Power-law Decays and Thermalization in Isolated Many-Body Quantum Systems

Lea F. Santos
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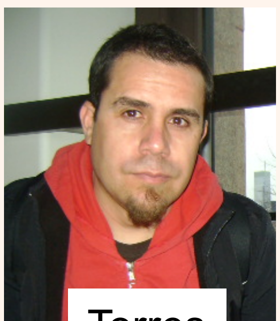
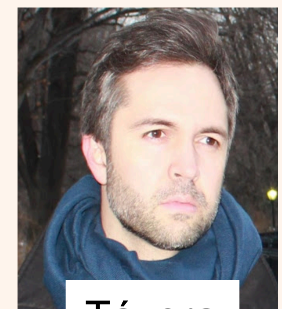

Torres

Marco Távora
E. Jonathan Torres-Herrera


Távora

Quantum chaos and thermalization in isolated systems of interacting particles
Borgonovi, Izrailev, LFS, Zelevinsky
Physics Reports **626**, 1 (2016)

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How fast can isolated interacting quantum systems evolve?

Dynamics

How does the evolution depend on the initial state, perturbation?

How does the dynamics depend on the time scale?

Is the dynamics affected by critical points?

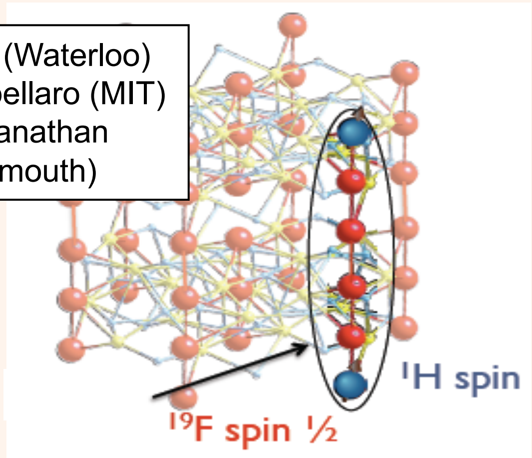
How does the dynamics depend on the Hamiltonian? (interactions, chaos)

Coherent Evolution in Experiments

NMR

Solid state NMR: nuclear positions are fixed;
They are collectively addressed with magnetic pulses;
Very slow relaxation

Cory (Waterloo)
Cappellaro (MIT)
Ramanathan (Dartmouth)

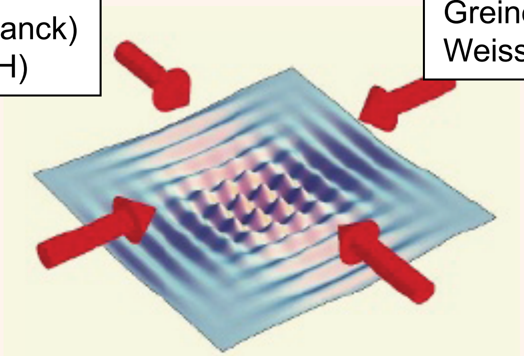


Ultracold Gases

Dynamics under designed potentials.

Bloch (Max Planck)
Esslinger (ETH)

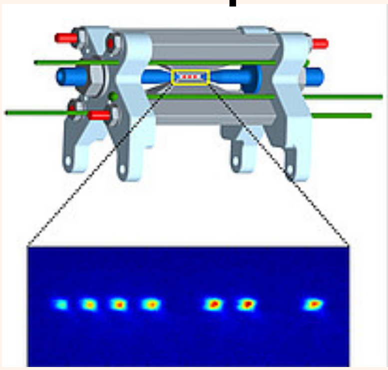
Greiner (Harvard)
Weiss (Penn Sate)



- highly controllable systems – interactions, level of disorder, 1,2,3D
  (simple models)
- quasi-isolated -- study evolution for very long time

Ion Traps

Ions trapped via electric and magnetic fields.
Laser used to induce couplings.
Isolated from an external environment.



Blatt (Innsbrück)

Monroe (Maryland)

SYSTEM MODELS
1D spin-1/2

Hardcore bosons

Integrable system:

XXZ model (1D)

$$H = \sum_{n=1}^{L-1} \frac{J}{4} \left(\Delta \sigma_n^z \sigma_{n+1}^z + \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y \right)$$

$$(b_n^+ b_n)(b_{n+1}^+ b_{n+1}) \qquad \left(b_n^+ b_{n+1} + h.c. \right)$$

Holstein-Primakoff

$$\sigma_j^z = \hat{b}_j^\dagger \hat{b}_j - 1/2,$$

Jordan-Wigner

$$\sigma_j^z = \hat{f}_j^\dagger \hat{f}_j - 1/2.$$

Holstein-Primakoff

$$\sigma_j^+ = \hat{b}_j^\dagger \sqrt{1 - \hat{b}_j^\dagger \hat{b}_j}, \quad \sigma_j^- = \sqrt{1 - \hat{b}_j^\dagger \hat{b}_j}\, \hat{b}_j,$$

Jordan-Wigner

$$\sigma_j^+ = \hat{f}_j^\dagger \, e^{-i\pi \sum_{k<j} \hat{f}_k^\dagger \hat{f}_k}, \quad \sigma_j^- = e^{i\pi \sum_{k<j} \hat{f}_k^\dagger \hat{f}_k} \, \hat{f}_j,$$

Map into hardcore bosons:

$$H = \sum_{n=1}^{L} \left[V \left(b_n^+ b_n - \frac{1}{2} \right) \left(b_{n+1}^+ b_{n+1} - \frac{1}{2} \right) - t \left(b_n^+ b_{n+1} + h.c. \right) \right]$$

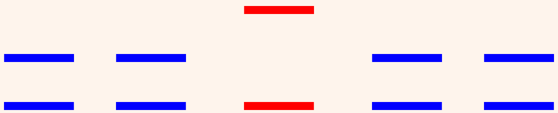
Chaotic Models

$$H = \sum_{n=1}^{L-1} \frac{J}{4} (\Delta \sigma_n^z \sigma_{n+1}^z + \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y)$$

Breaking the integrability of the 1D XXZ model

Defect model

LFS,
JPA (2004)



$$H = \frac{Jd}{2}\sigma_{L/2}^z + \sum_{n=1}^{L-1} \frac{J}{4} (\Delta \sigma_n^z \sigma_{n+1}^z + \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y)$$

Chaotic Models

$$H=\sum_{n=1}^{L-1}\frac{J}{4}(\Delta\sigma_n^z\sigma_{n+1}^z+\sigma_n^x\sigma_{n+1}^x+\sigma_n^y\sigma_{n+1}^y)$$

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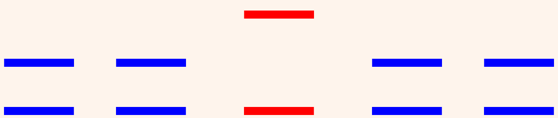
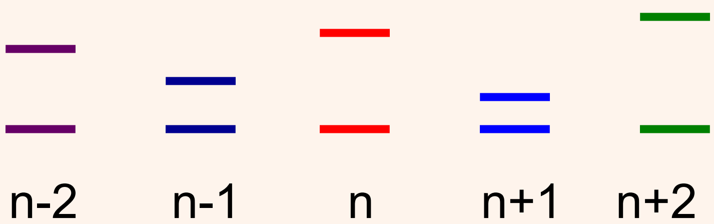


$$H=\frac{Jd}{2}\sigma_{L/2}^z+\sum_{n=1}^{L-1}\frac{J}{4}(\Delta\sigma_n^z\sigma_{n+1}^z+\sigma_n^x\sigma_{n+1}^x+\sigma_n^y\sigma_{n+1}^y)$$

Disordered model



$$H=\sum_{n=1}^{L}\frac{h_n}{2}\sigma_n^z+\sum_{n=1}^{L-1}\frac{J}{4}(\Delta\sigma_n^z\sigma_{n+1}^z+\sigma_n^x\sigma_{n+1}^x+\sigma_n^y\sigma_{n+1}^y)$$

Chaotic Models

$$H = \sum_{n=1}^{L-1} \frac{J}{4} (\Delta \sigma_n^z \sigma_{n+1}^z + \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y)$$

Breaking the integrability of the 1D XXZ model

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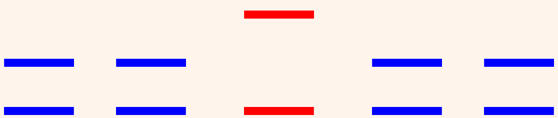
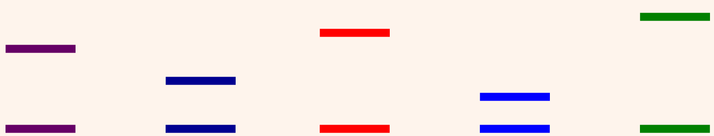


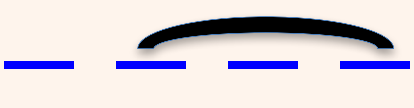
$$H = \frac{Jd}{2} \sigma_{L/2}^z + \sum_{n=1}^{L-1} \frac{J}{4} (\Delta \sigma_n^z \sigma_{n+1}^z + \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y)$$

Disordered model



$$H = \sum_{n=1}^{L} \frac{h_n}{2} \sigma_n^z + \sum_{n=1}^{L-1} \frac{J}{4} (\Delta \sigma_n^z \sigma_{n+1}^z + \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y)$$

NNN model



$$H_{NN} + H_{NNN} = \sum_{n=1}^{L-1} \frac{J}{4} (\Delta \sigma_n^z \sigma_{n+1}^z + \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y) + \lambda \sum_{n=1}^{L-2} \frac{J}{4} (\Delta \sigma_n^z \sigma_{n+2}^z + \sigma_n^x \sigma_{n+2}^x + \sigma_n^y \sigma_{n+2}^y)$$

QUANTUM CHAOS

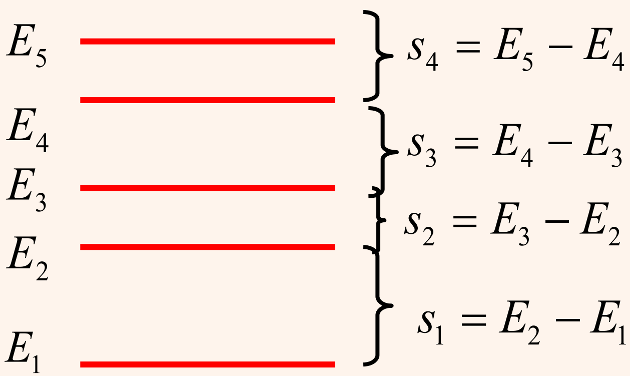
FULL RANDOM MATRICES
vs
TWO-BODY INTERACTIONS

Quantum Chaos: Level Repulsion

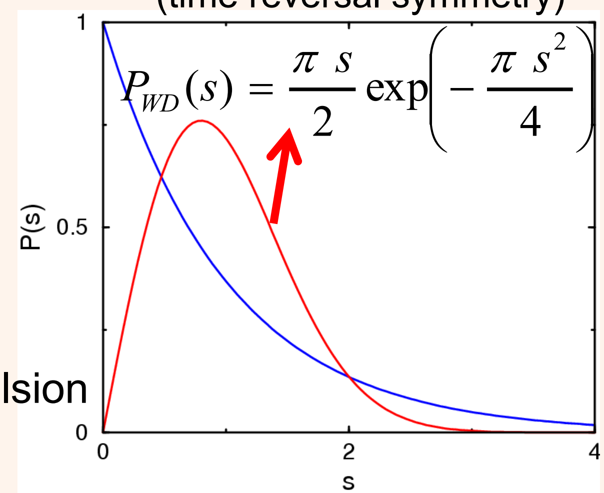
Full random matrices:
Matrices filled with random numbers and respecting the symmetries of the system.

Wigner in the 1950's used random matrices to study the spectrum of heavy nuclei
(atoms, molecules, quantum dots)

Level spacing distribution



Wigner-Dyson distribution
(time reversal symmetry)



Level repulsion

(i) Time-reversal invariant systems with rotational symmetry :
<u>Hamiltonians are real and symmetric</u>
Gaussian Orthogonal Ensemble (GOE)

Level repulsion = quantum chaos

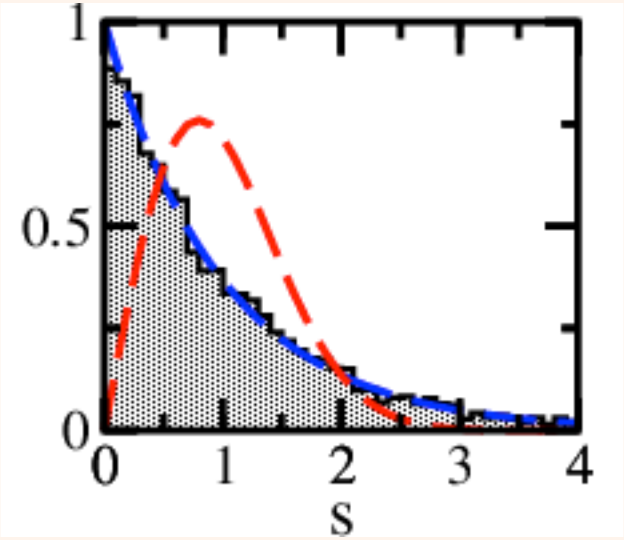
(ii) Systems without invariance under time reversal (atom in an external magnetic field)
Gaussian Unitary Ensemble (GUE)
<u>Hamiltonians are Hermitian</u>)

(iii) Time-reversal invariant systems,
half-integer spin, broken rotational symmetry
Gaussian Sympletic Ensemble (GSE)

Level Spacing Distribution: spin systems

Integrable

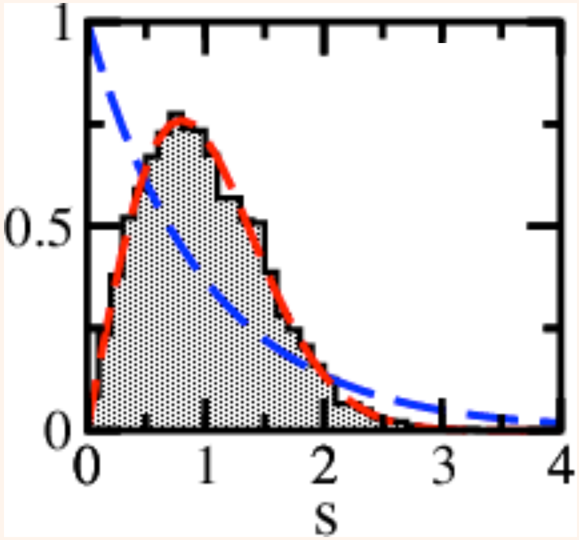
XXZ model



$$H=\sum_{n=1}^{L-1}\frac{J}{4}(\Delta\sigma_n^z\sigma_{n+1}^z+\sigma_n^x\sigma_{n+1}^x+\sigma_n^y\sigma_{n+1}^y)$$

Chaotic

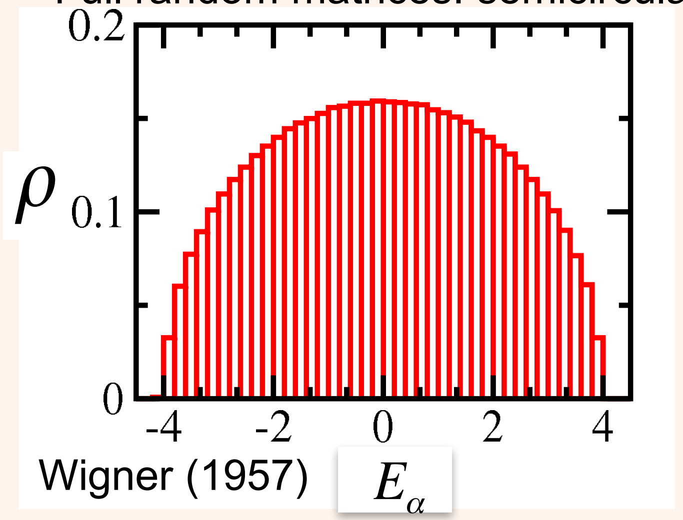
NNN model



$$H=\sum_{n=1}^{L-1}\frac{J}{4}(\Delta\sigma_n^z\sigma_{n+1}^z+\sigma_n^x\sigma_{n+1}^x+\sigma_n^y\sigma_{n+1}^y)+$$
$$+\lambda\sum_{n=1}^{L-2}\frac{J}{4}(\Delta\sigma_n^z\sigma_{n+2}^z+\sigma_n^x\sigma_{n+2}^x+\sigma_n^y\sigma_{n+2}^y)$$

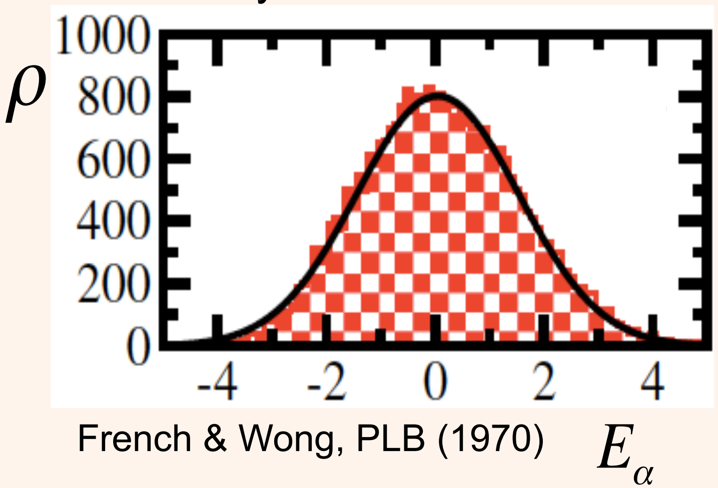
Full Random Matrices vs Two-Body Interaction

Full random matrices: semicircular



Wigner (1957)

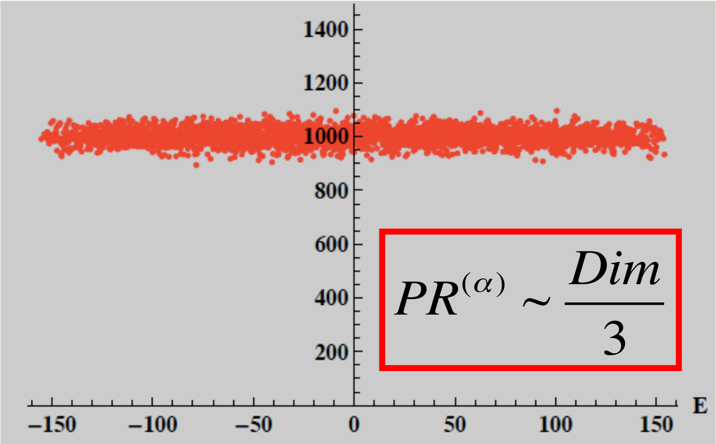
Two-body interactions: Gaussian



French & Wong, PLB (1970)

Full Random Matrices vs Two-Body Interaction

Full random matrices: random vectors



$$PR^{(\alpha)} \sim \frac{Dim}{3}$$

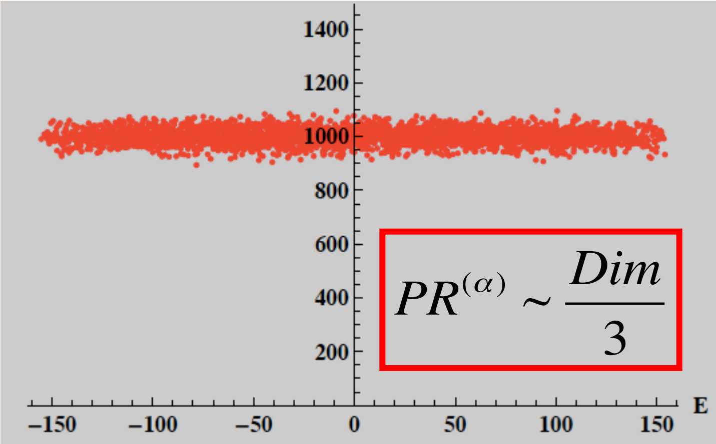
Participation Ratio

$$PR^{(\alpha)} \equiv \frac{1}{\sum_{i=1}^{D} |c_i^{(\alpha)}|^4}$$

$$\psi^{(\alpha)} = \sum_{i=1}^{D} c_i^{(\alpha)} \phi_i$$

Full Random Matrices vs Two-Body Interaction

Full random matrices: random vectors



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Shannon (information) entropy

$$Sh^{(\alpha)} \sim \ln(0.48 Dim)$$

$$Sh^{(\alpha)} = -\sum_i \left|C_i^{(\alpha)}\right|^2 \ln\left|C_i^{(\alpha)}\right|^2$$

