Nonequilibrium Physics of Correlated Electron Materials II:

Theory and Computation

Concepts and Challenges

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Experiments

Steady-state drive system in high-T phase though physical T low

Transient perturbation => long-duration change of state

\[ \text{Ca}_2\text{RuO}_4 \]

\[ \text{VO}_2 \]
This talk:

- Quench
- Open System: path integral
- Numerics
``Quench'' (change Hamiltonian)

\[ t < 0, \quad H = H_0 \quad \text{and} \quad t > 0, \quad H = H_1 \]
``Quench'' (change Hamiltonian)

\[ t < 0, \ H = H_0 \quad t > 0, \ H = H_1 \]

Example

\[
H(h) = -J \sum_{j=1}^{L} \left[ \sigma_j^x \sigma_{j+1}^x + h \sigma_j^z \right]
\]
``Quench'' (change Hamiltonian)

t<0, \ H=H_0 \quad t>0, \ H=H_1

Example

\[ H(h) = -J \sum_{j=1}^{L} \left[ \sigma_j^x \sigma_{j+1}^x + h \sigma_j^z \right] \]

Equilibrium Phase Diagram
``Quench'' (change Hamiltonian)

\[ t < 0, \ H = H_0 \quad t > 0, \ H = H_1 \]

Example

\[
H(h) = -J \sum_{j=1}^{L} \left[ \sigma_j^x \sigma_{j+1}^x + h \sigma_j^z \right]
\]

\[ \langle \sigma_x \rangle \]

Equilibrium Phase Diagram

FM

What happens if suddenly change \( h \)?
How to think about a quench
How to think about a quench

Non-thermal initial condition: at $t=0^+$ the system is in a superposition of eigenstates
How to think about a quench

Non-thermal initial condition: at $t=0^+$ the system is in a superposition of eigenstates

$$|\psi(t)\rangle = \sum_n e^{-iE_n t} |n\rangle \langle n| \psi(t = 0^-)\rangle$$
How to think about a quench

Non-thermal initial condition: at $t=0^+$ the system is in a superposition of eigenstates

$$\left| \psi(t) \right\rangle = \sum_n e^{-iE_n t} \left| n \right\rangle \left\langle n \right| \psi(t = 0^-)$$

Non-thermal: \[ \left| \left\langle n \right| \psi(t = 0^-) \right\rangle \right|^2 \neq \frac{e^{-\frac{E_n}{T}}}{Z} \]
How to think about a quench

Non-thermal initial condition: at $t=0^+$ the system is in a superposition of eigenstates

$$\ket{\psi(t)} = \sum_n e^{-iE_n t} \ket{n} \bra{n} \psi(t = 0^-)$$

Non-thermal:

$$\left| \bra{n} \psi(t = 0^-) \right|^2 \neq \frac{e^{-\frac{E_n}{T}}}{Z}$$

Mean energy:

$$\bar{E} \equiv \bra{H(t = 0^+)} = \sum_n E_n \left| \bra{n} \psi(t = 0^-) \right|^2$$
Dynamics: ‘simply’ evolve \( t=0 \) state forward in time

\[
|\psi(t)\rangle = \sum_n e^{-iE_nt} |n\rangle \langle n| \psi(t = 0)\rangle
\]
Dynamics: `simply’ evolve $t=0$ state forward in time

$$|\psi(t)\rangle = \sum_n e^{-iE_nt} |n\rangle \langle n|\psi(t = 0)\rangle$$

question: at long times does the system thermalize in the sense that local observables take the values expected from thermal ensemble corresponding to mean energy
Dynamics: `simply’ evolve $t=0$ state forward in time

$$|\psi(t)\rangle = \sum_n e^{-iE_n t} |n\rangle \langle n|\psi(t = 0)\rangle$$

$$\rho(t) = \sum_{nm} e^{-i(E_n - E_m)t} |n\rangle \langle m| |n\rangle \langle n|\psi(t = 0)\rangle \langle \psi(t = 0) |m\rangle$$

$$\rightarrow \rho(t) = \sum_n |n\rangle |\psi_n(t = 0)|^2 \langle n|$$

Density matrix becomes diagonal
eigenstate thermalization hypothesis

For generic (non-integrable) system, belief is that a typical eigenstate of energy $E_n$ gives same local expectation values as thermal state of same mean energy:

$$
\langle n | \mathcal{O} | n \rangle = \frac{1}{Z} \sum_m e^{-\frac{E_m}{T}} \langle m | \mathcal{O} | m \rangle
$$

if

$$
E_n = \frac{1}{Z} \sum_m e^{-\frac{E_m}{T}} E_m
$$

Fails if system has too many conservation laws.
Thermalization sometimes works: experimental quench a one dimensional charge density wave

