Thermalization of electron-boson systems described by a pure state

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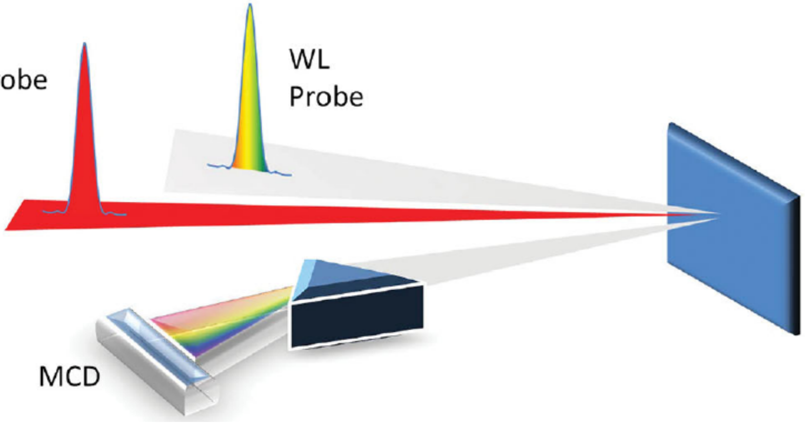
“Next generation” @ ICTP, September 26, 2016

Keywords in recent talks

Quantum

Nonequilibrium



Ultrafast experiments in condensed matter

Review: Giannetti *et al*, Adv. Phys. (2016)

$$|\psi(t)\rangle = e^{-i\hat{H}t}|\psi_0\rangle$$

Two nontrivial outcomes of unitary time evolution

Generate **novel states**?

States that do not exist in
equilibrium phase diagram

Pathway to **ergodicity**

$$\langle\hat{O}(t)\rangle = \mathrm{Tr}\{\hat{\rho}_{\mathrm{stat}}\hat{O}\}$$

These two concepts are fundamentally different

It underlines the need to understand **when and how fast** does a condensed-matter system **thermalize**

Why is understanding of thermalization important in condensed matter?

- Common belief: undriven systems, at asymptotic times after perturbation, should approach a thermal state

- However, time-resolved experiments may now study the response at extremely short times after perturbation

(in particular ultrafast optics ...)

In a **short time interval**, the dynamics may be efficiently described by models taking into account only the most important interactions

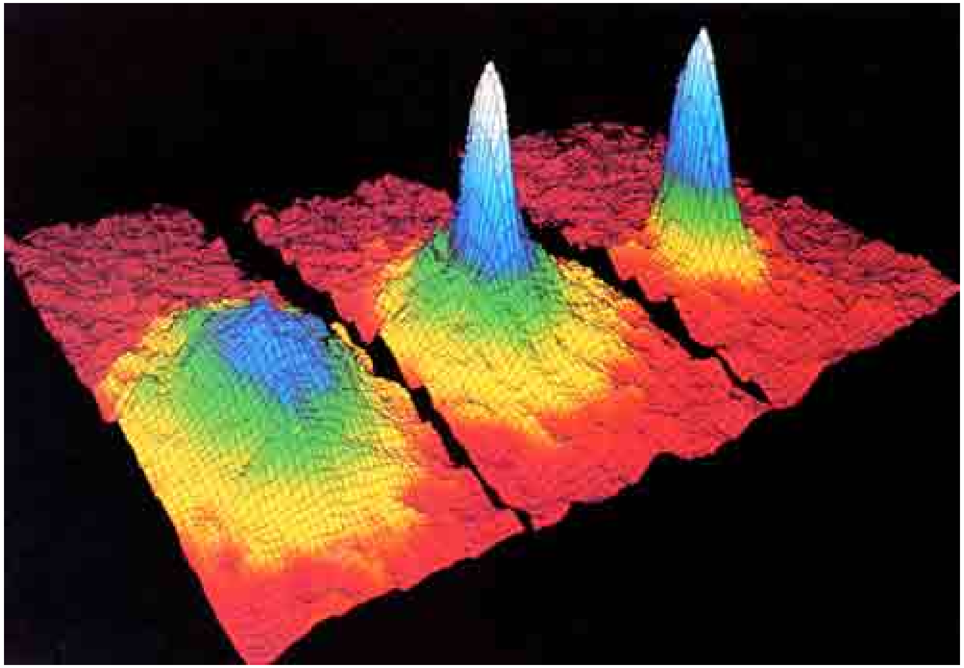
This implies that in a given time interval, the system behaves as a **closed quantum system**