Full Random Matrices vs Two-Body Interaction

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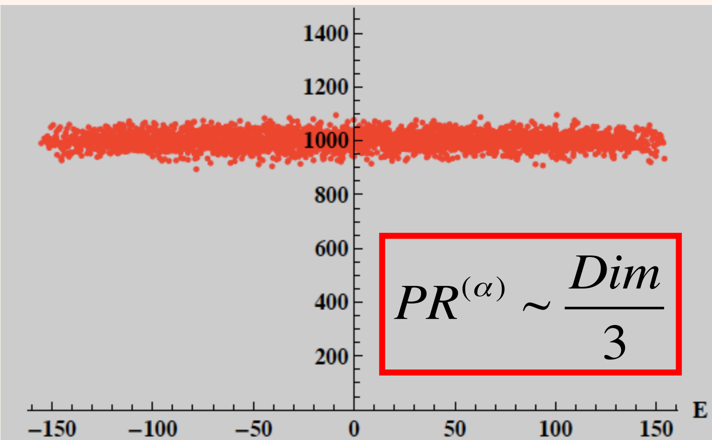

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Participation Ratio

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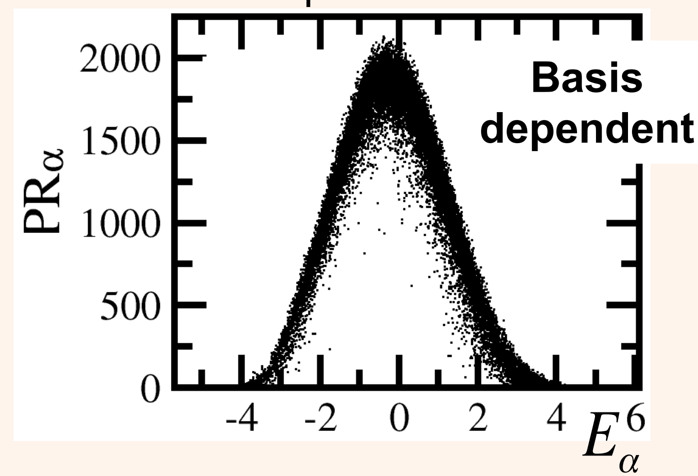
$$\psi^{(\alpha)} = \sum_{i=1}^{D} c_i^{(\alpha)} \phi_i$$

Two-body interactions: energy dependence



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$$Sh^{(\alpha)} \sim \ln(0.48 Dim)$$

$$Sh^{(\alpha)} = -\sum_i \left|C_i^{(\alpha)}\right|^2 \ln\left|C_i^{(\alpha)}\right|^2$$

Main Results

$$F(t) = \left| \langle \Psi(0) | \Psi(t) \rangle \right|^2$$

Survival Probability (= Fourier transform of the spectral autocorrelation function
= analytically continued partition function)

- Decays faster than exponential in chaotic and integrable models.
- Power-law decays at long times (delocalized and nearly localized systems). t^{-3}
- Unambiguous dynamical manifestation of level repulsion: correlation hole.
- Similarities between the entanglement and Shannon (information) entropy.
- Out-of-time correlators. t^{-6}

Analytical results for FRM

DYNAMICS

Quench

Initial state

$|\Psi(0)\rangle = |ini\rangle$ → $|\Psi(t)\rangle = \sum_{\alpha} C_{\alpha}^{ini} e^{-iE_{\alpha}t} |\alpha\rangle$

$H_{initial}$ —quench→ H_{final}

$|n\rangle$ → $|\alpha\rangle$

Survival Probability (Fidelity)

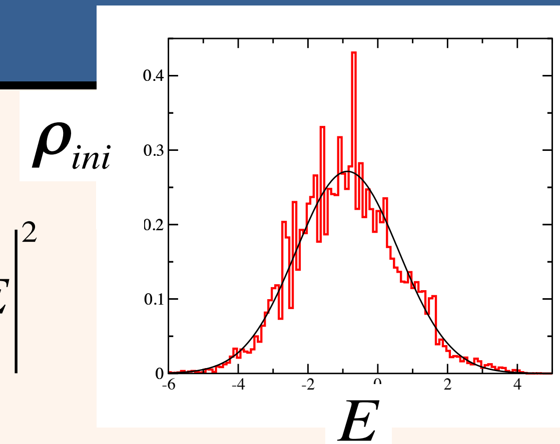
Overlap between the initial state and the evolved state

$$F(t) = \left| \langle \Psi(0) | \Psi(t) \rangle \right|^2 = \left| \sum_{\alpha} \left| C_{\alpha}^{ini} \right|^2 e^{-iE_{\alpha}t} \right|^2 \cong \left| \int_{-\infty}^{\infty} \rho_{ini}(E) e^{-iEt} \, dE \right|^2$$

$$|\Psi(0)\rangle = |ini\rangle = \sum_{\alpha} C_{\alpha}^{ini} |\alpha\rangle \qquad |\Psi(t)\rangle = \sum_{\alpha} C_{\alpha}^{ini} e^{-iE_{\alpha}t} |\alpha\rangle$$

Eigenvalues and eigenstates of the final Hamiltonian

Survival Probability (Fidelity)



Overlap between the initial state and the evolved state

$$F(t) = \left| \langle \Psi(0) | \Psi(t) \rangle \right|^2 = \left| \sum_{\alpha} \left| C_{\alpha}^{ini} \right|^2 e^{-iE_{\alpha}t} \right|^2 \cong \left| \int_{-\infty}^{\infty} \rho_{ini}(E) e^{-iEt} \, dE \right|^2$$

$$\Downarrow$$

$$\rho_{ini}(E) = \sum_{\alpha} \left| C_{\alpha}^{ini} \right|^2 \delta(E - E_{\alpha})$$

Fourier transform
- of the weighted energy distribution of the initial state
- of the LDOS (local density of states), strength function

$$| \Psi(0) \rangle = | ini \rangle = \sum_{\alpha} C_{\alpha}^{ini} | \alpha \rangle \qquad | \Psi(t) \rangle = \sum_{\alpha} C_{\alpha}^{ini} e^{-iE_{\alpha}t} | \alpha \rangle$$

Eigenvalues and eigenstates of the final Hamiltonian

Quench Dynamics

Integrable

XXZ model

$$H_{ini} = \sum_{n=1}^{L-1} \frac{J}{4} (\Delta \sigma_n^z \sigma_{n+1}^z + \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y) \longrightarrow$$

$$|\Psi(0)\rangle = |ini\rangle$$

Chaotic

NNN model

$$H = \sum_{n=1}^{L-1} \frac{J}{4} (\Delta \sigma_n^z \sigma_{n+1}^z + \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y) +$$

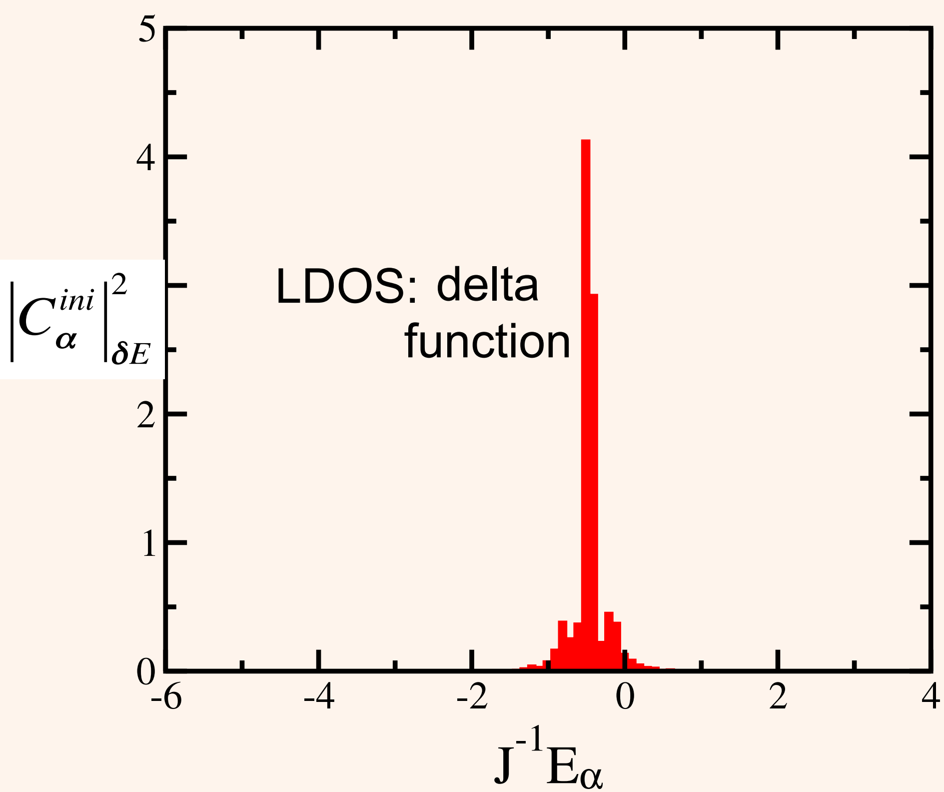
$$+ \lambda \sum_{n=1}^{L-2} \frac{J}{4} (\Delta \sigma_n^z \sigma_{n+2}^z + \sigma_n^x \sigma_{n+2}^x + \sigma_n^y \sigma_{n+2}^y)$$

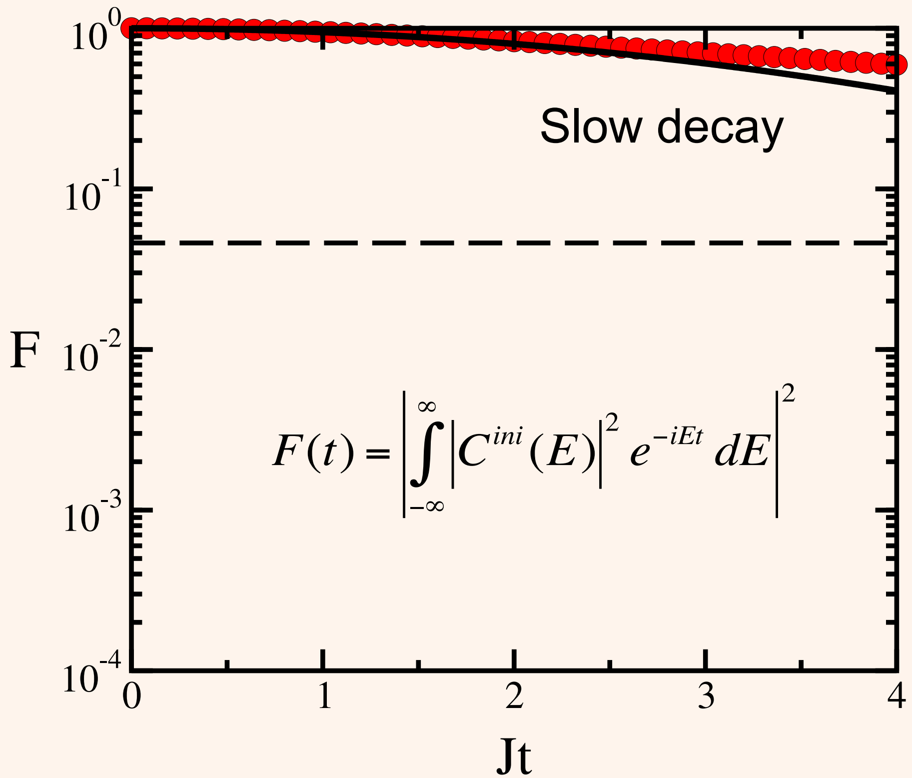
quench parameter

Perturbation increases Fidelity decays faster

$$H_{initial} = H_{XXZ} \xrightarrow{quench} H_{final} = H_{XXZ} + \lambda H_{NNN}$$

$$\lambda = 0.2$$





L=16, 8 up spins, T=7.1 $\Delta = 0.5$

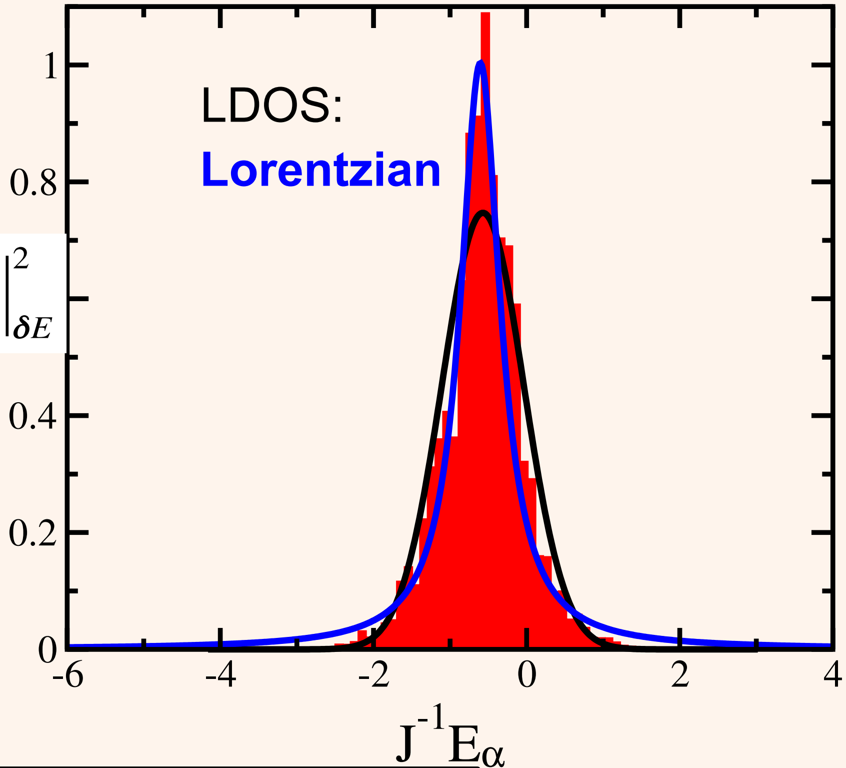
Exponential decay

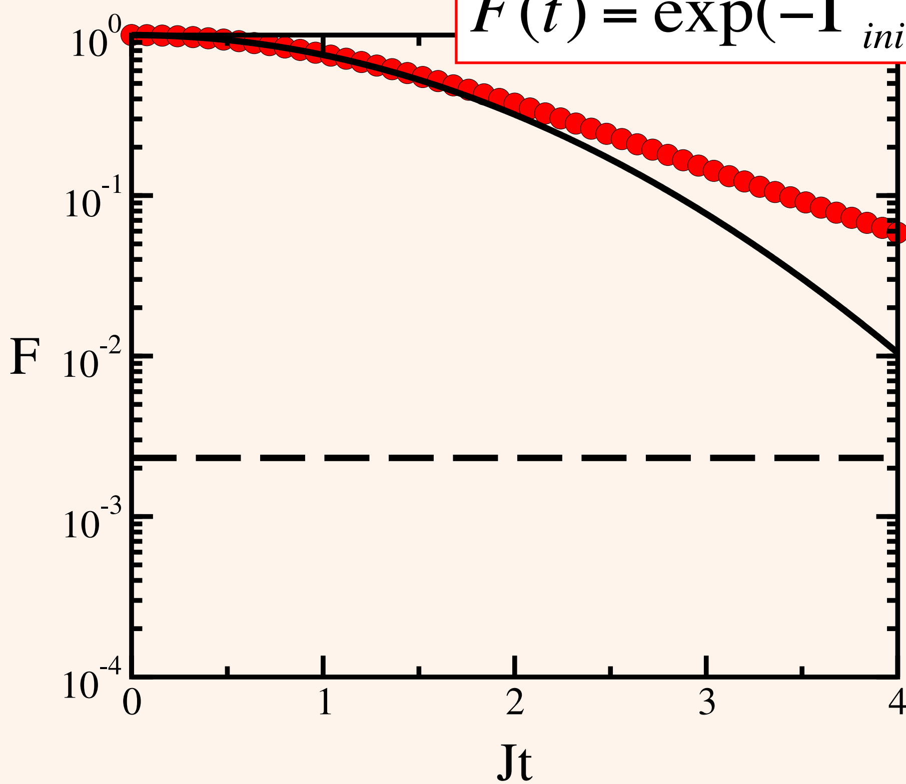
$$H_{initial} = H_{XXZ} \xrightarrow{quench} H_{final} = H_{XXZ} + \lambda H_{NNN}$$

$$\lambda = 0.45$$

$$\frac{1}{2\pi} \frac{\Gamma_{ini}}{(E_{ini} - E)^2 + \Gamma_{ini}^2 / 4}$$

$$F(t) = \exp(-\Gamma_{ini} t)$$





$|C_\alpha^{ini}|^2_{\delta E}$

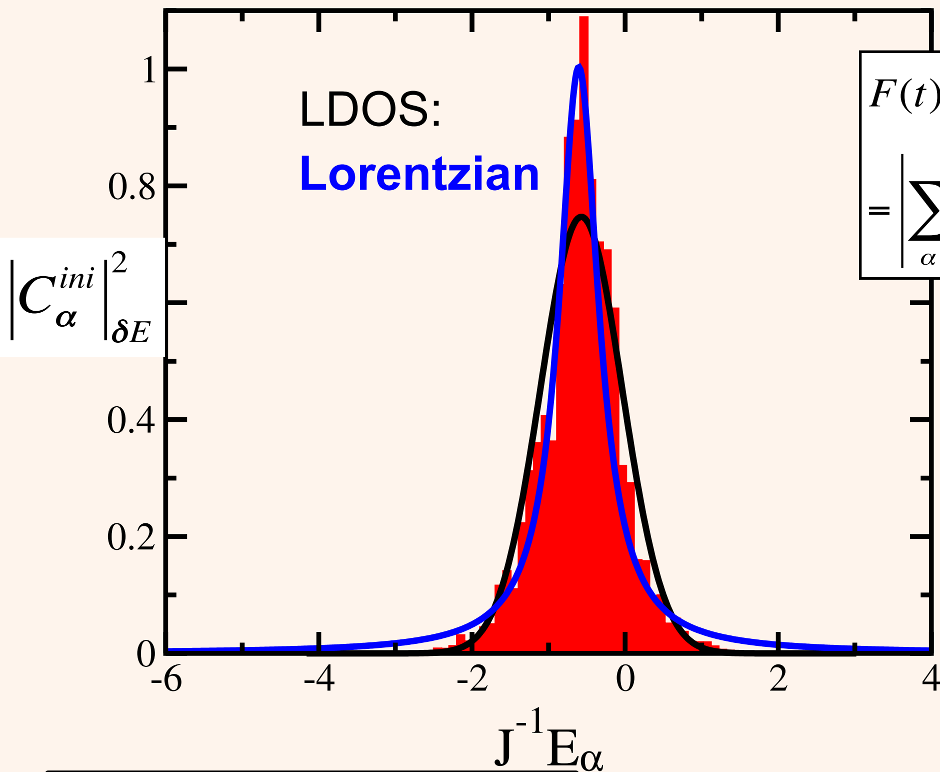
L=16, 8 up spins, T=7.1 $\Delta = 0.5$

Exponential decay

$$H_{initial} = H_{XXZ} \xrightarrow{quench} H_{final} = H_{XXZ} + \lambda H_{NNN}$$

$$\lambda = 0.45$$

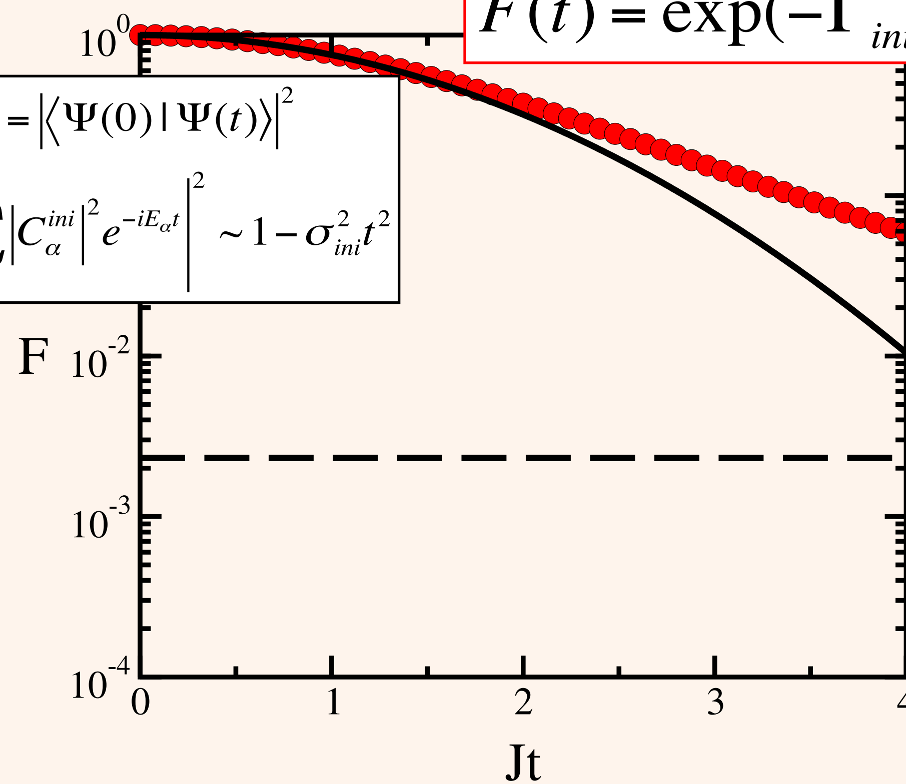
$$\frac{1}{2\pi}\frac{\Gamma_{ini}}{(E_{ini}-E)^2 + \Gamma_{ini}^2/4}$$



$$F(t) = \exp(-\Gamma_{ini} t)$$

$$F(t) = \left|\langle \Psi(0) | \Psi(t) \rangle\right|^2$$

$$= \left|\sum_{\alpha} \left|C_{\alpha}^{ini}\right|^2 e^{-iE_{\alpha}t}\right|^2 \sim 1 - \sigma_{ini}^2 t^2$$