Nat Phys v 8 p 325
Thermalization sometimes fails

``Quantum quench'' in infinite-d Hubbard model

DMFT study of Hubbard model with instantaneous change of interaction

\[ H(t) = \sum_{ij,\sigma} V_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U(t) \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) \]

Long-time state is not thermal one

Lack of equilibration attributed to conservation of `doublons’

Eckstein et al
arXiv:1208:0743

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Dynamical Mean Field Theory

Approximation to electron self energy of real problem from solution of:

• "impurity problem": a few sites coupled to non-interacting bath
• self-consistency condition

Figure: G. Cohen after A. Georges
Nonequilibrium DMFT

Original formulation:

- Schmidt and Monien, arXiv:cond-mat/0202046
- Freericks, Turkowski, and Zlatic, PRL 97, 266408

Nice description of modern understanding

Aoki, Tsuji, Eckstein, Kollar, Oka, Werner, (1310.5329 (RMP 2014)}
Computational task: solve impurity model

Impurity model action: local (on impurity) terms plus bath

\[ S = -i \int_C dt H_{imp}(t) - i \int_C dt_1 dt_2 \psi^\dagger(t_1) \Delta(t_1, t_2) \psi(t_2) \]

\[ \psi^\dagger \] creates state on impurity

\[ \Delta \] parametrizes hopping onto and off of bath
Key concept: prethermalization

Very often, system approaches state which is thermal given that some quantity (here, double occupancy) is approximately conserved. Long time scale associated with decay of approximately conserved quantity
Key concept: prethermalization

Very often, system approaches state which is thermal given that some quantity (here, double occupancy) is approximately conserved. Long time scale associated with decay of approximately conserved quantity or with metastability of ordered state.
Thermalization can fail (or be very slow) due to metastability of long ranged order

\[ U_{\text{init}} = 4 \quad T_{\text{init}} = 0.1 \]
\[ t_{\text{final}} = 0.11, 0.12, 0.7 \]

Werner et al, arXiv:1208.0743
Theory: Werner and Eckstein

Hubbard model coupled to phonons (frequency 1)

Small number (1%) of excited particle-hole pairs

If gap large relative to phonon frequency, then no relaxation

arXiv:1207.0402
Theory: Werner and Eckstein

Result: long-lived metallic state. Particle number increases slowly (Auger up-scattering) but coherence properties are not time dependent

arXiv:1207.0402
Experimental result not fully compatible with this picture.

Long-lived metallic state only for sufficiently high degree of excitation

is there a nonequilibrium phase
Long time behavior

• Partition function $\iff$ path integral

$$Z = \int \mathcal{D}\{\phi\} \ e^{-S[\{\phi(\tau)\}]}$$

• path integral dominated by most probably path (saddle point) + gaussian fluctuations

$$Z \to e^{-S^*} \int \mathcal{D}\psi_a \mathcal{D}\psi_b \ldots e^{-\frac{1}{2} \int d\tau_1 d\tau_2 \sum_{ab} \psi_a(\tau_1) \chi^{-1}(\tau_1 - \tau_2) \psi_b(\tau_2)}$$
thus

\[ S_{\text{gaussian}} = -\frac{1}{2} \int d\tau_1 d\tau_2 \sum_{ab} \psi_a(\tau_1) \chi^{-1}(\tau_1 - \tau_2) \psi_b(\tau_2) \]

- Identify fixed point (‘phase’)
- Identify important fluctuations (quasiparticles)
- Quasiparticle propagators \( \Leftrightarrow \) linear response susceptibilities
Path Integrals out of Equilibrium
(Schwinger, Kamenev)

To describe result of measurement of operator $O$ at time $t$ in system described by initial density matrix $\rho_{\text{init}}$

Compute:

$$\langle O(t) \rangle = Tr \left[ e^{-iHt} O e^{iHt} \rho_{\text{init}} \right]$$
Two time evolution operators implies two contours (Schwinger, Keldysh)

$$\langle \mathcal{O}(t) \rangle = Tr \left[ e^{-iHt} \mathcal{O} e^{iHt} \rho_{init} \right]$$

