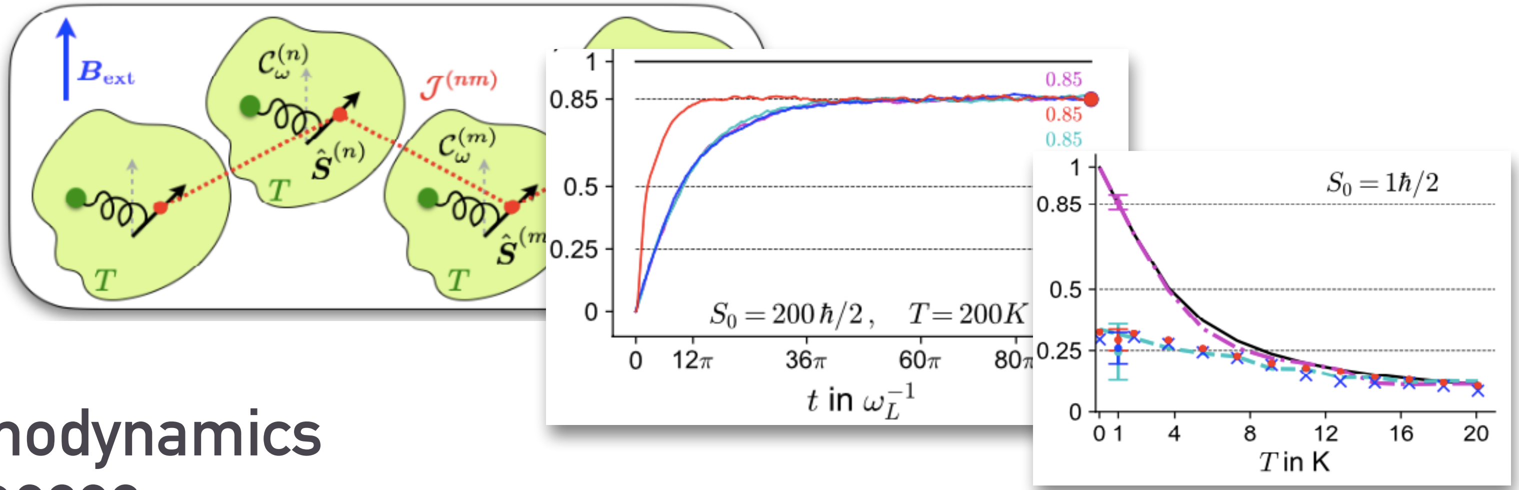

Quantum Thermodynamics
Conference QTD2020
(virtually in) Barcelona
21 Oct 2020

Versatile three-dimensional quantum spin dynamics equation with guaranteed fluctuation-dissipation link
Anders, Sait, Horsley, arxiv 2009.00600v1 (2020)

Deriving a generalised Landau-Lifschitz-Gilbert (LLG) equation from a system+bath Hamiltonian

Janet Anders
University of Exeter (part-time)
& University of Potsdam (part-time)

joint work with:
Simon Horsley
Connor Sait

UNIVERSITY OF EXETER
Universität Potsdam
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MOTIVATION

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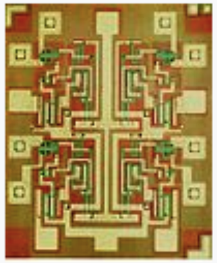
Semiconductor device fabrication



MOSFET scaling (process nodes)

- 10 µm – 1971
- 6 µm – 1974
- 3 µm – 1977
- 1.5 µm – 1981
- 1 µm – 1984
- 800 nm – 1987
- 600 nm – 1990
- 350 nm – 1993
- 250 nm – 1996
- 180 nm – 1999
- 130 nm – 2001
- 90 nm – 2003
- 65 nm – 2005
- 45 nm – 2007
- 32 nm – 2009
- 22 nm – 2012
- 14 nm – 2014
- 10 nm – 2016
- 7 nm – 2018
- 5 nm – 2020

Future

- 3 nm – *~2022*
- 2 nm – *~2023<*

cost

EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

Quantum Thermodynamics understanding will underpin future technologies at the nanoscale

MOTIVATION

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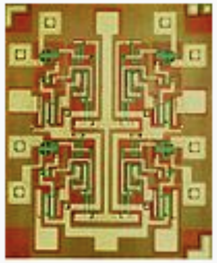
Semiconductor device fabrication



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cost

EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

Quantum Thermodynamics understanding will underpin future technologies at the nanoscale

In magnetism, the LLG equation has been used for 50 years+, but it is hitting its limits for some materials at short times

Article | Published: 28 September 2020

Inertial spin dynamics in ferromagnets

Kumar Neeraj, Nilesh Awari, Sergey Kovalev, Debanjan Polley, Nanna Zhou Hag

Nature Physics (2020) | Cite this article

1942 Accesses | **122** Altmetric | Metrics

Previous LLG extensions have struggled with how to consistently maintain the Fluct-Diss-Rel (FDR), and how to systematically go beyond LLG.

WHAT IS THE LLG EQUATION?

phenomenological equation that describes the damped dynamics of a spin $\boldsymbol{S}$ (implicit eq.)

Gilbert damping,
with damping η
(+)

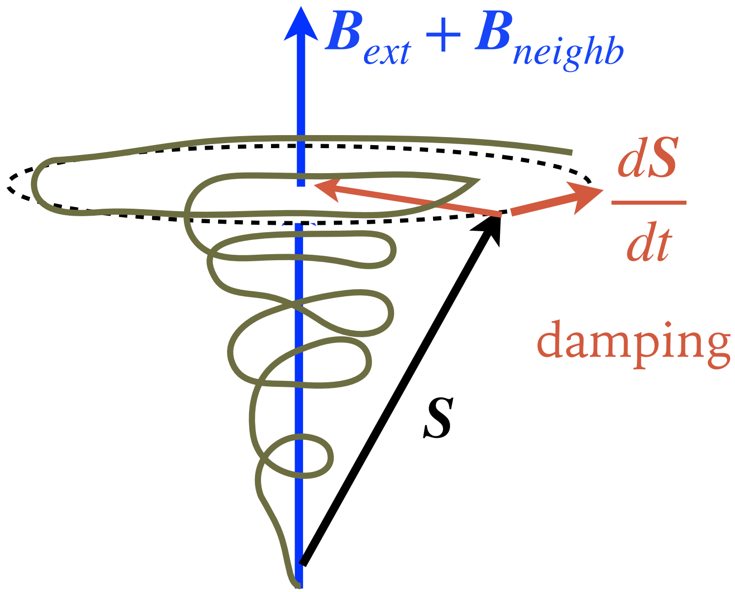
LLG

$$\frac{d\boldsymbol{S}}{dt} = \boldsymbol{S} \times \left(\gamma \boldsymbol{B}_{ext} + \gamma \boldsymbol{B}_{neighb} + \gamma \boldsymbol{b}_{th} - \gamma \eta \frac{d\boldsymbol{S}}{dt} \right)$$

gyromagnetic ratio γ
(can be +/-)

externally applied field + field from interaction with neighbours (exchange)

stochastic thermal field



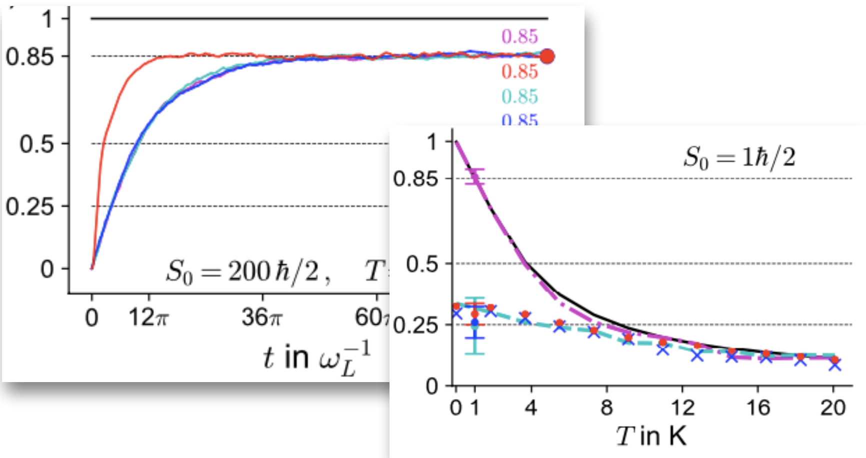
KEY MESSAGE

(different from Caldeira-Leggett and spin boson models)

