFT equations by iteration

- > DMFT iteration:
  - start from a hybridization function  $\,\Lambda\,$
  - obtain impurity Green function  $G(t, t') = -i\langle c(t)c^{\dagger}(t') \rangle$
  - obtain self-energy  $\Sigma$  from impurity Dyson equation
  - obtain new local Green function G(t, t') from lattice Dyson eq.
  - obtain new hybridization function  $\Lambda$
- Must solve Volterra-type integro-differential eqs.

see RMP 2014 & references

Can be implemented as time-propagation scheme

#### **Real-time impurity solvers**

- Many-body perturbation theory
  - Weak-coupling perturbation theory
    - [ sample code available as Supp.Mat. for RMP 86, 779 (2014) ]
  - Strong-coupling perturbation theory
- Continuous-time Quantum Monte Carlo
- Hamiltonian-based methods / exact diagonalization
- Falicov-Kimball model

see Lecture Notes for references

#### 4. Interaction quench in the Hubbard model

$$H = \sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U(t) \sum_{i} n_{i\uparrow} n_{i\downarrow}$$
$$= \sum_{k\sigma} \epsilon_{k} c_{k\sigma}^{\dagger} c_{k\sigma}$$

Strong-coupling regime: collaps-and-revival oscillations

#### Hubbard interaction quench: Collapse & revival



Collapse-and-revival oscillations due to vicinity of atomic limit ( $U = \infty$ ) Weak-coupling regime: metastable prethermalized state

#### Hubbard interaction quench: Prethermalization





Slow relaxation: *Prethermalization plateaus* due to vicinity of free system (U = 0) Berges et al. PRL '04 Moeckel & Kehrein PRL '08

#### Hubbard interaction quench from 0 to U

Eckstein et al., PRL '09



#### **Prethermalization regime**



#### Prethermalization in one and two dimensions

> Prethermalization less pronounced in low dimensions

Tsuji, Barmettler, Aoki, Werner, PRB '14

#### *d* = 1, *U* from 0 to 1

#### *d* = 2, *U* from 0 to 2



#### Prethermalization in one and two dimensions

> Prethermalization less pronounced in low dimensions

short-time expansion, Hamerla and Uhrig, PRB '14



perturbative correction does not reach a plateau

#### Intermediate-coupling regime: fast thermalization

#### Hubbard interaction quench: Thermalization

Hubbard model in DMFT: (bandwidth = 4, density n = 1)



Fast thermalization at intermediate Uboth prethermalization and oscillations disappear at  $U_c^{dyn} \approx 3.2$  $U_c^{dyn} \sim 3.4$  well-captured by time-dependent Gutzwiller approximation: Schiro & Fabrizio PRL 2010

## Summary and Outlook

#### **Summary and Outlook**

> Thermalization of correlated systems in nonequilibrium

- Eigenstate thermalization hypothesis:

Thermalization is due to energy eigenstates that contribute only according to their energy

- Thermalization does not occur in integrable systems
- > Nonequilibrium dynamical mean-field theory
  - Controlled approximation for nonequilibrium problems
  - Many applications:
     quenches, pulses, periodic driving, ...
     cluster extensions, ...
     magnetic phases; phonons; bosons; ...