Chaotic properties of spin lattices at high temperatures:

Lyapunov exponents, out-of-time-order correlators and beyond

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Definition of Lyapunov exponents

$$\mathcal{H} = \sum_{m<n}^{\mathrm{NN}} J_x\, S_m^x S_n^x + J_y\, S_m^y S_n^y + J_z\, S_m^z S_n^z$$

Equations of motion: $\dot{\mathbf{S}}_n = \mathbf{S}_n \times \mathbf{h}_n$

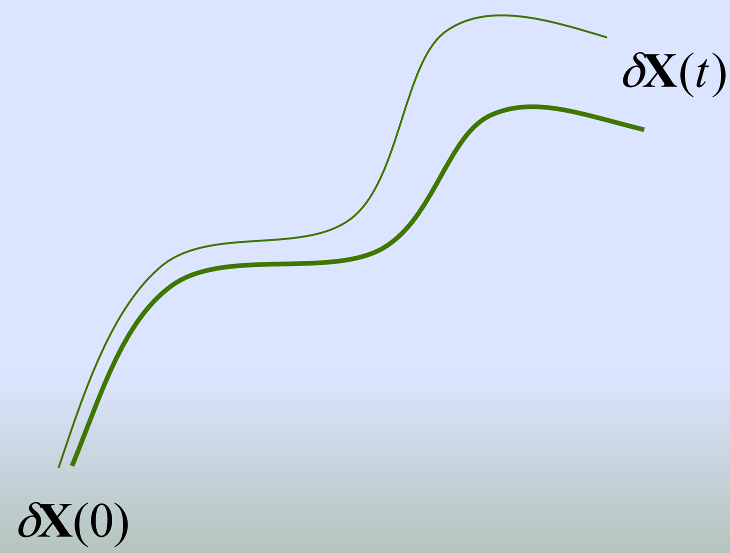
Local fields: $$\mathbf{h}_n = \sum_m^{\mathrm{NN}} \begin{pmatrix} J_x S_{mx} \\ J_y S_{my} \\ J_z S_{mz} \end{pmatrix}$$

Small deviations: $\delta\dot{\mathbf{S}}_n = \delta\mathbf{S}_n \times \mathbf{h}_n + \mathbf{S}_n \times \delta\mathbf{h}_n$

$$\delta\mathbf{h}_n = \sum_m^{\mathrm{NN}} \begin{pmatrix} J_x\ \delta S_{mx} \\ J_y\ \delta S_{my} \\ J_z\ \delta S_{mz} \end{pmatrix}$$

Phase space vectors:

$$\mathbf{X} = \begin{pmatrix} S_{1x} \\ S_{1y} \\ S_{1z} \\ S_{2x} \\ S_{2y} \\ S_{2z} \\ \vdots \\ S_{Nx} \\ S_{Ny} \\ S_{Nz} \end{pmatrix} \qquad \delta\mathbf{X} = \begin{pmatrix} \delta S_{1x} \\ \delta S_{1y} \\ \delta S_{1z} \\ \delta S_{2x} \\ \delta S_{2y} \\ \delta S_{2z} \\ \vdots \\ \delta S_{Nx} \\ \delta S_{Ny} \\ \delta S_{Nz} \end{pmatrix}$$



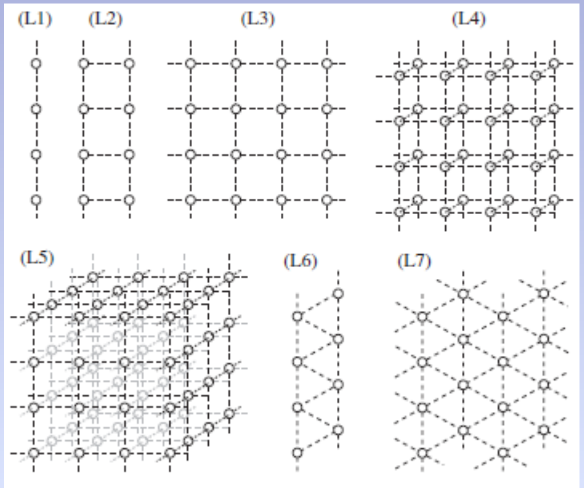
Largest Lyapunov exponent:

$$\boxed{\lambda_{\max} \equiv \lim_{\substack{t\to\infty \\ |\delta\mathbf{X}(0)|\to 0}} \frac{1}{t} \ln\left(\frac{|\delta\mathbf{X}(t)|}{|\delta\mathbf{X}(0)|}\right)}$$

Survey of the largest Lyapunov exponents

[A. de Wijn, B. Hess, and B. F., Phys. Rev. Lett. **109**, 034101 (2012)]

$$\mathcal{H} = \sum_{m<n}^{\mathrm{NN}} J_x S_m^x S_n^x + J_y S_m^y S_n^y + J_z S_m^z S_n^z$$



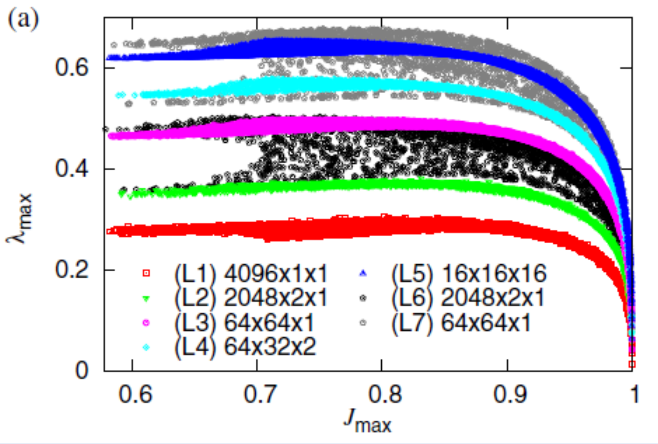
Interaction constants are randomly sampled

on a "sphere" $J_x^2 + J_y^2 + J_z^2 = 1$

Lessons learned:

- No integrable cases for large spin lattices besides the case of $J_x = J_y = 0;\ J_z = 1.$

- The largest Lyapunov exponent is mostly controlled by
$$J_{\max} = \max\left[|J_x|,\ |J_y|,\ |J_z| \right]$$



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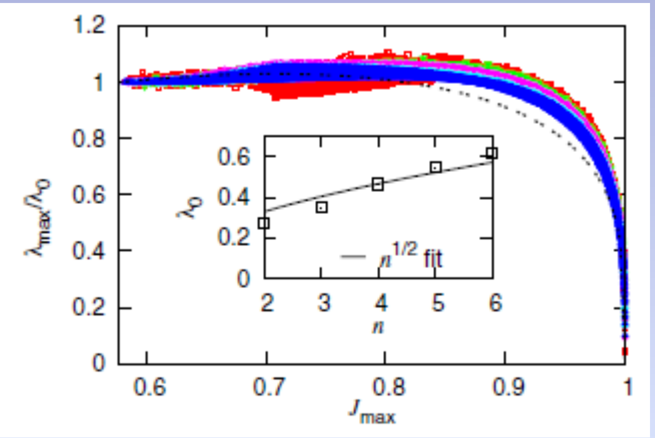