- Time $t=0$ $\leftarrow$ reverse evolution $\rightarrow$ Time $t$
- Initial, final states fixed by $\rho$
- Measure $\mathcal{O}$
- $e^{iHt}$

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Path integral interpretation: coherent states on each contour (Schwinger, Kamenev)

\[ e^{iHt} = \prod_{i=1}^{N} \int d\phi_1^+ ... d\phi_N^+ |\phi_N^+ \rangle \langle \phi_N^+ | e^{i\Delta t H} |\phi_{N-1}^+ \rangle . \]

\[ \times \langle \phi_{N-1}^+ | e^{i\Delta t H} | ... \phi_1^+ \rangle \langle \phi_1^+ | \]

\[ e^{-iHt} = \prod_{i=1}^{N} \int d\phi_1^- ... d\phi_N^- |\phi_N^- \rangle \langle \phi_N^- | e^{-i\Delta t H} |... \]

\[ \times |\phi_{N-1}^- \rangle \langle \phi_{N-1}^- | e^{-i\Delta t H} |\phi_N^- \rangle \]
Measure operator

\[ e^{iHt} = \Pi_{i=1,...,N} \int d\phi_N^+ ... d\phi_1^+ |\phi_N^+ > < \phi_N^+ | e^{i\Delta t H} | \phi_{N-1}^+ > \cdot \]
\[ \times < \phi_{N-1}^+ | e^{i\Delta t H} | ... \phi_1^+ > < \phi_1^- + \]

\[ e^{-iHt} = \Pi_{i=1,...,N} \int d\phi_1^- ... d\phi_N^- |\phi_1^- > < \phi_1^- | e^{-i\Delta t H} | ... \]
\[ \times |\phi_{N-1}^- > < \phi_{N-1}^- | e^{-i\Delta t H} | \phi_N^- > < \phi_N^- | \]
Measure operator

\[
e^{iHt} = \Pi_{i=1,...,N} \int \ d\phi_N^+ ... d\phi_1^+ |\phi_N^+ \rangle \langle \phi_N^+ | e^{i\Delta tH} |\phi_{N-1}^+ \rangle \cdot
\]
\[
\times \quad <\phi_{N-1}^+ | e^{i\Delta tH} |\ldots \phi_1^+ \rangle <\phi_1^- +
\]
\[
e^{-iHt} = \Pi_{i=1,...,N} \int \ d\phi_1^- ... d\phi_N^- |\phi_1^- \rangle \langle \phi_1^- | e^{-i\Delta tH} |\ldots \rangle
\]
\[
\times \quad |\phi_{N-1}^- \rangle <\phi_{N-1}^- | e^{-i\Delta tH} |\phi_N^- \rangle <\phi_N^- |
\]

\[
\left< \mathcal{O}(t) \right> = Tr \left[ e^{-iHt} \mathcal{O} e^{iHt} \rho_{\text{init}} \right]
\]
Measure operator

\[ e^{iHt} = \prod_{i=1}^{N} \int d\phi_N^+ ... d\phi_1^+ |\phi_N^+ \rangle \langle \phi_N^+| e^{i\Delta tH} \cdot \langle \phi_{N-1}^+ |. \]

\[ \times < \phi_{N-1}^+ |e^{i\Delta tH}|...\phi_1^+ > < \phi_1^- + \]

\[ e^{-iHt} = \prod_{i=1}^{N} \int d\phi_1^- ... d\phi_N^- |\phi_1^- \rangle \langle \phi_1^-| e^{-i\Delta tH} \cdot \]

\[ \times |\phi_{N-1}^- > < \phi_{N-1}^- |e^{-i\Delta tH}|\phi_N^- > < \phi_N^-| \]

Crucial factor

\[ < \phi_N^- |\mathcal{O}|\phi_N^+ > \]
\[
\begin{align*}
\rho_{\text{init}} & = e^{iHt} = \Pi_{i=1,...,N} \int d\phi_N^+ ... d\phi_1^+ \phi_N^+ <\phi_N^+ | e^{i\Delta t H} | \phi_{N-1}^+ > \\
& \times < \phi_{N-1}^+ | e^{i\Delta t H} | .... \phi_1^+ > < \phi_1^- + \\
\rho_{\text{init}} & = e^{-iHt} = \Pi_{i=1,...,N} \int d\phi_1^- ... d\phi_N^- \phi_1^- <\phi_1^- | e^{-i\Delta t H} | ..... \\
& \times | \phi_{N-1}^- > < \phi_{N-1}^- | e^{-i\Delta t H} | \phi_N^- > < \phi_N^- |
\end{align*}
\]

