Title: (Lea Santos) General Features of the Relaxation Dynamics of Isolated Interacting Quantum Systems

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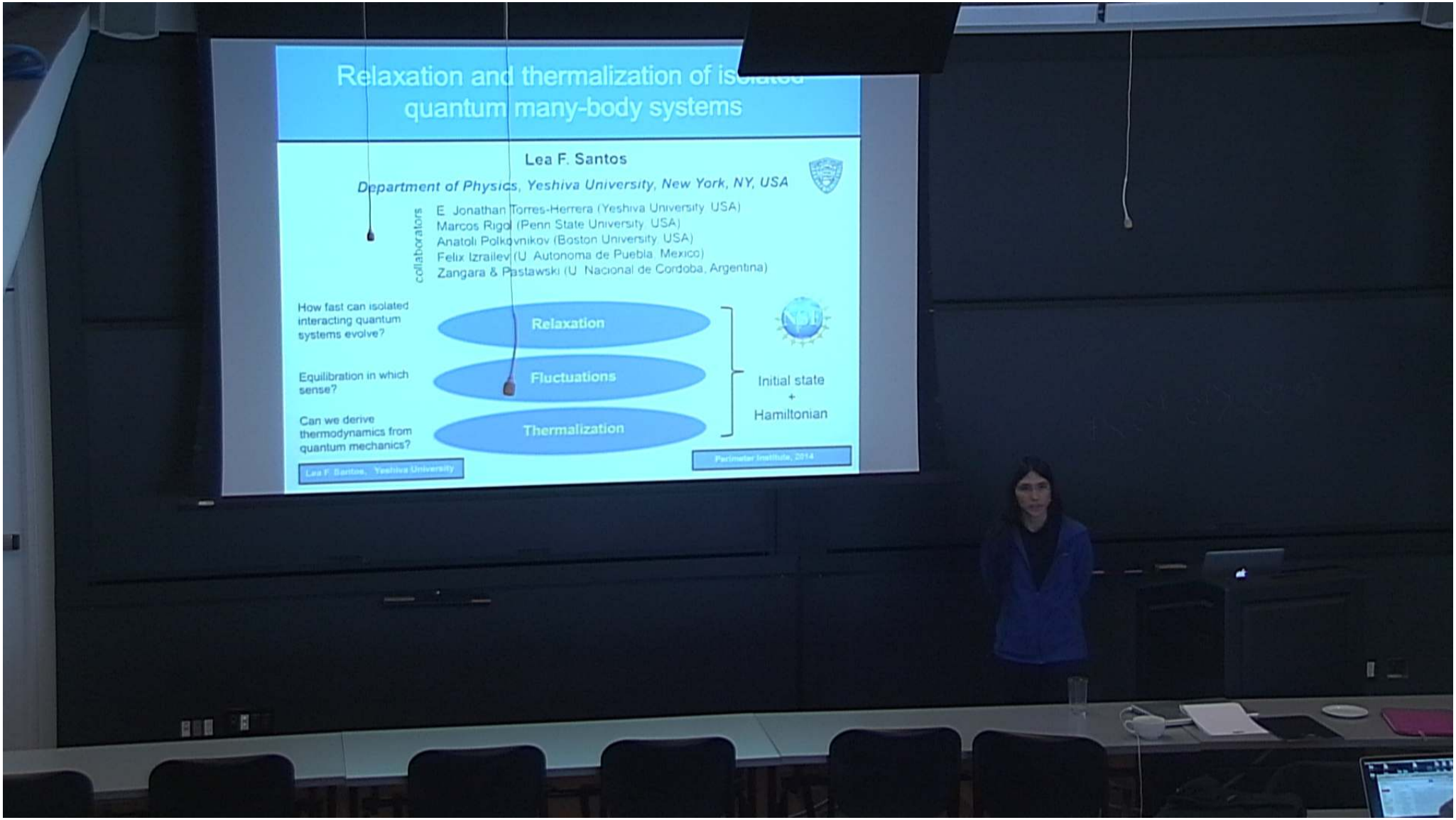
Abstract: We consider isolated interacting quantum systems that are taken out of equilibrium instantaneously (quenched). We study numerically and analytically the probability of finding the initial state later on in time (the so-called fidelity or Loschmidt echo), the relaxation time of the system, and the evolution of few-body observables. The fidelity decays fastest for systems described by full random matrices, where simultaneous many-body interactions are implied. In the realm of realistic systems with two-body interactions, the dynamics is slower and dependent on the energy of the initial state. The fastest fidelity decay in this case is Gaussian and can persist until saturation. The fidelity also plays a central role in the short-time dynamics of few-body observables that commute with the system Hamiltonian before the quench. Our analyses are mainly developed for initial states that can be prepared in experiments with cold atoms in optical lattices.