$$|\psi(t)\rangle = e^{-i\hat{H}t}|\psi_0\rangle$$

Closed quantum systems are peculiar:

Many of their properties are implicitly assumed, but rarely verified

Challenges for “Next generation” (1)

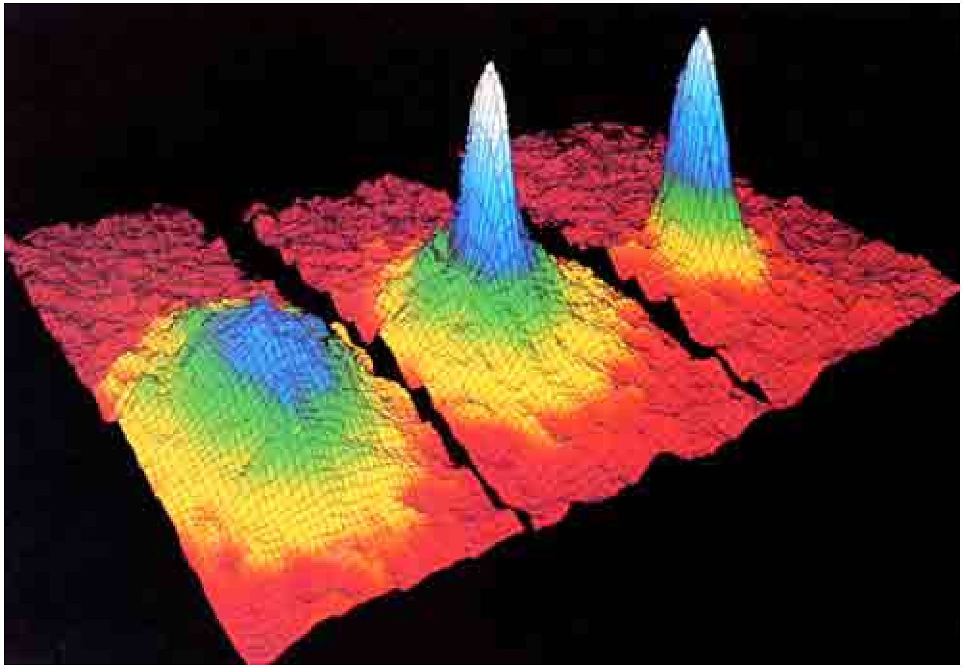


Nobel prize 2001

Experimental realization of
Bose-Einstein condensation
(1995)

“Ultracold atoms in perfectly isolated environment at temperature 20 nK”

Challenges for “Next generation” (1)



Nobel prize 2001

Experimental realization of
Bose-Einstein condensation
(1995)

“Ultracold atoms in **perfectly isolated** environment at **temperature** 20 nK”

Challenges for “Next generation” (2)

“A closed quantum system can never thermalize”

“It is described by a pure state, hence its entropy is always zero”