Crucial factor

\[
< \phi_1^+ | \rho_{\text{init}} | \phi_1^- >
\]
Path integral

\[ \rho_{\text{init}} \xrightarrow{\text{time } t=0} \xrightarrow{\text{time evolution}} \xrightarrow{\text{time } t} O \]

\[ \langle O \rangle = \int d\phi_+ d\phi_- \rho_{\text{init}}(\phi_+, \phi_-) \int D\phi_+(t) D\phi_-(t) W_0(\{\phi_+, \phi_-\}) \]

(1) Fix start (on + line) and stop (on -) values \( \phi^\pm \)
(2) Sum over all paths connecting start and stop values. Weight paths by action \( W \) (dep on operator \( O \))
(3) Sum over all start and stop values, weighted by \( \rho_{\text{init}} \)
Steady State

At long times: system forgets initial condition

\[ \Rightarrow ? \]

replace initial density matrix by steady state one

\[
\langle \mathcal{O} \rangle = \int d\phi_+ d\phi_- \rho_{SS}(\phi_+, \phi_-) \int \mathcal{D}\phi_+(t)\mathcal{D}\phi_-(t) W_0(\{\phi_+, \phi_-\})
\]

Notes:
• steady state density matrix must be determined
• Initial conditions may not be (fully) forgotten
Steady State

At long times: system forgets initial condition

=>

replace initial density matrix by steady state one

\[ \langle \mathcal{O} \rangle = \int d\phi_+ d\phi_- \rho_{SS}(\phi_+, \phi_-) \int \mathcal{D}\phi_+(t)\mathcal{D}\phi_-(t) W_0(\{\phi_+, \phi_-\}) \]

Steady state density matrix must be determined e.g. as solution of kinetic equation

\[ \rho_{SS} = e^{iHt} \rho_{SS} e^{-iHt} \]
Identification of Important Paths

In equilibrium

\[ Z = \text{Tr} \left[ e^{-\frac{H}{T}} \right] \]

Important paths are those that dominate the path integral for the partition function

\[ Z^\ast = \int \mathcal{D} \{ \phi \} \ e^{-S[\{ \phi(\tau) \}]} \]
Out of equilibrium

If operator $O=1$ then

$$\langle O(t) \rangle = Tr \left[ e^{-iHt} O e^{iHt} \rho_{init} \right] = Tr[\rho_{init}] = 1$$

No basis for selecting paths

$=>$ "Important paths" $\iff$ paths making important contribution to specific operator.
Most important case: steady-state density matrix seek paths that maximize the density matrix

$$\rho_{SS} \rightarrow \approx \rho_{SS}(\phi_+, \phi_-)$$
Stationary path approximation

\[ \rho_{ss} \quad \text{time } t=0 \quad \Rightarrow \text{time evolution} \Rightarrow \text{time } t \]

\[ \langle \mathcal{O}(t) \rangle = Tr \left[ e^{-iHt} \mathcal{O} e^{iHt} \rho_{init} \right] \]

Stationary path configuration must be the same on outbound and inbound time contour (so oscillations cancel) and must extremize the diagonal component of the density matrix
local polaron

\[ H = H_{\text{dot}} + H_{\text{lead}} + H_{\text{mix}} \]

\[ H_{\text{lead}} = \sum_{k,a=L,R} \varepsilon_k c_{k,a}^\dagger c_{k,a}. \]

\[ H_{\text{mix}} = \sum_{k,a=L,R} V_{k,a}^a c_{k,a}^\dagger d + H.c. \]

\[ H_{\text{dot}} = \varepsilon' d^\dagger d + \lambda q d^\dagger d + \frac{K}{2} q^2 + \frac{1}{2M} p^2. \]

