From quantum quenches to microwave refrigerator

Andrea De Luca
in collaboration with Alberto Rosso
Phys. Rev. Lett. 115, 080401

28/09/2015
Classical Thermalization?

Time evolution inside the phase space
Classical Thermalization?

Time evolution inside the phase space

Average over the entire phase space

Ergodic Hypothesis
Quantum dynamics

\[ i\hbar \frac{d\Psi}{dt} = H\Psi \]

\[ \Psi(t) = \sum_{n} c_{n} e^{-iE_{n}t}|E\rangle \rightarrow \text{unitary dynamics} \]

Any closed quantum system has a discrete spectrum

How can relaxation occur?
Density matrix formulation

\[ |\Psi(t)\rangle = \sum_{n=1}^{N} c_n e^{-iE_nt} |E_n\rangle \]

\[ \rho(t) \equiv |\Psi(t)\rangle \langle \Psi(t)| = \begin{pmatrix} |c_1|^2 & \cdots & c_1^* c_N e^{i(E_1-E_N)t} \\ \vdots & \ddots & \vdots \\ c_1 c_N^* e^{i(E_N-E_1)t} & \cdots & |c_N|^2 \end{pmatrix} \]

Fundamental question

\[ \rho(t) \xrightarrow{?} \rho_{\text{Gibbs}} = \frac{e^{-\beta \hat{H}}}{Z} \]
Dephasing

Time-dependence cannot disappear in general...

$$\rho(t) = \begin{pmatrix}
|c_1|^2 & \cdots & c_1^*c_N e^{i(E_1-E_N)t} \\
\vdots & \ddots & \vdots \\
\end{pmatrix}$$

$$\rho(\infty) = \begin{pmatrix}
|c_1|^2 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & |c_N|^2 \\
\end{pmatrix}$$

For local observable, fast phase oscillations are averaged to zero...

28/09/2015
Relaxation... but thermalization?

- Dephasing explains relaxation, but how do we arrive at Gibbs distribution?

\[ \rho(\infty) \approx \begin{pmatrix} |c_1|^2 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & |c_n|^2 \end{pmatrix} \overset{?}{=} \frac{1}{Z} \begin{pmatrix} e^{-\beta E_1} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & e^{-\beta E_n} \end{pmatrix} \]

- How can memory be lost if the asymptotic states depend on the initial condition?

**Extreme example.** Start from an eigenstate...

\[ \Psi \simeq |E_n\rangle \longrightarrow \Psi(t) \simeq e^{-iE_nt}|E_n\rangle \]
The average of local observables does not fluctuate between close eigenstates.
Two spin example

\[ H = \epsilon S_z^1 - \epsilon S_z^2 + U (S_+^1 S_-^2 + S_+^2 S_-^1) \]

Factorized states

\[ |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle \]

"LOC"

\[ \langle n | S_z^1 | n \rangle = \pm \frac{1}{2} \]

High entanglement

\[ \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle) \]

"ETH"

\[ \langle n | S_z^1 | n \rangle = 0 \]
Simple numerical test of ETH

\[ H = \sum_{i=1}^{N} \omega_i \hat{S}_z^i + \sum_{i<j} A_{ij} (\hat{S}_+^i \hat{S}_-^j + c.c.) \]

- \( \omega_i \) random field
- \( A_{ij} \) random coupling \( \overline{A_{ij}} = 0 \)

\[ \frac{\sigma_A^2}{\sigma_h^2} \gg 1 \]
\[ \frac{\sigma_A^2}{\sigma_h^2} \ll 1 \]
\[ \frac{\sigma_A^2}{\sigma_h^2} \simeq 1 \]
Interesting... but is it observable?

Not at equilibrium...

\[ \rho_\beta = e^{-\beta H} \rightarrow \overline{S}_z^i = \text{Tr}(\hat{S}_z^i \rho_\beta) = Z^{-1} \sum_n e^{-\beta E_n} \langle E_n | \hat{S}_z^i | E_n \rangle \]
Dynamical observations

Quantum quenches in cold atoms experiments: change suddenly the system Hamiltonian

\[ H(\lambda = \lambda_0) \rightarrow H(\lambda = \lambda_1) \]

- Isolated quantum dynamics for sufficiently long times

- Lacks of thermalization for 1d systems close to integrable points.