Closed quantum systems ***do*** thermalize

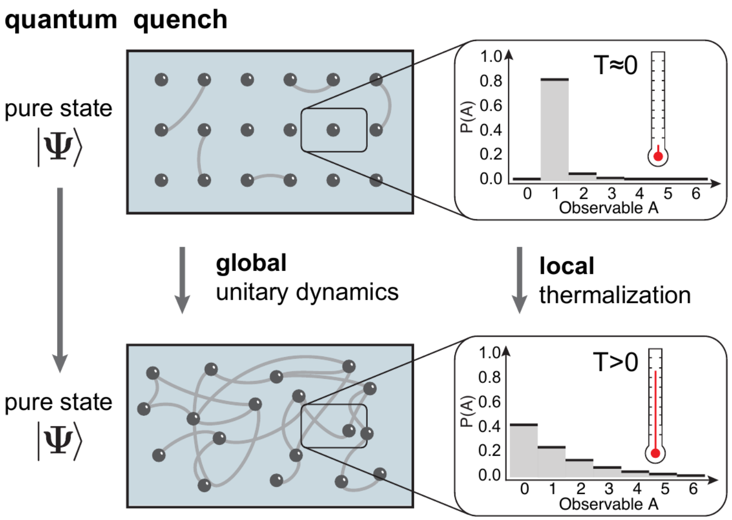
- The notion of **temperature** is valid for generic quantum systems

  Review: d'Alessio, Kafri, Polkovnikov, Rigol, Adv. Phys. (2016); and many others

- The total entropy of a pure state remains zero forever, however, the **entanglement entropy** between subsystems increases and reach thermal predictions

  Verified experimentally with ultracold bosons

  Kaufman *et al*, Science (2016)



How about condensed-matter systems in pump-probe experiments?

Two extreme views:

- “The pump pulse creates a thermal electronic distribution, at elevated temperature”

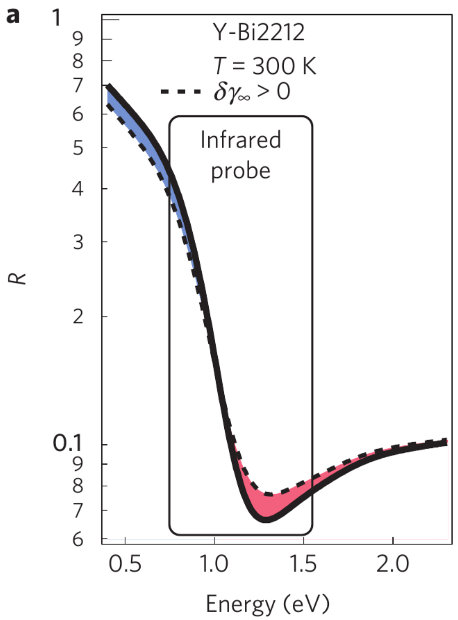
  (Not entirely correct. However, thermalization can occur very fast ...)

- “Electrons reach a thermal distribution only after completion of the whole hierarchy of relaxation processes”

  (Probably too conservative ...)

Motivation: ultrafast optics

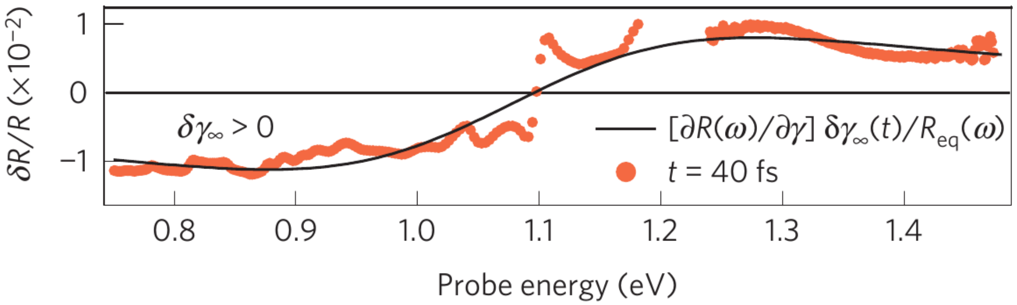
State-of-the-art: Width of the pump pulse ~ 15 fs, Broadband probe at a delay of ~40fs



Snapshots of the retarded interaction of charge carriers with ultrafast fluctuations in cuprates

S. Dal Conte[1★†], L. Vidmar[2,3★†], D. Golež[3], M. Mierzejewski[4], G. Soavi[1], S. Peli[5,6], F. Banfi[5,7], G. Ferrini[5,7], R. Comin[8,9], B. M. Ludbrook[8,9], L. Chauviere[8,9,10], N. D. Zhigadlo[11], H. Eisaki[12], M. Greven[13], S. Lupi[14], A. Damascelli[8,9], D. Brida[1,15], M. Capone[16], J. Bonča[3,17], G. Cerullo[1] and C. Giannetti[5,7★]