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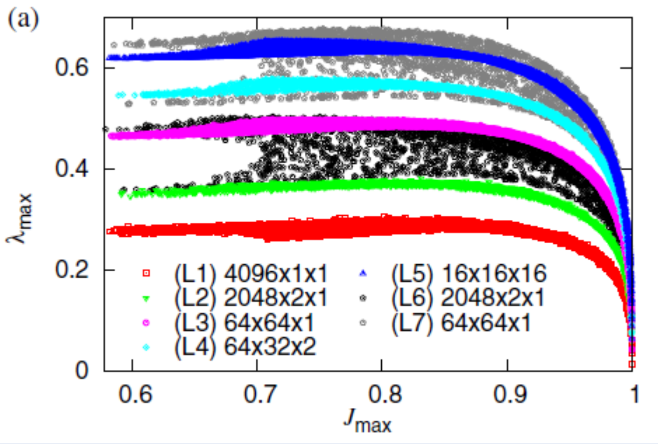
- The largest Lyapunov exponent is mostly controlled by $$J_{\max} = \max\left[|J_x|,\ |J_y|,\ |J_z|\right]$$

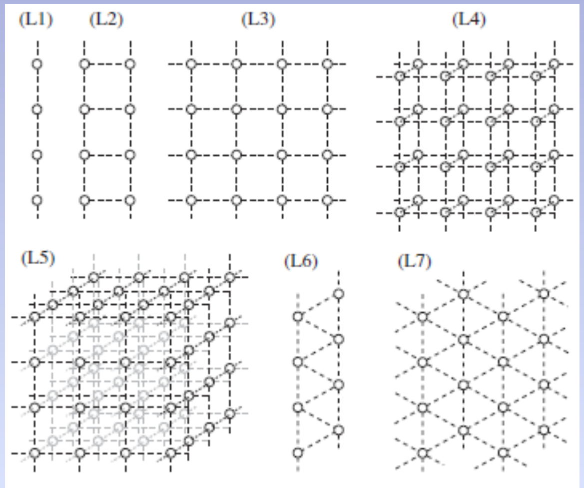
- The dependence on $J_{\max}$ is universal for bipartite lattices. For $J_{\max} < 0.85,$ it is nearly flat.



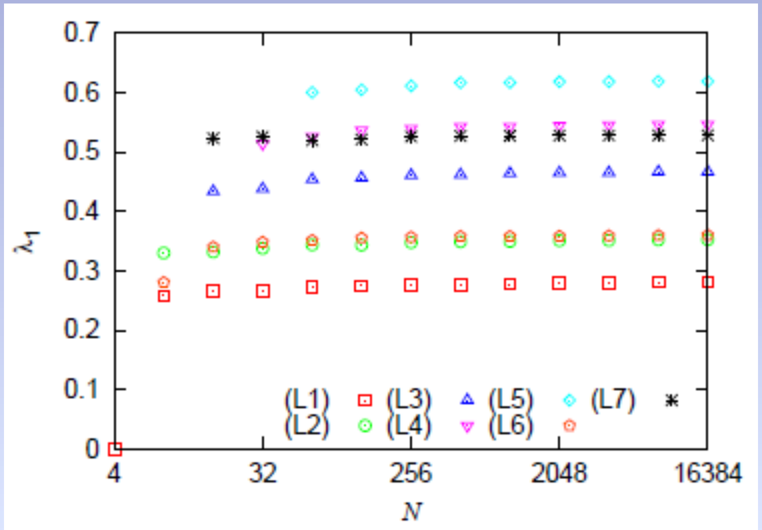
Investigations of Lyapunov spectra in classical spin systems

[A. de Wijn, B. Hess, and B. F., J. Phys. A: Math. Theor. **46** 254012, (2013)]

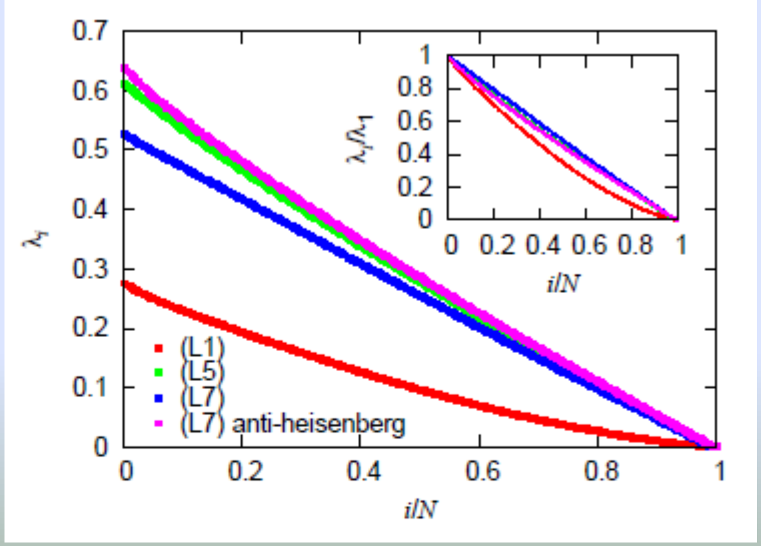
Lattices considered



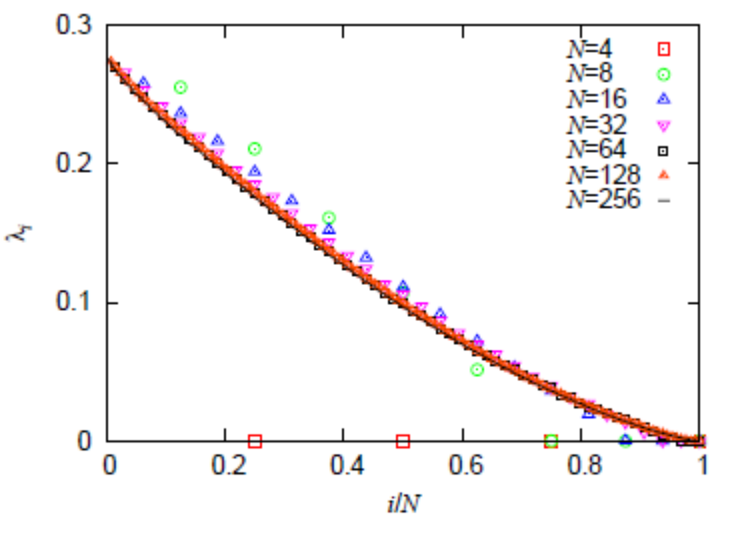
Size dependence of $\lambda_{\max}$ (Heisenberg Hamiltonian)



Lyapunov spectra for four different lattices



Size dependence of the entire spectra (Heisenberg chains)

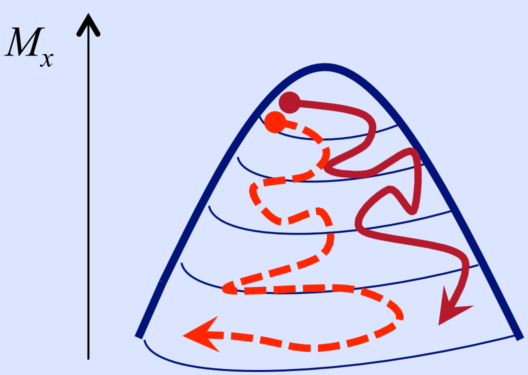


How to extract Lyapunov exponent from the observable behavior of a many-particle system?