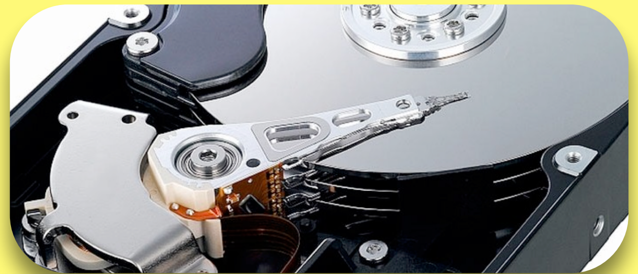
Based on system+bath Hamiltonian, derived general three-dimensional spin dynamics equation

$$\frac{\mathrm{d}\hat{\boldsymbol{S}}^{(n)}(t)}{\mathrm{d}t} = \hat{\boldsymbol{S}}^{(n)}(t) \times \Big[\gamma \boldsymbol{B}_{\text{ext}} + \sum_{m\neq n} \bar{\mathcal{J}}^{(nm)} \cdot \hat{\boldsymbol{S}}^{(m)}(t) + \gamma\, \hat{\boldsymbol{b}}^{(n)}(t) + \gamma^2 \int_{-\infty}^{t} \mathrm{d}t'\, \mathcal{K}^{(n)}(t-t') \cdot \hat{\boldsymbol{S}}^{(n)}(t')\Big], \quad (11)$$

Beyond LLG dynamics:
faster magnetisation equilibration and non-Gibbs steady state



A quantum thermodynamic model directly relevant to current magnetism technology (hard drives)



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OUTLINE

- ➤ System+bath Hamiltonian
- ➤ General spin dynamics equation
- ➤ LLG and Lorentzian coupling
- ➤ Short-time dynamics
- ➤ Equilibration
- ➤ Steady state magnetisation
- ➤ Conclusions and open questions

SYSTEM+BATH HAMILTONIAN

$$\hat{H} = \hat{H}_S + \hat{H}_R + \hat{V}_{\text{int}}$$

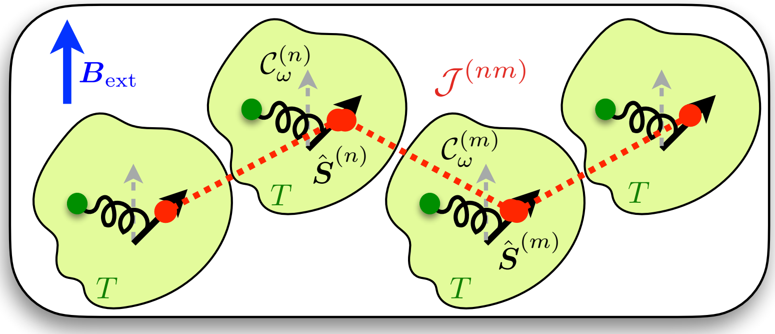
free Larmor frequency

$$\omega_L = |\gamma \boldsymbol{B}_{\text{ext}}|$$

system Hamiltonian

$$\hat{H}_S = -\gamma \sum_n \hat{\boldsymbol{S}}^{(n)} \cdot \boldsymbol{B}_{\text{ext}} - \frac{1}{2} \sum_{n \neq m} \hat{\boldsymbol{S}}^{(n)} \cdot \mathcal{J}^{(nm)} \cdot \hat{\boldsymbol{S}}^{(m)}$$

spin vector operator
at lattice site n $\quad [\hat{S}_j^{(n)}, \hat{S}_k^{(m)}] = \mathrm{i}\hbar\,\delta_{mn} \sum_k \epsilon_{jkl} \hat{S}_l^{(n)}$



bath Hamiltonian

$$\hat{H}_R = \frac{1}{2} \sum_n \int_0^\infty \mathrm{d}\omega \left[\left(\hat{\boldsymbol{\Pi}}_\omega^{(n)} \right)^2 + \omega^2 \left(\hat{\boldsymbol{X}}_\omega^{(n)} \right)^2 \right]$$

continuous bath of (3D) harmonic oscillators
(one for each site *n*)

Huttner, Barnett,
PRA **46** 4306 (1992)

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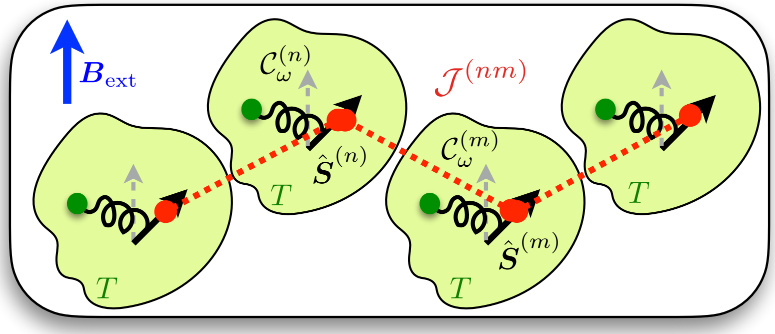

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continuous bath of (3D) harmonic oscillators
(one for each site n)

linear interaction

$$\hat{V}_{\text{int}} = -\gamma \sum_n \hat{\boldsymbol{S}}^{(n)} \cdot \int_0^\infty \mathrm{d}\omega\, \mathcal{C}_\omega^{(n)} \cdot \hat{\boldsymbol{X}}_\omega^{(n)}$$

coupling function (tensor)
(one for each site n)

Huttner, Barnett,
PRA **46** 4306 (1992)

GENERAL SPIN DYNAMICS EQUATION

… Heisenberg picture equation for the spin vector operator at site *n*:

$$\frac{\mathrm{d}\hat{\boldsymbol{S}}^{(n)}(t)}{\mathrm{d}t} = \hat{\boldsymbol{S}}^{(n)}(t) \times \Big[\gamma \boldsymbol{B}_{\mathrm{ext}} + \sum_{m\neq n} \mathcal{J}^{(nm)} \cdot \hat{\boldsymbol{S}}^{(m)}(t) + \gamma\, \hat{\boldsymbol{b}}^{(n)}(t) + \gamma^2 \int_{-\infty}^{t} \mathrm{d}t'\, \mathcal{K}^{(n)}(t-t') \cdot \hat{\boldsymbol{S}}^{(n)}(t')\Big]$$

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stochastic noise field: $\hat{\boldsymbol{b}}^{(n)}(t) = \int_0^\infty \mathrm{d}\omega \sqrt{\frac{\hbar}{2\omega}}\, \mathcal{C}_\omega^{(n)} \cdot \left(\hat{\boldsymbol{a}}_\omega^{(n)} e^{-\mathrm{i}\omega t} + \hat{\boldsymbol{a}}_\omega^{(n)\,\dagger} e^{+\mathrm{i}\omega t} \right)$

memory kernel: $\mathcal{K}^{(n)}(\tau) = \Theta(\tau) \int_0^\infty \mathrm{d}\omega\, \frac{\mathcal{C}_\omega^{(n)} \cdot \mathcal{C}_\omega^{(n)\,\mathrm{T}}}{\omega} \sin(\omega\tau)$

b and *K* fulfil a fluctuation dissipation relation

FLUCTUATION-DISSIPATION RELATION

Kubo (1966)