Relaxation and thermalization of isolated quantum many-body systems
Lea F. Santos
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collaborators
E. Jonathan Torres-Herrera (Yeshiva University, USA)
Marcos Rigol (Penn State University, USA)
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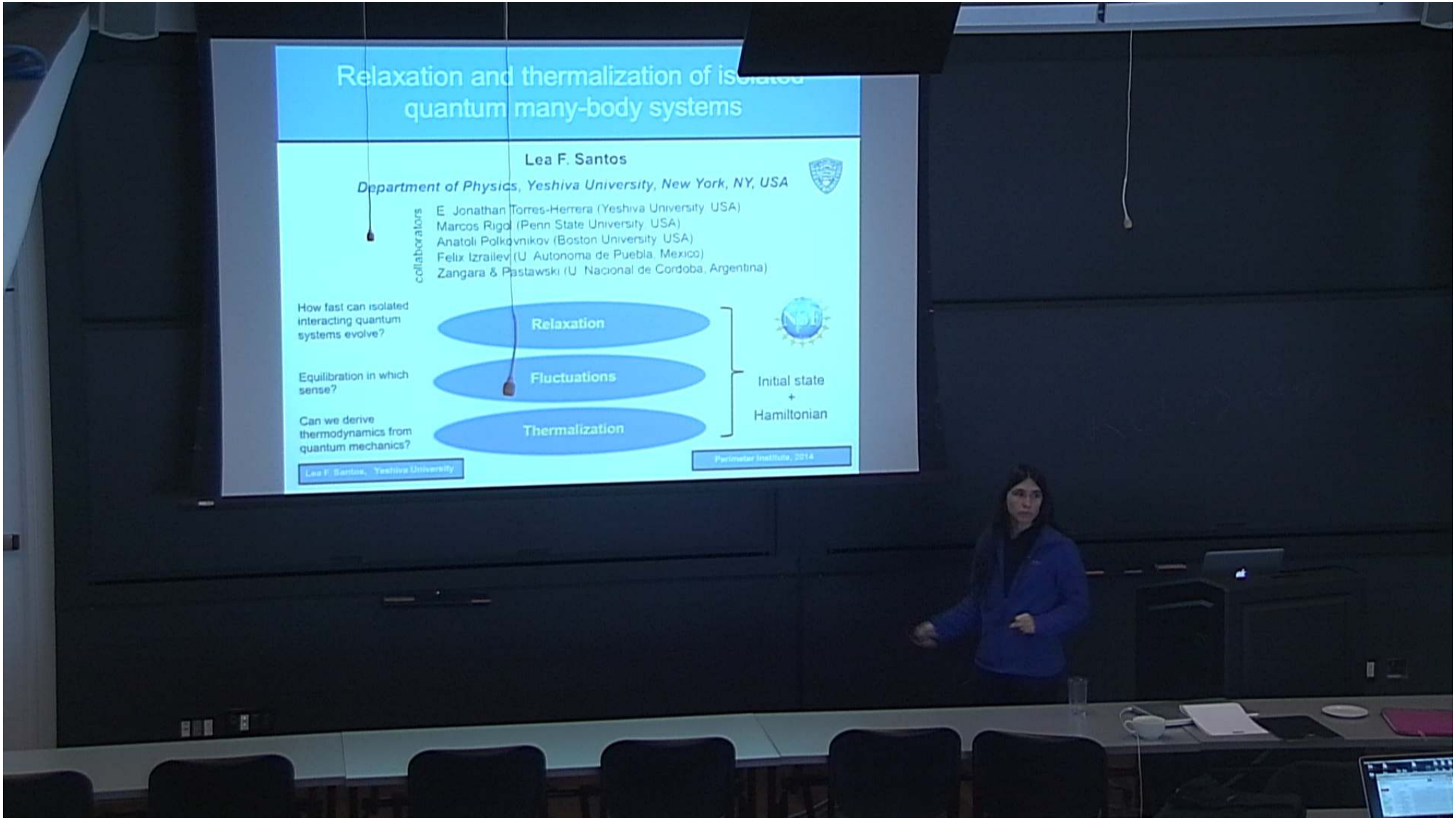
Zangara & Prastawski (U. Nacional de Cordoba, Argentina)
How fast can isolated interacting quantum systems evolve?
Relaxation
Equilibration in which sense?
Fluctuations
Can we derive thermodynamics from quantum mechanics?
Thermalization
Initial state
+
Hamiltonian
Lea F. Santos, Yeshiva University
Perimeter Institute, 2014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QUANTUM CHAOS