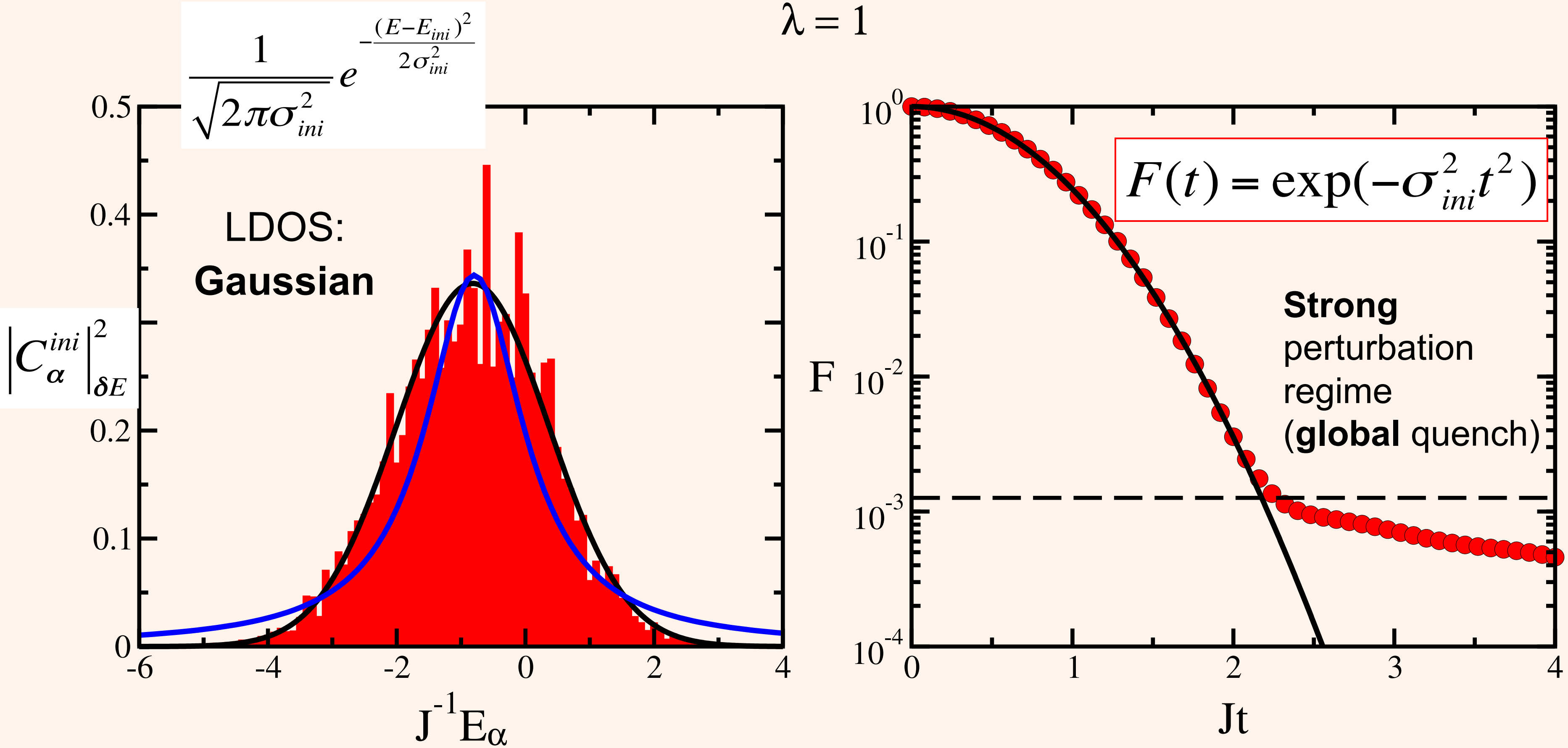
L=16, 8 up spins, T=7.1

$\Delta = 0.5$

Faster than exponential: Gaussian

$$H_{initial} = H_{XXZ} \xrightarrow{quench} H_{final} = H_{XXZ} + \lambda H_{NNN}$$

$\lambda = 1$

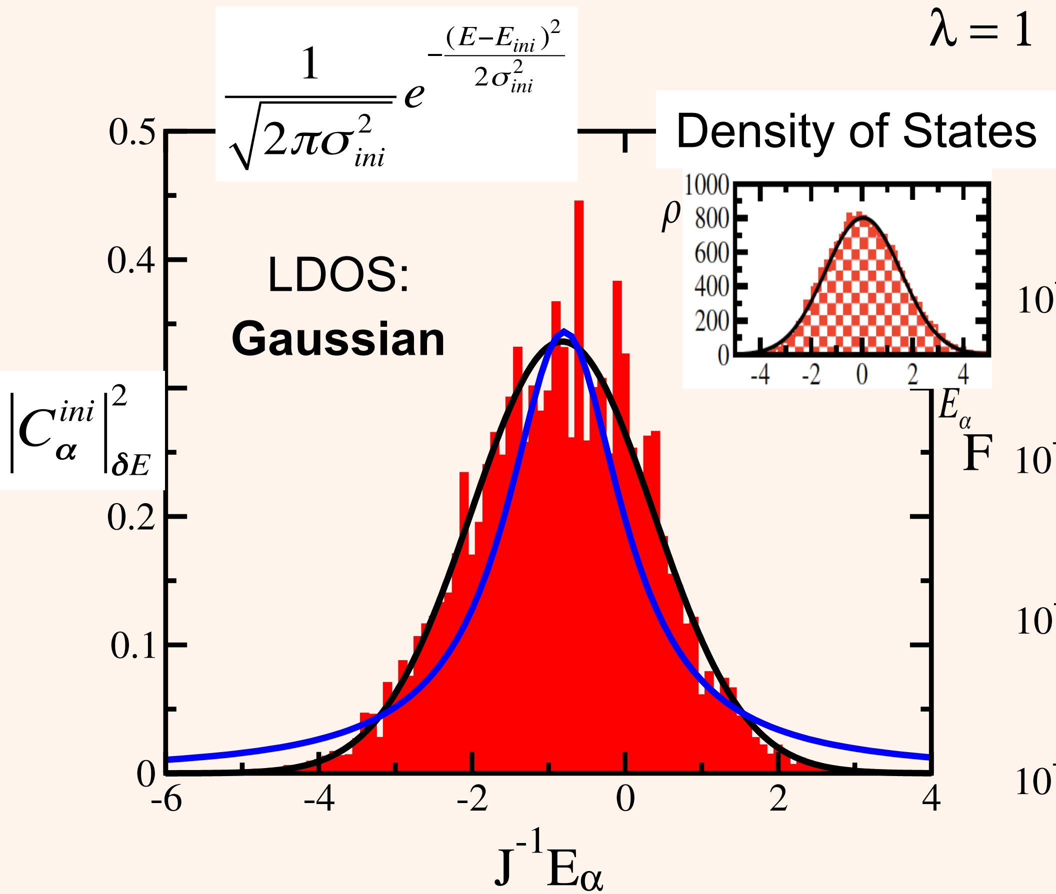


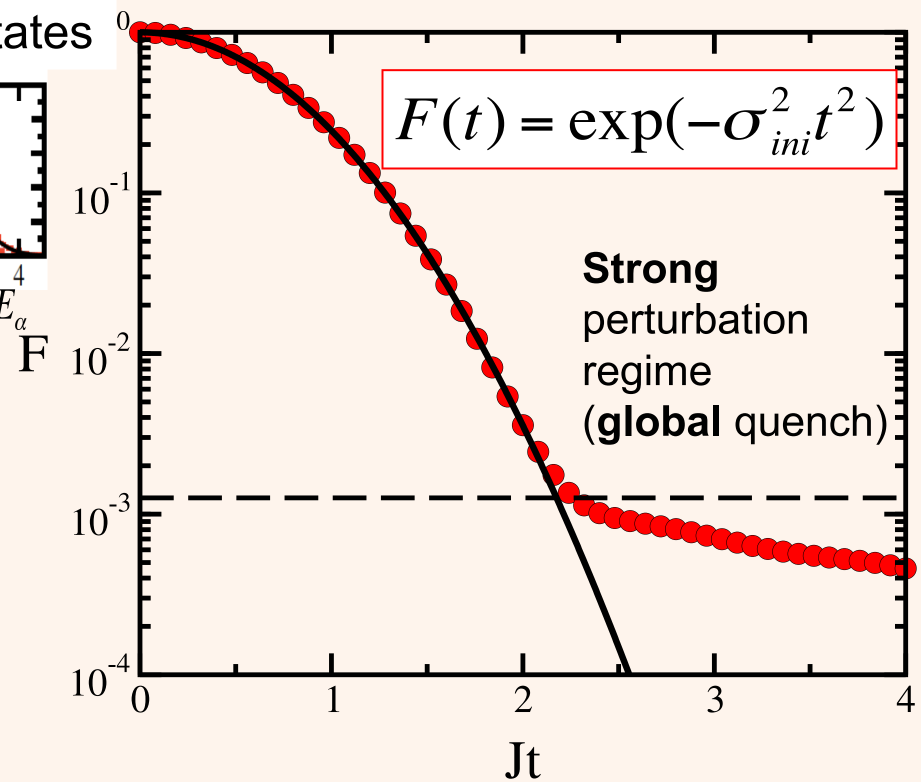
L=16, 8 up spins, T=7.1 $\Delta = 0.5$

Gaussian decay
Gaussian DOS & LDOS

$$H_{initial} = H_{XXZ} \xrightarrow{quench} H_{final} = H_{XXZ} + \lambda H_{NNN}$$

$$\lambda = 1$$





Lea F. Santos, Yeshiva University

L=16, 8 up spins, T=7.1

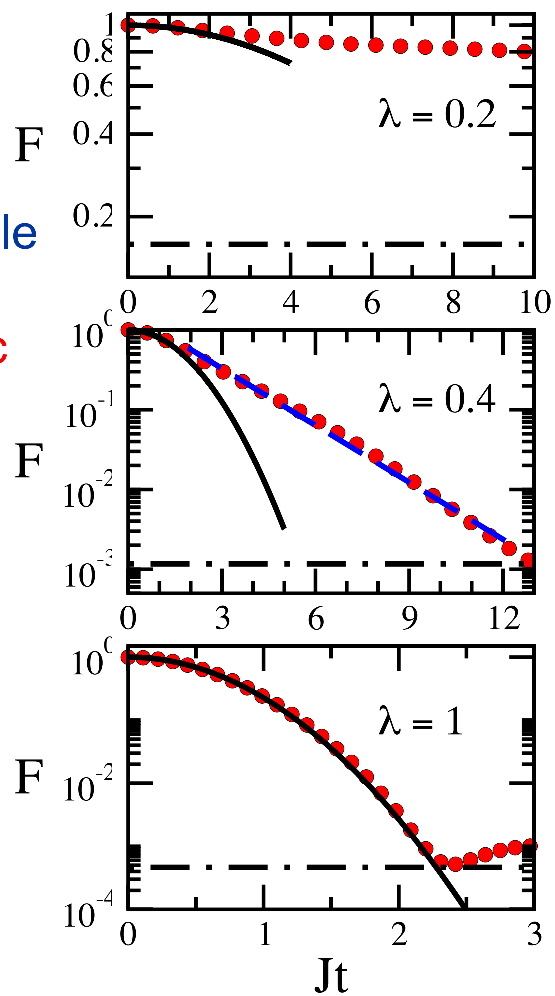
$\Delta = 0.5$

NMP17, East Lansing, MI

Exponential and Gaussian F(t)
H^{final}: Chaotic or Integrable

$$H_{XXZ} \xrightarrow{\lambda} H_{XXZ} + \lambda H_{NNN}$$

Integrable
to
chaotic



Torres & LFS
PRA **89** (2014)

Torres, Vyas, LFS
NJP **16** (2014)

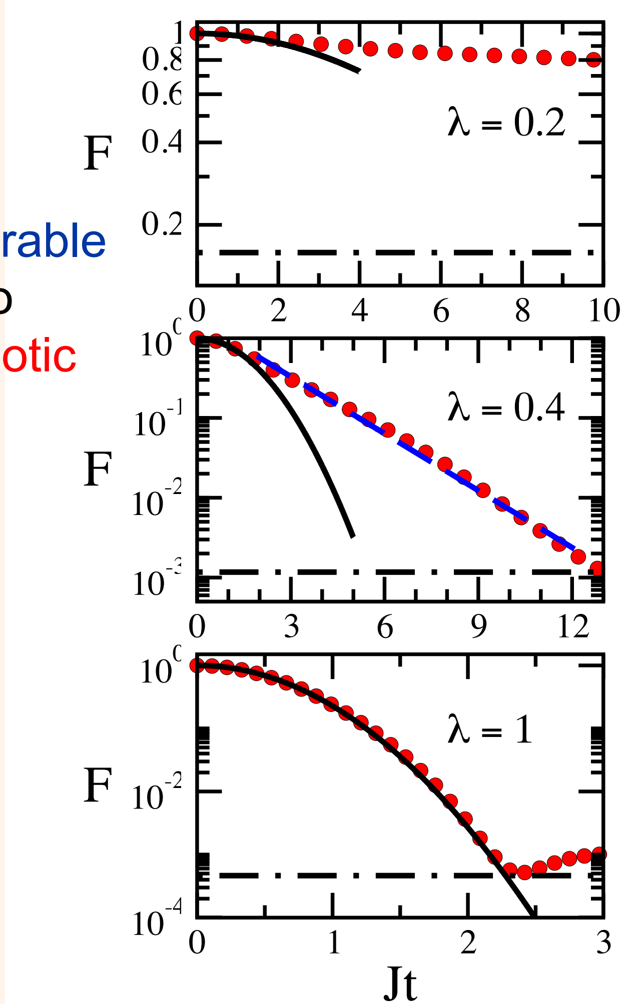
Torres & LFS
PRA **90** (2014)

L=18, 6 up spins

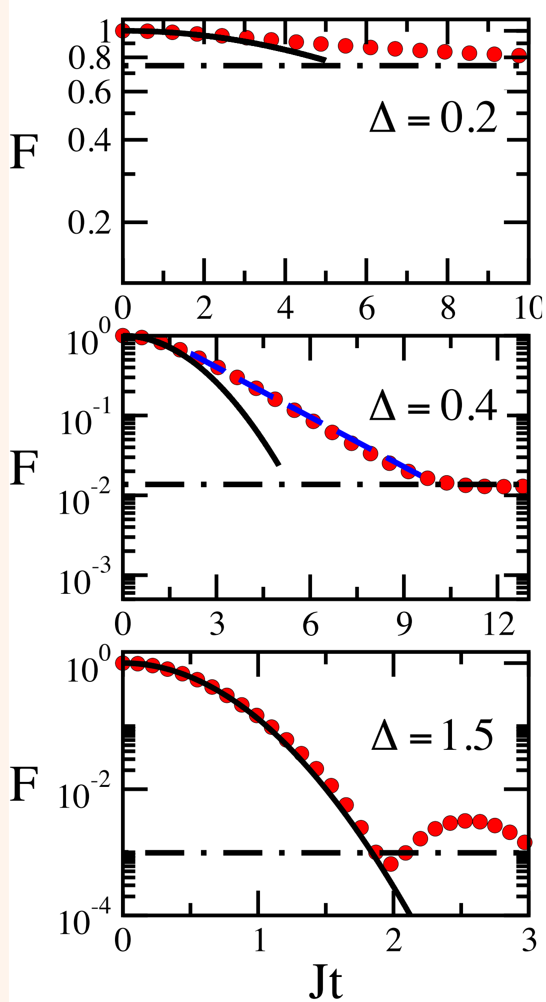
Exponential and Gaussian F(t)
H^{final}: Chaotic or Integrable

$H_{XXZ} \xrightarrow{\lambda} H_{XXZ} + \lambda H_{NNN}$

Integrable
to
chaotic



$H_{XX} \xrightarrow{\Delta} H_{XXZ}$



Integrable
to
integrable

$$\sum_{n=1}^{L-1} \frac{J}{4} (\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y)$$

$$\downarrow \Delta$$

$$\sum_{n=1}^{L-1} \frac{J}{4} (\Delta \sigma_n^z \sigma_{n+1}^z + \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y)$$

Torres & LFS
PRA **89** (2014)

Torres, Vyas, LFS
NJP **16** (2014)

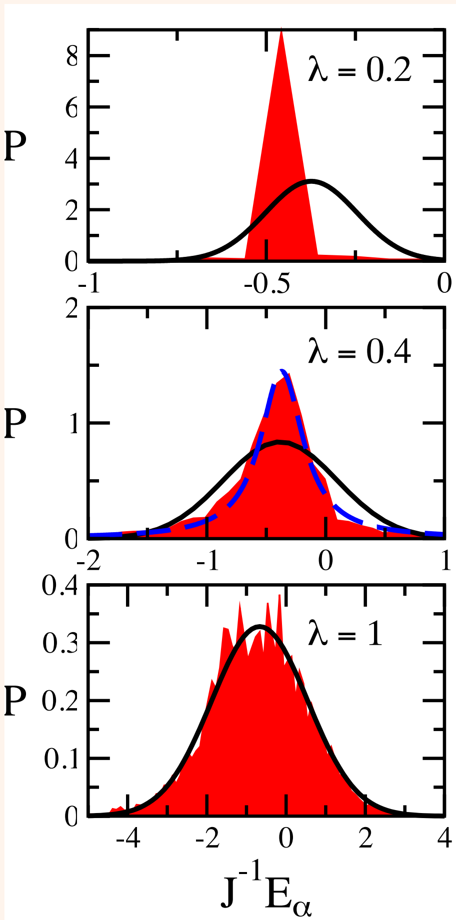
Torres & LFS
PRA **90** (2014)

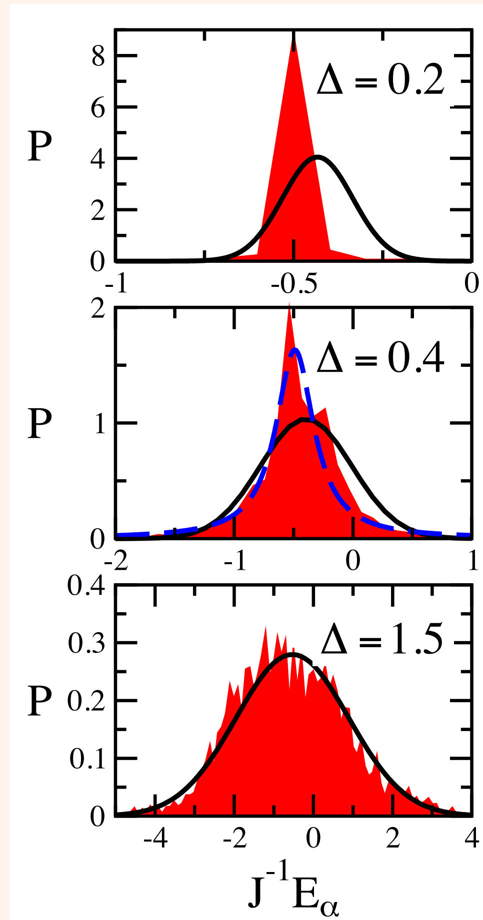
L=18, 6 up spins

Exponential and Gaussian F(t)
H^{final}: Chaotic or Integrable

$$H_{XXZ} \xrightarrow{\lambda} H_{XXZ} + \lambda H_{NNN} \qquad H_{XX} \xrightarrow{\Delta} H_{XXZ}$$

Integrable
to
chaotic





Integrable
to
integrable

Torres & LFS
PRA **89** (2014)

Torres, Vyas, LFS
NJP **16** (2014)

Torres & LFS
PRA **90** (2014)

