

Nonequilibrium electron dynamics near Mott transition

Sharareh Sayyad

In collaboration with: Martin Eckstein

Max Planck Institute for the Structure and Dynamics of Matter,
University of Hamburg-CFEL, Hamburg, Germany

September 27, 2016

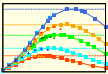
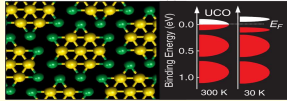
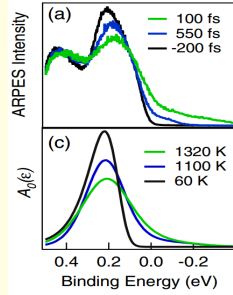
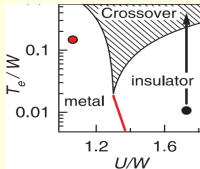


Photo induced Mott transition in $1T - TaS_2$

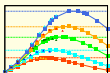


- Mott insulator at $T=30$ K
- Preparation of an excited state in crossover region
 \leftrightarrow Induced **insulator-to-metal** transition



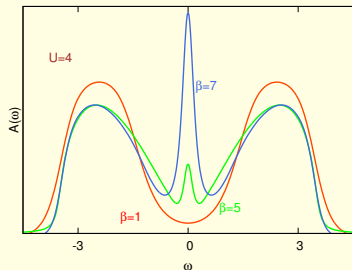
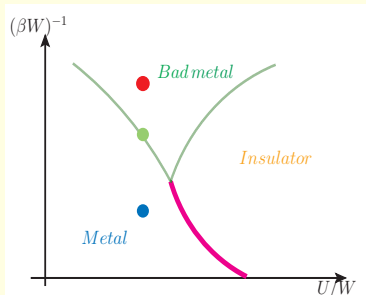
- Creation of **hot carriers**
- **Collapse** of the gap < 100 fs
- **Fast thermalization** < 100 fs
- Relaxation of the excited state > 500 fs
- **Electronic** relaxation timescale
 $<$ **electron-lattice** relaxation timescale

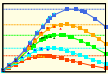
■ L. Perfetti, *et al.*, Phys. Rev. Lett. **97**, 067402 (2006).



Mott transition in the half-filled Hubbard model

$$H = -J \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + U \sum_{i=1}^N n_{i\uparrow} n_{i\downarrow}$$






Relaxation to the Fermi liquid?

$$H = -J \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + U \sum_{i=1}^N n_{i\uparrow} n_{i\downarrow}$$



Preparing the system in the **crossover region**:

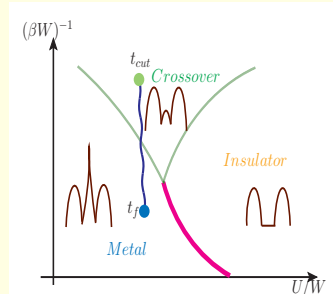
- Excitation (quench)
 - Phys. Rev. Lett. **117**, 096403(2016).
- 
- Fast thermalization
 - Phys. Rev. B **84**, 035122(2011).

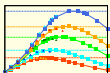


Studying the **relaxation dynamics** of the excited state

+ electrons coupled to the environment

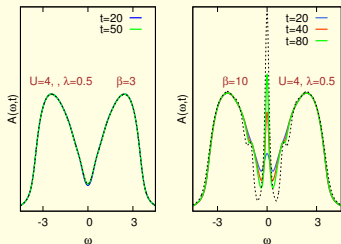
$$\Sigma_{eb} = \lambda \text{ (diagram of a self-energy loop with a wavy line and an arrow)}$$





Slow-relaxing electronic characteristic timescale

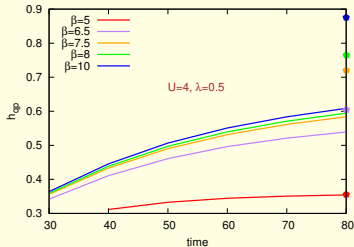
Solved by DMFT:



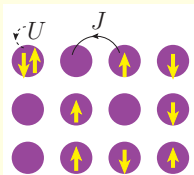
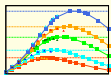
Bottleneck of dynamics (large β):

temperature-independent evolution of h_{qp}

- ✓ **Hubbard Bands** :: **Fast thermalization**
- inverse **One-body** energy-scales [$\frac{1}{4}$]
- ✗ **Quasiparticle peak** :: **Slow retrieval** (for $\beta > 5$)
- timescale
 - >> inverse **One-body** energy-scales [$\frac{1}{4}$]
 - >> inverse **quasiparticle** bandwidth [$\frac{1}{0.8}$]