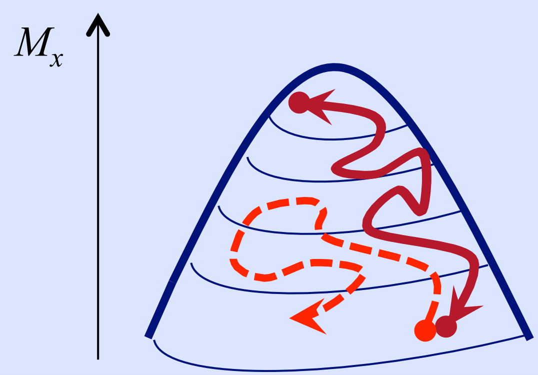
Difficulties:

- We cannot experimentally observe phase space coordinates of every particle
- We cannot controllably prepare two close initial conditions in a many-particle phase space
- Statistical behavior of many-particle systems masks Lyapunov instabilities

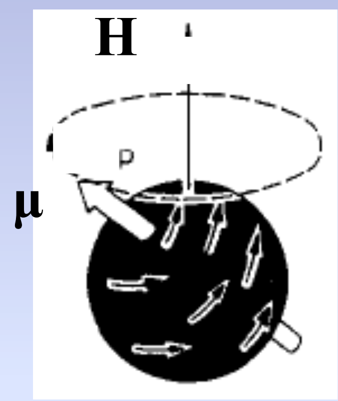
Relaxation path in many-body phase space

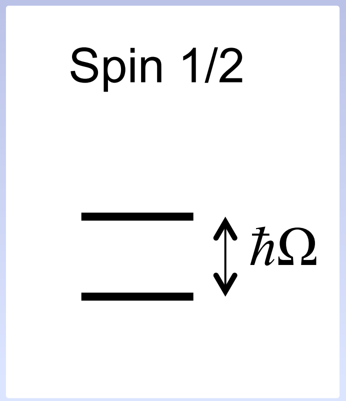


Solution: time-reversal of relaxation! (Loschmidt echo)



Nuclear Magnetic Resonance (NMR)



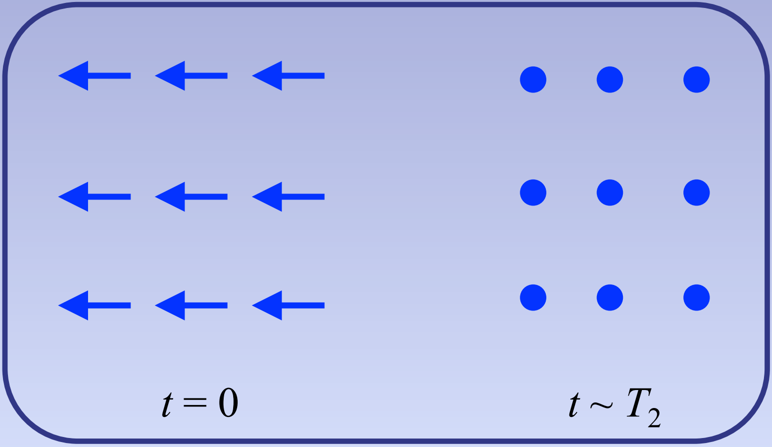


Larmor precession

$$\mathbf{\Omega} = \gamma\,\mathbf{H}$$

NMR free induction decay

$$\mathcal{H} = \sum_{m<n} J^z_{mn}\, S^z_m S^z_n + J^{\perp}_{mn} \left(S^x_m S^x_n + S^y_m S^y_n \right)$$



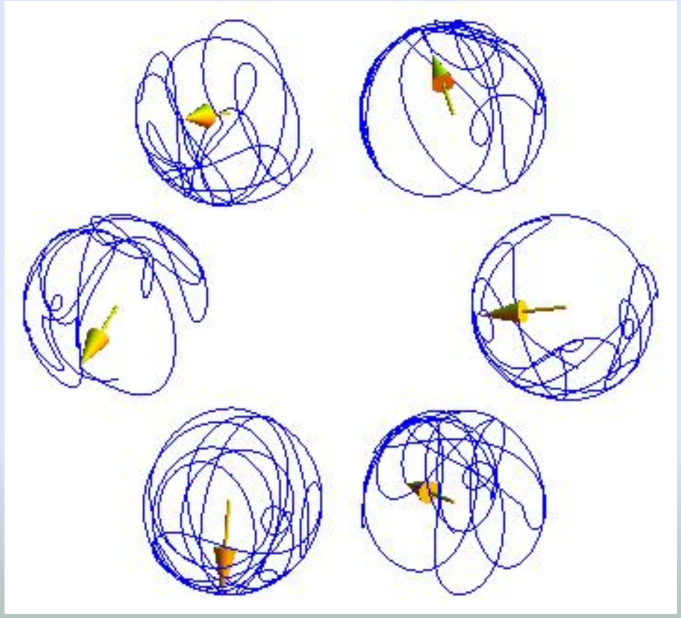
magnetic dipolar interaction:

$$J^z_{mn} = -2\,J^{\perp}_{mn} = \frac{g^2\hbar^2\left(1 - 3\cos^2\theta_{mn}\right)}{r^3_{mn}}$$

$$J^z_{mn}\,,\; J^{\perp}_{mn} \quad << \quad k_B T$$

<u>Quantity of interest:</u>

$$G(t) = \left\langle M_x(t)\, M_x(0) \right\rangle_{T=\infty} = \mathrm{Tr}\left\{ e^{i\mathcal{H}t} \sum_n S^x_n \, e^{-i\mathcal{H}t} \sum_m S^x_m \right\}$$



Sensitivity of Loschmidt echoes to small perturbations

VOLUME 25, NUMBER 4 PHYSICAL REVIEW LETTERS 27 JULY 1970

VIOLATION OF THE SPIN-TEMPERATURE HYPOTHESIS*

W.-K. Rhim, A. Pines,† and J. S. Waugh
Department of Chemistry and Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 5 May 1970)

A "Loschmidt demon" is exhibited which effectively reverses the spin-spin relaxation