Nature Physics (2015)



Modeling of the data consistent with ultrafast relaxation of charge carriers with strongly-coupled excitations of bosonic origin

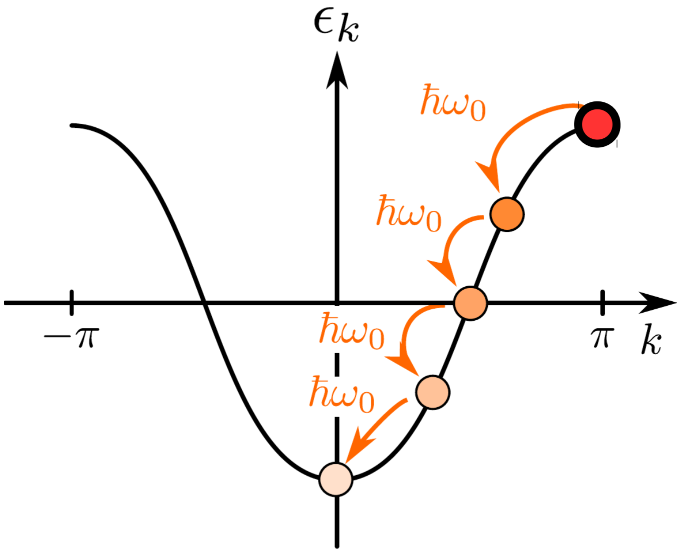
Thermalization of charrge carriers strongly coupled to a single branch of bosonic excitations ("local" bosons) occurred within 40 fs?

Case studied in the following:

Strongly-coupled boson = **dispersionless phonon**

Kogoj, Vidmar, Mierzejewski, Trugman, Bonča, PRB (2016)

Holstein model (single electron)



Electron in the initial state

$$\hat{H} = -t_0 \sum_j (\hat{c}_j^\dagger \hat{c}_{j+1} + \mathrm{h.c.}) \; + \; g \sum_j \hat{c}_j^\dagger \hat{c}_j (\hat{b}_j + \hat{b}_j^\dagger) \; + \; \omega_0 \sum_j \hat{b}_j^\dagger \hat{b}_j$$

Can phonons act as a reservoir/bath?

- Does their spectrum from a continuum?
- Is their intrinsic time scale much shorter than the typical electron time scale?

The system nevertheless does thermalize

“Thinking about thermalization in terms of system + bath is old fashioned”

- Electron and phonons form a closed quantum system
- Simply solve the time-dependent Schroedinger equation exactly

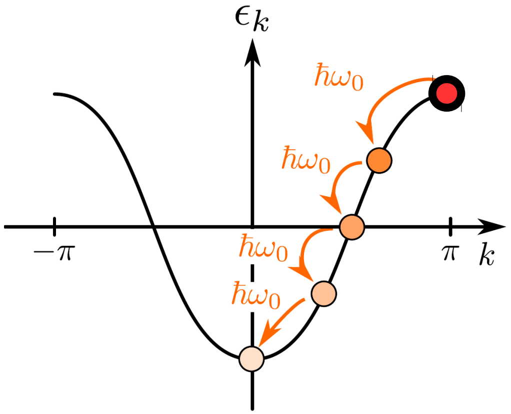
$$|\psi(t)\rangle = e^{-i\hat{H}t}|\psi_0\rangle$$

$$\langle\psi(t)|\hat{O}|\psi(t)\rangle = \mathrm{Tr}\{\hat{\rho}_{\mathrm{stat}}\hat{O}\}$$