FDR

$$\tilde{P}^{(nn)}_{jk}(\omega) = \hbar\,\mathrm{Im}[\tilde{\mathcal{K}}^{(n)}_{jk}(\omega)]\;\coth\frac{\beta\hbar\omega}{2}$$

noise present at 0K

fluctuations in noise ($\hat{\boldsymbol{b}}$)

dissipation (damping)

quantum (thermal) noise

approximation for high T/low ω:

$k_B T \gg \frac{\hbar\omega}{2}$

$$\tilde{P}^{(nn)}_{jk}(\omega) = \hbar\,\mathrm{Im}[\tilde{\mathcal{K}}^{(n)}_{jk}(\omega)]\;\frac{2}{\beta\hbar\omega}$$

no 0K noise

(classical) white noise

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fluctuations in noise ($\hat{\boldsymbol{b}}$)

dissipation (damping)

quantum (thermal) noise

for any coupling function $C_\omega^{(n)}$

approximation for high T/low ω:

$k_B T \gg \frac{\hbar\omega}{2}$

$$\tilde{P}_{jk}^{(nn)}(\omega) = \hbar\,\mathrm{Im}[\tilde{\mathcal{K}}_{jk}^{(n)}(\omega)]\ \frac{2}{\beta\hbar\omega}$$

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LLG AND LORENTZIAN COUPLING

choose for all n

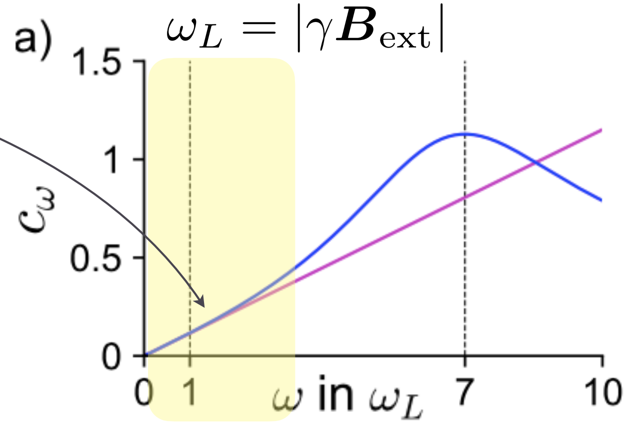
linear coupling in ω:

$$c_\omega^{\mathsf{LLG}} = \sqrt{\frac{2\eta\,\cos(\omega\epsilon^+)}{\pi}}\,\frac{\omega}{\omega_L}$$

(Ohmic)

(unit-free)

$\epsilon^+ = 0^\downarrow$



LLG

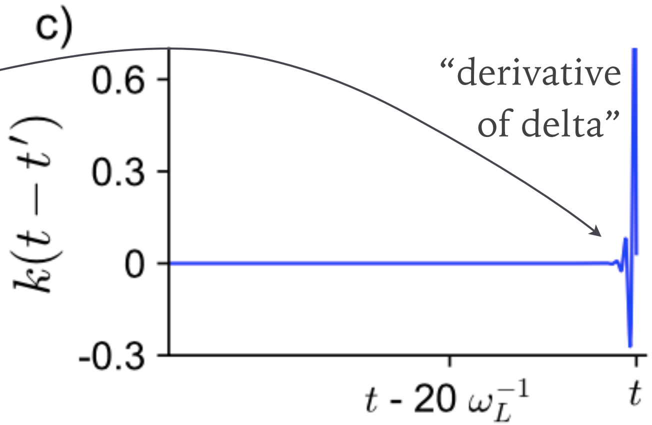
linear

get **instantaneous** memory kernel:

$t^- = t - \epsilon^+$

$$k^{\mathsf{LLG}}(t-t') = \frac{\eta}{\omega_L^2}\,\partial_{t'}\delta(t^- - t')$$

(unit-free)



no memory

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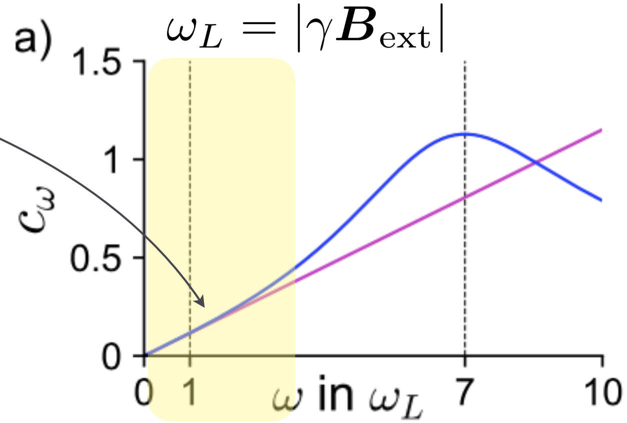

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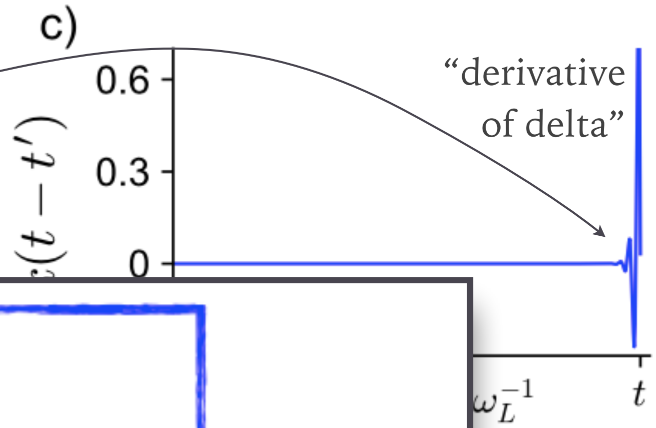

no memory

$$\frac{\mathrm{d}\hat{\boldsymbol{S}}^{(n)}(t)}{\mathrm{d}t} = \hat{\boldsymbol{S}}^{(n)}(t) \times \Big[\gamma \boldsymbol{B}_{\mathrm{ext}} + \sum_{m\neq n} \mathcal{J}^{(nm)} \cdot \hat{\boldsymbol{S}}^{(m)}(t) + \gamma \hat{\boldsymbol{b}}^{(n)}(t) + \gamma^2 \int_{-\infty}^{t} \mathrm{d}t'\,\mathcal{K}^{(n)}(t-t') \cdot \hat{\boldsymbol{S}}^{(n)}(t')\Big]$$

get: $\int_{-\infty}^{t} \mathrm{d}t'\,\mathcal{K}^{(n)}(t-t') \cdot \hat{\boldsymbol{S}}^{(n)}(t') \;\propto\; \int_{-\infty}^{t} dt'\,\eta\,\partial_{t'}\delta(t^- - t')\,\boldsymbol{S}(t') \;\propto\; -\eta\,\partial_t \boldsymbol{S}(t)$

recover:

LLG $\quad \dfrac{d\boldsymbol{S}}{dt} = \boldsymbol{S} \times \left(\gamma \boldsymbol{B}_{ext} + \gamma \boldsymbol{B}_{neighb} + \gamma \boldsymbol{b}_{th} - \gamma\eta \dfrac{d\boldsymbol{S}}{dt}\right)$ ✓

LLG AND LORENTZIAN COUPLING

choose for all n

linear coupling in ω:

$$c_\omega^{\mathsf{LLG}} = \sqrt{\frac{2\eta\cos(\omega\epsilon^+)}{\pi}}\,\frac{\omega}{\omega_L}$$

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(unit-free)

$\epsilon^+ = 0^\downarrow$

get **instantaneous** memory kernel:

$t^- = t - \epsilon^+$

$$k^{\mathsf{LLG}}(t-t') = \frac{\eta}{\omega_L^2}\,\partial_{t'}\delta(t^- - t')$$

(unit-free)

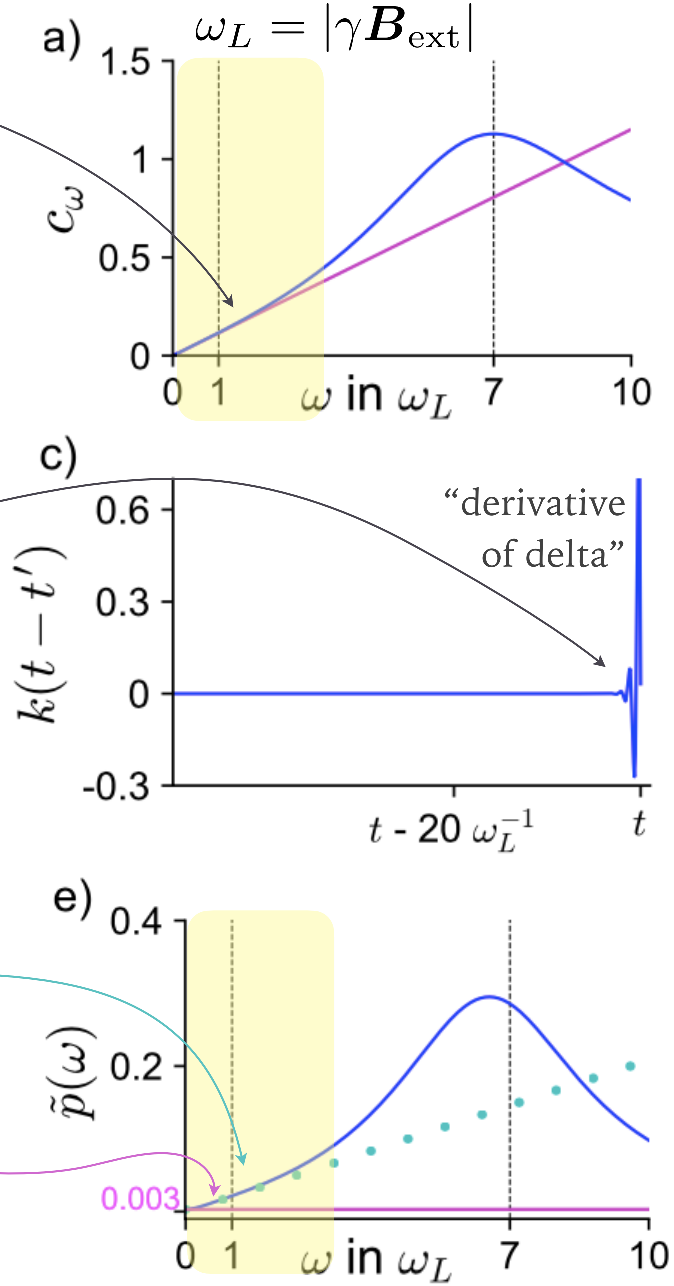
and **monotonic** power spectrum:

$$\tilde{p}_{\mathsf{qu}}^{\mathsf{LLG}}(\omega) = \frac{\eta\hbar\omega}{\hbar\omega_L}\coth\left(\frac{\beta\hbar\omega}{2}\right)$$

(unit-free)

$$k_BT \gg \hbar\omega : \tilde{p}_{\mathsf{cl}}^{\mathsf{LLG}}(\omega) = \eta\,\frac{2k_BT}{\hbar\omega_L}$$

"white noise"



LLG

linear

no memory

$T = 1K$

linear

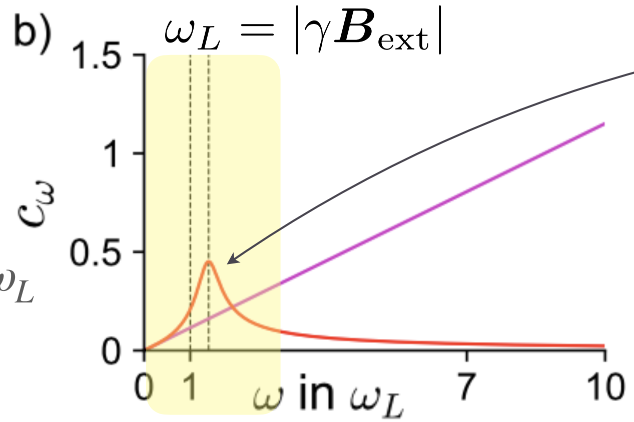
flat

LLG AND LORENTZIAN COUPLING

LORENTZIAN

peaked

$\omega_0 = 1.4\,\omega_L$

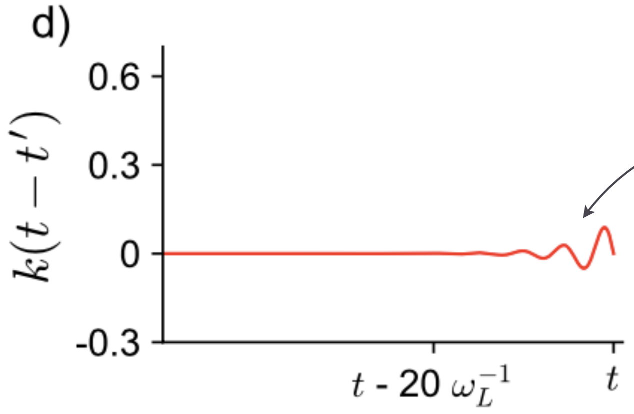


choose for all n

Lorentzian coupling in ω:

$$c_\omega^{\text{Lor}} = \sqrt{\frac{2\alpha\Gamma}{\pi}\frac{\omega^2}{(\omega_0^2-\omega^2)^2+\omega^2\Gamma^2}}$$

memory



get **oscillating and decaying** memory kernel:

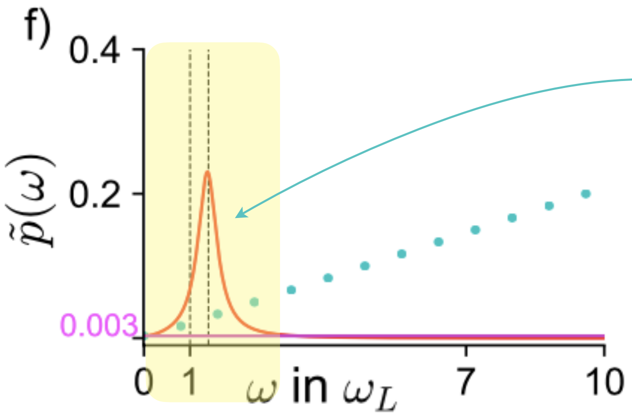
$$k^{\text{Lor}}(\tau) = \Theta(\tau)\,\alpha\,e^{-\Gamma\tau/2}\,\frac{\sin(\omega_1\tau)}{\omega_1}$$

$\tau = t - t'$

$\omega_1 = \sqrt{\omega_0^2 - \Gamma^2/4}$

$T = 1K$

peaked



and **peaked** power spectrum:

$$\tilde{p}_{\text{qu}}^{\text{Lor}}(\omega) = \frac{\alpha\Gamma\omega_L\,\omega}{(\omega_0^2-\omega^2)^2+\omega^2\Gamma^2}\;\coth\frac{\beta\hbar\omega}{2}$$

SHORT TIME DYNAMICS

stochastic dynamics of a single classical spin vector (no exchange)