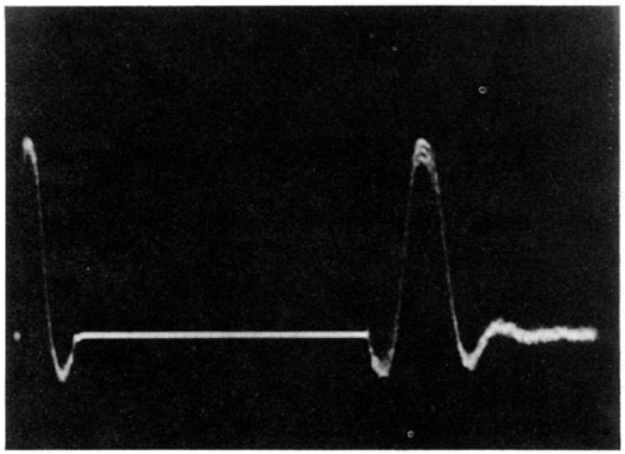


FIG. 1. Transient NMR of the ^{19}F nuclei in solid CaF_2. Following a normal Bloch decay, an rf burst

A nuclear magnetic resonance answer to the Boltzmann–Loschmidt controversy?

H.M. Pastawski[a,*], P.R. Levstein[a], G. Usaj[a], J. Raya[b], J. Hirschinger[b]

Physica A **283**, 166 (2000)

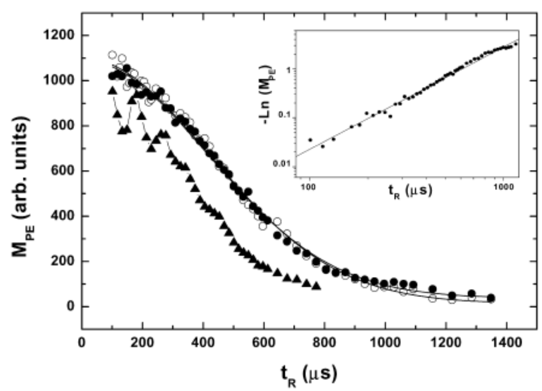
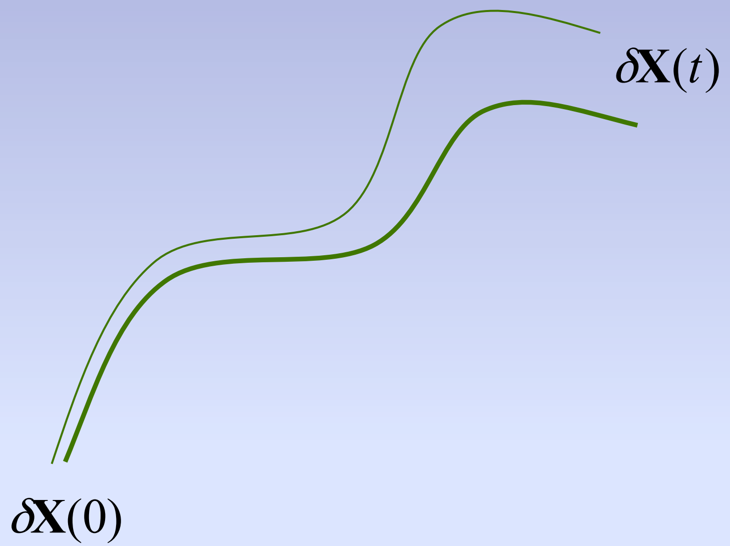
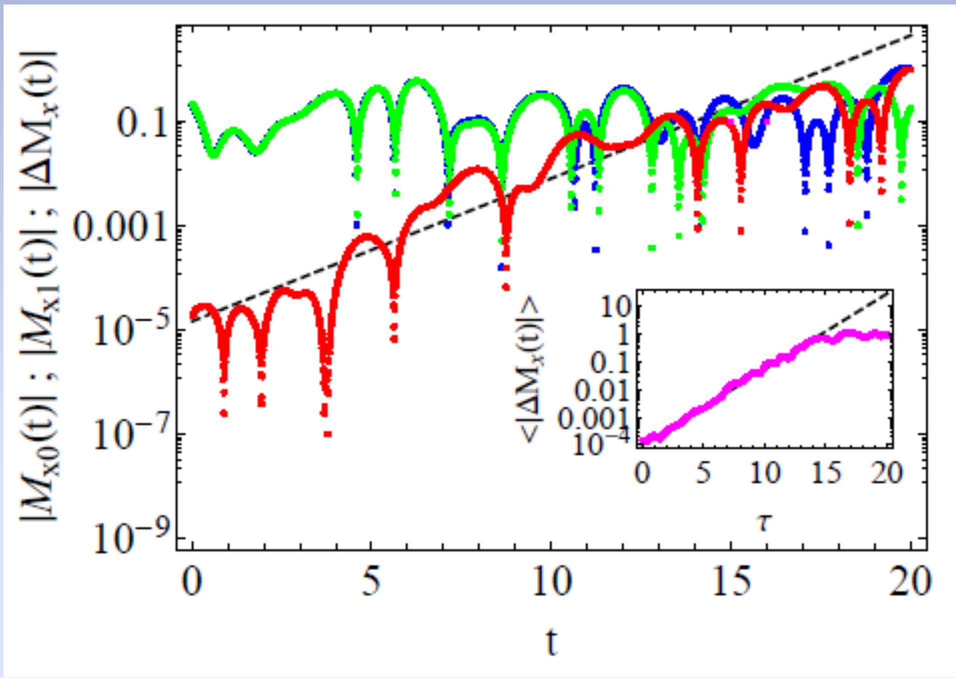


Fig. 1. Attenuation of the polarization echoes as a function of t_R in a single crystal of ferrocene, with

Time reversal of magnetization noise



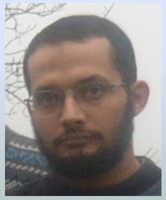


$$\langle|M_x(t_0-\tau)-M_x(t_0+\tau)|\rangle \sim e^{\lambda_{\max}\tau}$$

$$\langle[M_x(t_0-\tau)-M_x(t_0+\tau)]^2\rangle \cong e^{2\lambda_{\max}\tau}$$

$$\frac{\langle M_x(t_0-\tau)M_x(t_0+\tau)\rangle}{\langle M_x^2\rangle} = 1 - Ce^{2\lambda_{\max}\tau}$$

B.V. Fine, T.A. Elsayed, C. M. Kropf, and A.S. de Wijn,
Phys. Rev. E **89**, 012923 (2014)



Observable exponential sensitivity of classical spin systems to small perturbations