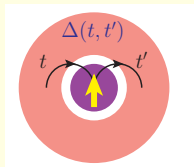


Dynamical mean field theory

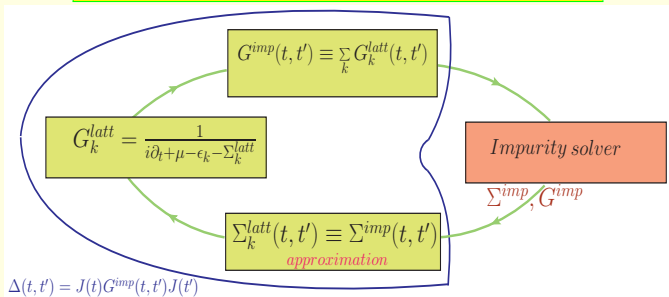


lattice problem \rightarrow impurity-bath problem

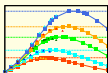
❓ Solving the impurity problem



DMFT self-consistency on Bethe lattice



Review on NEDMFT: Rev. Mod. Phys. 86, 779 (2014).



Impurity solver: U(1) slave-rotor

$$\underbrace{c_{\sigma}^{\dagger}}_{\text{electron}} = \underbrace{e^{i\theta}}_{X:\text{rotor}} \underbrace{f_{\sigma}^{\dagger}}_{\text{spinon}} \quad \Leftrightarrow \quad G_e = G_X \cdot G_f$$

Atomic model:

$$\underbrace{\{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}}_{\text{electron}} \equiv \underbrace{\{|l = -1\rangle, |l = 0\rangle, |l = 0\rangle, |l = 1\rangle\}}_{\text{Charge conservation: } l = n_f - 1} \otimes \underbrace{\{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}}_{\text{Spinon}}$$

On the impurity site:

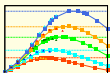
$$\left\{ \begin{array}{l} \text{Solving Dyson equations for} \\ \text{Imposing constraints} \end{array} \right. \left\{ \begin{array}{l} G_X \quad \text{with } \Sigma_X = \Delta \cdot G_f \\ G_f \quad \text{with } \Sigma_f = \Delta \cdot G_X \\ \text{Charge conservation} \\ |X|^2 = 1 \end{array} \right.$$

? Why slave-rotor impurity solver:

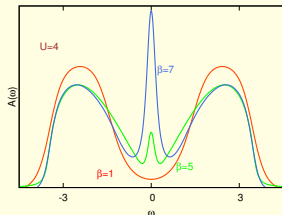
- ✓ Accessibility of long time-evolution (Similar to NCA)
- ✓ Accurate phase diagram near Mott transition (not the case in NCA)

■ **Equilibrium study:** S. Florens and A. Georges, *Phys. Rev. B* **66** 165111 (2002).

■ **Nonequilibrium study:** Sh. S and M. Eckstein, *Phys. Rev. Lett.* **117**, 096403 (2016).



Equilibrium Physics: Slave-rotor Language



By decreasing the temperature:



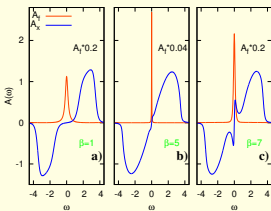
Electron: height of the quasiparticle peak enhanced.



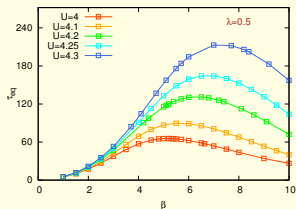
Rotor: density at zero frequency formed.



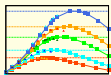
Spinon: nonmonotonous behavior as a function of β



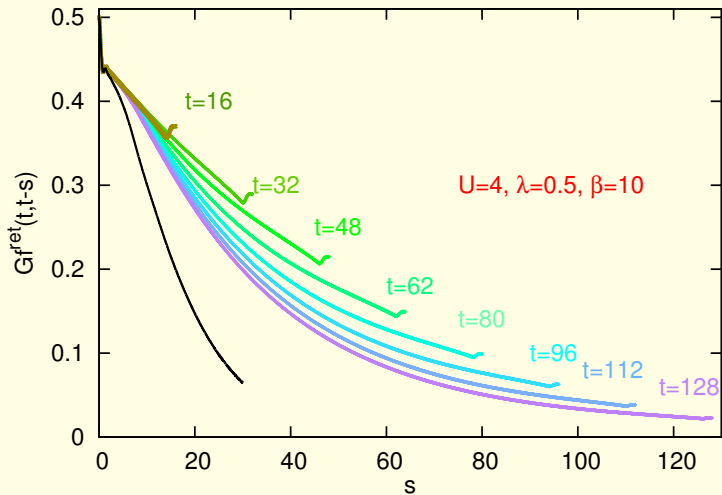
Maximum in the spinon inverse bandwidth

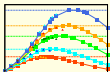


Footprint of this nonmonotonous response out of equilibrium ?