Any other possibility?
Dynamic nuclear polarization

Solid material doped with unpaired localized electrons.

\[ H_0 = 1 \text{Tesla}, \beta^{-1} = 1.2K \]
\[ P_e = 94\%, \quad P_C = 0.086\% \]

But in presence of microwave irradiation...

\[ P_C \approx 40\% \]
Dynamic nuclear polarization

Solid material doped with

Anatomical 1H image  $^{13}$C-pyruvate  $^{13}$C-alanine  $^{13}$C-lactate

$P_C \approx 40\%$

28/09/2015  12/27
Thermal mixing regime

Different nuclear species achieve different levels of polarization

Jannin et al. (J. Phys. D 2008) - Tempo

But they are all described by a single parameter

\[
P_H = \tanh\left(\frac{\beta_s \omega_H}{2}\right) \quad P_C = \tanh\left(\frac{\beta_s \omega_C}{2}\right)
\]
**Intuitive explanation**

- The interaction between unpaired electrons is the fastest time-scale.
- Electrons are constantly at their own equilibrium.
- In the stationary state,
  \[ P_e = \text{Tr}(e^{-\beta_e(t)(S_z - \omega_0 S_z)}) = \tanh(\beta_e(t)(\omega_e - \omega_0(t)))) \]

All the nuclear species in contact with the electrons reach electron temperature.
Quantum jumps and spin-temperature

In the limit of fast decoherence, the electrons system is jumping from an eigenstate to the other...

\[ P_e(t) = \langle n(t) | S_z^1 | n(t) \rangle \approx \tanh(\beta(t) \omega_e - \omega_0(t)) \]

- fast decoherence
- thermal eigenstates (ETH)
Single-spin with reservoir

\[ \mathcal{H} = \hat{H}_S + \hat{H}_{\text{bath}} + \lambda \hat{H}_{\text{int}} \]

Weak coupling approximation: \( \lambda \ll 1 \)

Lindblad equation

\[ \frac{d\rho}{dt} = -i[\hat{H}_S, \rho] + \lambda^2 \mathcal{L}_\rho \]
Reservoir induced transitions

\[ \frac{d\rho}{dt} = -i[\hat{H}, \rho] + \lambda^2 L\rho \]

\[ \frac{h(\omega)}{h(-\omega)} = e^{\beta\omega} \]

\[
\begin{pmatrix}
\rho_{11} & \rho_{12} \\
\rho_{21} & \rho_{22}
\end{pmatrix}
\]

\[
\rightarrow
\begin{pmatrix}
\rho_{11} & 0 \\
0 & \rho_{22}
\end{pmatrix}
\]

\[
\rightarrow
\begin{pmatrix}
e^{\beta\omega/2} & 0 \\
0 & e^{-\beta\omega/2}
\end{pmatrix}
\]
Single spin with MW irradiation

\[ \hat{H}_{\text{MW}} = (\omega_e + \Delta)\hat{S}_z + \hat{H}_{\text{bath}} + \omega_1 \cos(\omega_{\text{MW}} t) \hat{S}_x \]

local inhomogeneities

reservoir at \( \beta = 1\,\text{K} \)
Single spin with MW irradiation

\[ \hat{H}_{ \text{MW}} = (\omega_e + \Delta) \hat{S}_z + \hat{H}_\text{bath} + \omega_1 \cos(\omega_{\text{MW}} t) \hat{S}_x \]

local inhomogeneities

reservoir at \( \beta = 1\)K
Mean-field interacting model

\[ H = \sum_{i=1}^{N} (\omega + \Delta_i) \hat{S}_z^i + \sum_{i<j} A_{ij} (\hat{S}_+^i \hat{S}_-^j + c.c.) \]

\[ \overline{A_{ij}} = 0, \quad \overline{A_{ij}^2} = U^2 / N \]

\[ W_{n\rightarrow n'} = h(\omega_{nn'}) W_{nn'}^{\text{bath}} + W_{nn'}^{\text{MW}} \]

reservoir induced transitions

MW induced transitions
Interaction tsunami

\[ 0 = \frac{dp_n^{\text{stat}}}{dt} = \sum_{n'} [W_{n' \rightarrow n} p_{n'}^{\text{stat}} - W_{n \rightarrow n'} p_n^{\text{stat}}]\]