Initial state and numerical method

Initial state

Interaction quench



$$|\psi_0\rangle = \hat{c}^\dagger_{k=\pi}|\emptyset\rangle$$

Field quench

Drive by a constant electric field *F* in a time interval

$$t \in [-t_{\rm i}, 0]$$

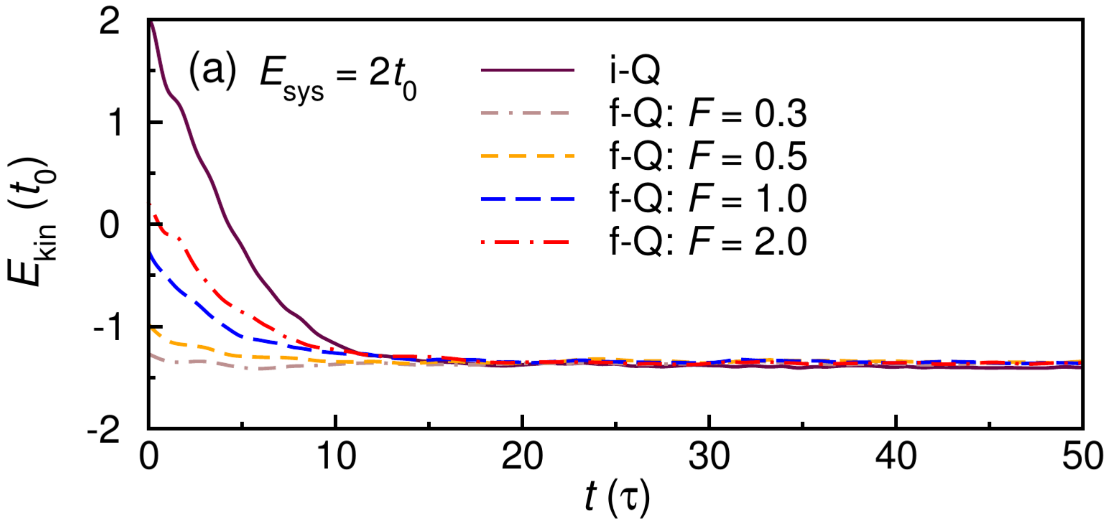
to reach the same target energy

- Unitary time evolution $|\psi(t)\rangle = e^{-i\hat{H}t}|\psi_0\rangle$

$$\hat{H} = -t_0 \sum_j (\hat{c}^\dagger_j \hat{c}_{j+1} + \text{h.c.}) \;+\; g\sum_j \hat{c}^\dagger_j \hat{c}_j (\hat{b}_j + \hat{b}^\dagger_j) \;+\; \omega_0 \sum_j \hat{b}^\dagger_j \hat{b}_j$$

- Ground-state properties — Bonča, Trugman, Batistić, PRB (1999)
- Nonequilibrium dynamics — Vidmar, Bonča, Mierzejewski, Prelovšek, Trugman, PRB (2011)
- Finite-temperature equilibrium — Kogoj, Vidmar, Mierzejewski, Trugman, Bonča, PRB (2016)

Independence of initial state



$$\lambda = g^2/(2t_0\omega_0) = 0.5$$

$$\omega_0/t_0 = 0.75$$

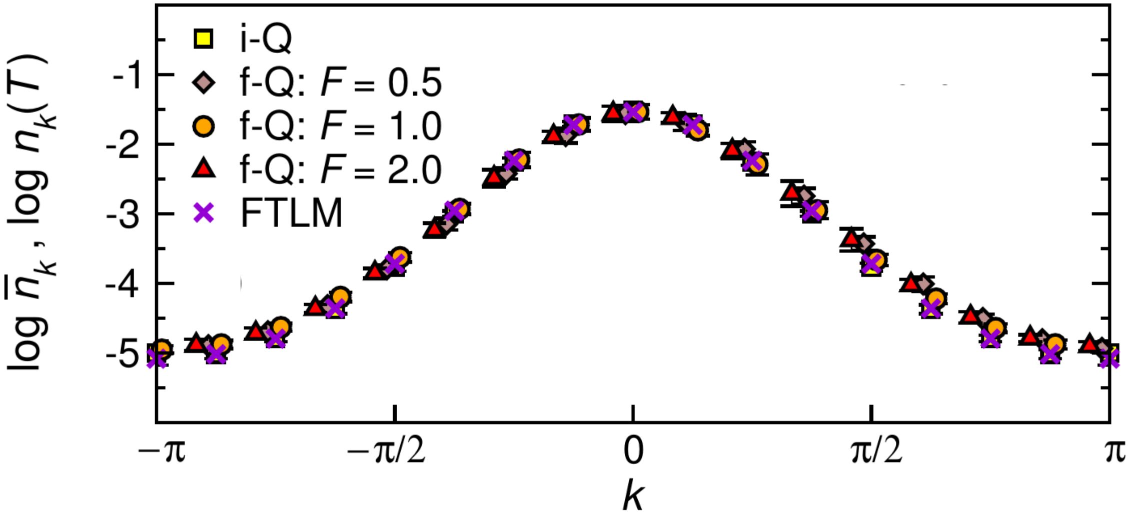
$$\hat{H}_{\text{kin}} = -t_0 \sum_j (\hat{c}_j^\dagger \hat{c}_{j+1} + \text{h.c.})$$

