From quantum quenches to microwave refrigerator

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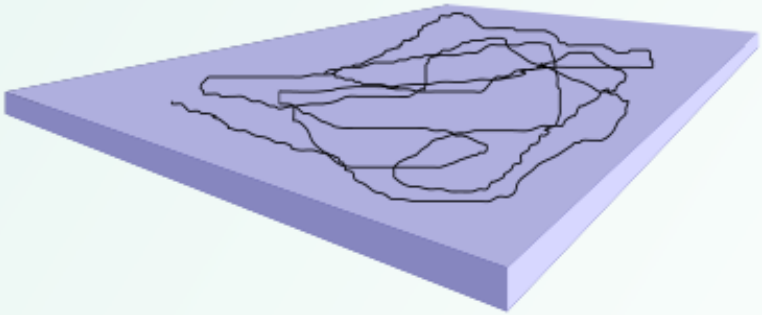
Classical Thermalization?

Time evolution inside the phase space



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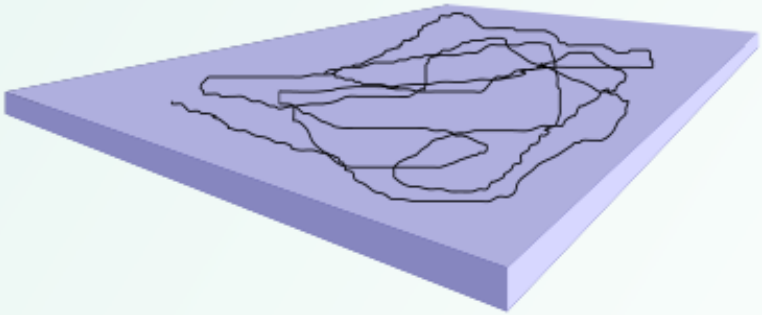


Average over the entire phase space

Quantum case

Quantum dynamics

$$i\hbar \frac{d\Psi}{dt} = H\Psi$$

$$\Psi(t) = \sum_n c_n e^{-iE_n t} |E\rangle \quad \rightarrow \quad \text{unitary dynamics}$$

Any closed quantum system has a discrete spectrum

How can relaxation occurs?

Density matrix formulation

$$|\Psi(t)\rangle = \sum_{n=1}^{N} c_n e^{-iE_n t} |E_n\rangle$$

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

Fundamental question

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

Dephasing

Time-dependence cannot disappear in general...

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

$$\downarrow$$

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

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

Relaxation... but thermalization?

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

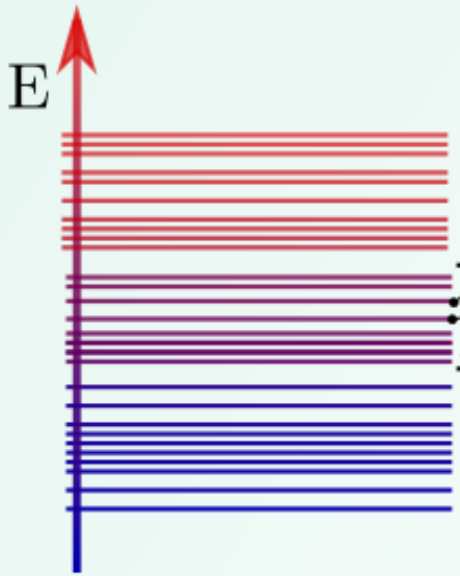
$$\rho(\infty) \simeq \begin{pmatrix} |c_1|^2 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & |c_n|^2 \end{pmatrix} \stackrel{?}{=} \frac{1}{Z} \begin{pmatrix} e^{-\beta E_1} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & e^{-\beta E_n} \end{pmatrix}$$

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

Extreme example. Start from an eigenstate...

$$\Psi \simeq |E_n\rangle \longrightarrow \Psi(t) \simeq e^{-iE_n t}|E_n\rangle$$

Eigenstate thermalization hypothesis



$$\langle E_n|O|E_n\rangle \simeq \langle E_{n+1}|O|E_{n+1}\rangle$$
$$\simeq \overline{O}_E$$

The average of local observables does not fluctuate between close eigenstates

Two spin example

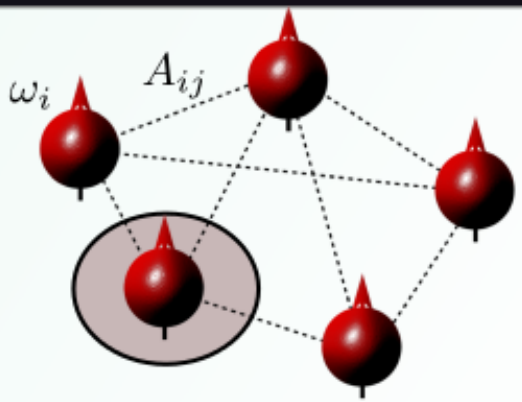
$$H = \epsilon S_z^1 - \epsilon S_z^2 + U(S_+^1 S_-^2 + S_+^2 S_-^1)$$

Factorized states	High entanglement
$\lvert\uparrow\downarrow\rangle, \lvert\downarrow\uparrow\rangle$	$\frac{1}{\sqrt{2}}(\lvert\uparrow\downarrow\rangle \pm \lvert\downarrow\uparrow\rangle)$
"LOC"	"ETH"
$\langle n\lvert S_z^1\rvert n\rangle = \pm\frac{1}{2}$	$\langle n\lvert S_z^1\rvert n\rangle = 0$