FULL RANDOM MATRICES
vs
TWO-BODY INTERACTIONS

Lea F. Santos, Yeshiva University

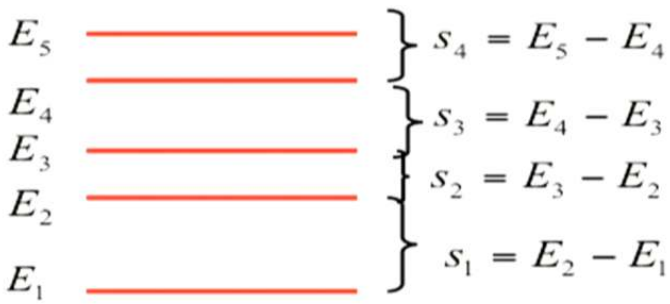
Perimeter Institute, 2014

Full Random Matrices

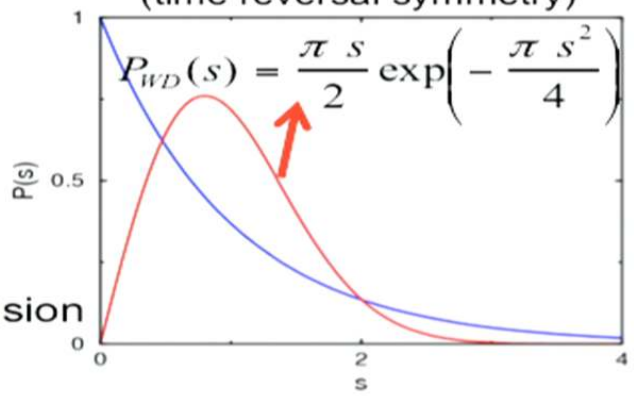
Matrices filled with random numbers and respecting the symmetries of the system.

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 :
Hamiltonians are real and symmetric
Gaussian Orthogonal Ensemble (GOE)

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

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

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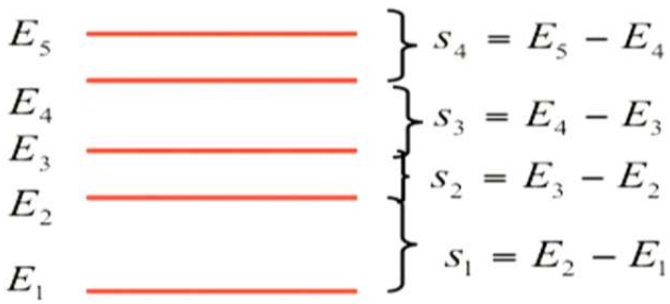

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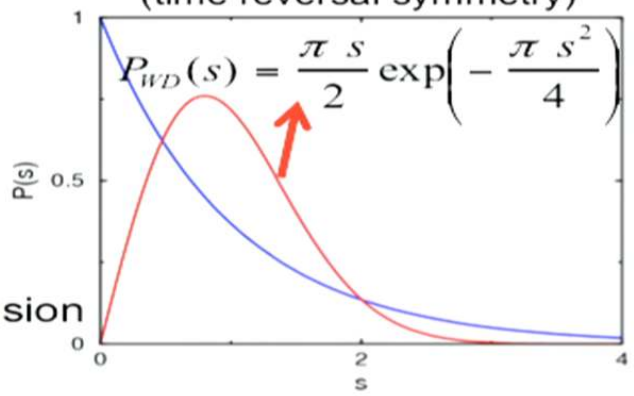

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Signatures of chaos: eigenvectors

Chaotic eigenstates

delocalized states; large number of uncorrelated components, described statistically; **pseudo-random vectors**

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

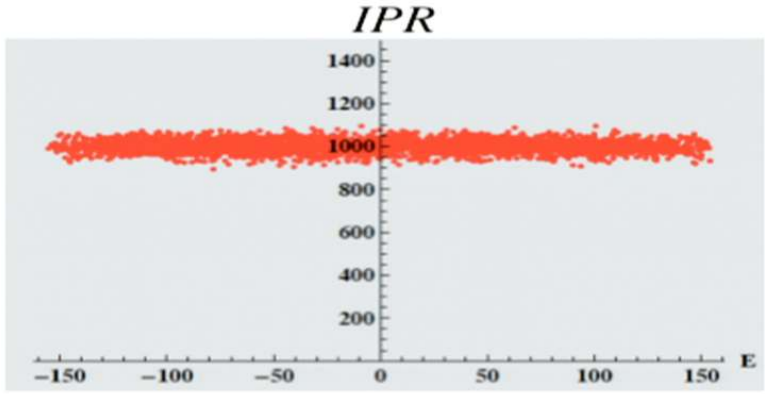
In random matrix ensembles,

- the amplitudes of the eigenstates become random variables;
- eigenstates are completely delocalized