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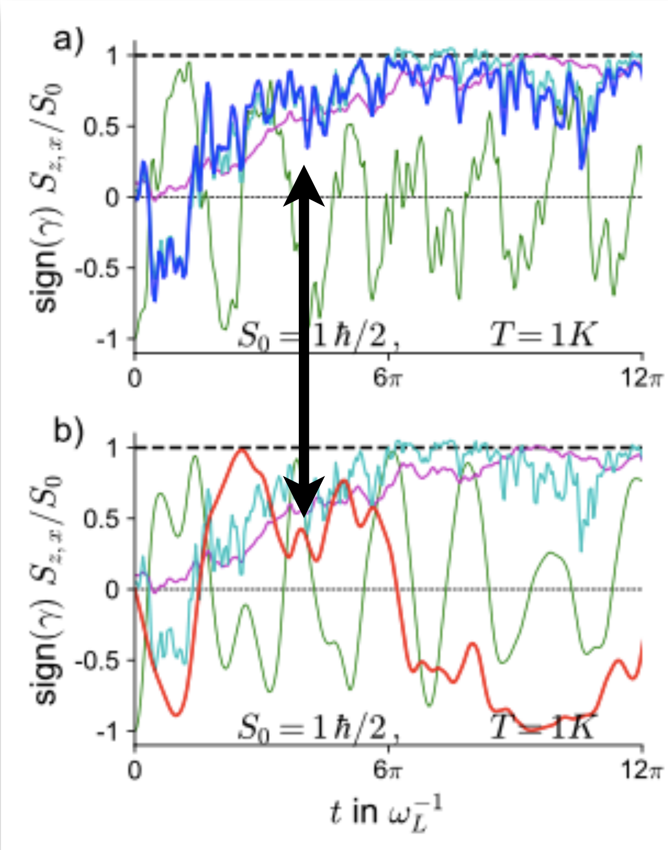
S_z in time for LLG-like and Lorentzian coupling with same linear η:

small spin $|S| = 1 \frac{\hbar}{2}$

at T=1K

S_z and S_x for LLG-like coupling

S_z and S_x for Lorentzian coupling



memory effects make dynamics completely different!

(offset to see deviations)

(same in upper+lower panels)

S_z in linear LLG approx. with quantum noise

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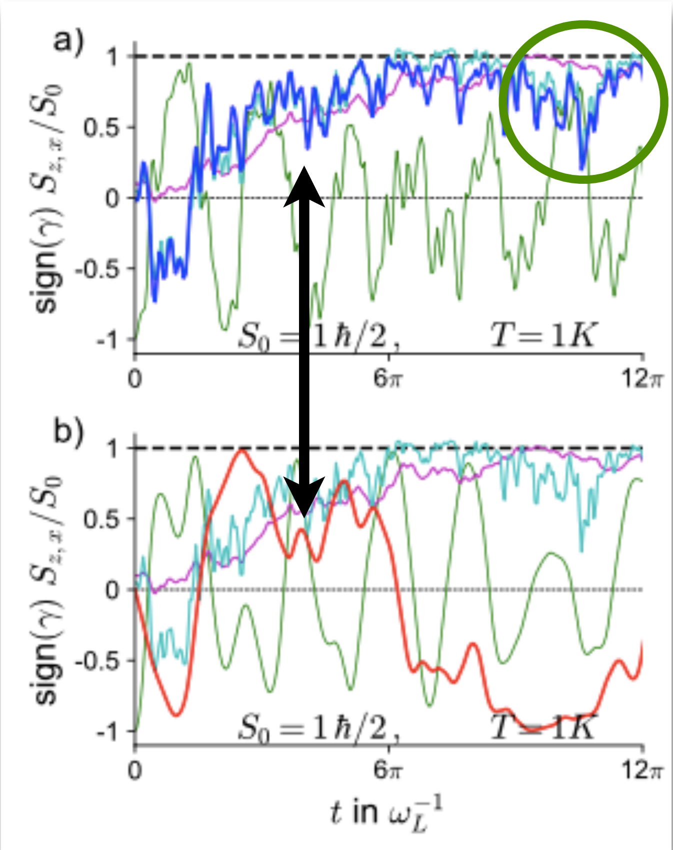


quantum noise makes even LLG-like dynamics different

memory effects make dynamics completely different!

(offset to see deviations)
(same in upper+lower panels)

S_z in linear LLG approx. with quantum noise

S_z in linear LLG approx. with white noise

(double offset to see deviations)
(same in all four subpanelds)

SHORT TIME DYNAMICS

stochastic dynamics of a single classical spin vector (no exchange)

UNIVERSITY OF EXETER

Universität Potsdam

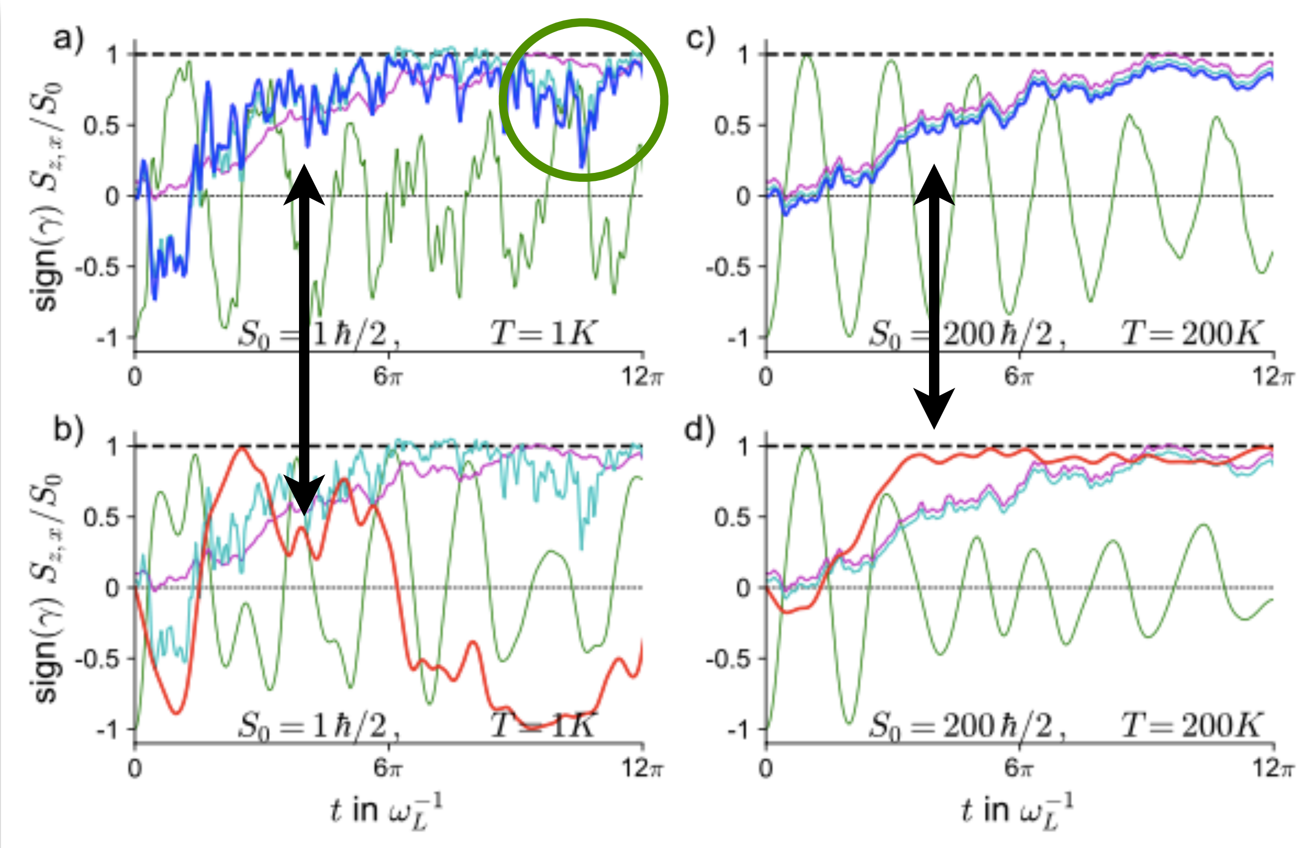
S_z in time for LLG-like and Lorentzian coupling with same linear η:

small spin $|S| = 1\,\frac{\hbar}{2}$ at T=1K

mesoscopic spin $|S| = 200\,\frac{\hbar}{2}$ at T=200K

S_z and S_x for LLG-like coupling

S_z and S_x for Lorentzian coupling



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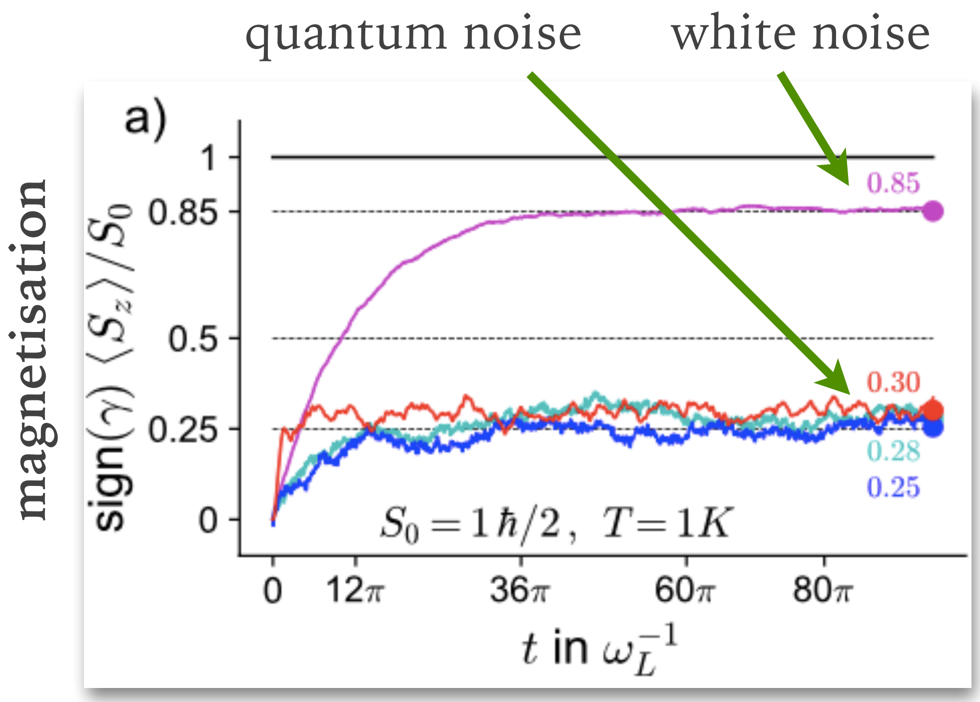
OUTLINE

- ➤ System+bath Hamiltonian
- ➤ General spin dynamics equation
- ➤ LLG and Lorentzian coupling
- ➤ Short-time dynamics
- ➤ Equilibration
- ➤ Steady state magnetisation
- ➤ Conclusions and open questions

EQUILIBRATION

ensemble average dynamics

small spin



LLG-like coupling

Lorentzian coupling

linear approx. with quantum noise

or linear approx. with white noise

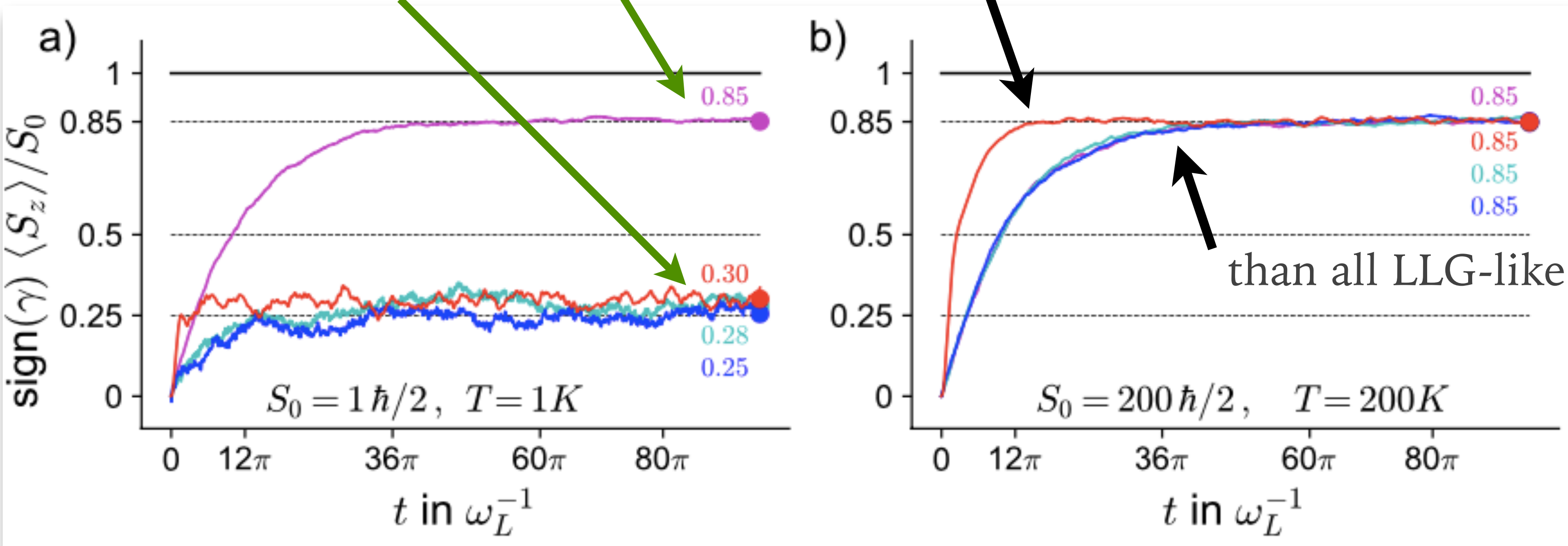
EQUILIBRATION

ensemble average dynamics

small spin | **mesoscopic spin**

quantum noise | white noise | Lorentzian: quicker equilibration

magnetisation



than all LLG-like couplings

LLG-like coupling
Lorentzian coupling

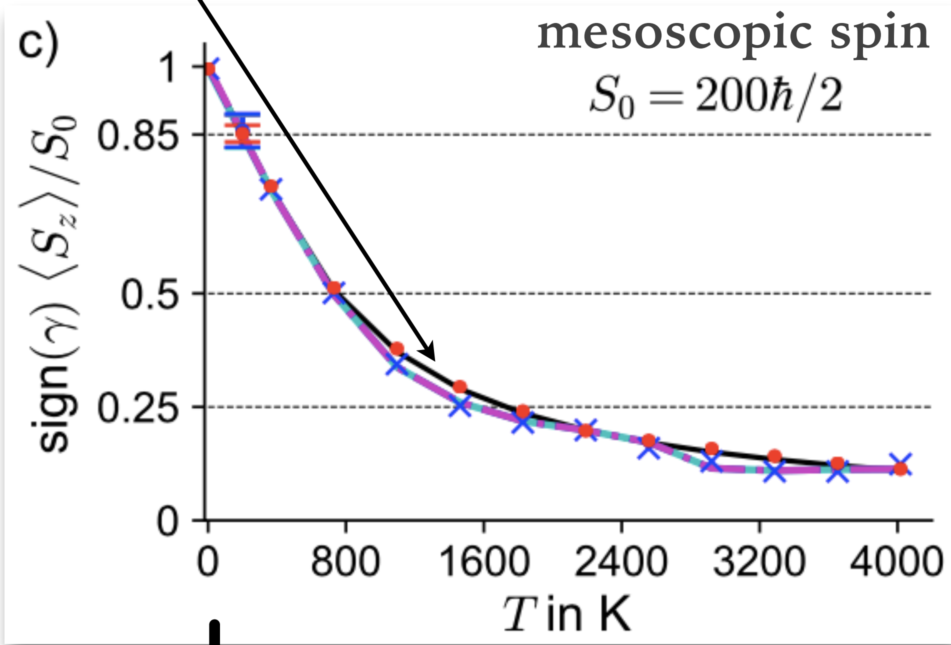
linear approx. with quantum noise
or linear approx. with white noise