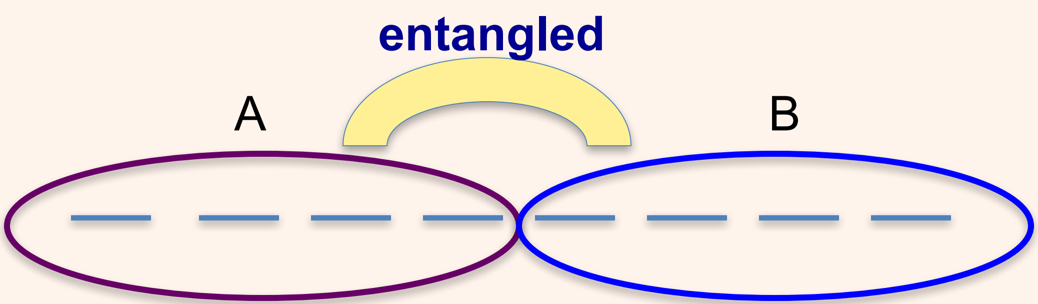
L=18, 6 up spins

LFS, Borgonovi, Izrailev
PRL **108** (2012), PRE **85** (2012)

Evolution of Entropies

Entanglement Entropy: von Neumann entropy of the reduced density matrix

$$Sv(t) = -Tr[\rho_A(t) \ln \rho_A(t)]$$



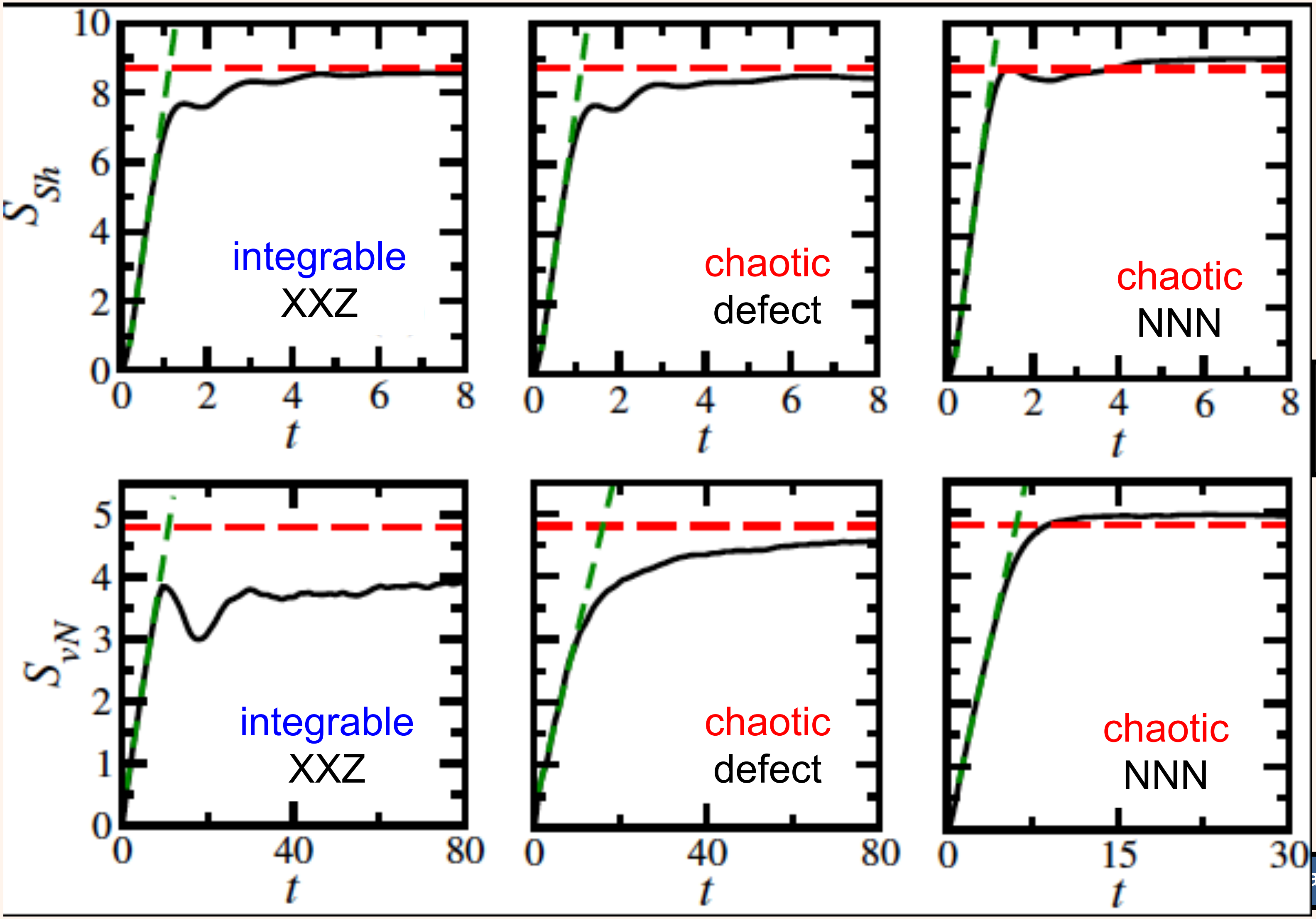
Shannon Entropy:

$$Sh(t) = -\sum_n W_n(t) \ln W_n(t)$$

$$W_n(t) = \left| \langle \phi_n | e^{-iHt} | \Psi(0) \rangle \right|^2$$

Torres et al,
Entropy **18**, 359 (2016)

Integrable and Chaotic Models



$|\Psi(0)\rangle$

Néel state

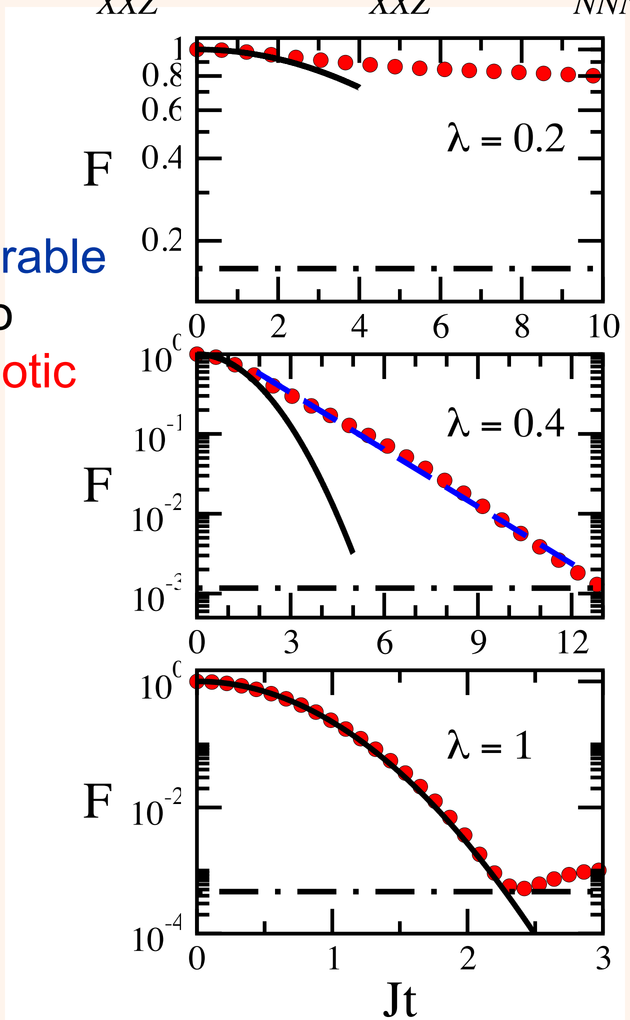
LFS, Borgonovi, Izrailev
PRL **108**, 094102 (2012)
PRE **85**, 036209 (2012)

Torres et al,
Entropy (2016)

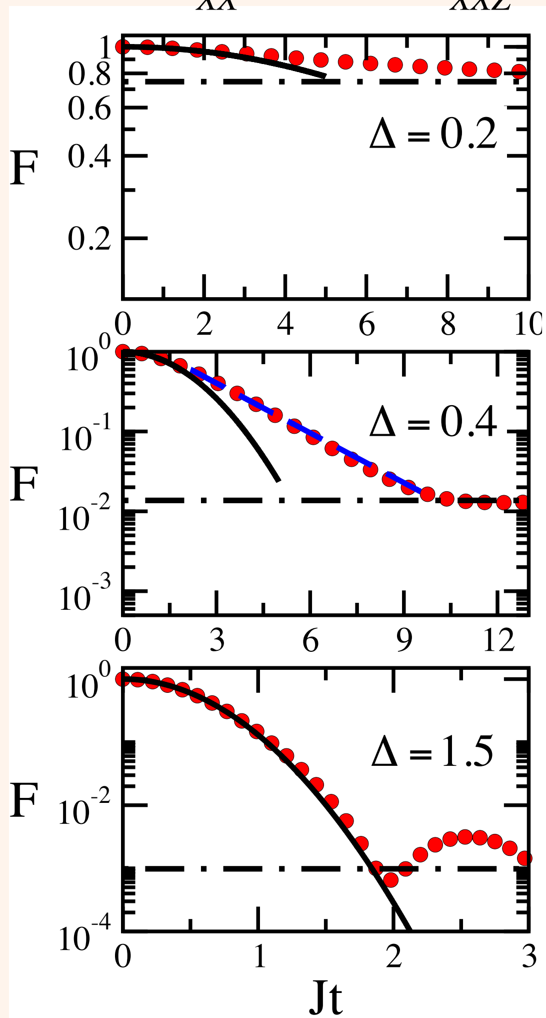
Exponential and Gaussian F(t)
H^{final}: Chaotic or Integrable

$$H_{XXZ} \xrightarrow{\lambda} H_{XXZ} + \lambda H_{NNN}$$

Integrable
to
chaotic



$$H_{XX} \xrightarrow{\Delta} H_{XXZ}$$



Integrable
to
integrable

$$\sum_{n=1}^{L-1} \frac{J}{4} (\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y)$$

$$\downarrow \Delta$$

$$\sum_{n=1}^{L-1} \frac{J}{4} (\Delta \sigma_n^z \sigma_{n+1}^z + \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y)$$

Torres & LFS
PRA **89** (2014)

Torres, Vyas, LFS
NJP **16** (2014)

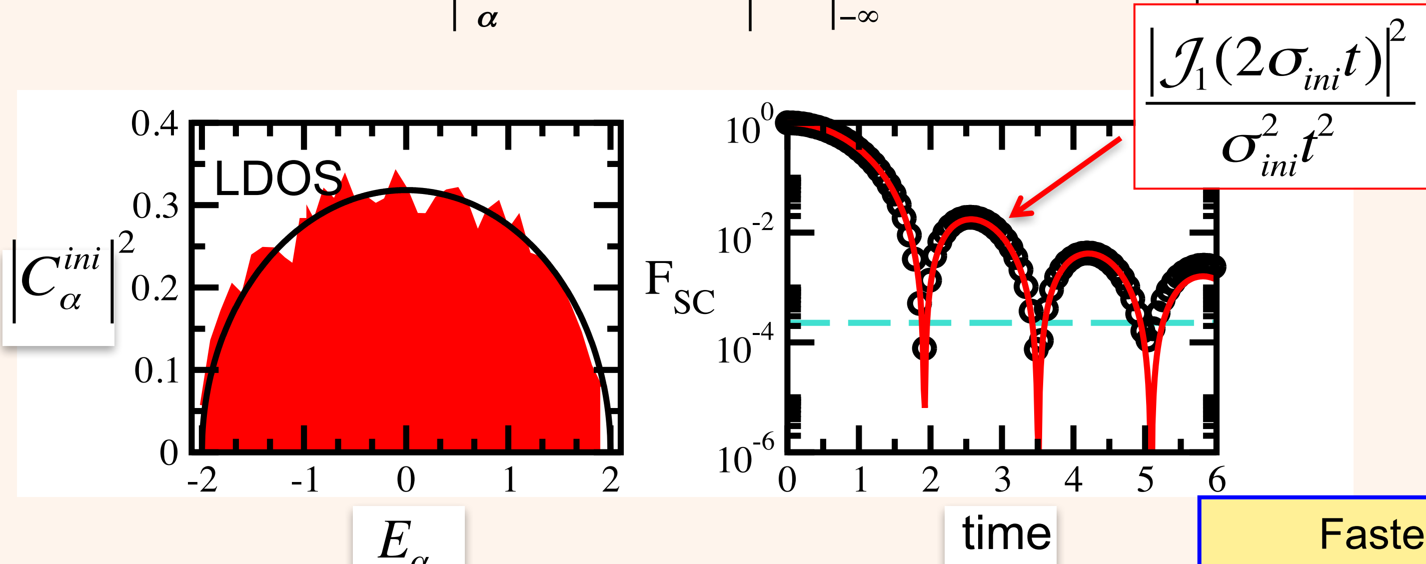
Torres & LFS
PRA **90** (2014)

L=18, 6 up spins

Dynamics under full random matrices

Distribution of $\left|C_\alpha^{ini}\right|^2$ for initial state projected into random matrices: semicircular

$$F(t) = \left|\langle \Psi(0) | \Psi(t) \rangle\right|^2 = \left|\sum_\alpha \left|C_\alpha^{ini}\right|^2 e^{-iE_\alpha t}\right|^2 \cong \left|\int_{-\infty}^{\infty} P_{ini}(E) e^{-iEt}\, dE\right|^2$$



Faster decay in:
Torres & LFS
PRA **90** (2014)
(quantum speed limit)

Torres & LFS
PRA **89** (2014)

Torres, Vyas, LFS
NJP **16** (2014)

Dynamics under full random matrices

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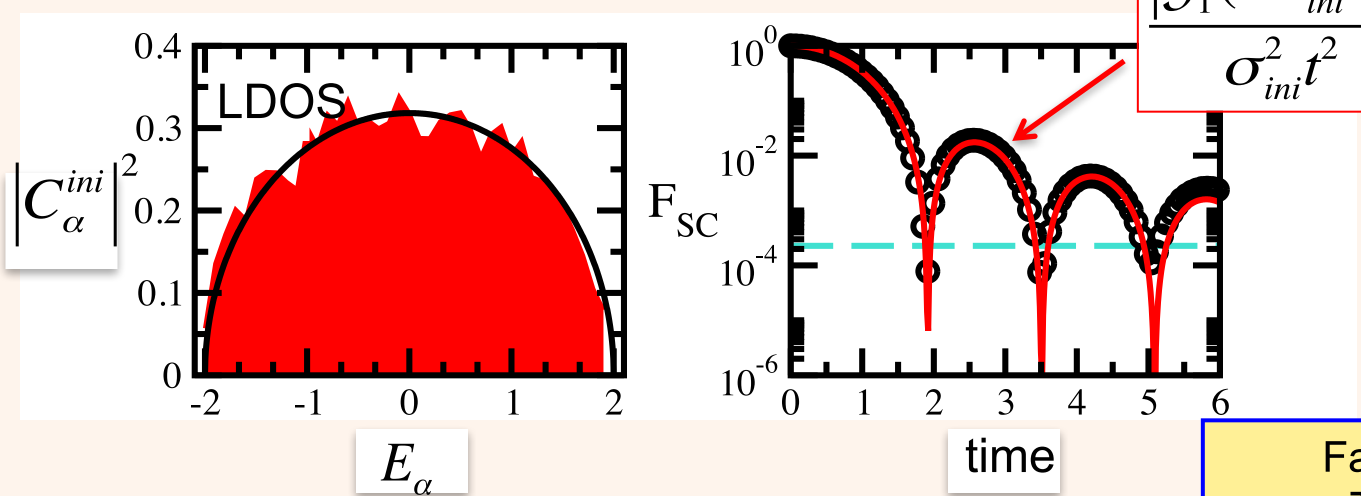
$$\frac{\left|\mathcal{J}_1(2\sigma_{ini} t)\right|^2}{\sigma_{ini}^2 t^2} \rightarrow t^{-3} \frac{1-\sin(4\sigma t)}{2\pi\sigma^3}$$



Faster decay in:
Torres & LFS
PRA **90** (2014)
(quantum speed limit)

Torres & LFS
PRA **89** (2014)

Torres, Vyas, LFS
NJP **16** (2014)

LONG-TIME DYNAMICS

Távora, Torres, LFS
PRA **94**, 041603R (2016)

Távora, Torres, LFS
PRA **95**, 013604 (2017)

Quench: Disordered Hamiltonian

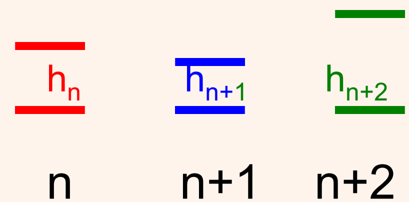
Site-basis vectors

↑↓↑↓↑↓↑↓

↑↓↑↑↓↓↑↓

Strong perturbation

$$H_{final} = \sum_{n=1}^{L} h_n S_n^z + \sum_{n=1}^{L} J(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + S_n^z S_{n+1}^z)$$



Anderson localization

↑↓↑↓↑↓↑↓

↑↓↑↑↓↓↑↓

$$H_{final} = \sum_{n=1}^{L} h_n S_n^z + \sum_{n=1}^{L} J(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \cancel{S_n^z S_{n+1}^z})$$

Integrable-chaos-integrable

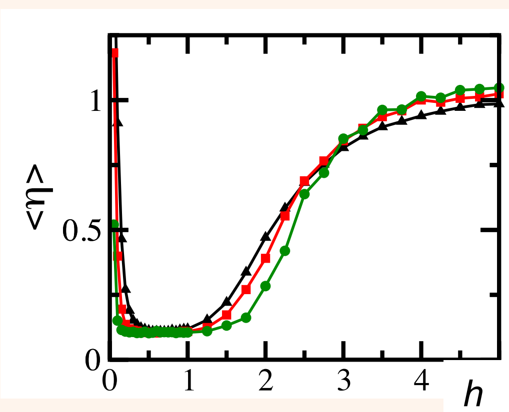
Intermediate level statistics: h>J (nonergodic delocalized states)

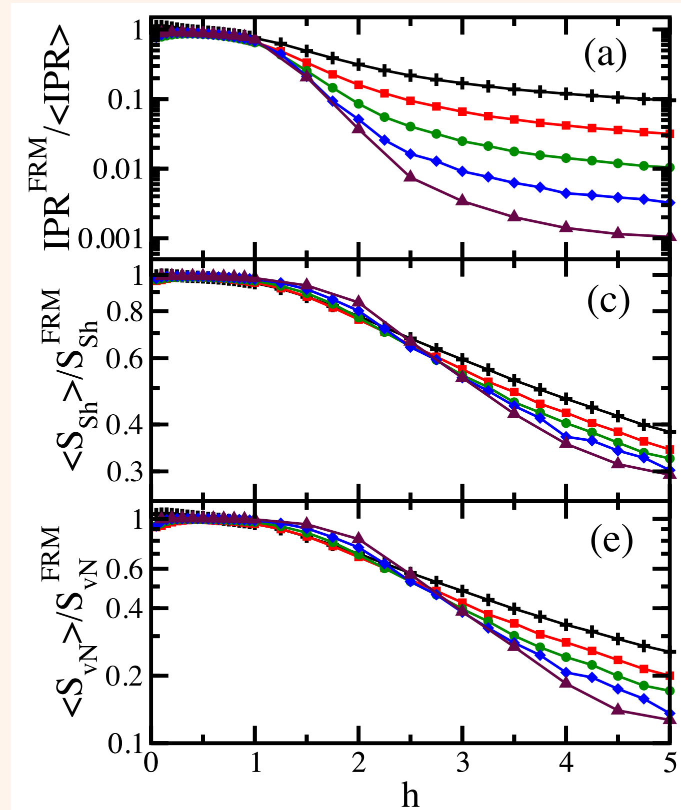
$$H_{final} = \sum_{n=1}^{L} h_n S_n^z + \sum_{n=1}^{L} J(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + S_n^z S_{n+1}^z)$$

$$PR^{(\alpha)} \propto Dim^{D_2}$$

$$D_2 < 1$$

$$\eta = \frac{\int_0^{s_0} [P(s) - P_{WD}(s)]ds}{\int_0^{s_0} [P_P(s) - P_{WD}(s)]ds},$$





LFS, J. Phys. A **37,** 4723 (2004)
LFS, Rigolin, Escobar PRA (2004)