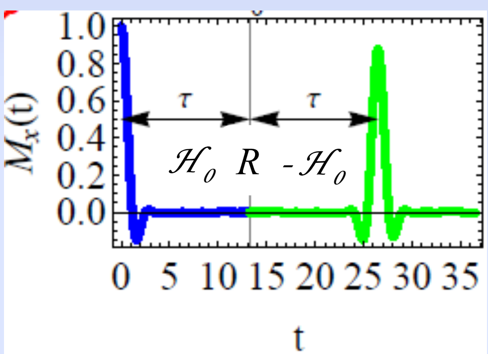
B. V. Fine, T.A. Elsayed, C. M. Kropf, and A.S. de Wijn, Phys. Rev. E **89**, 012923 (2014)

$$\mathcal{H}_0 = \sum_{i<j}^{\mathrm{NN}} J_x S_{ix} S_{jx} + J_y S_{iy} S_{jy} + J_z S_{iz} S_{jz}$$

cubic lattice of $16 \times 16 \times 16$ classical spins

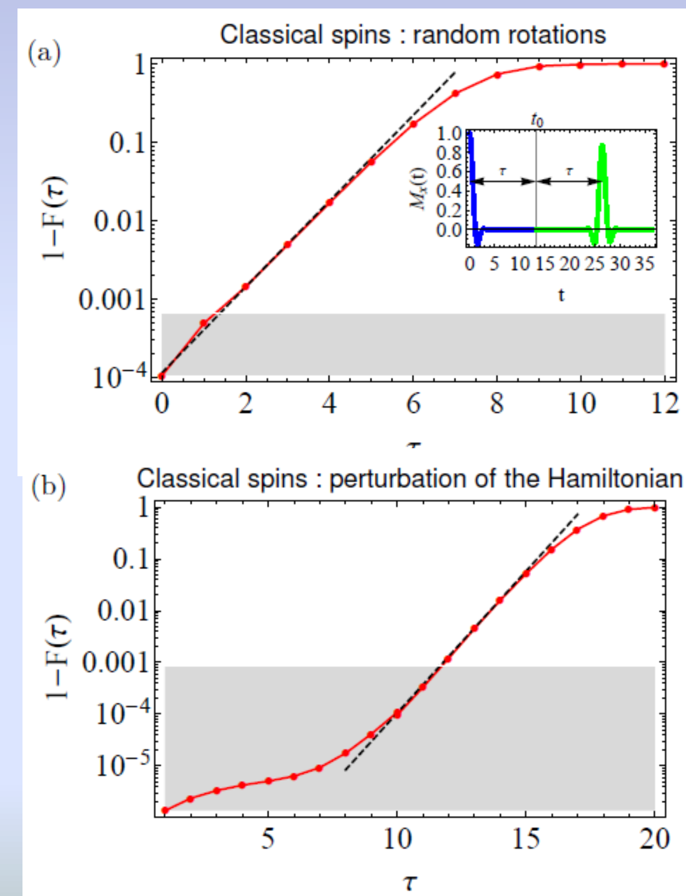
$$J_x = -0.41,\ J_y = -0.41,\ J_z = 0.82$$

$$\rho_0 \cong e^{-\alpha M_x}$$



$$\rho_1 = \hat{U}_{-\mathcal{H}_0}(\tau)\ \hat{U}_R\ \hat{U}_{\mathcal{H}_0}(\tau)\ \rho_0$$

$$F(\tau) = \frac{\langle M_x \rangle_{\rho_1}}{\langle M_x \rangle_{\rho_0}} = 1 - C\ e^{2\lambda_{\max}\tau}$$



Absence of exponential sensitivity to small perturbations in nonintegrable systems of spins 1/2

B.F., T.A. Elsayed, C. M. Kropf, and A.S. de Wijn, Phys. Rev. E **89**, 012923 (2014)

$$\mathcal{H}_0 = \sum_{i<j}^{\mathrm{NN}} J_x S_{ix} S_{jx} + J_y S_{iy} S_{jy} + J_z S_{iz} S_{jz}$$

$$F(\tau) \cong \mathrm{Tr}\left\{ e^{i\mathcal{H}_0 \tau}\ R^\dagger\ e^{-i\mathcal{H}_0 \tau}\ M_x\ e^{i\mathcal{H}_0 \tau}\ R\ e^{-i\mathcal{H}_0 \tau}\ \rho_0 \right\}$$

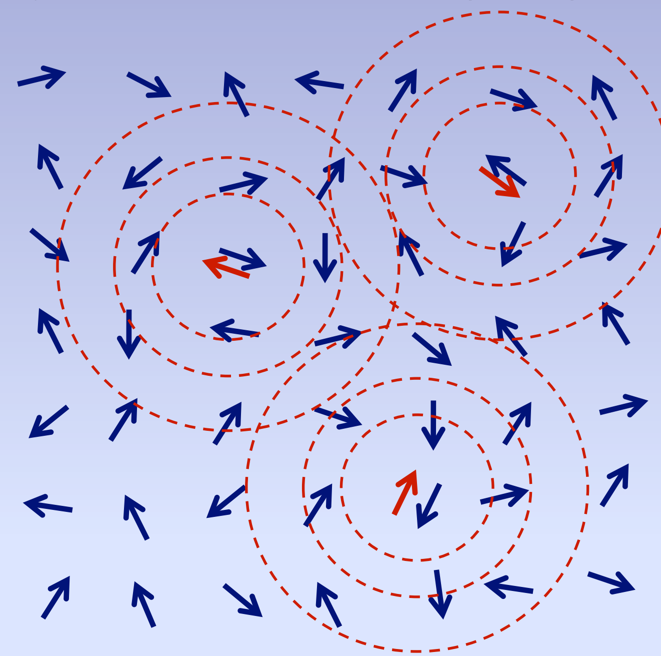
Out-of-time-order correlator

$$R = \prod_k e^{-i\delta\theta_k S_{kz}} \approx \prod_k (\mathbb{1} - i\delta\theta_k S_{kz})$$

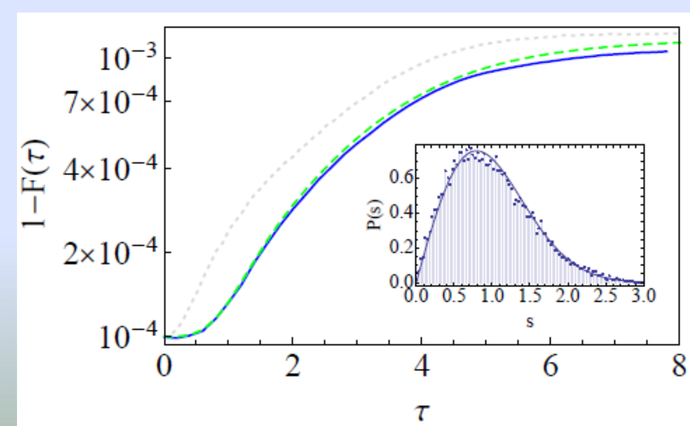
$$\Psi_+ \equiv R\Psi_- = \sum_\nu \Psi_\nu$$