U/ϵ

Simple numerical test of ETH

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

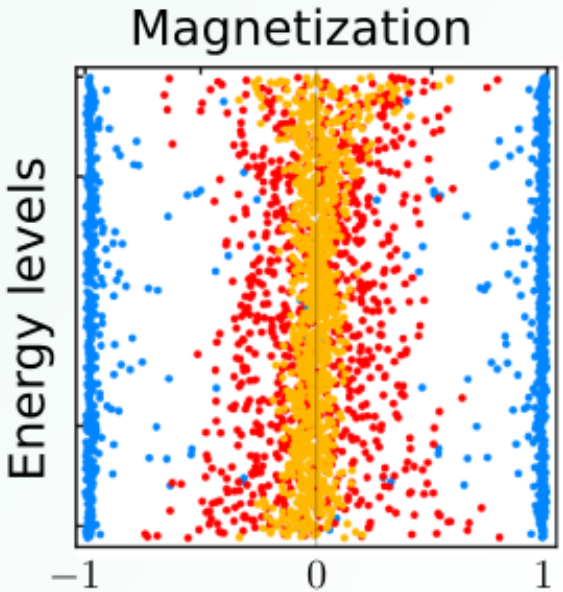


- ω_i random field
- A_{ij} random coupling $\overline{A_{ij}} = 0$

$$\frac{\sigma_A^2}{\sigma_h^2} \gg 1$$

$$\frac{\sigma_A^2}{\sigma_h^2} \ll 1$$

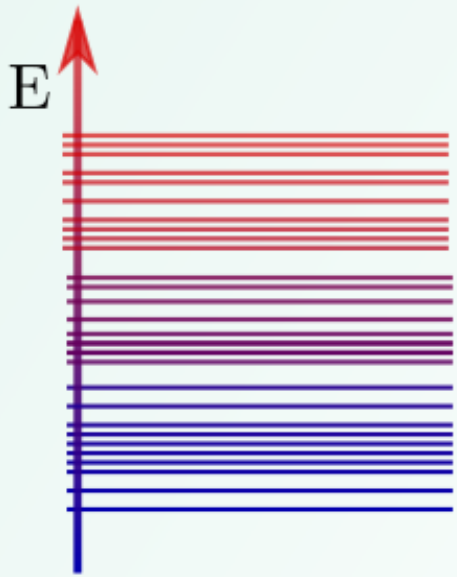
$$\frac{\sigma_A^2}{\sigma_h^2} \simeq 1$$



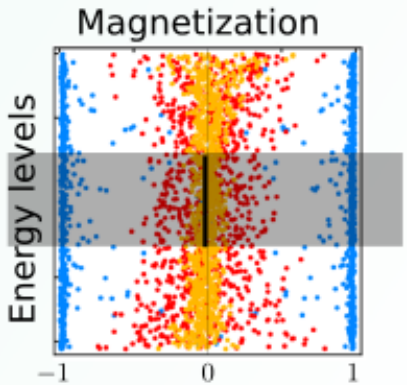
Interesting... but is it observable?

Not at equilibrium...

$$\rho_\beta = e^{-\beta H} \rightarrow \overline{S_z^i} = \mathrm{Tr}(\hat{S}_z^i \rho_\beta) = Z^{-1} \sum_n e^{-\beta E_n} \langle E_n | \hat{S}_z^i | E_n \rangle$$

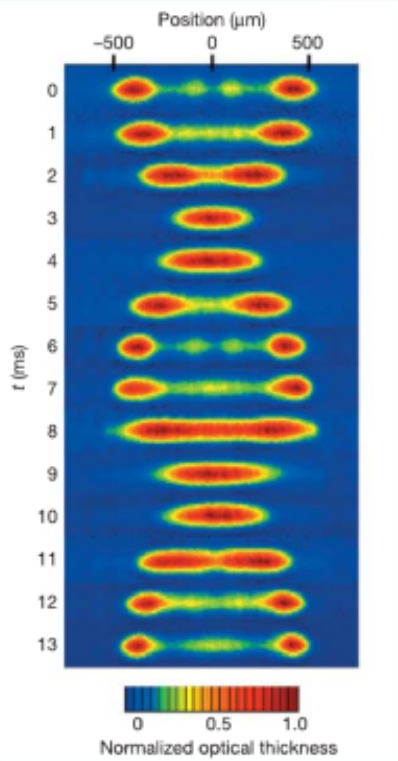


$$E_{n+1} - E_n \simeq 1/2^N$$



Dynamical observations

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



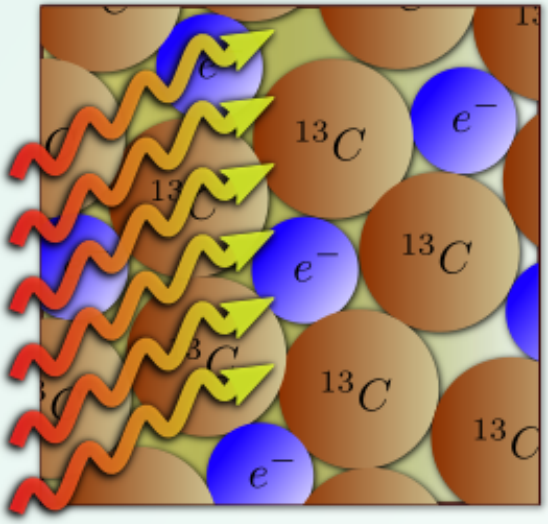
$$H(\lambda = \lambda_0) \to H(\lambda = \lambda_1)$$

- Isolated quantum dynamics for sufficiently long times

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

Any other possibility?

Dynamic nuclear polarization



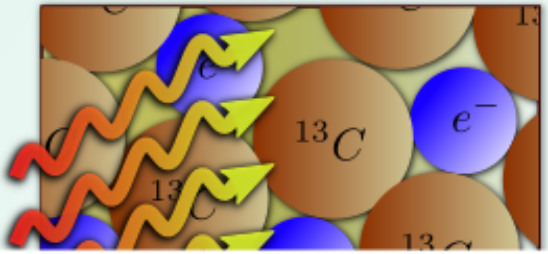
Solid material doped with unpaired localized electrons.