However:

- Independence of initial state is only a necessary condition
- Demonstrated only for one observable

One-particle density matrix

Goal: to make a statement about all static one-particle correlations



$$\bar{n}_k = \langle \psi(t) | \hat{n}_k | \psi(t) \rangle_t$$

$n_k(T)$ Calculated in the Gibbs ensemble

FTLM: Finite-temperature Lanczos method

- Momentum distribution function $\hat{n}_k = \frac{1}{L} \sum_{j,l} e^{-i(j-l)k} \hat{c}_j^\dagger \hat{c}_l$

- Eigenvalues of the fermionic one-particle density matrix

Thermalization of static electronic correlations on the **entire lattice**

Dynamic correlations

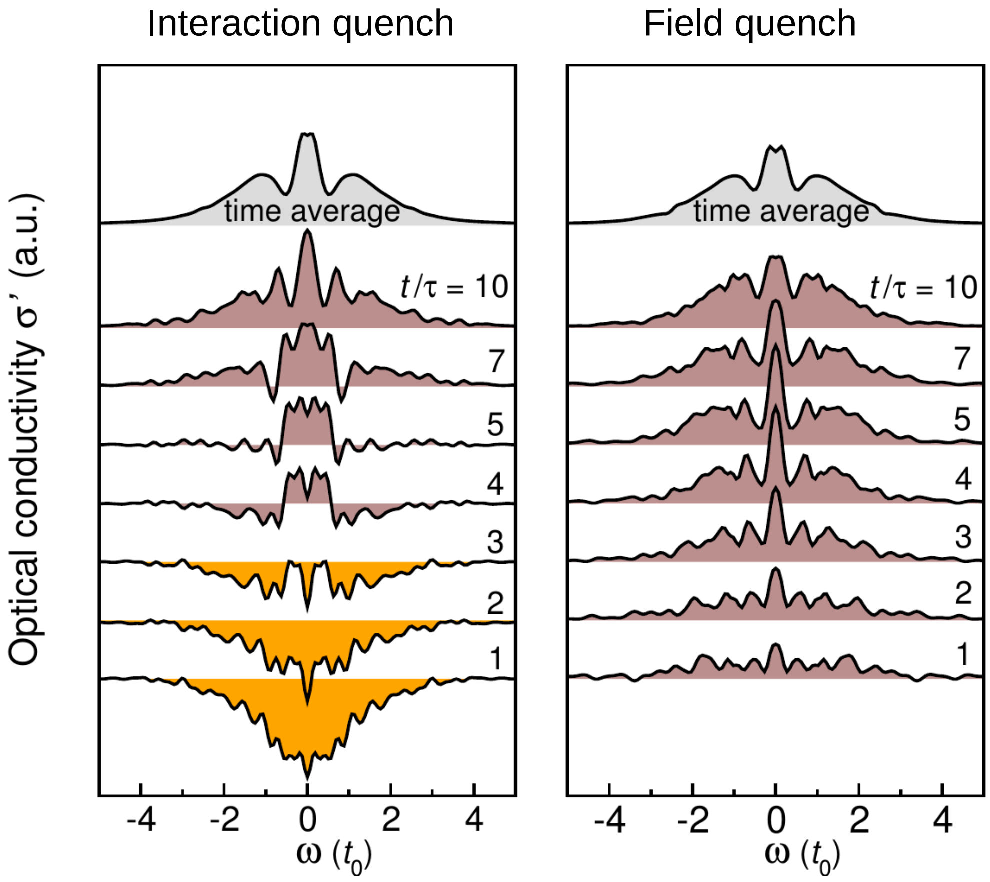
Result on static observables does not immediately extend to dynamic observables