Each Ψ_ν is obtained from Ψ_- by complete flipping of a small fraction of spins

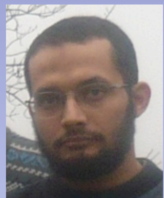
No exponential growth in the regime 1-F(τ) << 1



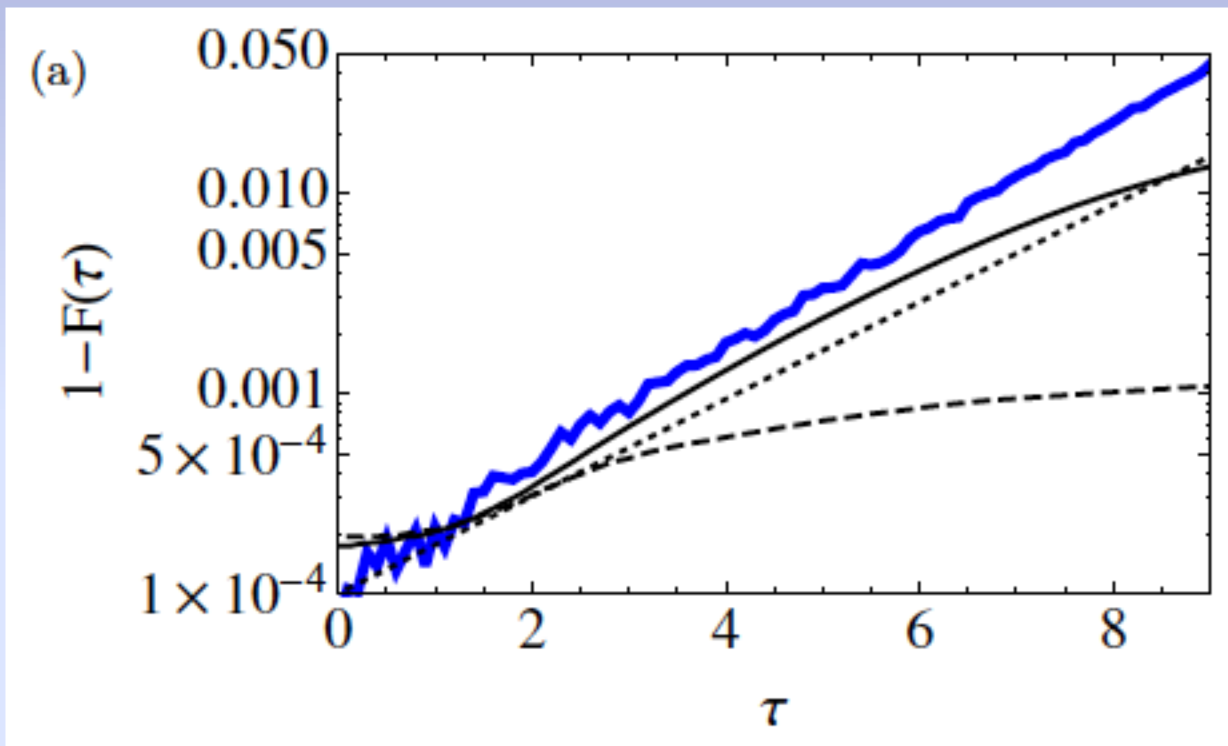
5x5 lattice of spins 1/2



Larger quantum spins



T.A. Elsayed, B. F., Physica Scripta **T165**, 014011 (2015)



Blue: 6 classical spins

Solid black: 6 spins 15/2

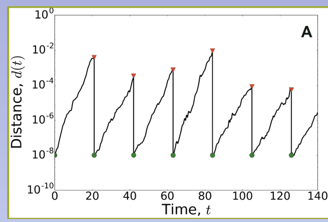
Dashed: 26 spins 1/2

Dotted: $2\,\lambda_{max}\,\tau$

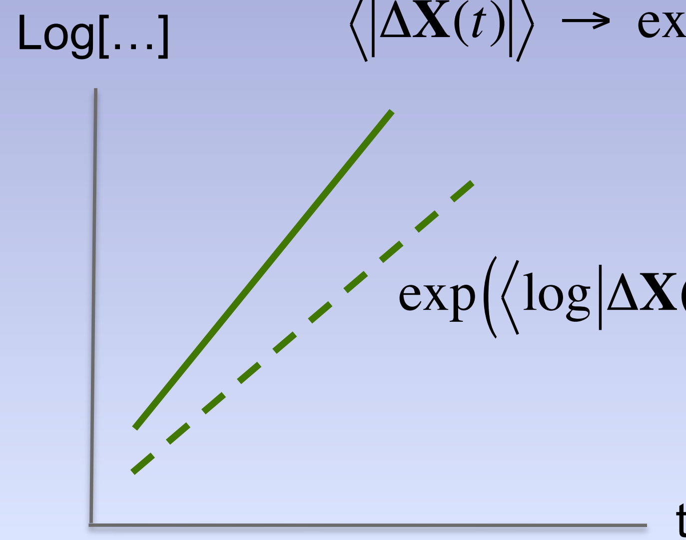
Demonstration of the Lyapunov regime for an out-of-time-order quantum correlator.

Extracting ergodization time from Loschmidt echoes

[A. E. Tarkhov, B. V. Fine, New J. Phys. 20, 123021 (2018)]



$$\left\langle \left| \Delta \mathbf{X}(t) \right| \right\rangle \rightarrow \exp(\Lambda\, t)$$



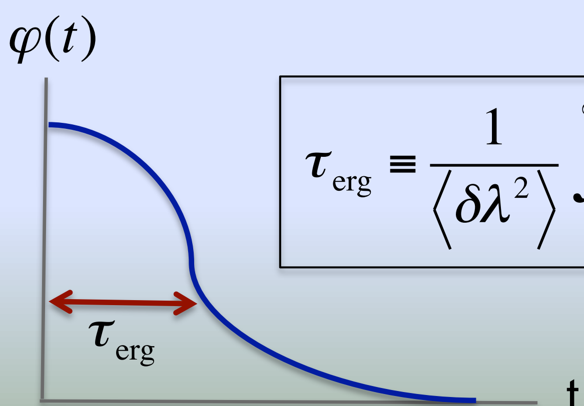
$$\exp\left(\left\langle \log \left| \Delta \mathbf{X}(t) \right| \right\rangle \right) \rightarrow \exp(\lambda_{\max}\, t)$$

$$\lambda_{\max} = \lim_{t \to \infty} \frac{1}{t} \int_0^t \lambda(t')\, dt'$$

$$\lambda(t) = \lambda_{\max} + \delta\lambda(t)$$

$$\varphi(t) \equiv \langle \delta\lambda(t) \delta\lambda(0) \rangle$$

$$\exp[(\Lambda - \lambda_{\max})\, t] = \left\langle \exp\left[\int_0^t \delta\lambda(t')\, dt' \right] \right\rangle = \exp\left[t \int_0^\infty \varphi(t')\, dt' \right]$$



$$\tau_{\mathrm{erg}} \equiv \frac{1}{\langle \delta\lambda^2 \rangle} \int_0^\infty \varphi(t)\, dt$$

$$\boxed{\tau_{\mathrm{erg}} \equiv \frac{\Lambda - \lambda_{\max}}{\langle \delta\lambda^2 \rangle}}$$