Inverse participation ratio

$$IPR^{(\alpha)} \equiv \frac{1}{\sum_{i=1}^{D} | c_i^{(\alpha)} |^4} \sim \frac{D}{3}$$

maximum delocalization
chaotic states - GOE



Izrailev, Phys. Rep.**196** 299 (1990)
Zelevinsky et al, Phys. Rep. **276** 85 (1996)

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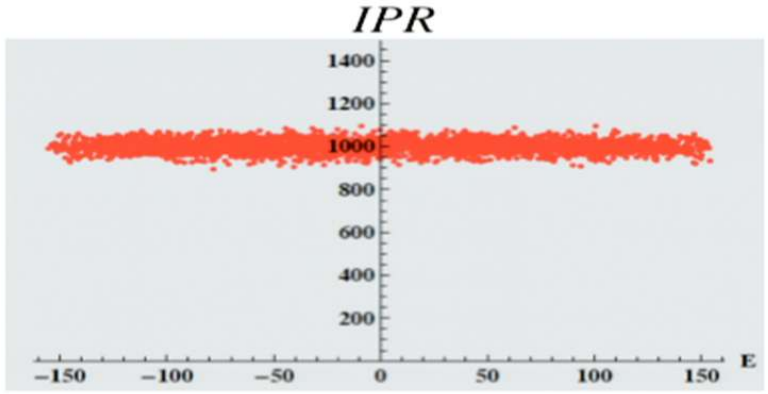

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1D Spin-1/2 systems

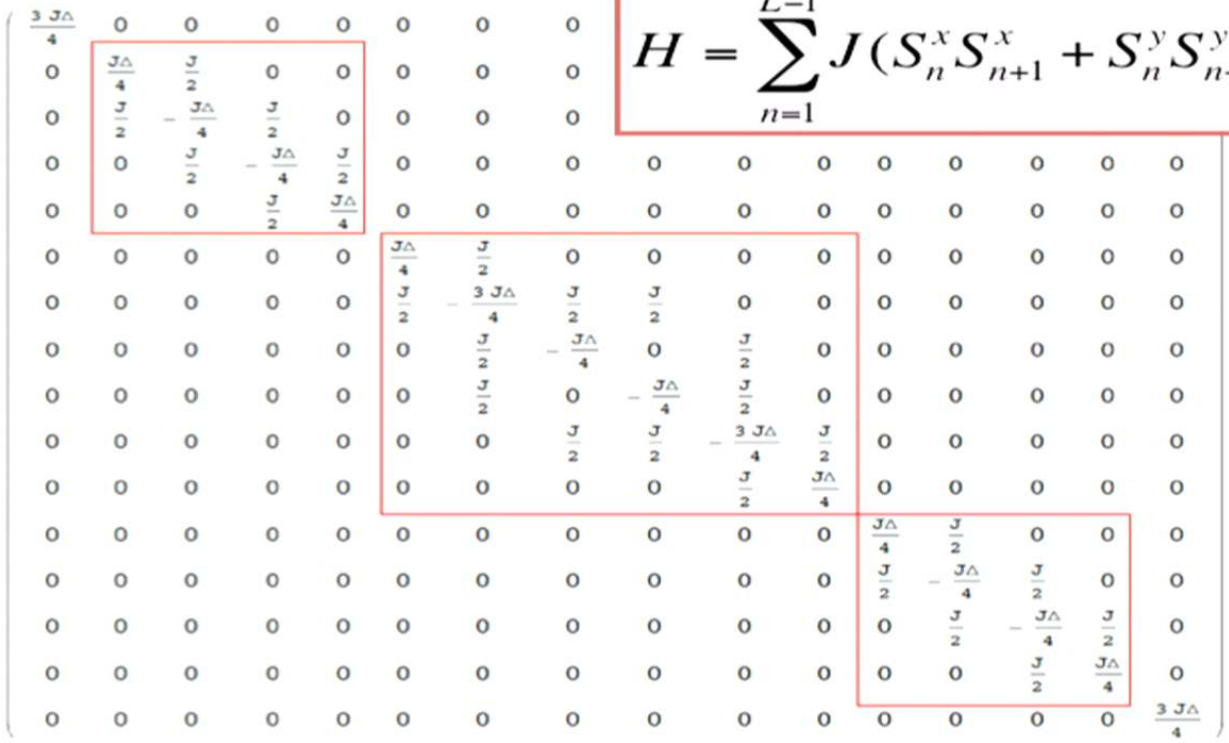
Real systems are not described by random matrices, they have few (two-)body interactions.
The Hamiltonian matrix is sparse

$$H = \sum_{n=1}^{L-1} J\left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z\right)$$