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

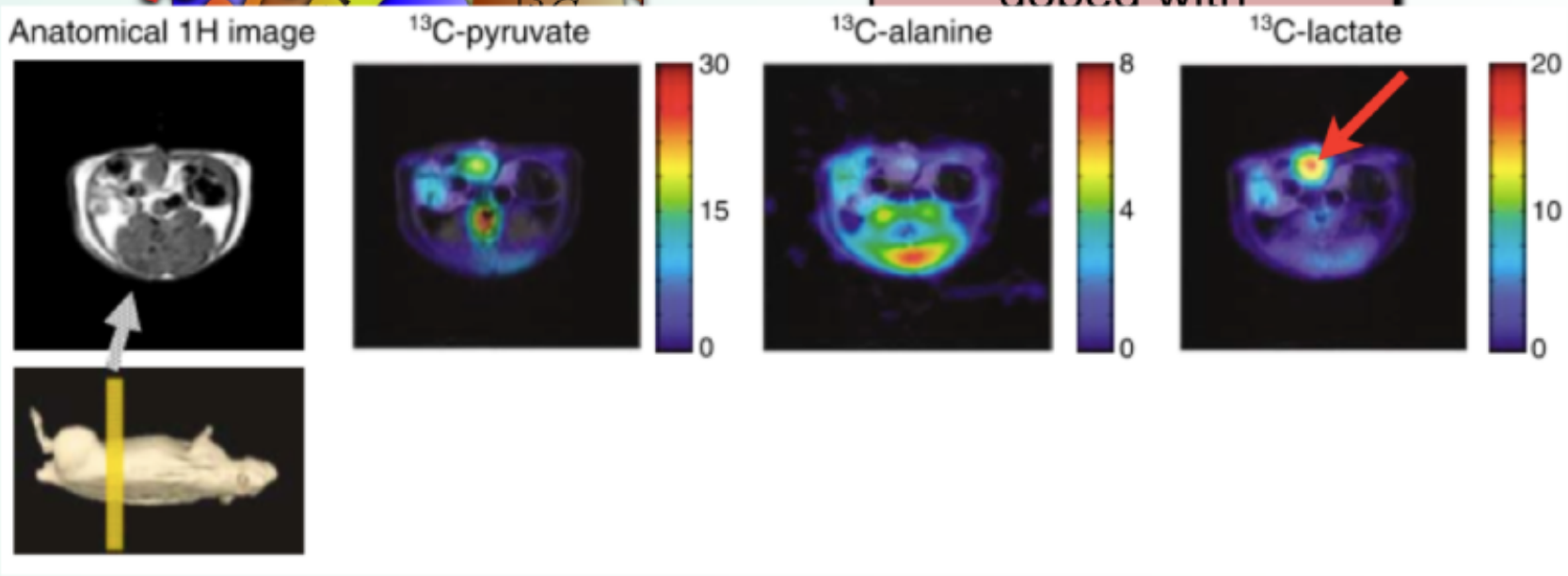
But in presence of microwave irradiation...

$$P_C \simeq 40\%$$

Dynamic nuclear polarization



Solid material doped with

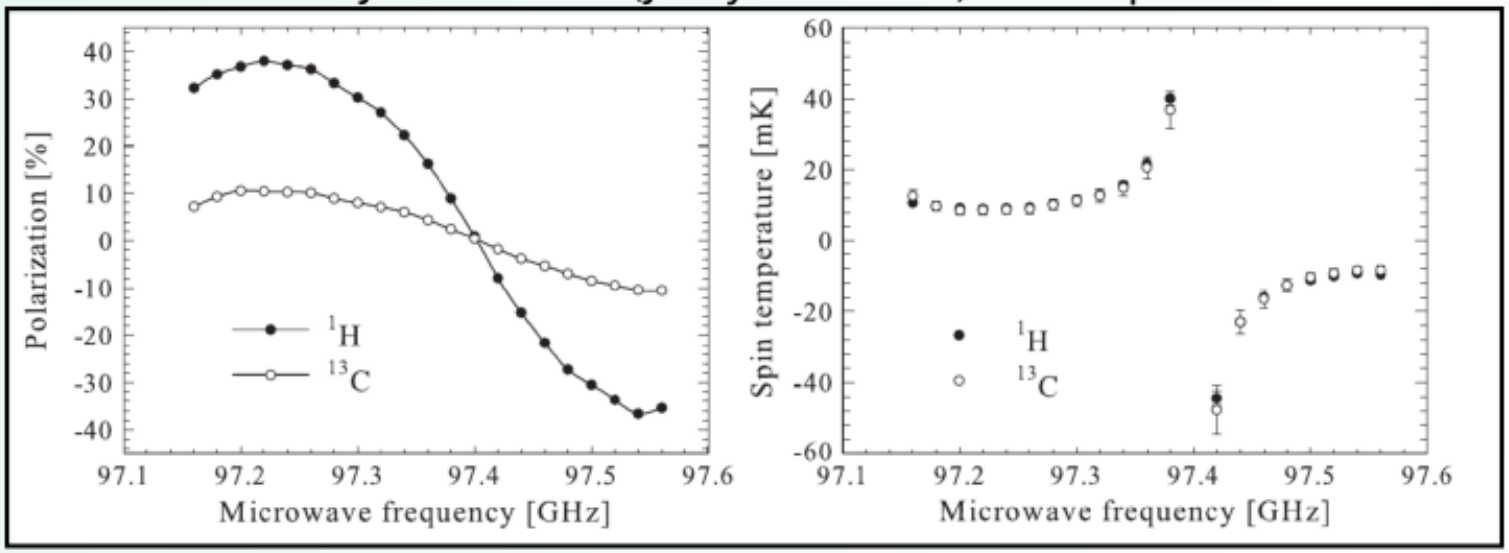


$$P_C \simeq 40\%$$

Thermal mixing regime

Different nuclear species achieve different levels of polarization

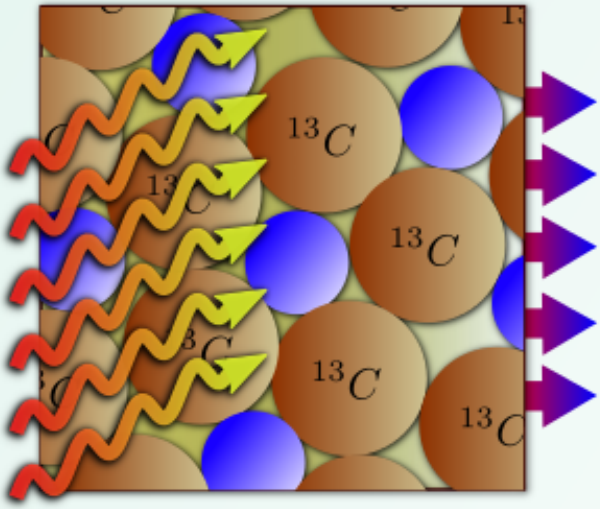
Jannin et al. (J.Phys. D 2008) - Tempo



But they are all described by a single parameter

$$P_H = \tanh(\beta_s \omega_H / 2) \qquad P_C = \tanh(\beta_s \omega_C / 2)$$

Intuitive explanation



- the interaction between unpaired electrons is the fastest time-scale
- electrons are constantly at their own equilibrium

$$P_e = \mathrm{Tr}(e^{-\beta_e(t)(S_z - \omega_0 S_z)}) = \tanh(\beta_e(t)(\omega_e - \omega_0(t)))$$