$$\langle \hat{j}(t)\hat{j}(0)\rangle$$

Calculate optical conductivity at time *t* after the quench without applying time-translation invariance

$$\sigma' = \mathrm{Re}\,\sigma(\omega,t)$$

Lenarčič, Golež, Bonča, Prelovšek, PRB (2014)



Dynamic correlations

Test thermalization without explicitly carrying out calculations in the Gibbs ensemble

- Thermal equilibrium

$$\sigma'_{\mathrm{reg}}(\omega) = \frac{1-e^{-\omega/T}}{\omega} C(\omega)$$

$$C(\omega) = \Re \int_0^\infty \mathrm{d}t e^{i\omega^+ t} \mathrm{Tr}\{\hat{\rho}_{\mathrm{sys}} \hat{\jmath}(t)\hat{\jmath}(0)\}$$

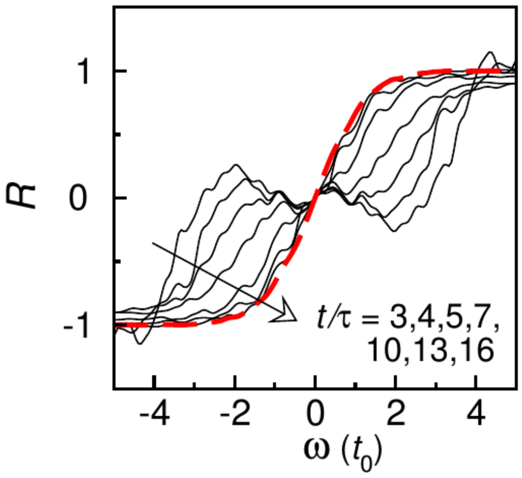
$$R(\omega) = \frac{C(\omega)-C(-\omega)}{C(\omega)+C(-\omega)} = \tanh\left(\frac{\omega}{2T}\right)$$

- Nonequilibrium

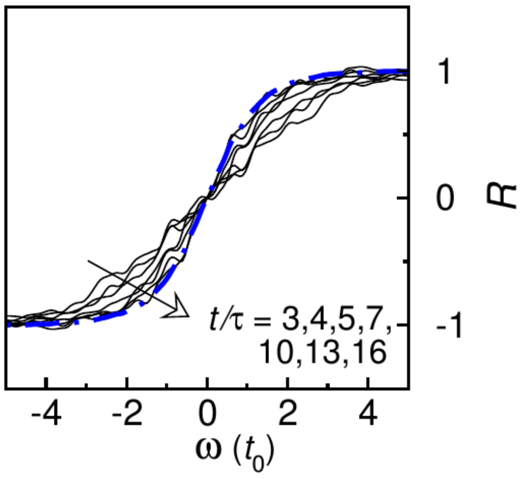
$$C(\omega,t) = \Re \int_0^\infty \mathrm{d}s e^{i\omega^+ s} \langle\psi_0|\hat{\jmath}(t+s)\hat{\jmath}(t)|\psi_0\rangle$$