Basis

$\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow$

$\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$



$$S^z = \sum_{n=1}^{L} S_n^z$$

$$[H, S^z] = 0$$

XXZ model
L=4 sites

Integrable vs chaos

Integrable system:

XXZ model (1D)

$$H = \sum_{n=1}^{L-1} J(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z)$$

Chaotic systems:

LFS, JPA (2004)

Impurity model

$$H = JdS_{L/2}^z + \sum_{n=1}^{L-1} J(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z)$$

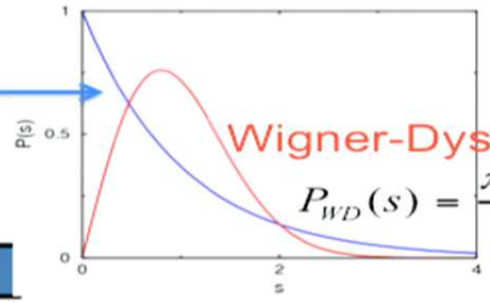
NNN model

$$H_{NN} + \lambda H_{NNN} = \sum_{n=1}^{L-1} J(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z) +$$

$$+\lambda \sum_{n=1}^{L-2} J(S_n^x S_{n+2}^x + S_n^y S_{n+2}^y + \Delta S_n^z S_{n+2}^z)$$

Poisson distribution

$$P_P(s) = \exp(-s)$$



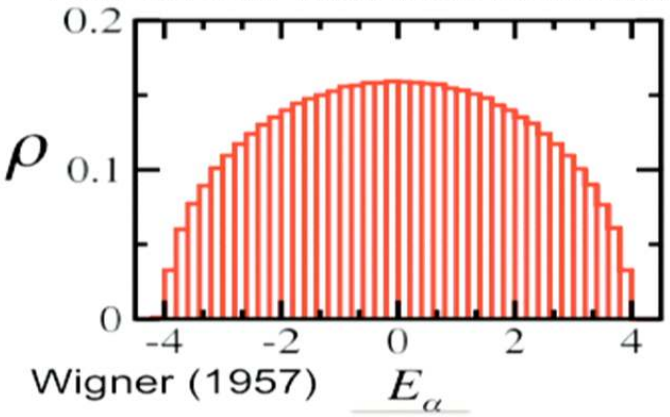
Wigner-Dyson distribution

$$P_{WD}(s) = \frac{\pi s}{2} \exp\left(-\frac{\pi s^2}{4}\right)$$

Full Random Matrices vs Two-Body Interaction

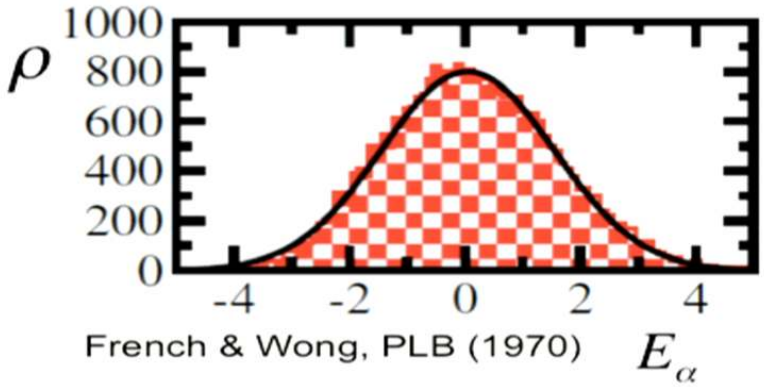
Density of States (Energy Distribution)

Full random matrices: semicircular



Wigner (1957)

Few-body interactions: Gaussian



French & Wong, PLB (1970)