\(p_n = \text{stationary occupation probability of the } n\text{-th eigenstate}\)

Numerical solution

\(N = 12\)

![Graph showing dramatic change induced by interactions]

28/09/2015
Collective cooling driven by MW

No interactions

Effective temperature description (Borghini 1970)

\[ P_e(\omega) = \tanh\left[ \frac{\beta_s}{2} (\omega - \omega_{MW}) \right] \]

for DNP \( \beta_s \gg \beta \)

\[ \omega_e \]

\[ \Delta \omega_e \]

28/09/2015
Collective cooling driven by MW

When interaction are turned on, electrons reach a steady state which looks like "equilibrium" with a temperature much lower than the environment.

No interactions

Effective temperature description (Borghini 1970)

\[ f(\omega) \tanh\left[ \frac{\beta}{2} (\omega - \omega_{MW}) \right] \]

for DNP \( \beta_s \gg \beta \)

\[ P_e(\omega) = \tanh\left[ \frac{\beta}{2} (\omega - \omega_{MW}) \right] \]
Summary

- Interactions trigger a radical change in the macroscopic behavior of the polarization profile

- The emergence of spin-temperature is associated to the presence of ETH

  ETH ensures a pseudo-thermal stationary state, the environment and microwave then fix the temperature

- A low spin-temperature induces DNP: nuclei thermalize to the effective temperature of the electron system

  Let's have a look to the nuclei...
Recipe to check thermal mixing

- numerical simulation: $N_e = 12$, $N_n = 1$
- match the stationary energy to get the effective temperature

$$
\sum_n p_n^{\text{stat}} \epsilon_n = \langle E \rangle = \frac{1}{Z} \sum_n e^{\beta_{el} \epsilon_n} \epsilon_n
$$

- system energy microcanonical
- temperature that produces this energy canonical

- compute the stationary nuclear polarization: $P_n = \sum_n p_n^{\text{stat}} \langle n|I_z|n \rangle$

- $P_n$ nuclear polarization in the simulation
- $\tanh \left( \frac{\beta_{el} \omega_n}{2} \right)$ polarization predicted by spin temperature

28/09/2015
Effect of interactions on the nuclei

\[ P_n = \tanh \left( \frac{\beta_{\text{el}} \omega_n}{2} \right) \]

- concentration
- interaction
- spin temperature

U = typical dipolar coupling

local hybridization vs. thermal mixing

28/09/2015
Effect of magnetic field on the nuclei

$tanh(\beta_{el} \omega_n / 2)$

$P_n$

thermal mixing

local hybridization

$h/h_0$

$P_n$

28/09/2015 25/27
Breaking ETH?

\[ H = \sum_{i=1}^{N} (\omega_e + \Delta_i) \hat{S}_z^i + \sum_{i<j} A_{ij} (\hat{S}_+^i \hat{S}_-^j + c.c.) \]

Failure of ETH for strong disorder similar to Anderson localization for single particles.

Many-body localization transition
Breaking ETH?

\[ H = \sum_{i=1}^{N} (\omega_e + \Delta_i) \hat{S}_z^i + \sum_{i<j} A_{ij} (\hat{S}_+^i \hat{S}_-^j + c.c.) \]

Failure of ETH for strong disorder similar to Anderson localization for single particles.

Many-body transition
Perspectives

• Simple quantum model for DNP as cooling by microwaves

• Take home message:

  fast decoherence + ETH \rightarrow effective thermal description

• Possibility to investigate microscopically how to optimize DNP

• Connections with fundamental physics

DNP to study Many-body localization?