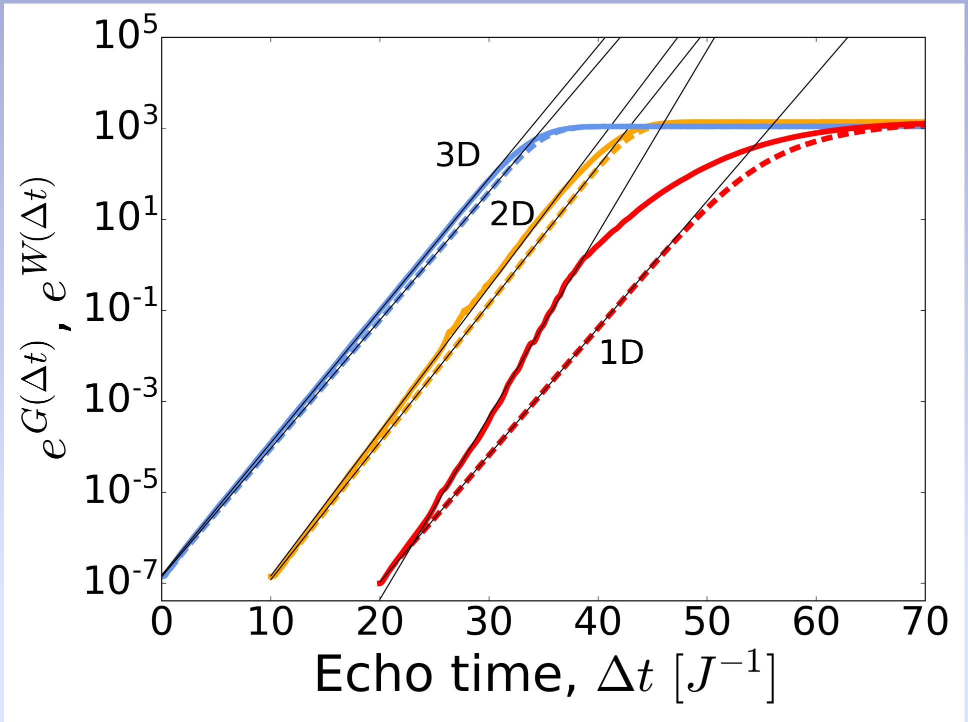
cf.

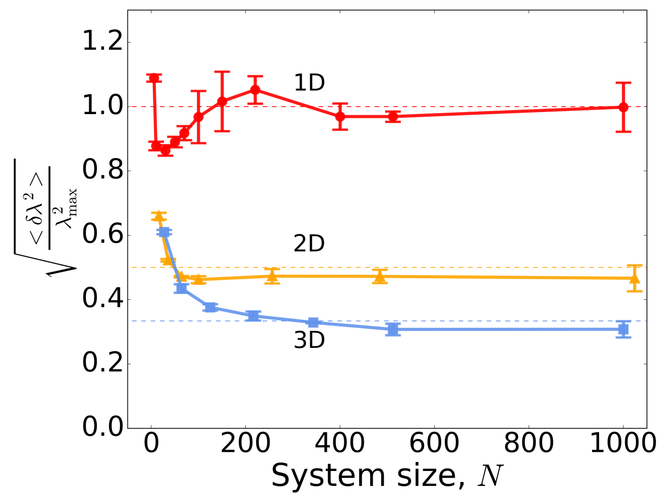
E. B. Rozenbaum et al., PRL **118**, 086801 (2017).

M. Serbyn and D.A. Abanin PRB **96**, 014202 (2017)

Extracting ergodization time from Loschmidt echoes: numerical tests

[A. E. Tarkhov, B. V. Fine, New J. Phys. **20**, 123021 (2018)]





$$\boxed{\tau_{\text{erg}} \equiv \frac{\Lambda - \lambda_{\max}}{\langle \delta\lambda^2 \rangle}}$$

$$\langle \delta\lambda^2 \rangle^{approx} \approx \frac{4\lambda^2_{\max}}{N_N^2}$$

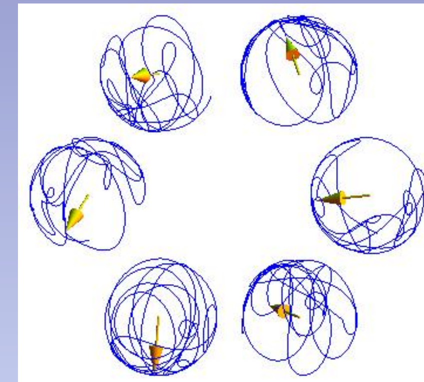
Lattice	N_N	$\lambda_{\max}$	Λ	$\langle \delta\lambda^2 \rangle$	$\langle \delta\lambda^2 \rangle^{approx}$	τ_{erg}^{LE}	τ_{erg}^{approx}	τ_{erg}
1D, $N = 100$	2	0.643	0.927	0.362	0.413	0.79	0.69	0.66 ± 0.05
2D, $N = 10 \times 10$	4	0.697	0.731	0.104	0.122	0.32	0.27	0.32 ± 0.02
3D, $N = 4 \times 4 \times 4$	6	0.649	0.669	0.080	0.047	0.25	0.43	0.26 ± 0.02

Generic long-time behavior of nuclear spin decays:
[*B. F.*, Int. J. Mod. Phys. B **18**, 1119 (2004)]