Quench

Ho: unperturbed Hamiltonian
noninteracting, quasiparticle, mean-field

H=Ho+V: perturbed (interacting) Hamiltonian

$H_{initial}$ $|n\rangle$ —quench→ H_{final} $|\psi_\alpha\rangle$

Initial state

$|\Psi(0)\rangle = |ini\rangle$ →

$$|\Psi(0)\rangle = |ini\rangle = \sum_\alpha C_\alpha^{ini} |\psi_\alpha\rangle$$

$$\Downarrow$$

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

(not ground state from $H_{initial}$ nor H_{final})

$$E_{ini} = \langle ini | H_{final} | ini \rangle = \sum_\alpha |C_\alpha|^2 E_\alpha$$

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Ho: unperturbed Hamiltonian
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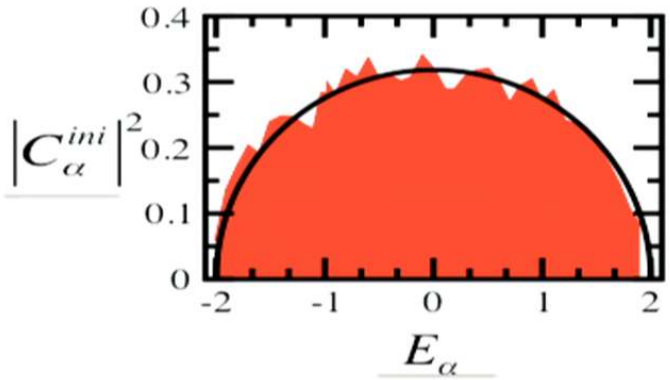
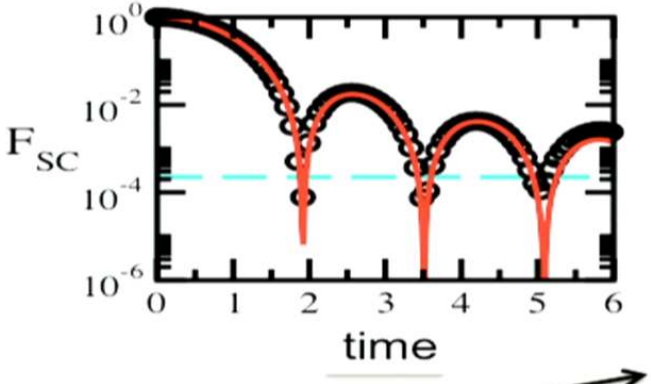
Energy distribution of the initial state in random matrices

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





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

$$F(t) = \left| \int_{-\infty}^{\infty} \left|C^{ini}(E)\right|^2 e^{-iEt}\, dE \right|^2$$

$$C_{SC}^{ini}(E) = \frac{2}{\pi\varepsilon}\sqrt{1-\left(\frac{E}{\varepsilon}\right)^2}$$

$$F_{SC}(t) = \frac{\left|\mathcal{J}_1(2\sigma_{ini}t)\right|^2}{\sigma_{ini}^2 t^2}$$

Bessel function of first order

$$\sigma_{ini} = \sqrt{\int_{-\varepsilon}^{\varepsilon} C_{SC}^{ini}(E) E^2\, dE} = \frac{\varepsilon}{2}$$

Lea F. Santos, Yeshiva University

Torres & LFS PRA (2014)

Torres, Manan, LFS NJP (2014)

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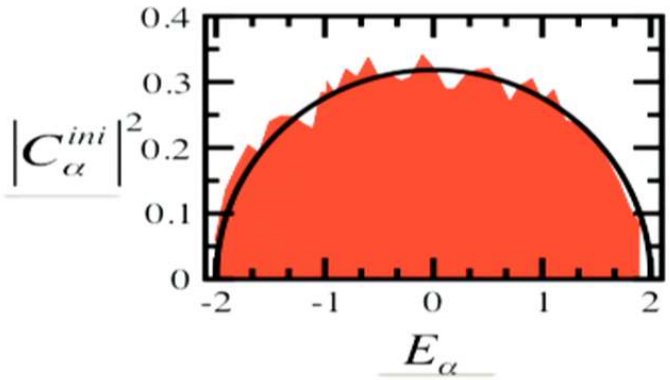
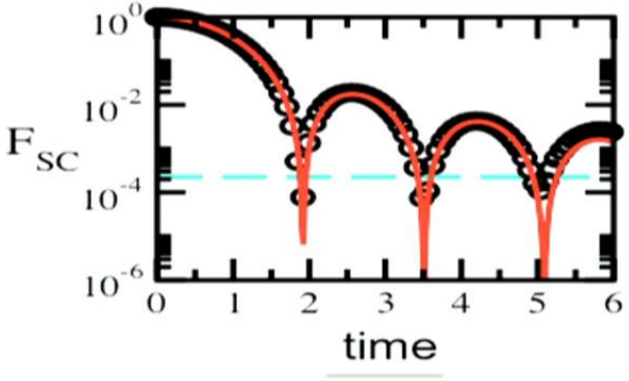
Relaxation time for random matrices