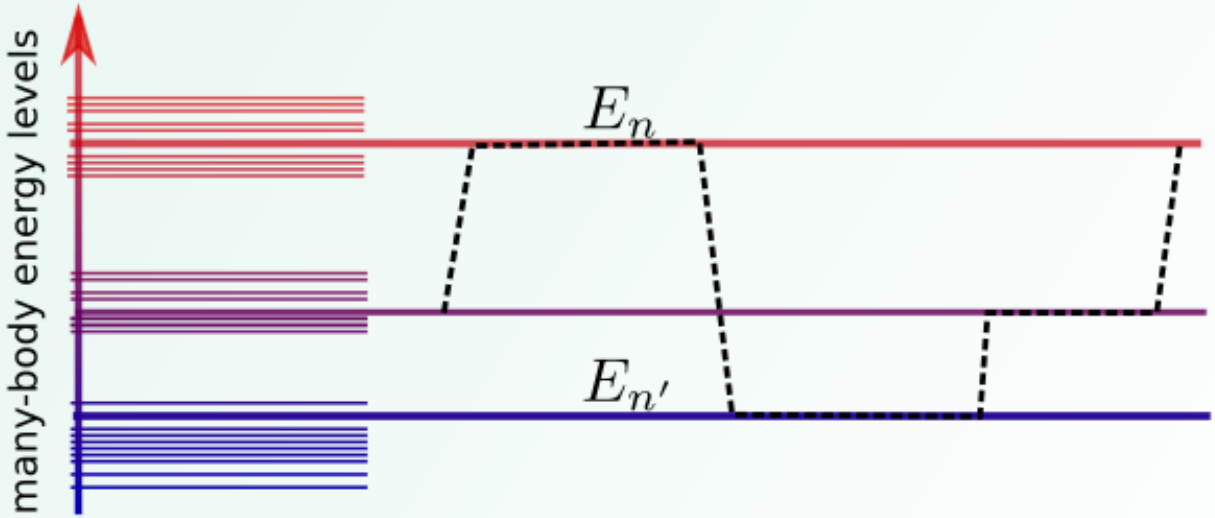
- in the stationary state

$$\beta_e(t) \to \beta_s$$

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...



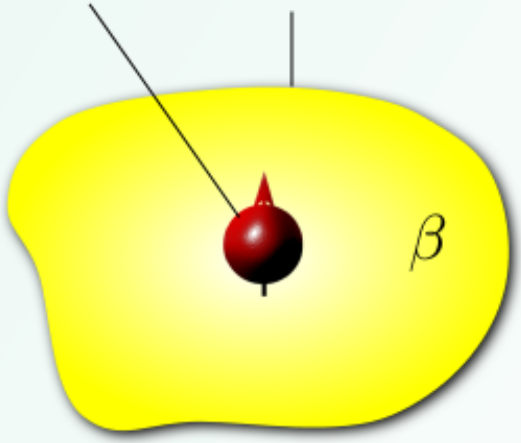
$$P_e(t) = \langle n(t)|S_z^1|n(t)\rangle \simeq \tanh(\beta(t)\omega_e - \omega_0(t))$$

fast decoherence

thermal eigenstates (ETH)

Single-spin with reservoir

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



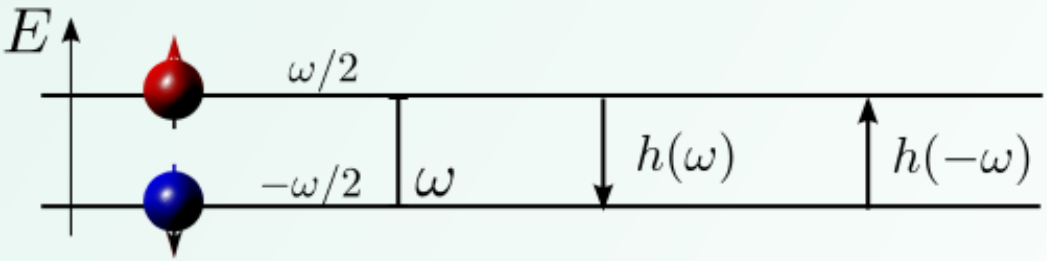
Weak coupling approximation: $\lambda \ll 1$

Lindblad equation

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

Reservoir induced transitions

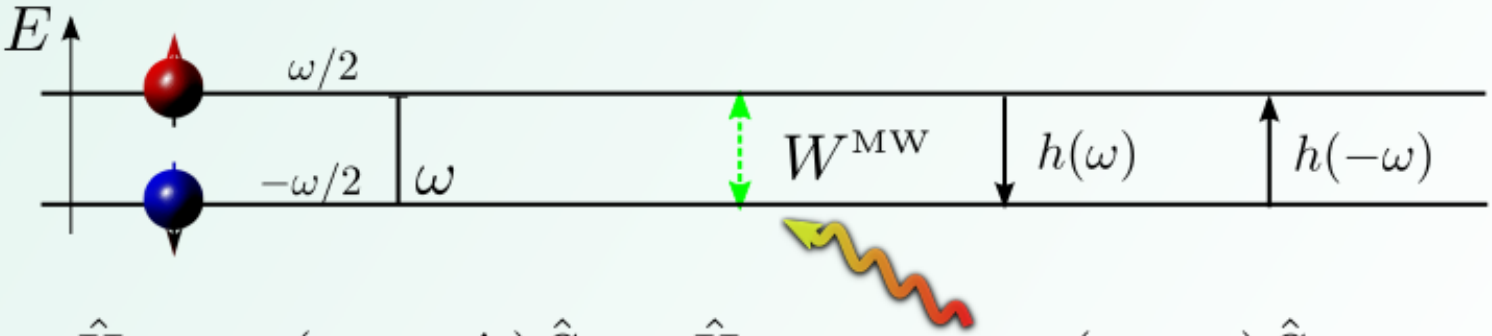
$$\frac{d\rho}{dt} = -i[\hat{H}, \rho] + \lambda^2 \mathcal{L}\rho$$



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

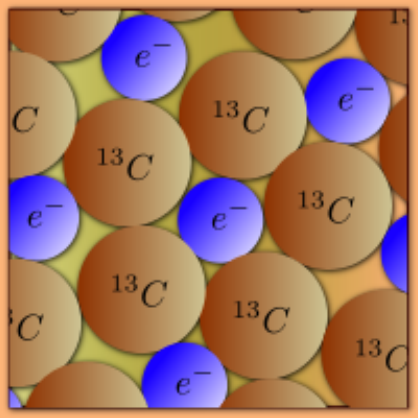
$$\begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} \xrightarrow{\text{dephasing}} \begin{pmatrix} \rho_{11} & 0 \\ 0 & \rho_{22} \end{pmatrix} \xrightarrow{\text{relaxation}} \begin{pmatrix} e^{\beta\omega/2} & 0 \\ 0 & e^{-\beta\omega/2} \end{pmatrix}$$