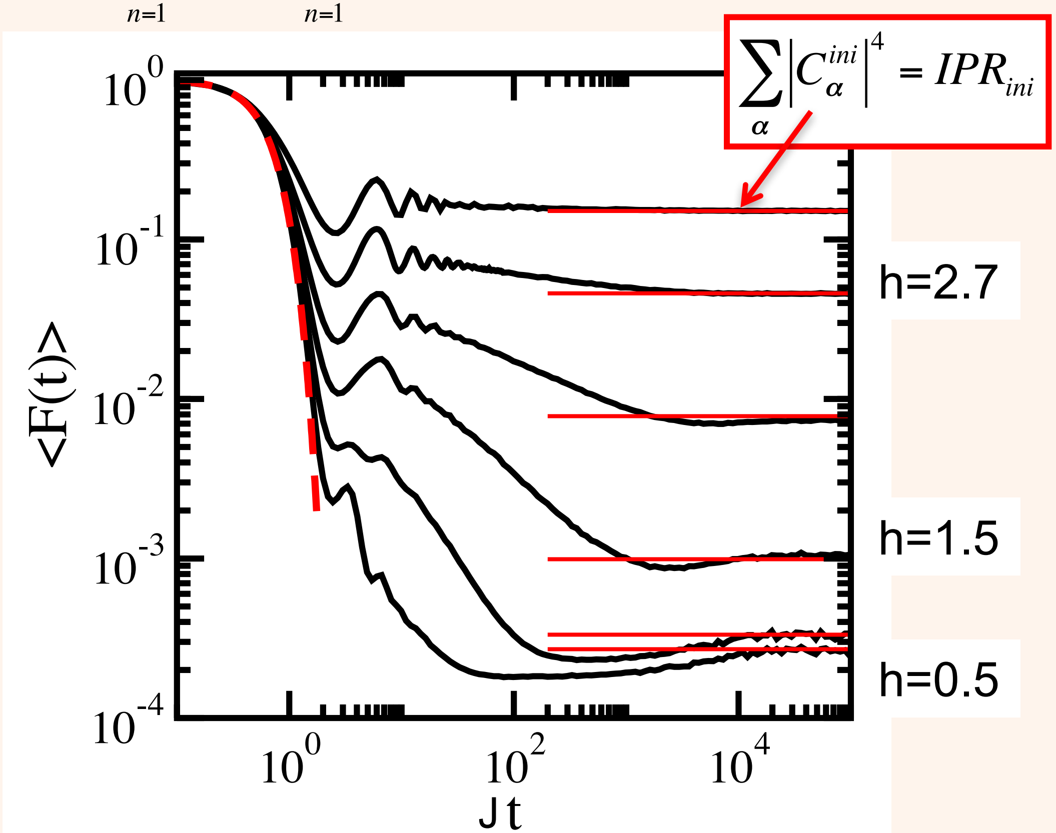
$$PR_q^{(\alpha)} \propto Dim^{(q-1)D_q}$$

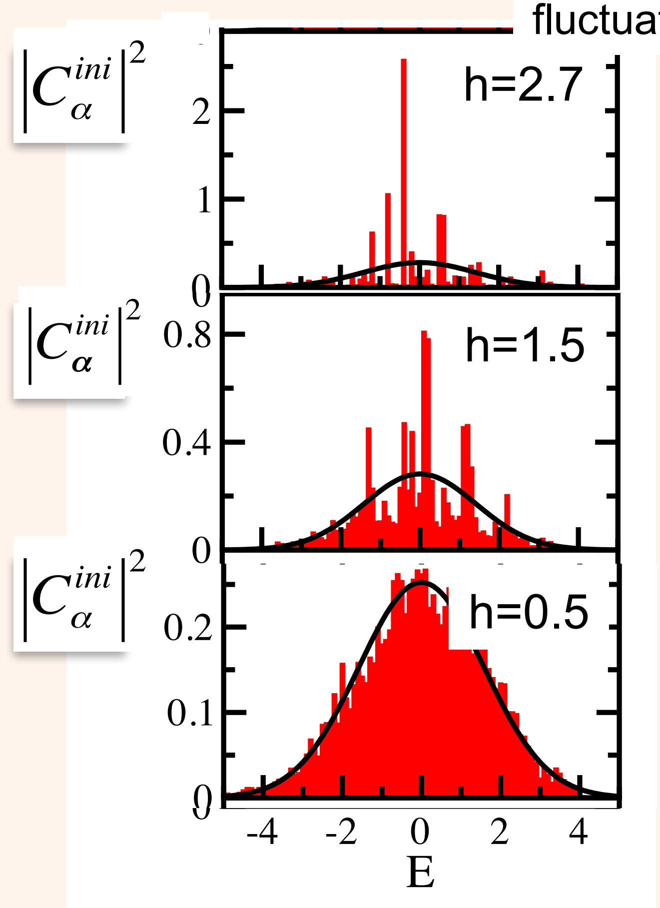
Multifractality = nonlinear dependence of the generalized dimension on q

Torres & LFS, Ann. Phys. (2017)

Sparse LDOS
System with strong disorder

$$H_{final} = \sum_{n=1}^{L} h_n S_n^z + \sum_{n=1}^{L} J(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + S_n^z S_{n+1}^z)$$





multifractal fluctuations

L=16, 8 up spins

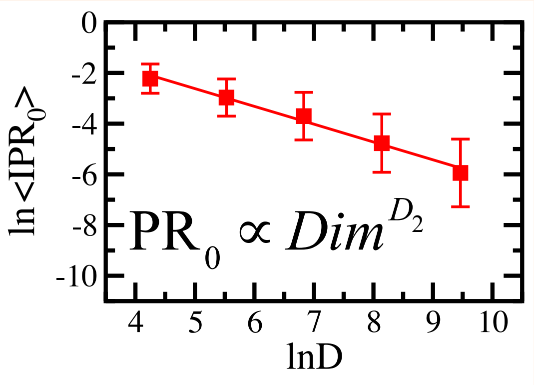
Torres & LFS
PRB **92**, 01420 (2015)

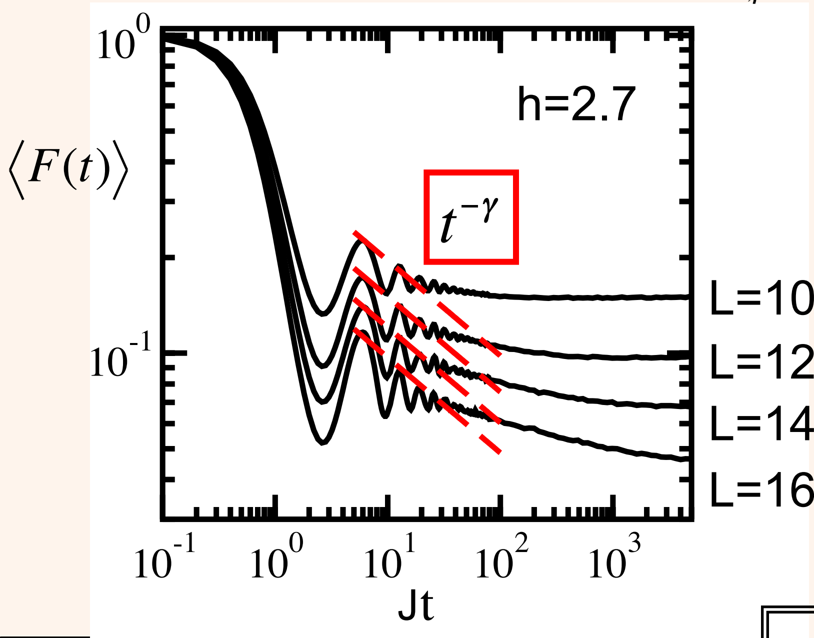
Power-law exponent: correlations

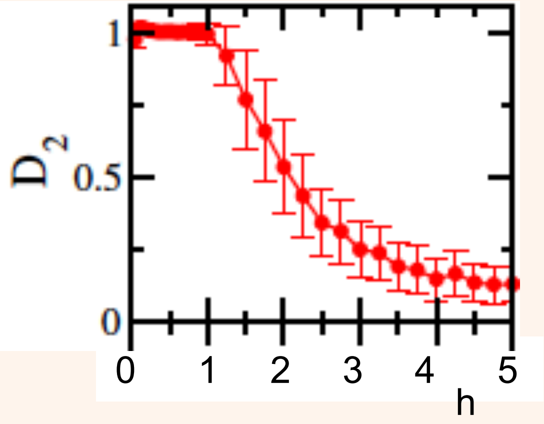
$$PR_0 = \frac{1}{\sum_{\alpha} \left| C_{\alpha}^{(0)} \right|^4} \propto (Dim)^{D_2} \Rightarrow D_2 < 1$$

$$F(t) = \sum_{\alpha,\beta} \left| C_{\alpha}^{(0)} \right|^2 \left| C_{\beta}^{(0)} \right|^2 e^{i(E_\beta - E_\alpha)t} \xrightarrow{\omega = E_\beta - E_\alpha} \int d\omega e^{i\omega t} C(\omega) \rightarrow t^{-\gamma}$$

$$C(\omega) = \sum_{\alpha,\beta} \left| C_{\alpha}^{(0)} \right|^2 \left| C_{\beta}^{(0)} \right|^2 \delta(E_\alpha - E_\beta - \omega) = |\omega|^{\gamma - 1}$$







Generalized dimension
Multifractal dimension

Torres & LFS
PRB **92**, 01420 (2015)

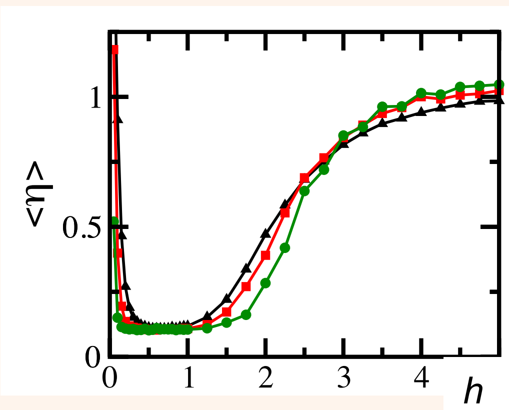
Entropies: log behavior

Intermediate level statistics: h>J

Nonergodic delocalized states: $PR^{(\alpha)} \propto Dim^{D_2}$

$D_2 < 1$

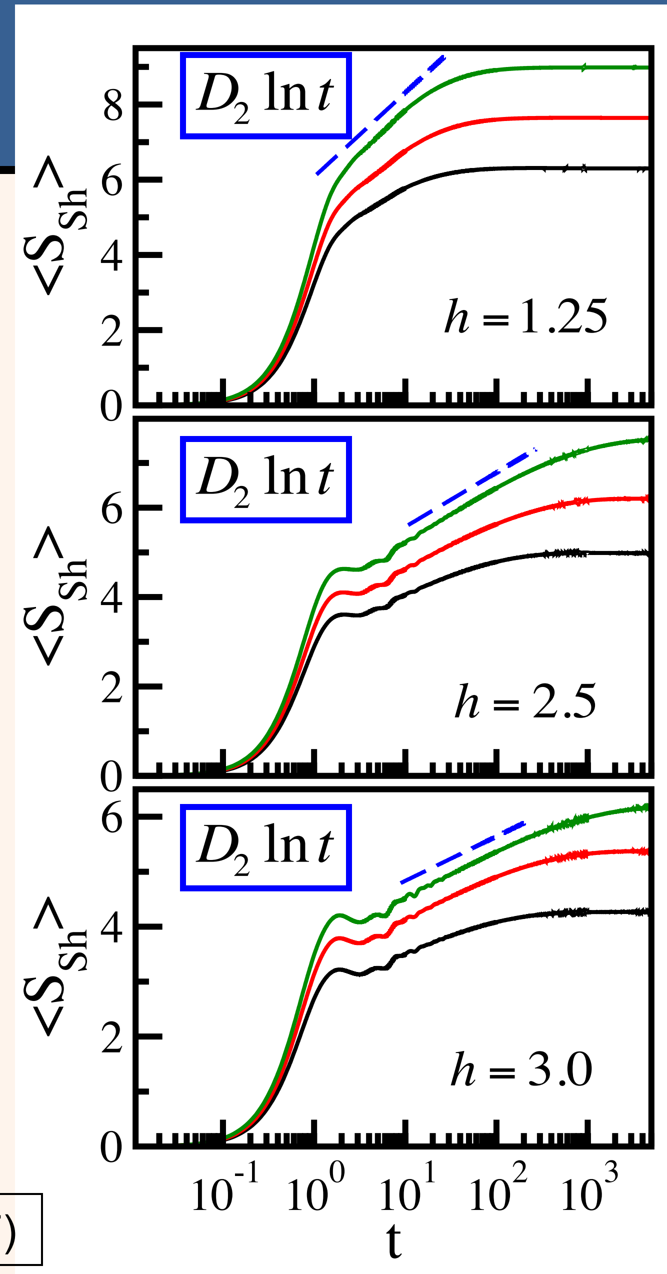
$$\eta = \frac{\int_0^{s_0}[P(s) - P_{WD}(s)]ds}{\int_0^{s_0}[P_P(s) - P_{WD}(s)]ds},$$



LFS, J. Phys. A **37**, 4723 (2004)

$$Sh(t) = -\sum_n W_n(t) \ln W_n(t)$$

$$W_n(t) = \left| \langle \phi_n | e^{-iHt} | \Psi(0) \rangle \right|^2$$



Lea F. Santos, Yeshiva University

Torres & LFS, Ann. Phys. (2017)

Power-law exponent: energy bounds

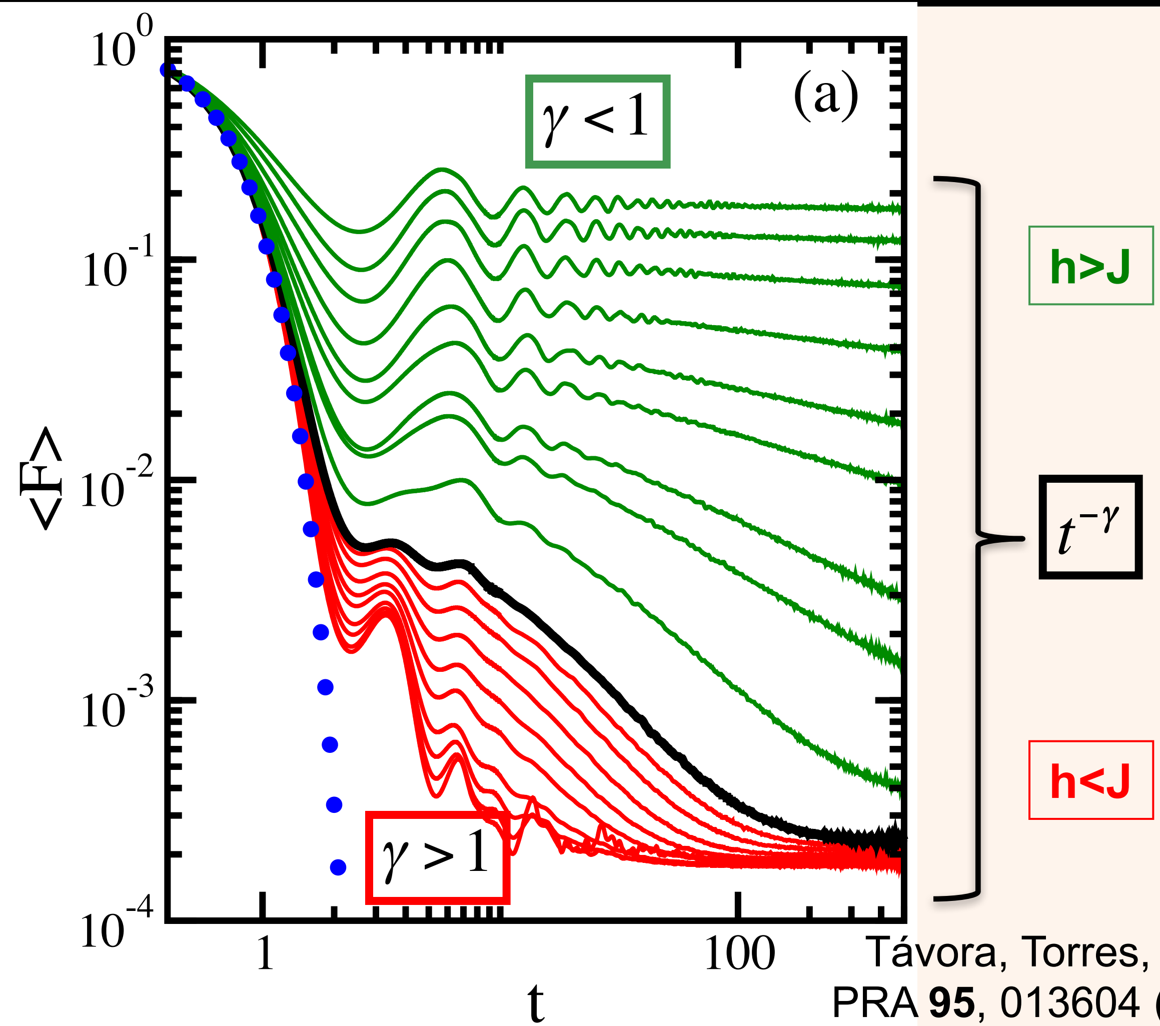
$$F(t) = \left| \langle \Psi(0) | \Psi(t) \rangle \right|^2$$

$$= \left| \int_{E_{\min}}^{E_{\max}} \rho_{ini}(E) e^{-iEt} \, dE \right|^2$$

$$\longrightarrow t^{-2}$$

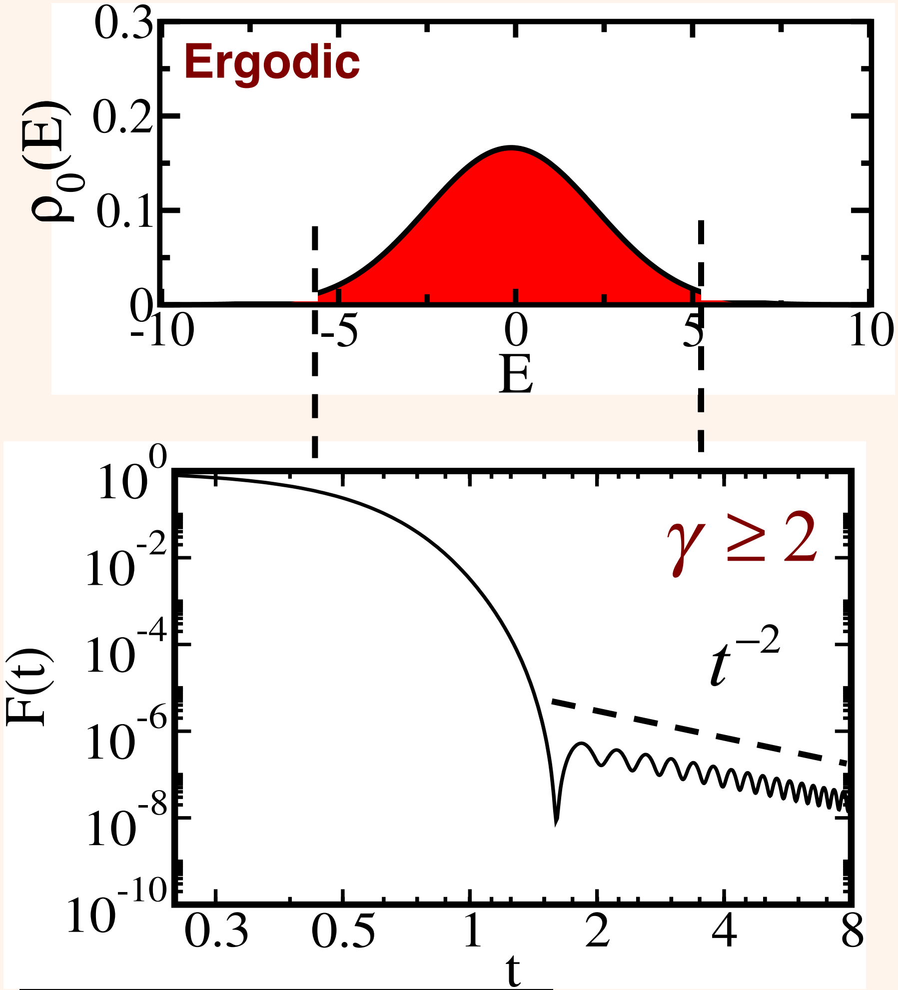
Criterion for Thermalization

Távora, Torres, LFS
PRA **94**, 041603R (2016)



Távora, Torres, LFS
PRA **95**, 013604 (2017)