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





D = dimension of the matrix

$$F(t) = \left| \int_{-\infty}^{\infty} \left|C^{ini}(E)\right|^2 e^{-iEt}\, dE \right|^2$$

Infinite time average

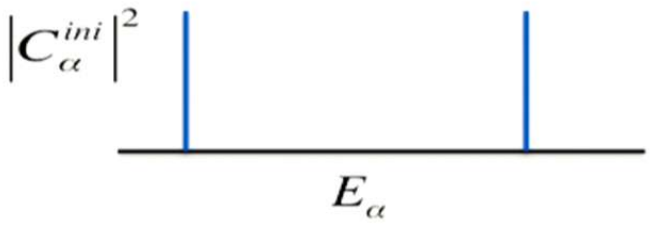
$$F(t) = \sum_\alpha \left|C_\alpha^{ini}\right|^4 + \sum_{\alpha \neq \beta} \left|C_\alpha^{ini}\right|^2 \left|C_\beta^{ini}\right|^2 e^{i(E_\alpha - E_\beta)t} \Rightarrow \overline{F} = \sum_\alpha \left|C_\alpha^{ini}\right|^4 = \frac{3}{D}$$

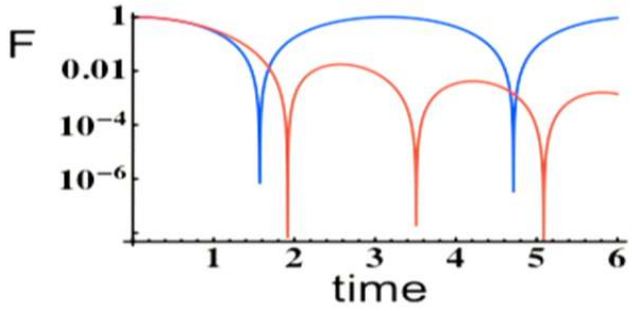
$$\frac{1}{\sum_\alpha \left|C_\alpha^{ini}\right|^4} = IPR_{ini}$$

Torres & LFS PRA (2014)

Torres, Manan, LFS NJP (2014)

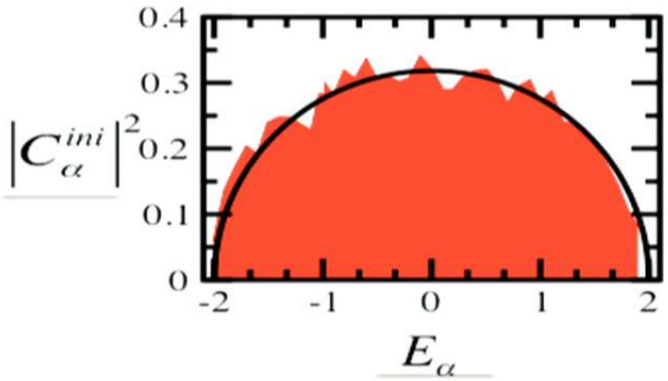
Lifetime bounded by the uncertainty in energy

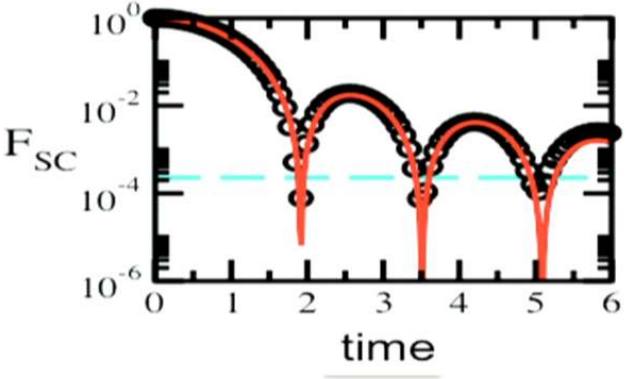




$$F(t) \geq \cos^2(\Delta E t)$$

Fleming (1973)
Bhattacharyya (1983)
Giovannetti, Lloyd, Maccone (2003)





$$F_{SC}(t) = \frac{|\mathcal{J}_1(2\sigma_{ini}t)|^2}{\sigma_{ini}^2 t^2}$$

$$\frac{|\mathcal{J}_1(2\sigma_{ini}t_R)|^2}{\sigma_{ini}^2 t_R^2} = \frac{3}{D}$$