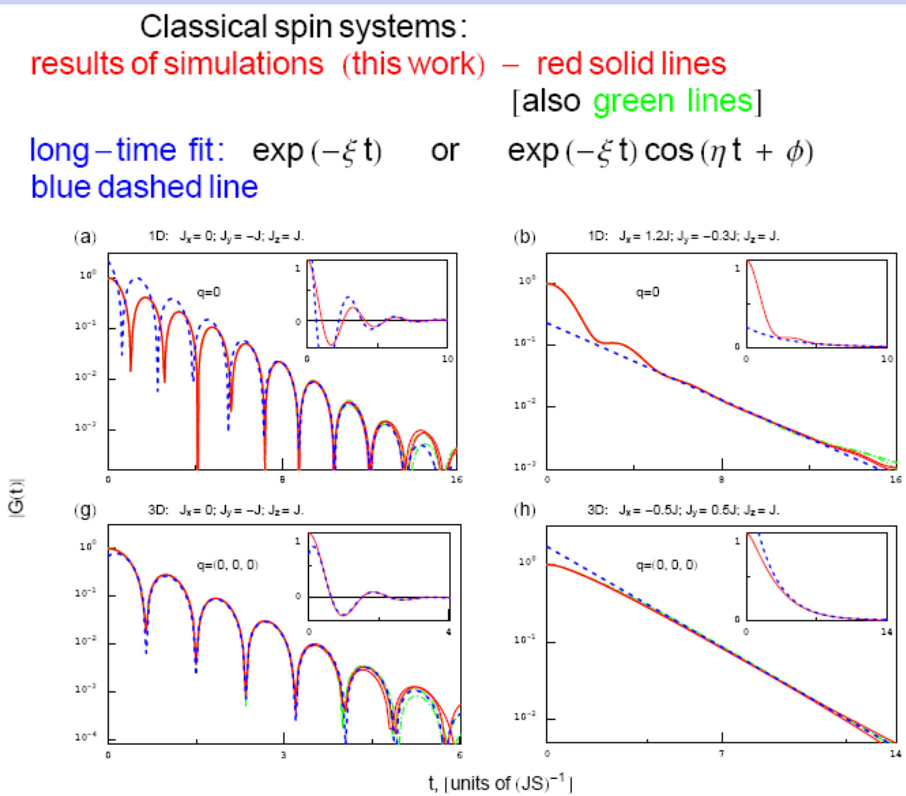
$$G(t) \sim e^{-\gamma t} \cos(\omega t + \phi), \qquad \text{where} \quad \gamma, \omega \sim J\sqrt{N_{nn}}$$

<u>Markovian behavior on non-Markovian time scale is a manifestation of chaos.</u>

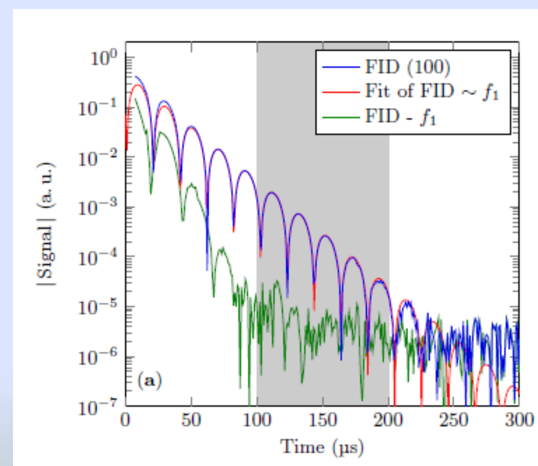
Chaotic eigenmodes of the time evolution operator:
Pollicott-Ruelle resonances [D. Ruelle, PRL **56**, 405 (1986)]



B.F., cond-mat/9911230 (1999)
C. Manderfeld et al., J.Phys.A **34**, 9893(2001)
T. Prosen, J.Phys.A **35**, L737(2002)



Spins 1/2, experiment
B. Meier et al., PRL **108**, 177602 (2012).



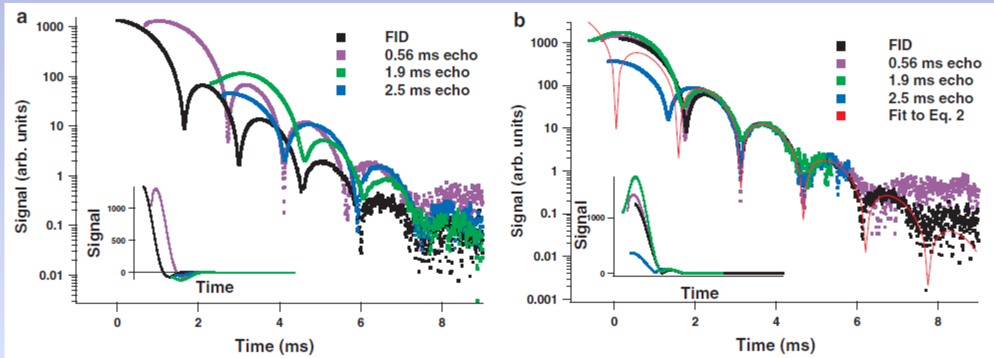
Quantitative relations between NMR free induction decays and spin echoes [B.F. PRL 94, 247601 (2005)]

Identical constants γ and ω in $e^{-\gamma t} \cos(\omega t + \phi)$

Asymptotic behavior of many-spin density matrices:

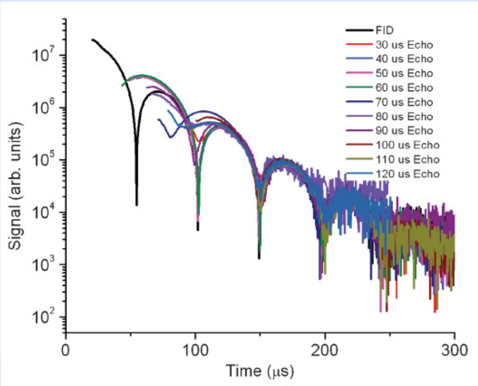
$$\rho_{kl}(t) = \rho_{0,kl}\, e^{-(\gamma + i\omega)t} + \rho^{+}_{0,kl}\, e^{-(\gamma - i\omega)t}$$

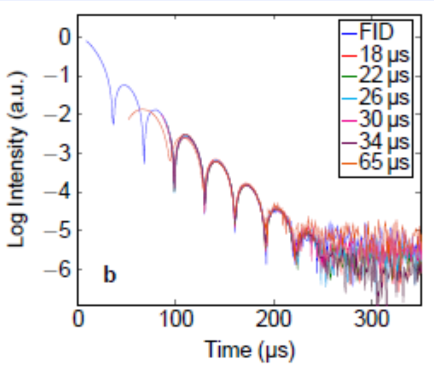
Experimental results for solid xenon:



S. W. Morgan et al, PRL **101**, 067601 (2008)

Experimental results for CaF_2:





E. G. Sorte et al,
PRB **83**, 064302 (2011)

B. Meier et al,
Univ. of Leipzig, unpublished

similar numerical results for Loschmidt echoes:
M. Schmitt and S. Kehrein
PRB **98**, 180301(R) (2018)

Summary:

1. Systematic investigation of Lyapunov exponents for classical spin lattices.

2. Loschmidt echoes in chaotic lattices of classical spins exhibit exponential sensitivity to small perturbations characterized by 2 λ_{max}.

3. **Lyapunov exponent cannot be defined for nonintegrable systems of spins 1/2 at high temperatures even for $N \rightarrow \infty$**
   ➔ Wigner-Dyson statistics and ETH without a classical chaotic limit

Generic ergodicity without exponential sensitivity to small perturbations.

4. OTOCs for lattices of large quantum spins exhibit Lyapunov growth over the time range ~ Log[S] / λ_{max}

5. $\Lambda - \lambda_{max}$ is proportional to the ergodization time of the system.

6. **Fast exponential long-time decays of non-conserved quantities are proposed as a universal indicator of chaos for classical and quantum systems.**