Phys. Rev. Lett. 94 07640
Density of states in absence of phonons
Energy scales

\[ \Gamma^a = \pi \sum_k |V_k^a|^2 \delta(\omega - \varepsilon_k) \quad 1/(\text{electron escape time}) \]

\[ \omega_{\text{phonon}} = \sqrt{\frac{K}{M}} \quad \ll \Gamma \quad (\text{adiabatic approx}) \]

polaron shift at \( \Gamma = 0 \) : \( \frac{\lambda^2}{K} \)
Polaron shift

Energy of isolated dot

$$\lambda q d\dagger d + \frac{K}{2} q^2$$

Implies extremum

$$\frac{\lambda \langle d\dagger d \rangle}{K} = q^*$$

$$\Rightarrow \varepsilon \rightarrow \varepsilon - \frac{\lambda^2 \langle d\dagger d \rangle^2}{2K}$$
In equilibrium

If \( \frac{\lambda^2}{K} \gtrless \Gamma \)

Then 2 extrema

\[ \varepsilon > \mu : \quad \langle d^\dagger d \rangle \approx 0; \quad q^* \approx 0 \]

\[ \varepsilon < \mu : \quad \langle d^\dagger d \rangle \approx 1; \quad q^* \approx \frac{\lambda}{K} \]
Equilibrium: two states for oscillator

\[ P_2 \sim e^{-\frac{E_2 - E_1}{T}} \]

\[ P(q - q_1) \sim e^{-\frac{K(q - q_1)^2}{\omega_0 \coth \frac{\omega_0}{2T}}} \]
Nonequilibrium local polaron

\[ H = H_{dot} + H_{lead} + H_{mix} \]

\[ H_{lead} = \sum_{k,a=L,R} \varepsilon_k c_{k,a}^{\dagger} c_{k,a} \]

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\[ H_{dot} = \varepsilon' d^{\dagger} d + \lambda q d^{\dagger} d + \frac{K}{2} q^2 + \frac{1}{2M} p^2 \]

Can be more or less completely solved
Nonequilibrium local polaron

\[ H = H_{\text{dot}} + H_{\text{lead}} + H_{\text{mix}} \]

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Open system: coupled to leads (reservoirs)
Nonequilibrium local polaron

\[ H = H_{dot} + H_{lead} + H_{mix} \]

\[ H_{lead} = \sum_{k,a=L,R} \varepsilon_k c_{k,a}^\dagger c_{k,a}. \]

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\[ H_{dot} = \varepsilon' d^\dagger d + \lambda q d^\dagger d + \frac{K}{2} q^2 + \frac{1}{2M} p^2 \]

Open system: coupled to leads (reservoirs) steady state exists and is unique
Nonequilibrium local polaron

\[ H = H_{\text{dot}} + H_{\text{lead}} + H_{\text{mix}} \]

\[ H_{\text{lead}} = \sum_{k,a=L,R} \varepsilon_k c_k^\dagger c_{k,a} \]

\[ H_{\text{mix}} = \sum_{k,a=L,R} V_k^a c_k^\dagger c_{k,a} d + H.c. \]

\[ H_{\text{dot}} = \varepsilon' d^\dagger d + \lambda q d^\dagger d + \frac{K}{2} q^2 + \frac{1}{2M} p^2 \]

Difference in chemical potential
\[ \Rightarrow \text{current across quantum dot} \]
Nonequilibrium results

\[ P_2 \sim e^{- \frac{E_2 - E_1}{T'_{\text{eff}}}} \]

\[ T'_{\text{eff}} \approx T_{\text{eff}} \ln \frac{E_2 - E_1}{T_{\text{eff}}} \]

\[ P(q - q_1) \sim e^{- \frac{K(q - q_1)^2}{\omega_0 \coth \frac{\omega_0}{2T_{\text{eff}}}}} \]
Key point

\[ T_{\text{eff}} \text{ a complicated function of current and } T \text{ of leads} \]

As \( T_{\text{reservoir}} \rightarrow 0 \)

\[ T_{\text{eff}} \sim \Delta \mu \]

Effective temperature of electron system proportional to current; \textbf{parametrically larger than } I^2 R

Effective temperature larger than physical temperature
Current-driven quantum criticality
nonequilibrium $\Rightarrow$ temperature without heating relative to reservoir

\[ T_{\text{eff}} \sim \Delta \mu \coth \left( \frac{\Delta \mu}{T} \right) \]
Effective temperature not equal to physical temperature
Important question: how well can we solve impurity models out of equilibrium