Ergodically filled LDOS
Power-law decay caused by energy bounds

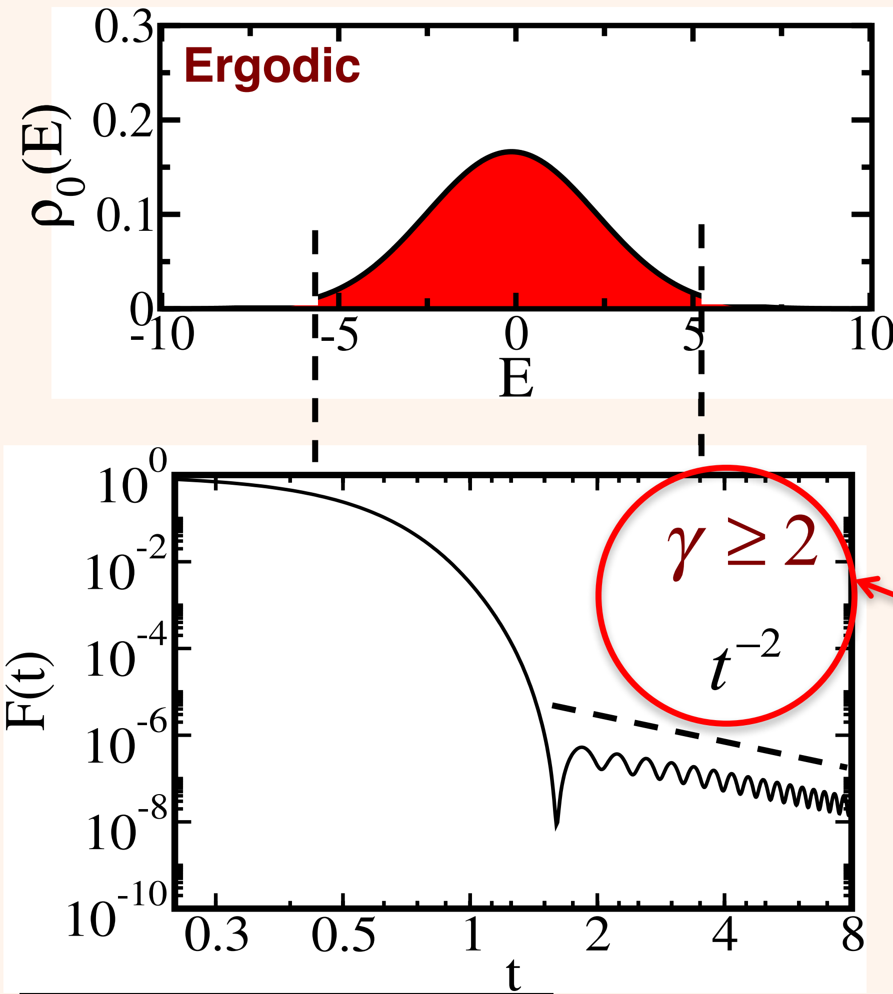


Khalfin (JETP, 1958)

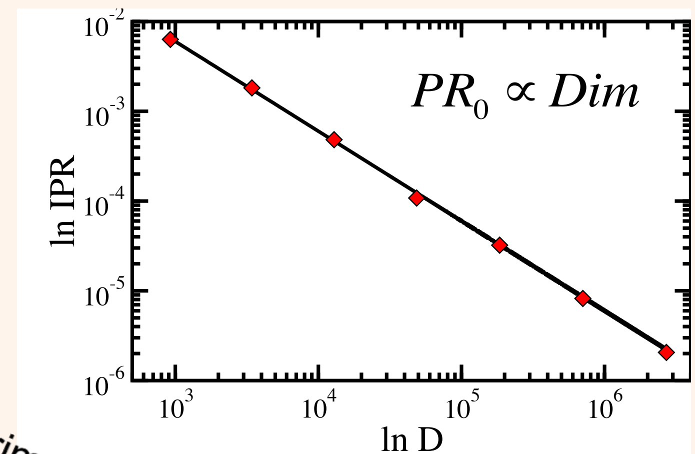
$$F(t) = \left| \frac{1}{\sqrt{2\pi\sigma_{ini}^2}} \int_{Elow}^{\infty} e^{-(E-E_{ini})^2/2\sigma_{ini}^2} e^{-iEt}\, dE \right|^2$$

$$\xrightarrow[t\to\infty]{} \propto \frac{1}{t^2}$$

Ergodically filled LDOS
Power-law decay caused by energy bounds



$$PR_0 \equiv \frac{1}{\sum_{\alpha=1}^{Dim} |C_\alpha^{(0)}|^4} \propto Dim$$



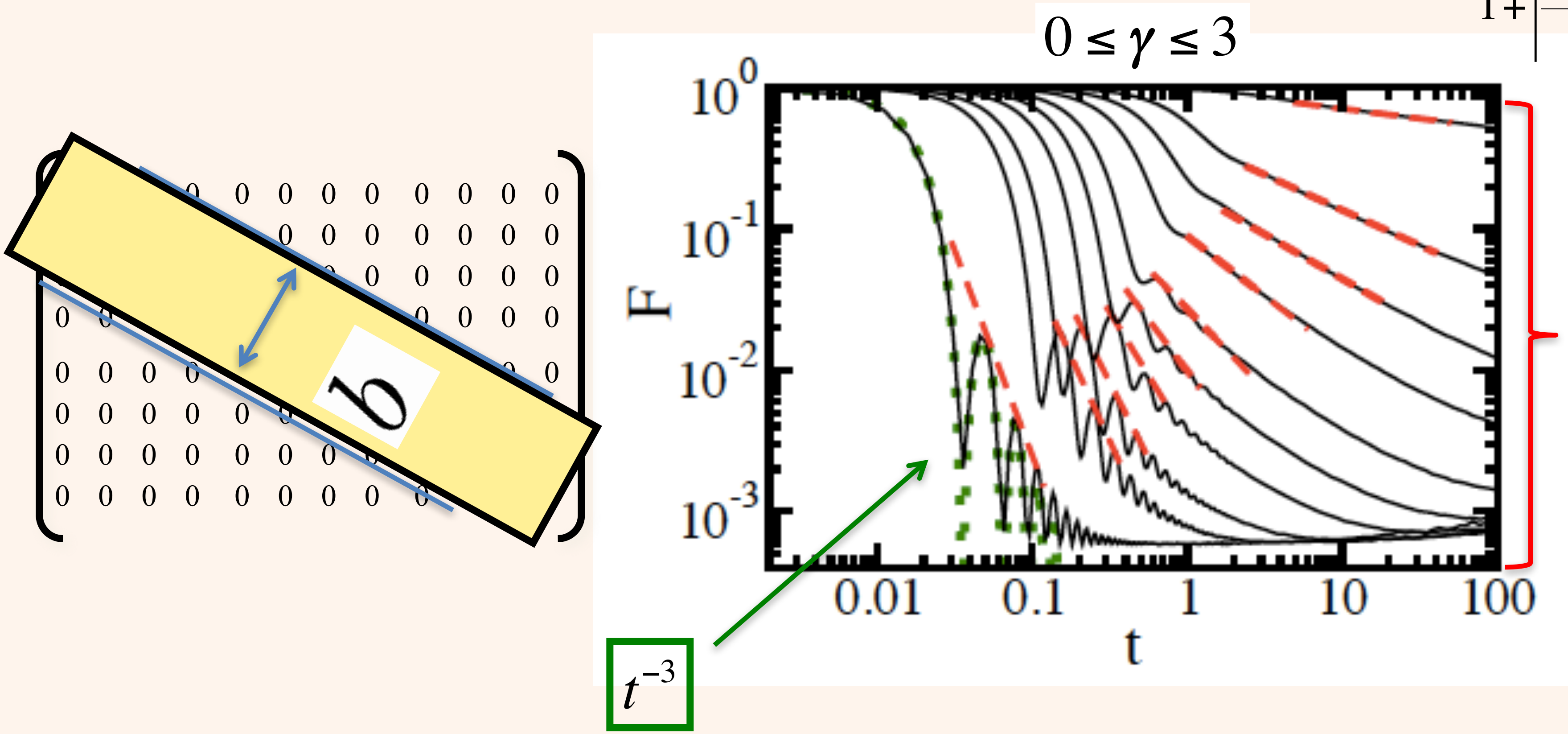
experiments

New Criterion for Thermalization

Távora, Torres, LFS
PRA **94**, 041603R (2016)

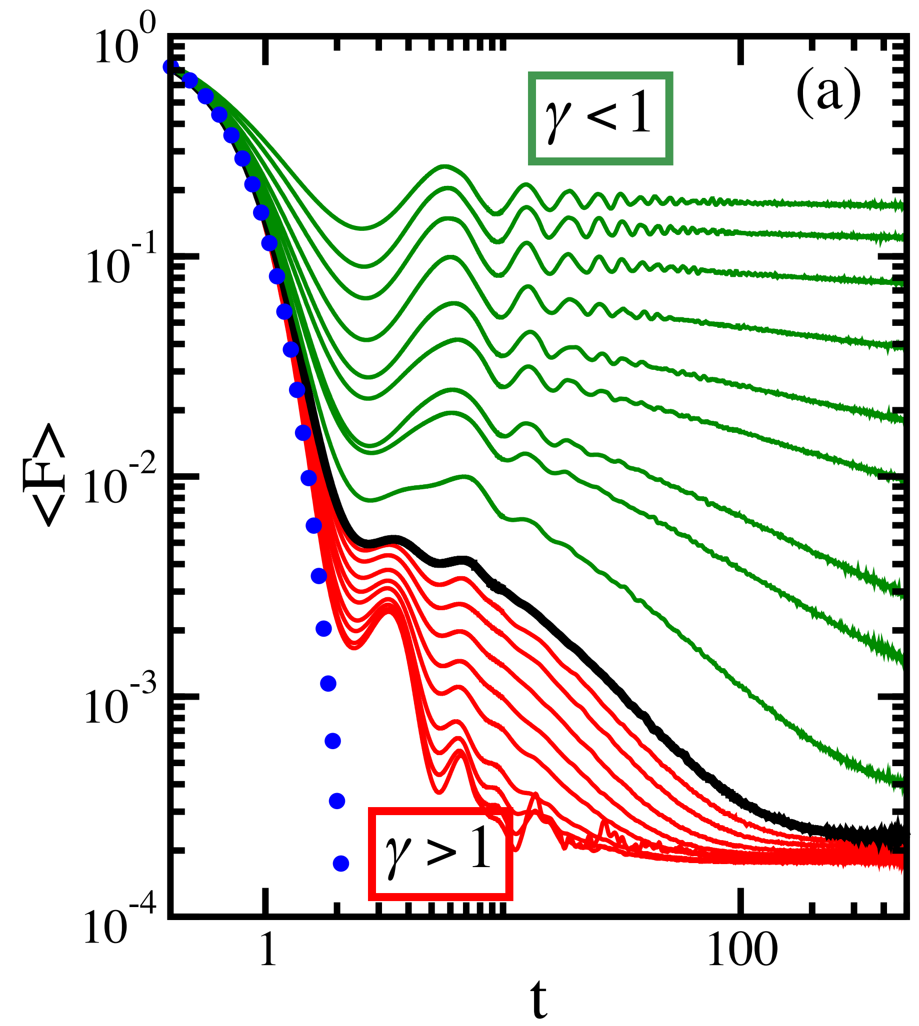
Band random matrices

Power-law band random matrices, Wigner band random matrices $\langle H_{nm}^2 \rangle = \dfrac{1}{1+\left|\dfrac{n-m}{b}\right|^2}$



Távora, Torres, LFS
PRA **94**, 041603**R** (2016)

After the power-law decay



h>J

$t^{-\gamma}$

h<J

$$F(t) = \left(\sum_\alpha |C_\alpha^{ini}|^2 e^{-iE_\alpha t}\right)\left(\sum_\beta |C_\beta^{ini}|^2 e^{-iE_\beta t}\right)$$

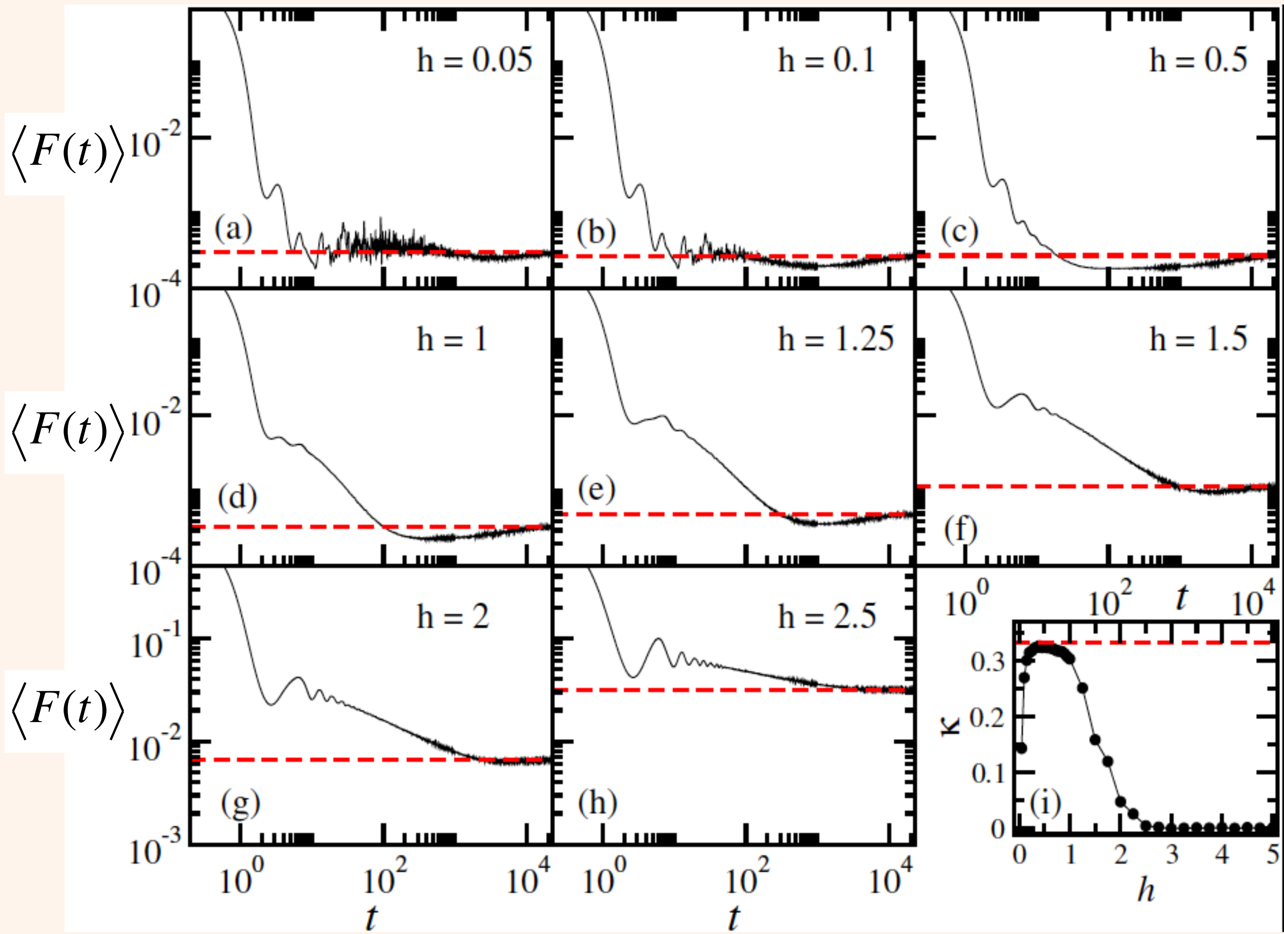
$$= \sum_\alpha |C_\alpha^{ini}|^4 + \sum_{\alpha \neq \beta} |C_\alpha^{ini}|^2 |C_\beta^{ini}|^2 e^{-i(E_\alpha - E_\beta)t}$$

Infinite time average

$$\overline{F} = \sum_\alpha |C_\alpha^{ini}|^4 = \frac{1}{PR_{ini}}$$

Távora, Torres, LFS
PRA **94**, 041603**R** (2016)

Correlation hole



Torres & LFS, arXiv:1702.04363

Correlation hole

VOLUME 56, NUMBER 23 PHYSICAL REVIEW LETTERS 9 JUNE 1986

Fourier Transform: A Tool to Measure Statistical Level Properties in Very Complex Spectra

Luc Leviandier, Maurice Lombardi, Rémi Jost, and Jean Paul Pique
Laboratoire de Spectrométrie Physique, Université Scientifique et Médicale de Grenoble, 38402 Saint Martin d'Hères, France, and Service National des Champs Intenses, Centre National de la Recherche Scientifique, 38042 Grenoble Cedex, France
(Received 27 November 1985)

VOLUME 58, NUMBER 5 PHYSICAL REVIEW LETTERS 2 FEBRUARY 1987

Chaos and Dynamics on 0.5–300-ps Time Scales in Vibrationally Excited Acetylene: Fourier Transform of Stimulated-Emission Pumping Spectrum

J. P. Pique,[a] Y. Chen, R. W. Field, and J. L. Kinsey
Department of Chemistry and George Harrison Spectroscopy Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 27 October 1986)

Chemical Physics 146 (1990) 21–38
North-Holland

Correlations in anticrossing spectra and scattering theory. Analytical aspects

T. Guhr and H.A. Weidenmüller
Max-Planck-Institut für Kernphysik, 6900 Heidelberg, FRG

Received 12 December 1989

Experimental results of anticrossing spectroscopy in molecules, in particular the correlation hole, are discussed in a theoretical model. The laser measurements are modelled in terms of the scattering matrix formalism originally developed for compound nucleus scattering. Random matrix theory is used in the framework of this model. The correlation hole is analytically derived for small singlet–triplet coupling. In the case of the data on methylglyoxal this limit is realistic if the spectrum is indeed a superposition of several pure sequences as one can conclude from the analysis of the measurements.

PHYSICAL REVIEW E, VOLUME 65, 026214

Signatures of the correlation hole in total and partial cross sections

T. Gorin* and T. H. Seligman
Centro de Ciencias Fisicas, University of Mexico (UNAM), CP 62210 Cuernavaca, Mexico
(Received 3 August 2001; published 24 January 2002)

In a complex scattering system with few open channels, say a quantum dot with leads, the correlation properties of the poles of the scattering matrix are most directly related to the internal dynamics of the system. We may ask how to extract these properties from an analysis of cross sections. In general this is very difficult, if we leave the domain of isolated resonances. We propose to consider the cross correlation function of two different elastic or total cross sections. For these we can show numerically and to some extent also analytically a significant dependence on the correlations between the scattering poles. The difference between uncorrelated and strongly correlated poles is clearly visible, even for strongly overlapping resonances.

PHYSICAL REVIEW A VOLUME 46, NUMBER 8 15 OCTOBER 1992

Spectral autocorrelation function in the statistical theory of energy levels

Y. Alhassid
Center for Theoretical Physics, Sloane Physics Laboratory, Yale University, New Haven, Connecticut 06511 and the A.W. Wright Nuclear Structure Laboratory, Yale University, New Haven, Connecticut 06511

R. D. Levine
The Fritz Haber Research Center for Molecular Dynamics, The Hebrew University, Jerusalem 91904, Israel
(Received 11 October 1991; revised manuscript received 5 May 1992)

Ensemble Average

$$F(t)=\left(\sum_{\alpha}\left|C_{\alpha}^{ini}\right|^{2}e^{-iE_{\alpha}t}\right)\left(\sum_{\beta}\left|C_{\beta}^{ini}\right|^{2}e^{-iE_{\beta}t}\right)=\sum_{\alpha}\left|C_{\alpha}^{ini}\right|^{4}+\sum_{\alpha\neq\beta}\left|C_{\alpha}^{ini}\right|^{2}\left|C_{\beta}^{ini}\right|^{2}e^{-i(E_{\alpha}-E_{\beta})t}=\sum_{\alpha}\left|C_{\alpha}^{ini}\right|^{4}+\int G(E)e^{-iEt}dE$$

Spectral autocorrelation function

$$\left\langle G(E)\right\rangle=\sum_{\alpha\neq\beta}\left\langle\left|C_{\alpha}^{ini}\right|^{2}\left|C_{\beta}^{ini}\right|^{2}\right\rangle\left\langle\delta\left(E-(E_{\alpha}-E_{\beta})\right)\right\rangle$$

Two-level correlation function

$$F(t)=\left(\sum_{\alpha}\left|C_{\alpha}^{ini}\right|^{2}e^{-iE_{\alpha}t}\right)\left(\sum_{\beta}\left|C_{\beta}^{ini}\right|^{2}e^{-iE_{\beta}t}\right)=\sum_{\alpha}\left|C_{\alpha}^{ini}\right|^{4}+\sum_{\alpha\neq\beta}\left|C_{\alpha}^{ini}\right|^{2}\left|C_{\beta}^{ini}\right|^{2}e^{-i(E_{\alpha}-E_{\beta})t}=\sum_{\alpha}\left|C_{\alpha}^{ini}\right|^{4}+\int G(E)e^{-iEt}dE$$

Spectral autocorrelation function

$$\langle G(E)\rangle=\sum_{\alpha\neq\beta}\left\langle\left|C_{\alpha}^{ini}\right|^{2}\left|C_{\beta}^{ini}\right|^{2}\right\rangle\left\langle\delta\left(E-(E_{\alpha}-E_{\beta})\right)\right\rangle$$

Two-level correlation function

$$\left\langle\delta\left(E-(E_{\alpha}-E_{\beta})\right)\right\rangle=\frac{1}{N(N-1)}\int\delta\left(E-(E_{1}-E_{2})\right)R_{2}(E_{1},E_{2})dE_{1}dE_{2}$$