STEADY STATE MAGNETISATION

$$\langle S_z \rangle = \int_{-S_0}^{+S_0} dS_z\, S_z \frac{e^{-\beta(-\gamma S_z B_{ext})}}{Z}$$

$$\frac{\langle S_z \rangle}{S_0} = \mathrm{sign}(\gamma) \left(\coth\left(\frac{S_0\,\omega_L}{k_B T}\right) - \frac{k_B T}{S_0\,\omega_L} \right)$$

where temperature is scaled by $S_0 = |\boldsymbol{S}|$



LLG-like coupling

Lorentzian coupling

linear approx. with quantum noise

or linear approx. with white noise

STEADY STATE MAGNETISATION

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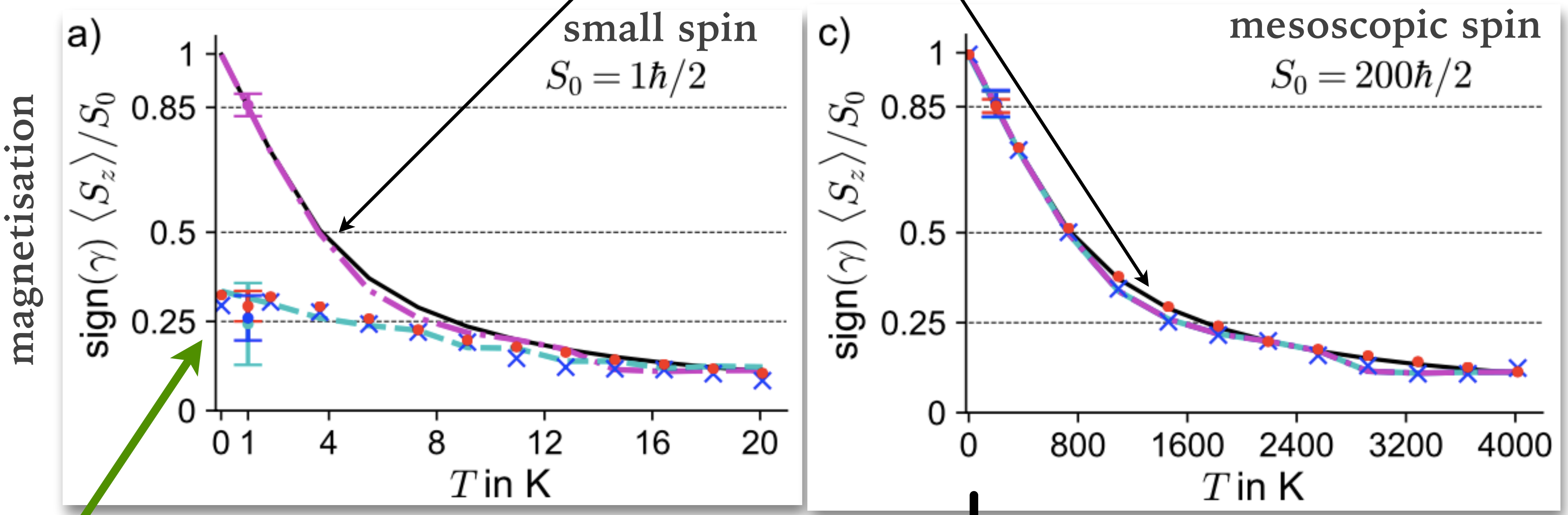

reduced magnetisation due to quantum noise even at 0K

LLG-like coupling

Lorentzian coupling

linear approx. with quantum noise

or linear approx. with white noise

OUTLINE

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- ➤ Steady state magnetisation
- ➤ Conclusions and open questions

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… beyond Caldeira-Leggett and Spin-boson

based on system+bath Hamiltonian, have derived **three-dimensional** general spin dynamics equation

$$\frac{\mathrm{d}\hat{\boldsymbol{S}}^{(n)}(t)}{\mathrm{d}t} = \hat{\boldsymbol{S}}^{(n)}(t) \times \Big[\gamma \boldsymbol{B}_{\mathrm{ext}} + \sum_{m\neq n} \bar{\mathcal{J}}^{(nm)} \cdot \hat{\boldsymbol{S}}^{(m)}(t) + \gamma\, \hat{\boldsymbol{b}}^{(n)}(t) + \gamma^2 \int_{-\infty}^{t} \mathrm{d}t'\, \mathcal{K}^{(n)}(t-t') \cdot \hat{\boldsymbol{S}}^{(n)}(t')\Big], \quad (11)$$

PHYSICAL REVIEW LETTERS **121**, 040401 (2018)

Rotational Friction and Diffusion of Quantum Rotors

Benjamin A. Stickler,* Björn Schrinski,† and Klaus Hornberger

Universit

(Receive

We present
diffusion, and
environment.
like thermal e
expected rotat

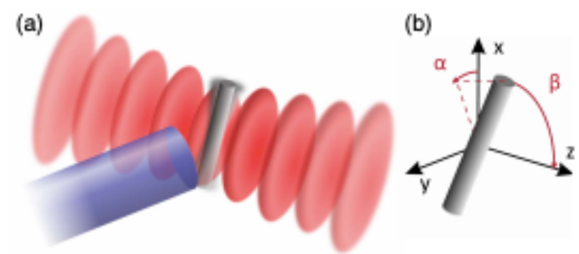
Research Article Vol. 4, No. 3 / March 2017 / Optica 356

optica

Full rotational control of levitated silicon nanorods

Stefan Kuhn,[1,*,†] Alon Kosloff,[2,†] Benjamin A. Stickler,[3] Fernando Patolsky,[2] Klaus Hornberger,[3] Markus Arndt,[1] and James Millen[1]

applicable for 3D rotational Brownian motion



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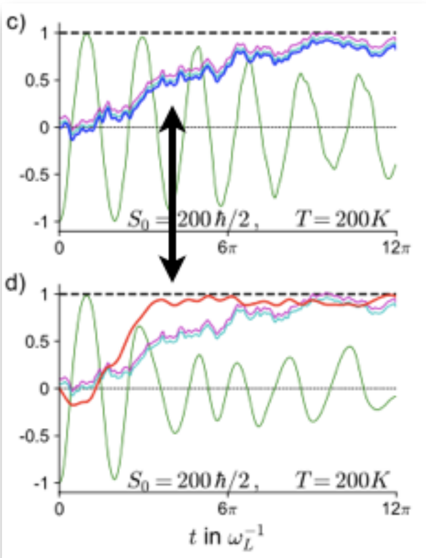
… beyond Caldeira-Leggett and Spin-boson

based on system+bath Hamiltonian, have derived **three-dimensional** general spin dynamics equation

$$\frac{\mathrm{d}\hat{\boldsymbol{S}}^{(n)}(t)}{\mathrm{d}t} = \hat{\boldsymbol{S}}^{(n)}(t) \times \Big[\gamma \boldsymbol{B}_{\text{ext}} + \sum_{m \neq n} \bar{\mathcal{J}}^{(nm)} \cdot \hat{\boldsymbol{S}}^{(m)}(t) + \gamma\, \hat{\boldsymbol{b}}^{(n)}(t) + \gamma^2 \int_{-\infty}^{t} \mathrm{d}t'\, \mathcal{K}^{(n)}(t-t') \cdot \hat{\boldsymbol{S}}^{(n)}(t')\Big], \quad (11)$$

magnetism:

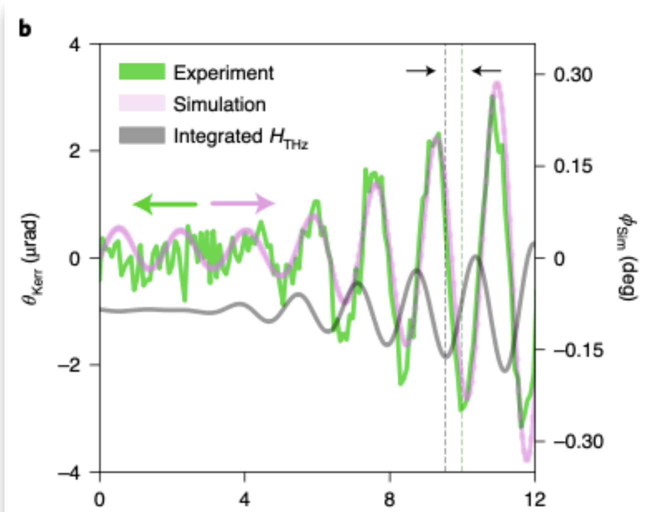


For linear coupling function (Ohmic), recover widely used LLG equation.

Lorentzian couplings allow to systematically study how memory kernels affect the short/long time dynamics.

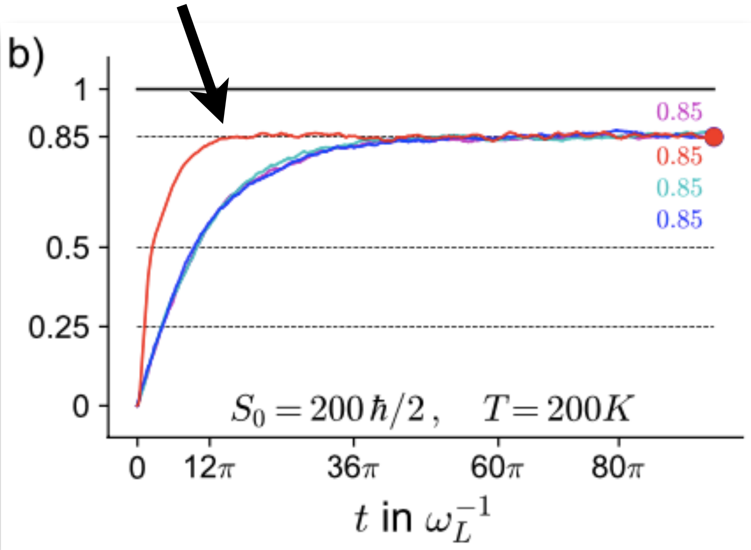
(with guaranteed FDR)

simulation with memory kernel fits very recent measurements:



Neeraj, et al., Bonetti, Nat. Phys. (2020)

Memory effects lead to faster
magnetisation equilibration.

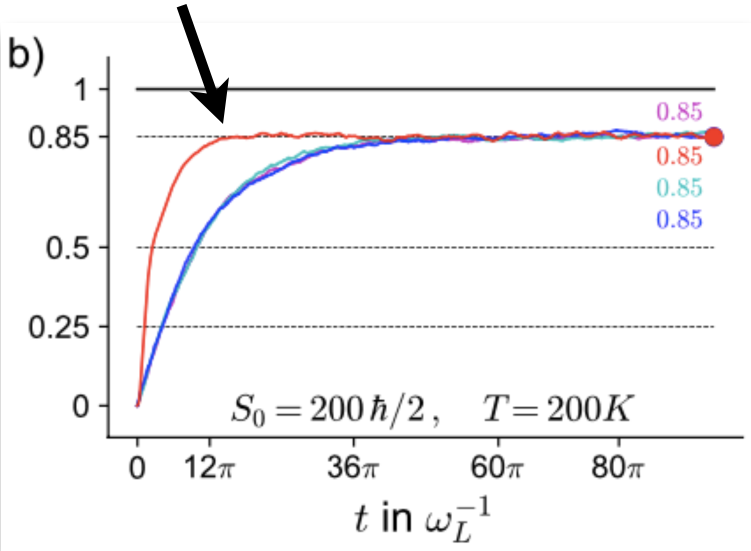


Predictions of the **short time dynamics** and **equilibration to steady state** strongly depend on the parameters of the Lorentzian coupling.

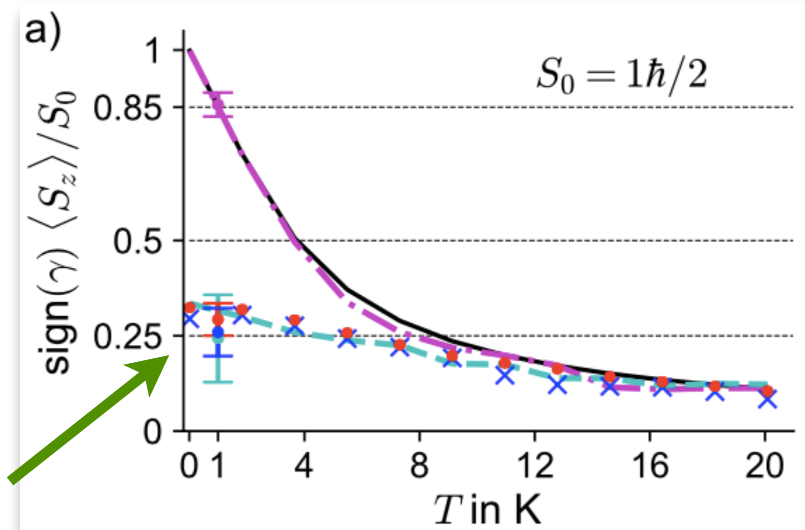
What is the precise link between
non-delta memory kernel
(non-Markovian dynamics)
and the equilibration time?

(please point out references)

Memory effects lead to faster magnetisation equilibration.



Non-Gibbs steady state due to quantum noise



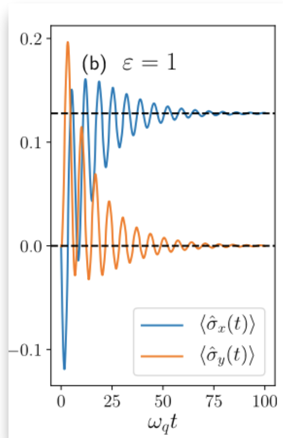
What is the precise link between non-delta memory kernel (non-Markovian dynamics) and the equilibration time?

(please point out references)

strong coupling thermodyn?

Link to Hamiltonian of mean force?

Purkayastha, et al., Goold, npj Quantum Information (2020)



FUTURE

Versatile three-dimensional quantum spin dynamics equation with guaranteed fluctuation-dissipation link
Anders, Sait, Horsley, arxiv 2009.00600v1 (2020)

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- timescale of equilibration and steady state?
- non-isotropic coupling tensors

$$\hat{V}_{\text{int}} = -\gamma \sum_n \hat{\boldsymbol{S}}^{(n)} \cdot \int_0^\infty \mathrm{d}\omega\, \mathcal{C}_\omega^{(n)} \cdot \hat{\boldsymbol{X}}_\omega^{(n)}$$

  - ➤ 3D vs 1D effects
  - ➤ thin magnetic layers
- differences between quantum and classical spin dynamics
- bath modes at different temperatures
  - ➤ heat transport
  - ➤ electron/phonon baths
- common baths? see Camille's talk
- including driving with EM fields/light in equations of motion
- replace LLG in micromagnetic/atomistic simulations with general spin dynamics equation

R. Evans - VAMPIRE (York)

Thank you!

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