Single spin with MW irradiation

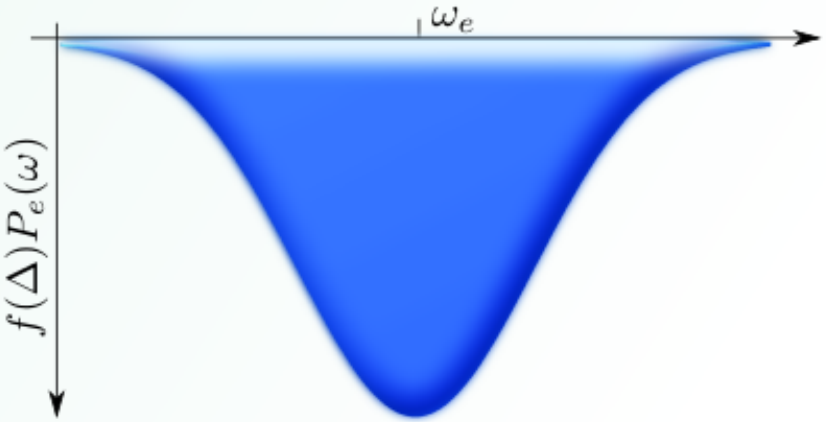


$$\hat{H}_{\mathrm{MW}} = (\omega_e + \Delta)\hat{S}_z + \hat{H}_{\mathrm{bath}} + \omega_1 \cos(\omega_{\mathrm{MW}} t)\hat{S}_x$$

local inhomogeneities



reservoir at $\beta = 1\mathrm{K}$



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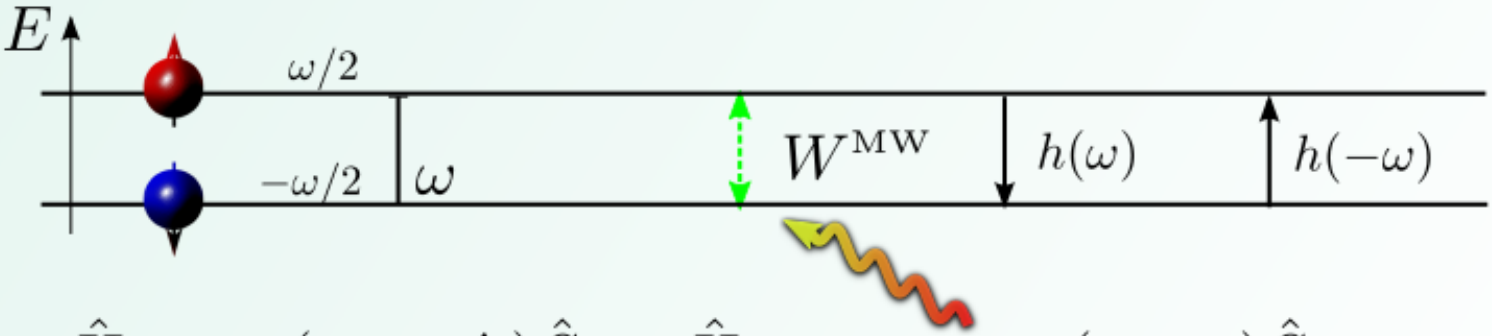

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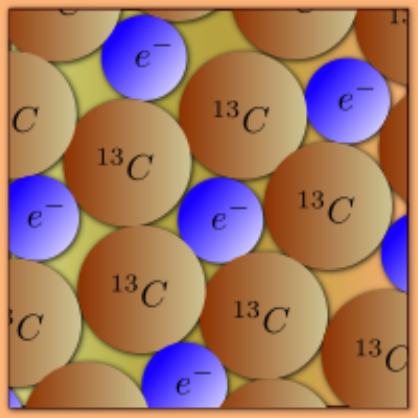

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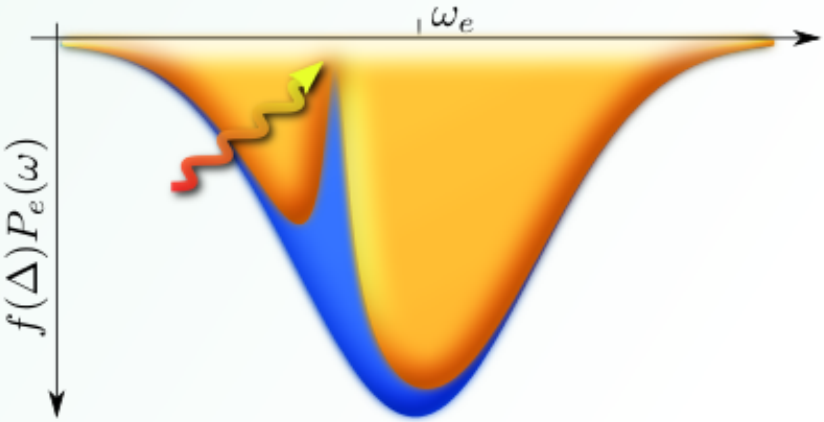
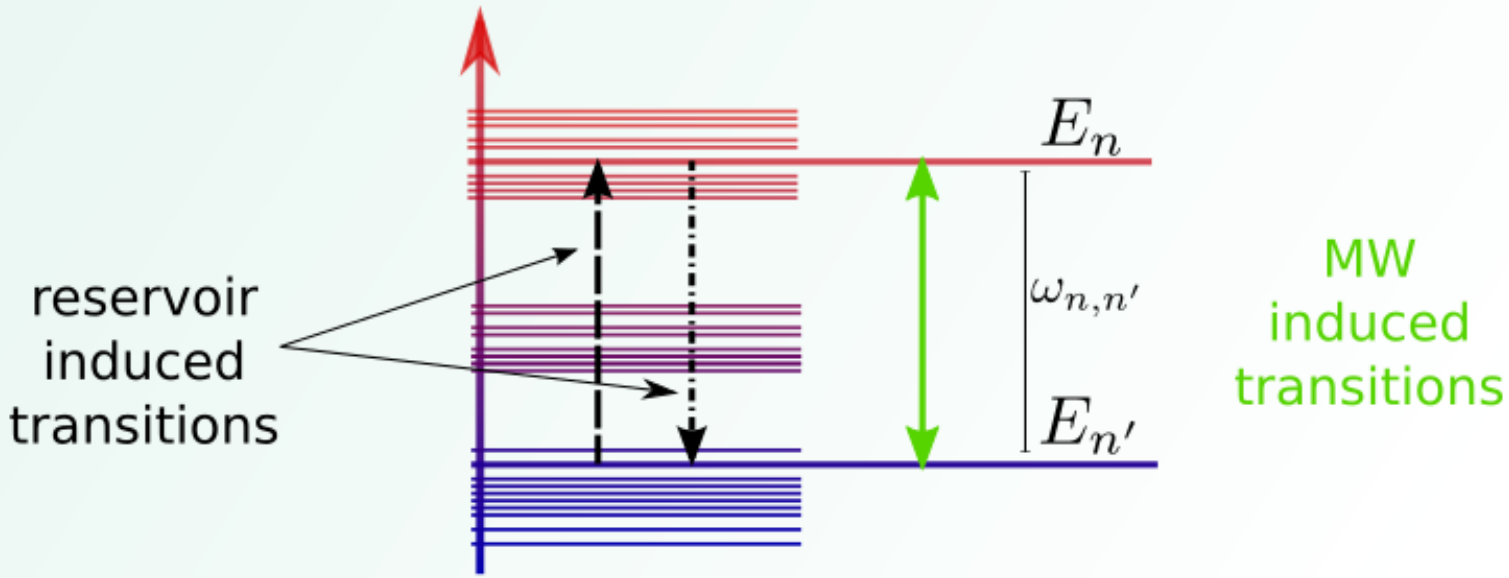