Two-level cluster function

DOS

$$R_{2}(E_{1},E_{2})=R_{1}(E_{1})R_{1}(E_{1})-T_{2}(E_{1},E_{2})$$

Correlation hole: linear increase

$$F(t)=\left(\sum_{\alpha}\left|C_{\alpha}^{ini}\right|^{2}e^{-iE_{\alpha}t}\right)\left(\sum_{\beta}\left|C_{\beta}^{ini}\right|^{2}e^{-iE_{\beta}t}\right)=\sum_{\alpha}\left|C_{\alpha}^{ini}\right|^{4}+\sum_{\alpha\neq\beta}\left|C_{\alpha}^{ini}\right|^{2}\left|C_{\beta}^{ini}\right|^{2}e^{-i(E_{\alpha}-E_{\beta})t}=\sum_{\alpha}\left|C_{\alpha}^{ini}\right|^{4}+\int G(E)e^{-iEt}dE$$

Spectral autocorrelation function

$$\langle G(E)\rangle=\sum_{\alpha\neq\beta}\left\langle\left|C_{\alpha}^{ini}\right|^{2}\left|C_{\beta}^{ini}\right|^{2}\right\rangle\left\langle\delta\left(E-(E_{\alpha}-E_{\beta})\right)\right\rangle$$

Two-level correlation function

$$\left\langle\delta\left(E-(E_{\alpha}-E_{\beta})\right)\right\rangle=\frac{1}{N(N-1)}\int\delta\left(E-(E_{1}-E_{2})\right)R_{2}(E_{1},E_{2})dE_{1}dE_{2}$$

Two-level cluster function

DOS

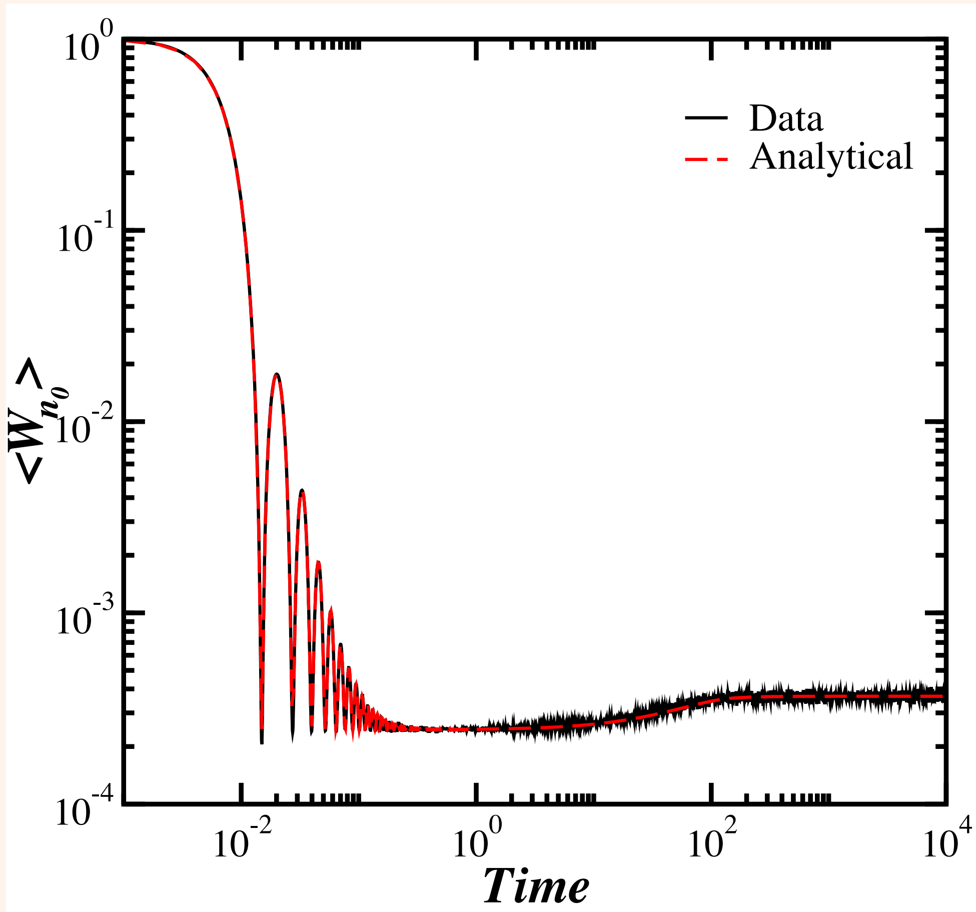
$$R_{2}(E_{1},E_{2})=R_{1}(E_{1})R_{1}(E_{1})-T_{2}(E_{1},E_{2})$$

Two-level form-factor

$$\frac{1}{N(N-1)}\int\delta\left(E-(E_{1}-E_{2})\right)T_{2}(E_{1},E_{2})dE_{1}dE_{2}=\frac{1}{(N-1)}b_{2}\left(\frac{t}{\sigma_{ini}}\right)$$

$$b_{2}\left(\frac{t}{\sigma_{ini}}\right)=1-\frac{2t}{\sigma_{ini}}+\frac{t}{\sigma_{ini}}\log\left(1+\frac{2t}{\sigma_{ini}}\right)\Theta+(\ldots)\Theta$$

Correlation Hole: Full Random Matrices



$$F_{FRM}(t) = \frac{N-3}{N(N-1)}\left[N\frac{\left|\mathcal{J}_1(2\sigma_{ini}t)\right|^2}{\sigma_{ini}^2 t^2} - b_2\left(\frac{t}{\sigma_{ini}}\right)\right] + \frac{3}{N}$$

Analytically Continued Partition Function

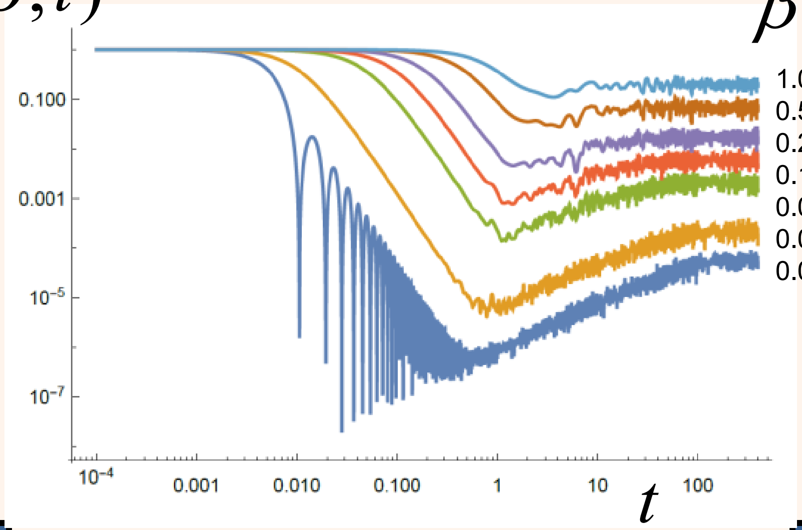
$$g(\beta,t) = \left|Z(\beta+it)\right|^2 = \sum_{a,b} \frac{e^{-\beta(E_a+E_b)}}{Z(\beta)^2} e^{-i(E_a-E_b)t}$$

$$F(t) = \sum_{a,b} \left|C_a^{ini}\right|^2 \left|C_b^{ini}\right|^2 e^{-i(E_a-E_b)t}$$

$$\left|C_a^{ini}\right|^2 = \frac{e^{-\beta E_a}}{Z(\beta)}$$

$g(\beta,t)$

$\beta = 1/T$



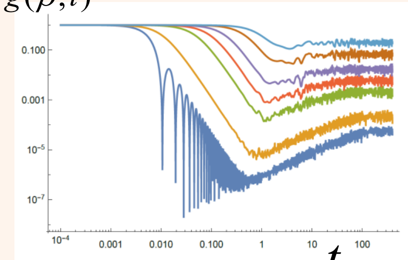
Analytically Continued Partition Function

$$g(\beta,t)=\left|Z(\beta+it)\right|^2=\sum_{a,b}\frac{e^{-\beta(E_a+E_b)}}{Z(\beta)^2}e^{-i(E_a-E_b)t}$$

$$F(t)=\sum_{a,b}\left|C_a^{ini}\right|^2\left|C_b^{ini}\right|^2 e^{-i(E_a-E_b)t}$$

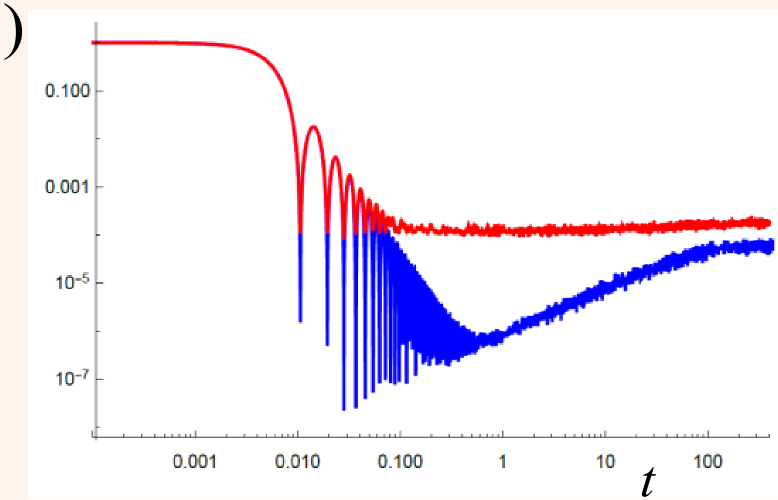
$$\left|C_a^{ini}\right|^2=\frac{e^{-\beta E_a}}{Z(\beta)}$$

$g(\beta,t)$



t

$F(t)$

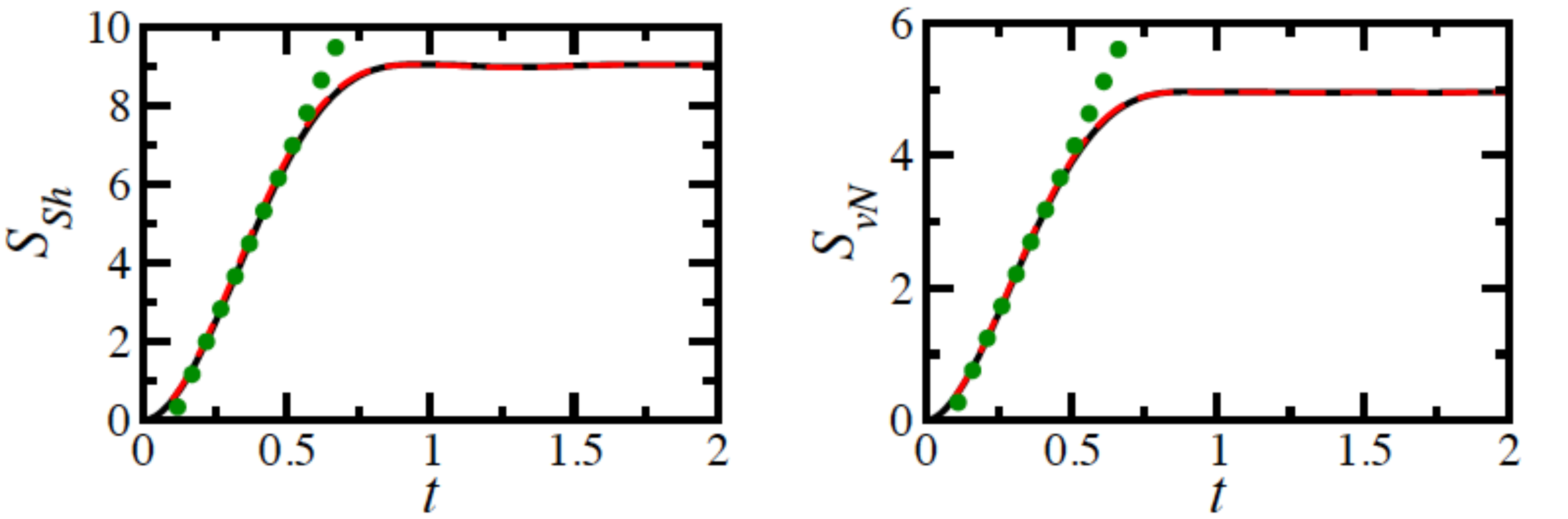


t

$$F_{FRM}(t)=\frac{N-3}{N(N-1)}\left[N\frac{\left|\mathcal{J}_1(2\sigma_{ini}t)\right|^2}{\sigma_{ini}^2t^2}-b_2\left(\frac{t}{\sigma_{ini}}\right)\right]+\frac{3}{N}$$

$$F_{T\to\infty}(t)=\frac{N-1}{N(N-1)}\left[N\frac{\left|\mathcal{J}_1(2\sigma_{ini}t)\right|^2}{\sigma_{ini}^2t^2}-b_2\left(\frac{t}{\sigma_{ini}}\right)\right]+\frac{1}{N}$$

Full Random Matrices: Analytical Expression



Flambaum & Izrailev PRE (2012)

$$S_{Sh}(t) = -W_{ini}(t)\ln W_{ini}(t) - \sum_{k\neq ini}^{\mathcal{D}} W_k(t)\ln W_k(t)$$
$$\sim -W_{ini}(t)\ln W_{ini}(t) - [1 - W_{ini}(t)]\ln\left[\frac{1 - W_{ini}(t)}{N_{pc}}\right],$$

$$W_n(t) = \left|\left\langle \phi_n | e^{-iHt} | \Psi(0) \right\rangle\right|^2$$

Torres et al, Entropy **18**, 359 (2016)

Summary

- Exponential/Gaussian decays appear in integrable and chaotic models.
  indicates **delocalized** initial states.
  determined by the **shape** and width of the LDOS.

- Power-law decay at longer times captures the **filling** of the LDOS.
  caused by energy **bounds** or **correlations**.
  A criterion to anticipate **thermalization** from the dynamics.

- **Correlation hole** emerges before saturation.
  is an unambiguous signature of **level repulsion**.
  is an indicator of the chaos-integrable transition.
  is an indicator of the delocalized-localized transition.

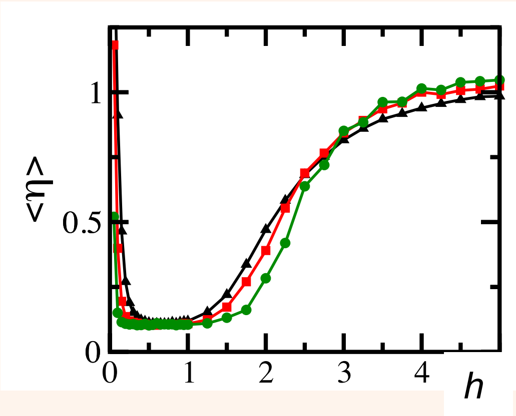
- **Analytical expressions** from full random matrices serve as bounds and references for the analysis of realistic models.

Entropies: Chaotic region

Wigner-Dyson level statistics: 0<h<J

Ergodic delocalized states: $PR^{(\alpha)} \propto Dim$

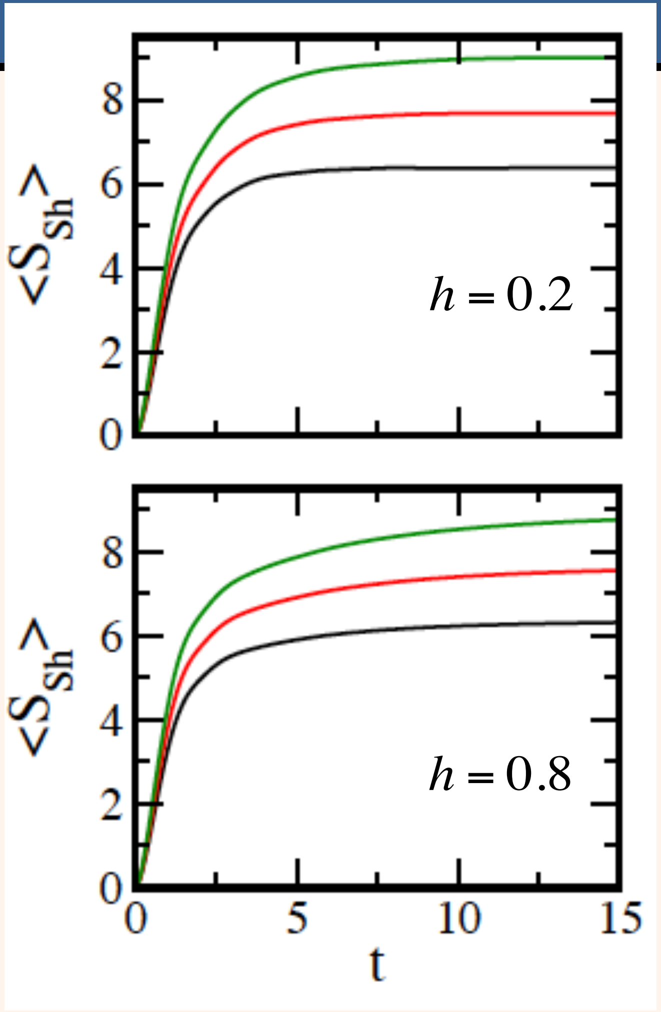
$$\eta = \frac{\int_0^{s_0} [P(s) - P_{WD}(s)]ds}{\int_0^{s_0} [P_P(s) - P_{WD}(s)]ds},$$



LFS, J. Phys. A **37**, 4723 (2004)

$$Sh(t) = -\sum_n W_n(t) \ln W_n(t)$$

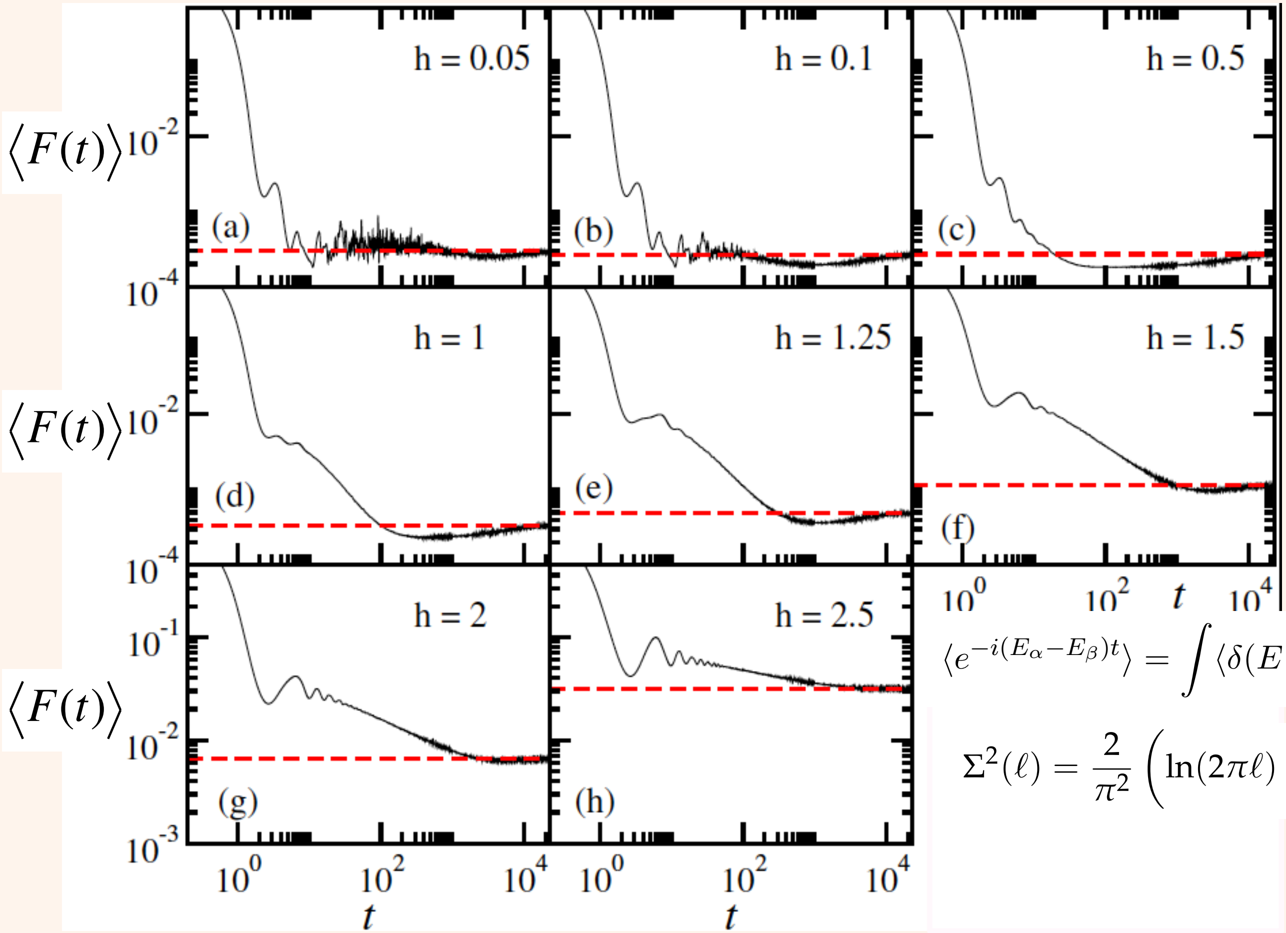
$$W_n(t) = \left| \langle \phi_n | e^{-iHt} | \Psi(0) \rangle \right|^2$$