$$R(\omega,t) = \frac{C(\omega,t)-C(-\omega,t)}{C(\omega,t)+C(-\omega,t)}$$

Interaction quench

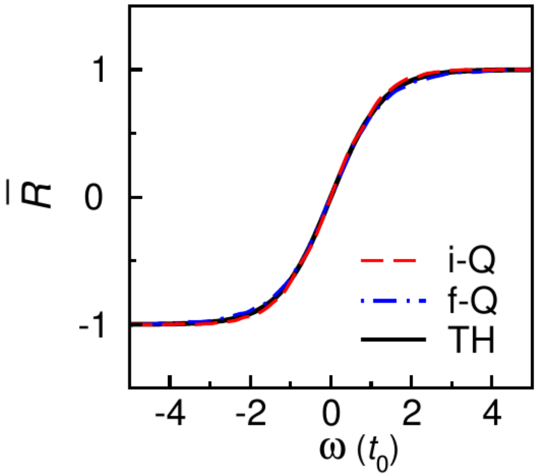


Field quench



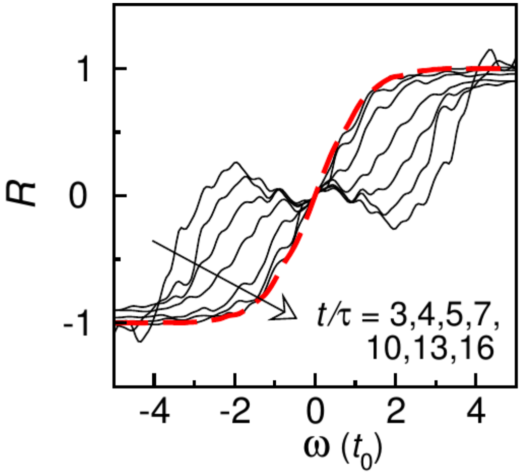
Dynamic correlations

Test thermalization without explicitly carrying out calculations in the Gibbs ensemble

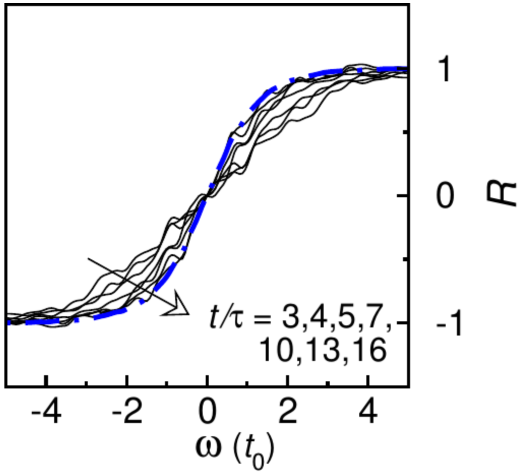


Interaction quench
Field quench
$\tanh(\omega/(2T))$

Interaction quench



Field quench

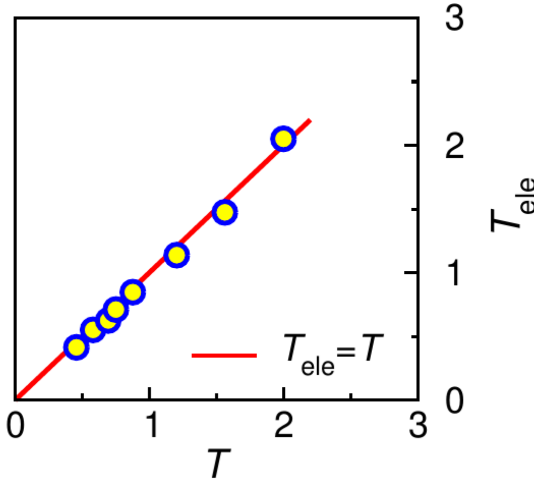


Static and dynamic correlations - Temperature

Static fermionic correlations: temperature obtained from the Gibbs ensemble by matching the electron kinetic energy

Dynamic correlations: temperature obtained by fitting $\langle R(\omega, t)\rangle_t$ with the thermal form $\tanh(\omega/(2T))$

Are these temperatures equal? **Yes!**



The temperature, measured in response functions, is the temperature of the closed electron-phonon system

Conclusions

- Simple, closed quantum systems may thermalize extremely fast

  (Useful input for ultrafast optical experiments)

- “Thinking about thermalization in terms of system + bath is old fashioned”

  (Is it really true? Find more examples ...)

Thank you!