Mean-field interacting model

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

$$\overline{A_{ij}} = 0, \qquad \overline{A_{ij}^2} = U^2/N$$

$$W_{n\to n'} = h(\omega_{nn'})W_{nn'}^{\text{bath}} + W_{nn'}^{\text{MW}}$$



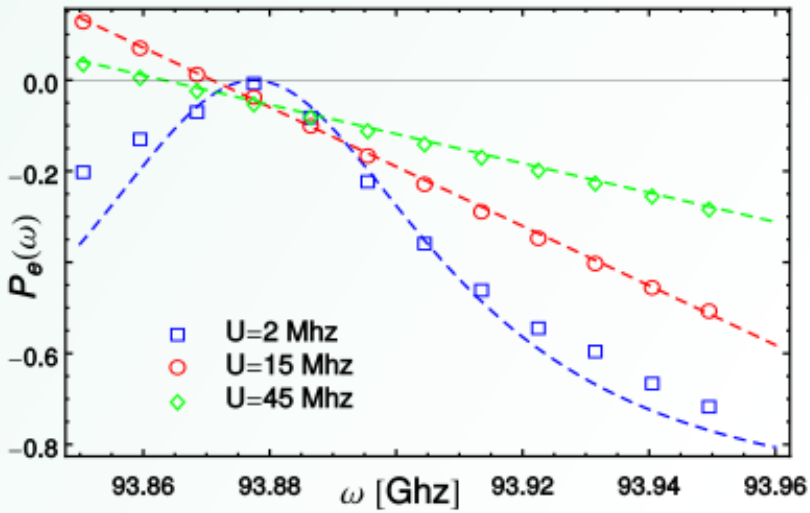
Interaction tsunami

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

p_n = stationary occupation probability of the n-th eigenstate

Numerical solution
N = 12

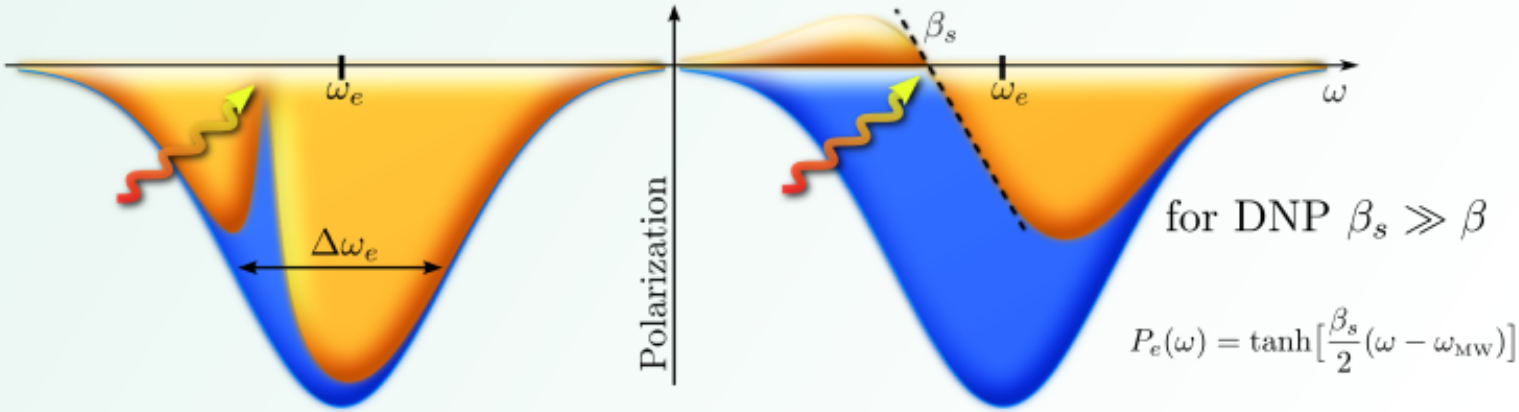
dramatic change induced by interactions



Collective cooling driven by MW

No interactions

Effective temperature description (Borghini 1970)



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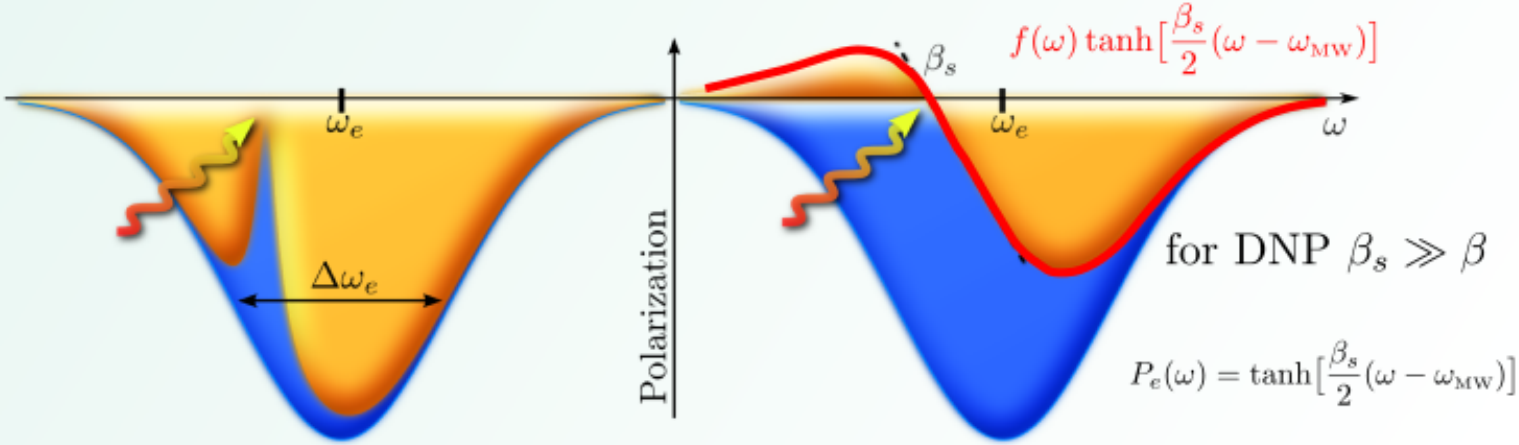