Torres & LFS, Ann. Phys. (2017)

$$Sv(t) = -Tr[\rho_A(t) \ln \rho_A(t)]$$

Correlation hole



$$\langle e^{-i(E_\alpha - E_\beta)t} \rangle = \int \langle \delta(E - E_\alpha + E_\beta) \rangle e^{-iEt} dE$$

$$\Sigma^2(\ell) = \frac{2}{\pi^2}\left(\ln(2\pi\ell) + \gamma_e + 1 - \frac{\pi^2}{8}\right)$$

$$F_{FRM}(t) = \frac{Dim-3}{Dim(Dim-1)}\left[Dim\frac{|\mathcal{J}_1(2\sigma_{ini}t)|^2}{\sigma_{ini}^2 t^2} - \left(1 - 2\frac{t}{\sigma_{ini}}\right)\right] + \frac{3}{Dim}$$

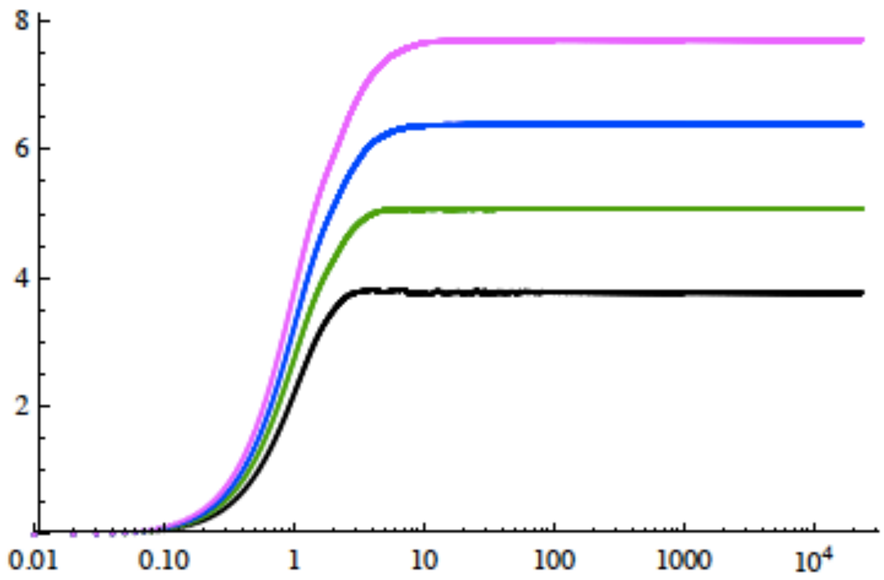
Shannon and Entanglement Entropy

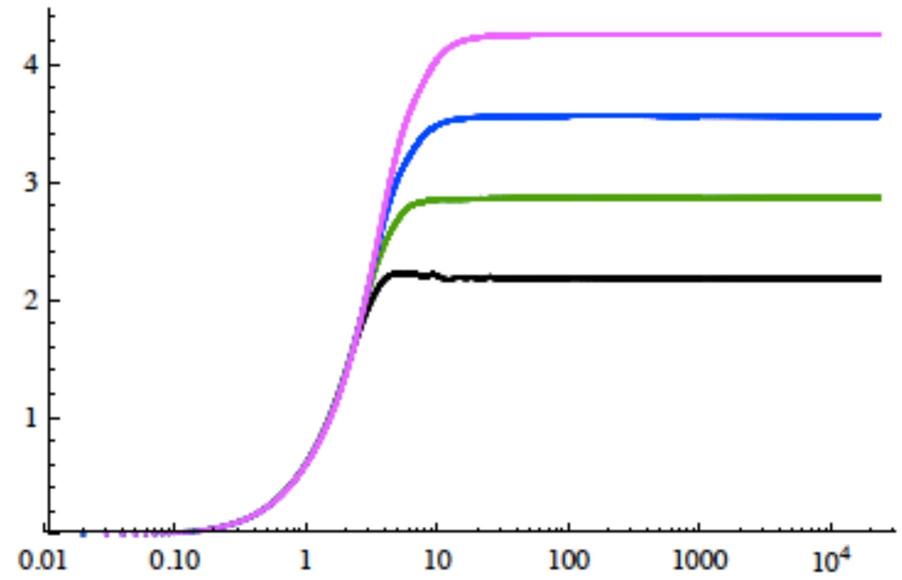
Shannon entropy

$$Sh(t) = \sum_k \left|C_k^{(ini)}(t)\right|^2 \ln \left|C_k^{(ini)}(t)\right|^2$$

Entanglement entropy

$$Sv(t) = -Tr[\rho_A(t) \ln \rho_A(t)]$$





h=0.3

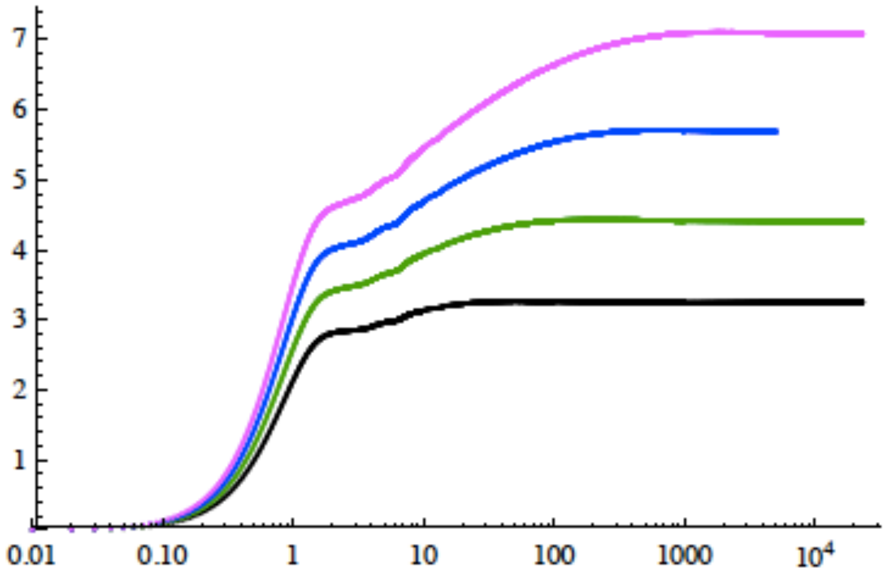
Shannon and Entanglement Entropy

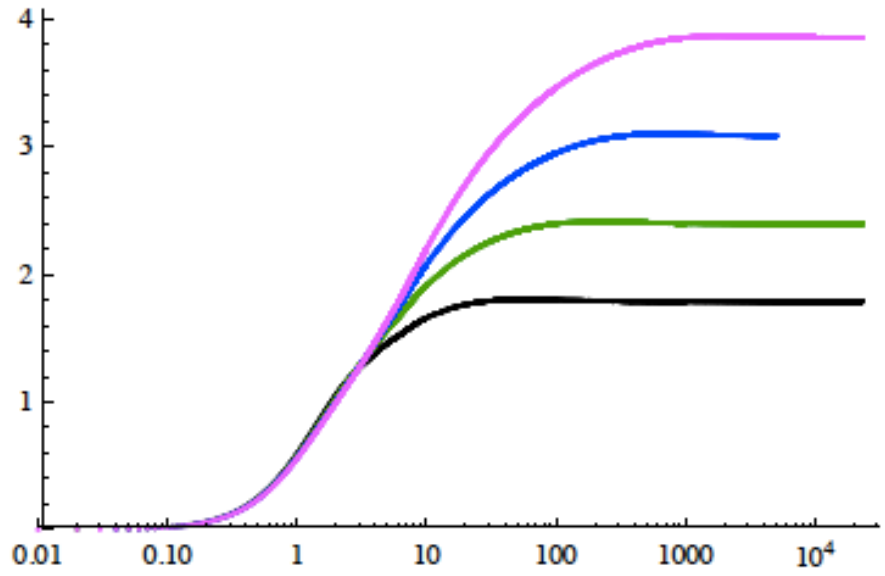
Shannon entropy

$$Sh(t) = \sum_k \left|C_k^{(ini)}(t)\right|^2 \ln\left|C_k^{(ini)}(t)\right|^2$$

Entanglement entropy

$$Sv(t) = -Tr[\rho_A(t)\ln\rho_A(t)]$$





Lea F. Santos, Yeshiva University

h=2.0

OTOC

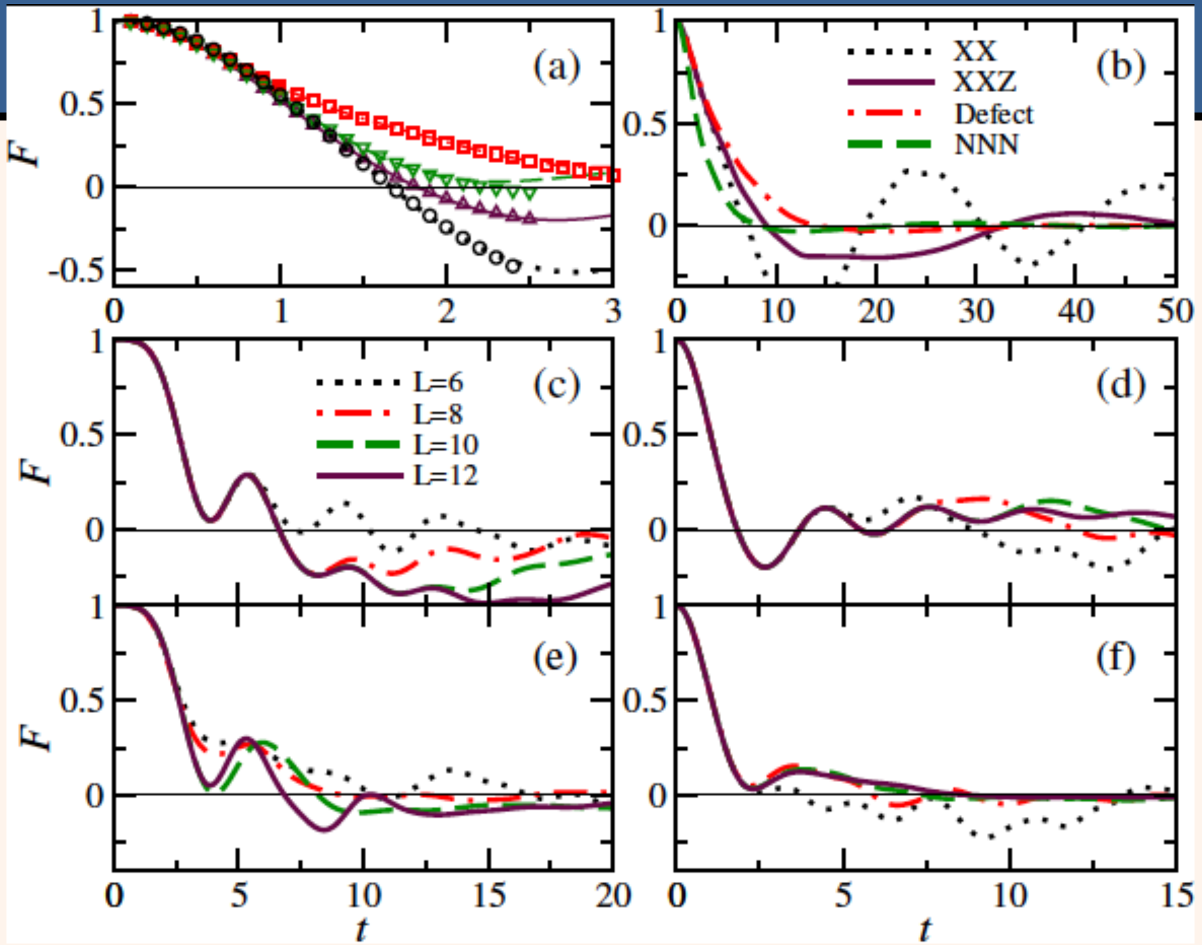
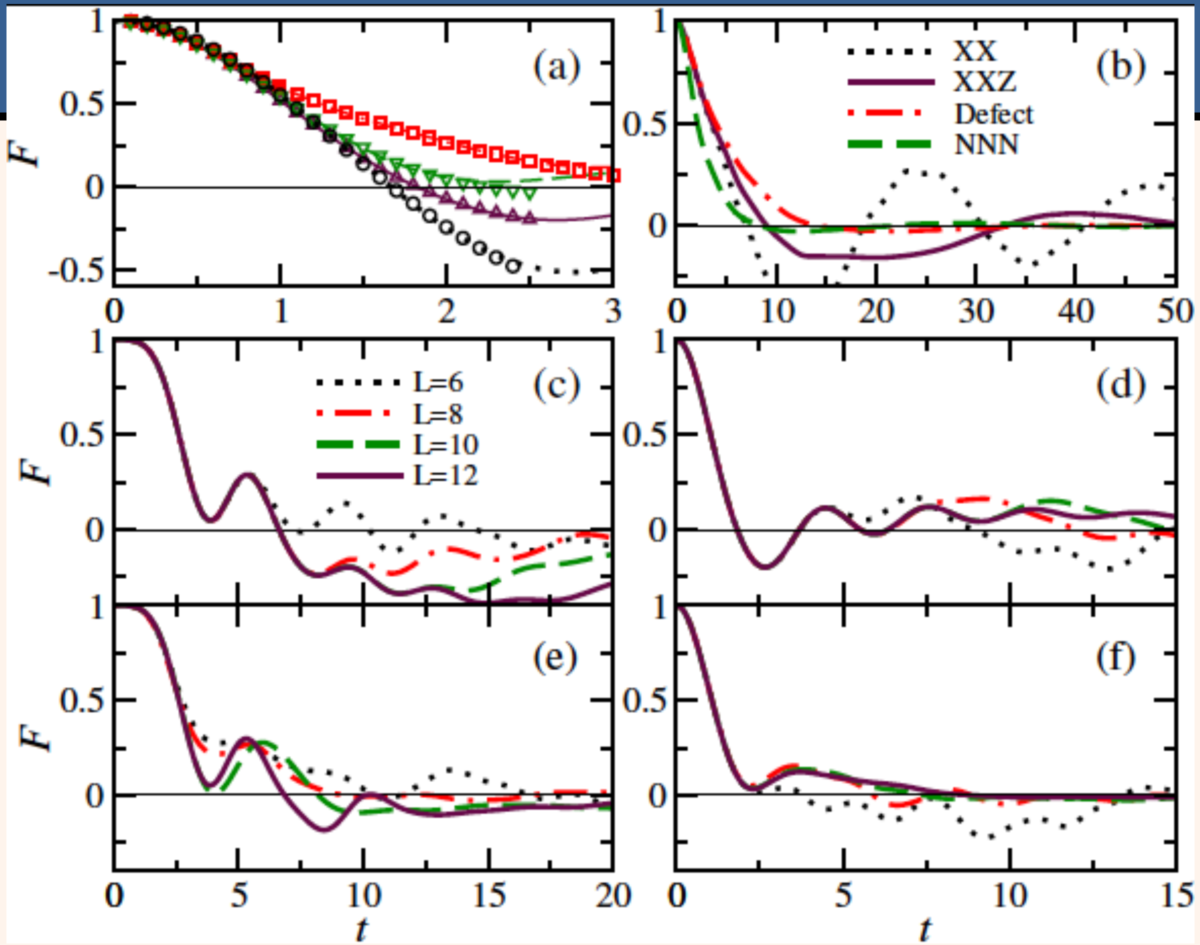


FIG. 2: OTOC decay averaged over all site-basis vectors as in Eq. (4). All four models in (a) and (b), XXZ model in (c) and (d), defect model in (e), and NNN model in (f). In (a): $L = 12$, $k = L/2$, $k' = L/2+1$. Lines represent numerical results and symbols are the fittings. Empty circles (XX), up triangles (XXZ), down triangles (NNN), and squares (defect) are for the Gaussian fit $F(t) = A + Be^{-Ct^2}$ and filled squares (defect) for the exponential fit $F(t) = A + Be^{-Ct}$, where A, B, C are constants. In (b): $L = 10$ and average over all pairs of sites $k' > k$; the legend indicates the models. In (c)-(f): comparison for different system sizes with legend in (c). In (c) and (e): $k = 2$, $k' = 4$. In (d) and (f): $k = L/2$, $k' = L/2+1$. All panels: a single random realization of border defects. The parameters are $\Delta = 0.48$, $d = 0.9$, $\lambda = 1$, $h = 0$; open boundaries.

OTOC



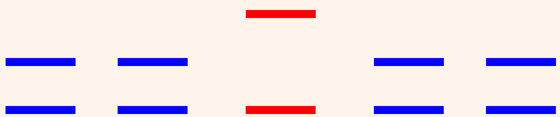
$$F(t) = \frac{1}{\mathcal{D}_H} \sum_{n=1}^{\mathcal{D}_H} \langle \phi_n | e^{iHt} \sigma_{k'}^x e^{-iHt} \sigma_k^x e^{iHt} \sigma_{k'}^x e^{-iHt} \sigma_k^x | \phi_n \rangle .$$

d>1, Effectively Break the Chain

integrable impurity model

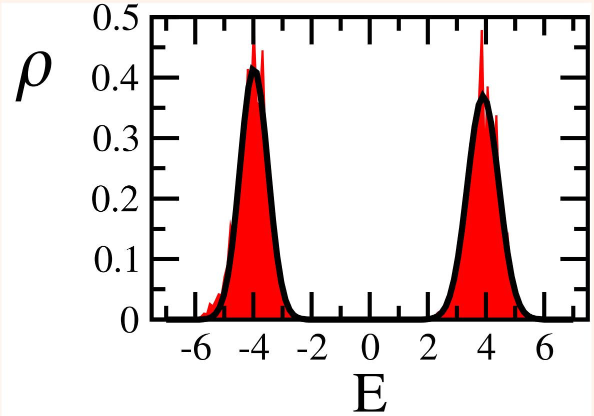
$$H_{initial} = H_{XXZ} = \sum_{n=1}^{L-1} J(\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \Delta \sigma_n^z \sigma_{n+1}^z) \longrightarrow H_{final} = H_{XXZ} + dJS_{L/2}^z$$

$d > 1$ breaks the chain



DENSITY OF STATES

$$|\psi_\alpha\rangle = c_1|1001\rangle + c_2|0101\rangle$$



$$|\psi_\alpha\rangle = c_1|0011\rangle + c_2|0110\rangle$$

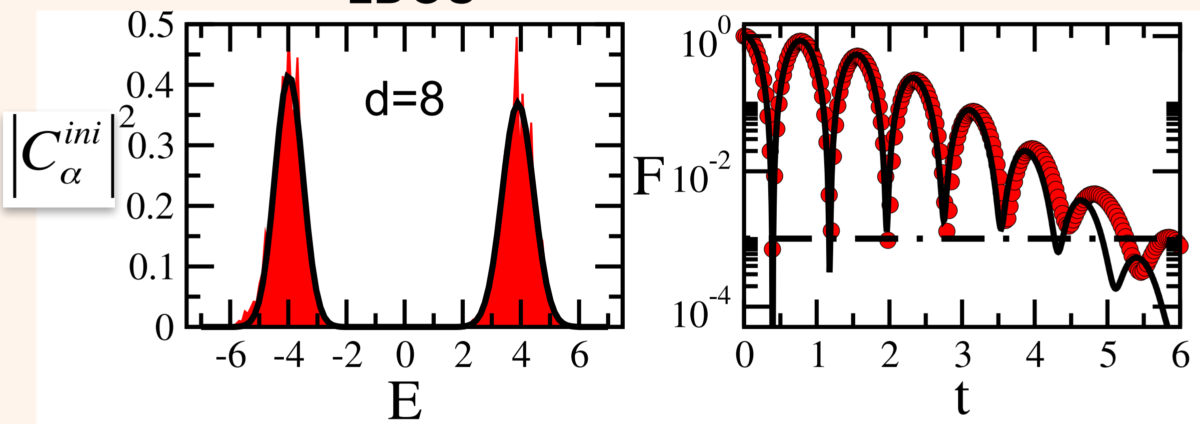
Lower bound
Energy-time uncertainty relation

integrable — impurity model

$$H_{initial} = H_{XXZ} = \sum_{n=1}^{L-1} J(\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \Delta \sigma_n^z \sigma_{n+1}^z) \longrightarrow H_{final} = H_{XXZ} + dJS_{L/2}^z$$

$$F(t) = \cos^2(dt/2)\exp(-\sigma^2 t^2)$$

LDOS



Mandelstam-Tamm relation

$$\sigma_H \sigma_A \geq \left| \frac{\langle [H,A] \rangle}{2i} \right| = \frac{1}{2} \left| \frac{d\langle A \rangle}{dt} \right|$$

$$F(t) \geq \cos^2(\sigma_{ini} t)$$

$$t < \pi / (2\sigma_{ini})$$

Torres & LFS
PRA **90** (2014)

L=16, 8 up spins $\Delta = 0.48$