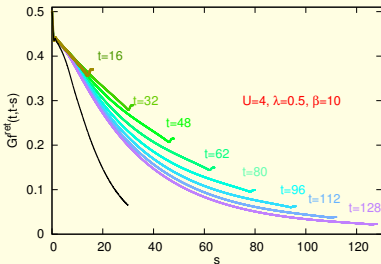


Spinon's response: presence of a “ \cap ” turn!





Spinon's response: presence of a “ \cap ” turn!



Nontrivial timescale:

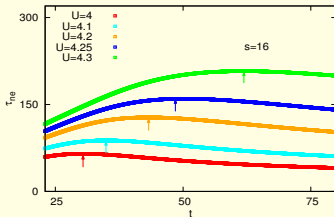
“ \cap ” turn: Bottleneck of dynamics at t_{\max}

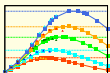
Quasiparticle retrieval only after $t = t_{\max}$

Time-evolution of G_f^{ret} :

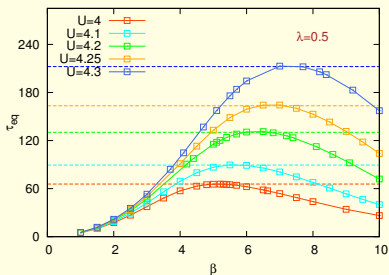
1. Evolving against equilibrium value initially
2. “ \cap ” turn: Reaching τ_{\max} at t_{\max}
3. Start evolving towards equilibrium value

$$\tau_{\text{ne}}^{-1} = -\partial_s G_f^{\text{ret}} / G_f^{\text{ret}}$$





Spinon “ \cap ” turn: equilibrium and nonequilibrium

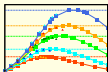


Spinon nontrivial response:

◎ Agreement between τ_{eq}^{\max} and τ_{neq}^{\max}

Spinon lifetime (t_{\max}) $\propto \tau_{eq}^{\max}$

Spinon lifetime reflected in **electronic bottleneck** of dynamics

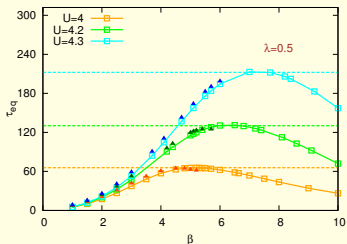


Reflection of spinon lifetime in other observables?

Assume : $\Im G_f(\omega) \approx \delta(\omega)/\pi$

$$\tau_{ne}^{-1} = -\Sigma_f''(\omega = 0) \approx -\pi J^2 \int d\omega \frac{A(\omega)A(\omega)}{\cosh^2(\beta\omega/2)}$$

✓ Emergence of a **correlation** timescale



Nontrivial spinon response in multi-orbital physics:



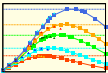
"Frozen" spin-spin correlation function

Ph. Werner, et al., Phys. Rev. Lett. 101, 166405 (2008).



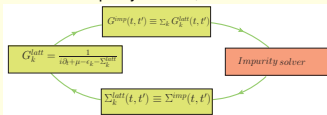
Non-Fermi-liquid behavior of optical conductivity in perovskite ruthenates ($\propto 1/\sqrt{\omega}$)

Y. S. Lee, et al., Phys. Rev. B 66, 041104 (2002).

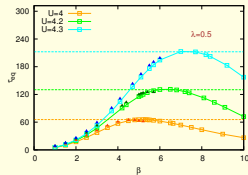


Conclusion and Summary

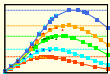
- Study the Hubbard model near Mott transition
- Investigate the system under a quick ramp
- slave-rotor impurity solver + DMFT



- Slow retrieval of the quasiparticle density
- Presence of a “∩” turn in the spinon retarded Green’s function
- Presence of a nonmonotonous spinon behavior in equilibrium
- Agreement between equilibrium and nonequilibrium spinon response



• Emergence of a **correlation** timescale



Thanks for your attention.