When interaction are turned on, electrons reach a steady state which looks like "equilibrium" with a temperature much lower than the environment

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

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

$$\underbrace{\langle E \rangle}_{\substack{\text{system energy} \\ \text{microcanonical}}} \longrightarrow \underbrace{\beta_{\text{el}}}_{\substack{\text{temperature that produces this energy} \\ \text{canonical}}}$$

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

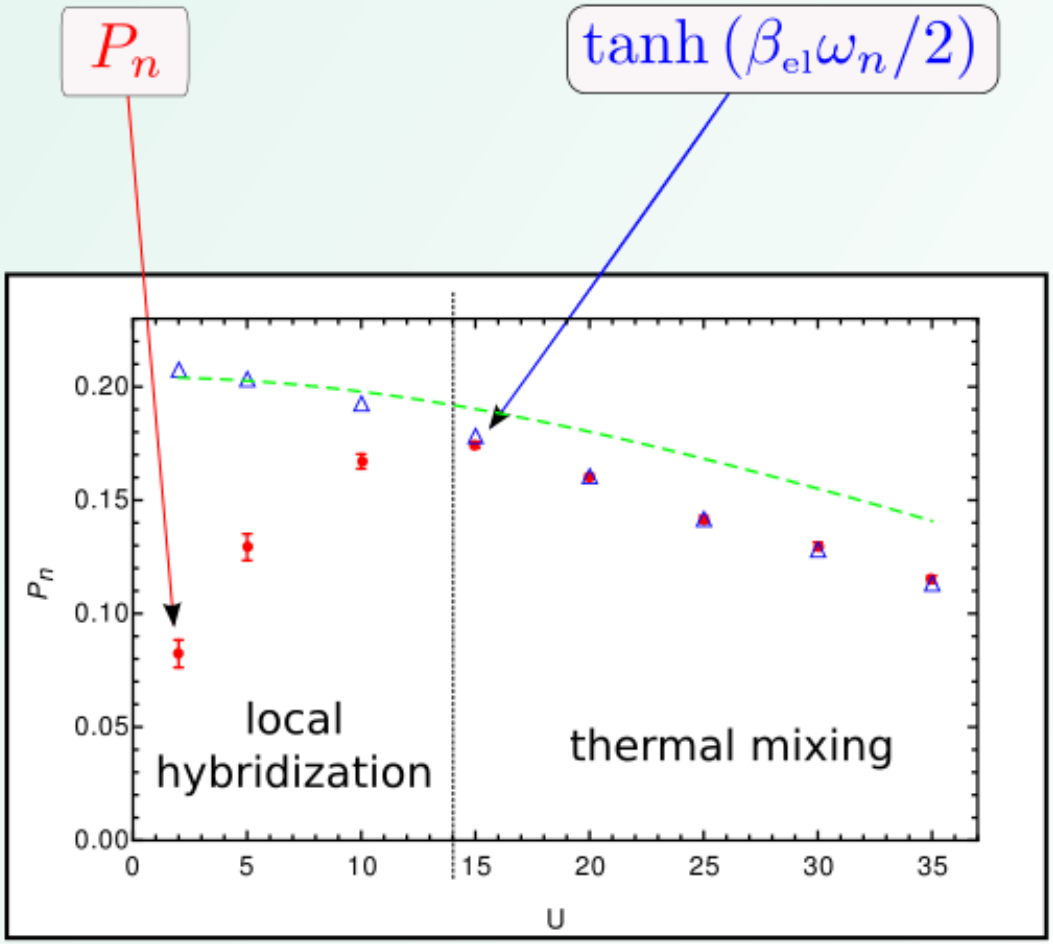
P_n

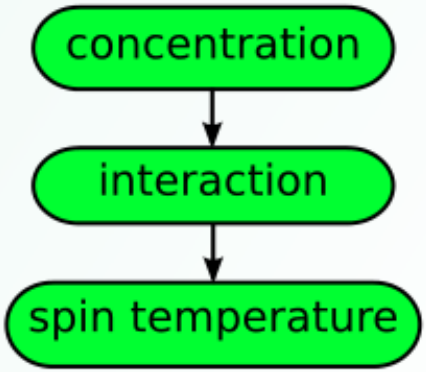
nuclear polarization
in the simulation

$\tanh\left(\frac{\beta_{\text{el}} \omega_n}{2}\right)$

polarization predicted
by spin temperature

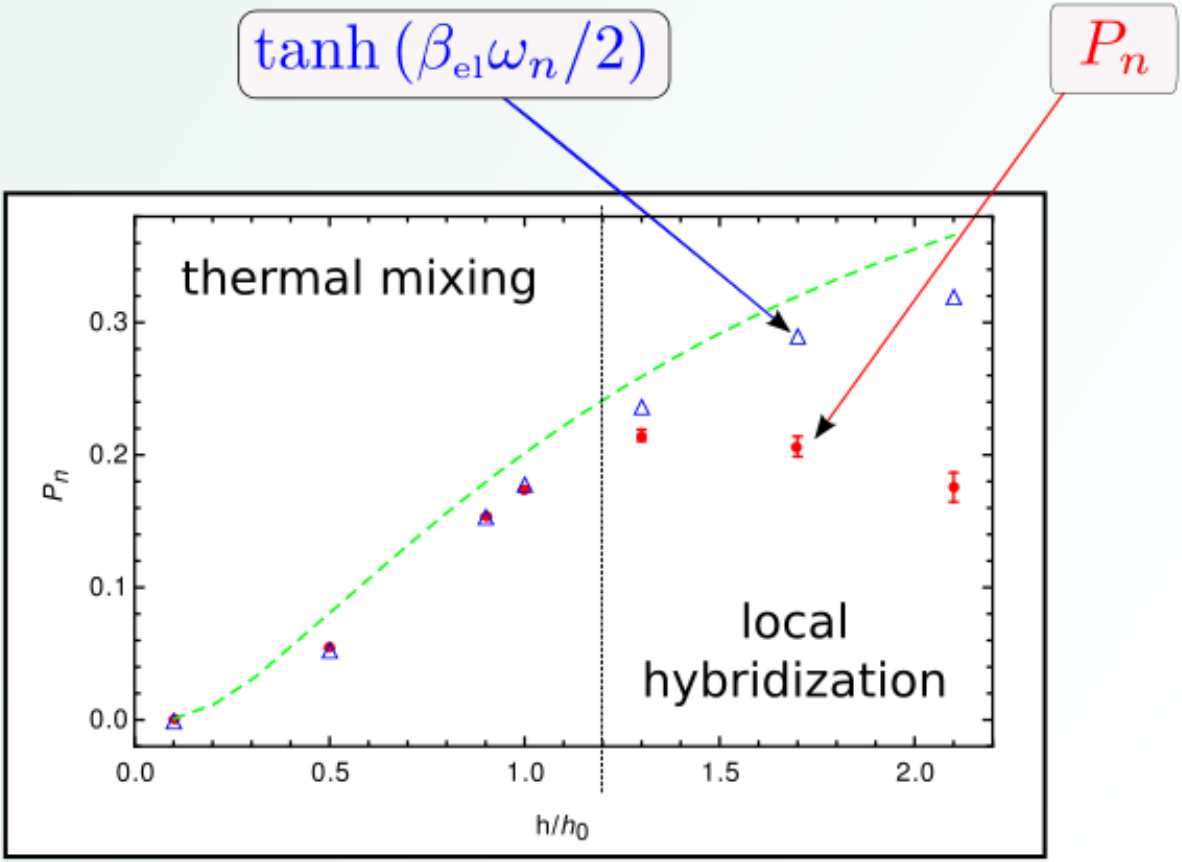
Effect of interactions on the nuclei





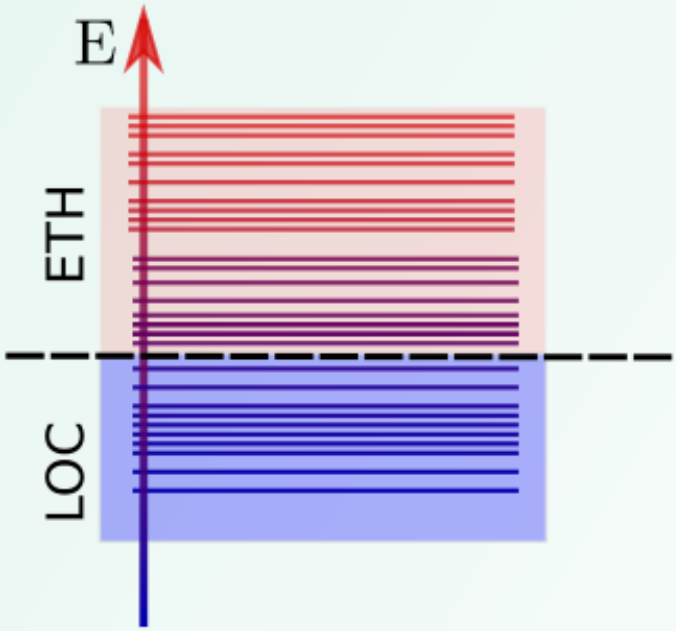
U = typical dipolar coupling

Effect of magnetic field on the nuclei



Breaking ETH?

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



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

Many-body localizion transition

Breaking ETH?

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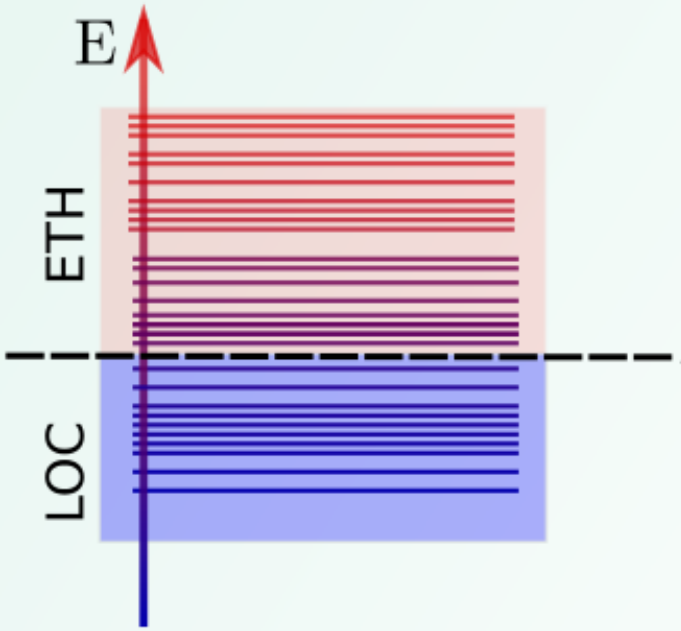
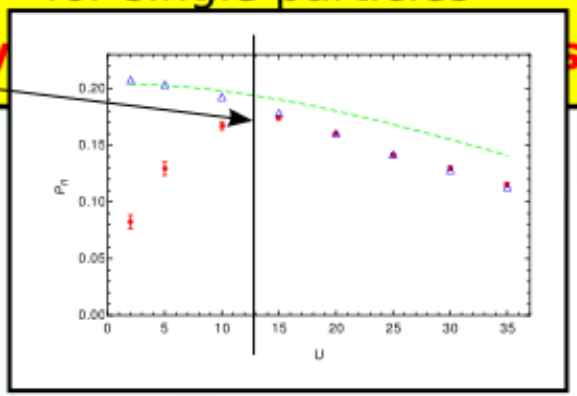


Failure of ETH for strong disorder similar to Anderson localization for single particles

Many **sition**



Perspectives

- Simple quantum model for DNP as **cooling by microwaves**

- Take home message:

fast decoherence + ETH → effective thermal description

- Possibility to investigate microscopically how to optimize DNP

- Connections with fundamental physics

DNP to study Many-body localization?