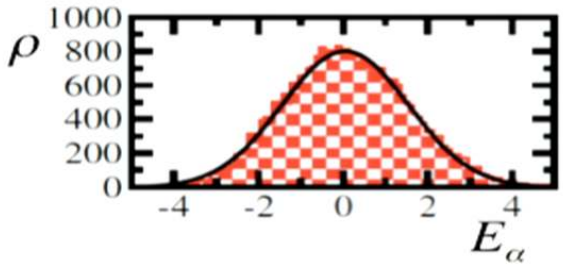
Realistic Systems: Energy Shell

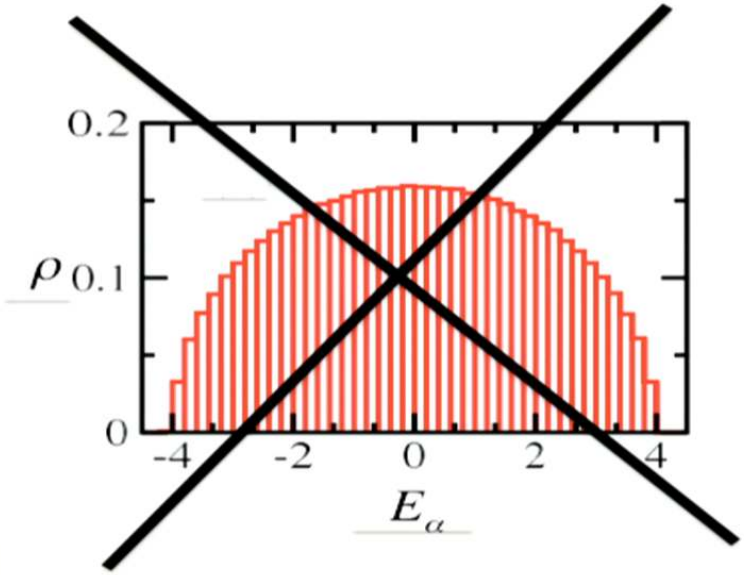
- Realistic systems are not described by full random matrices
They have with few(two)-body interactions.

- The density of states is Gaussian.

- The maximum spreading of the initial state is Gaussian.

French & Wong, PLB (1970)





Gaussian Fidelity Decay

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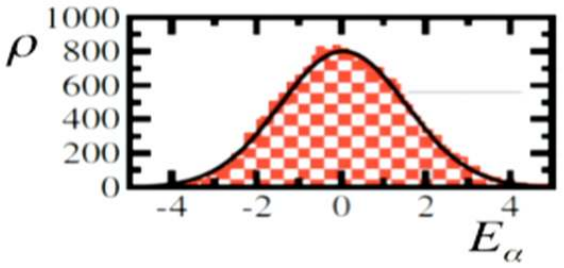
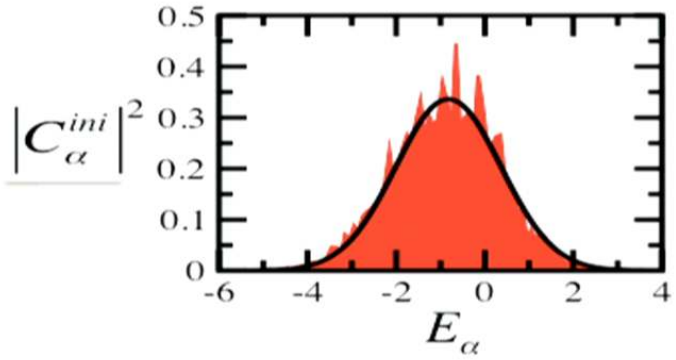
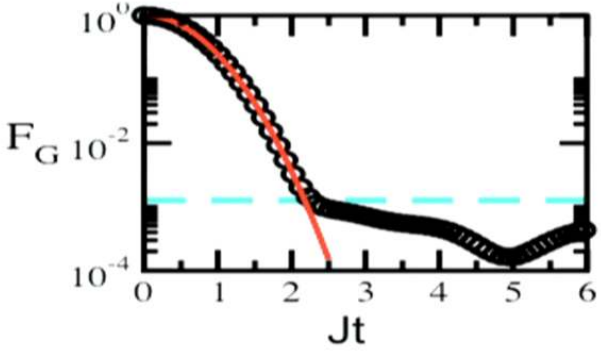






Flambaum (1999)
Flambaum & Izrailev (2001)
Castaneda & Izrailev (2006)

$$\sigma_{ini}^2 = \sum_\alpha |C_\alpha|^2 (E_\alpha - E_{ini})^2$$

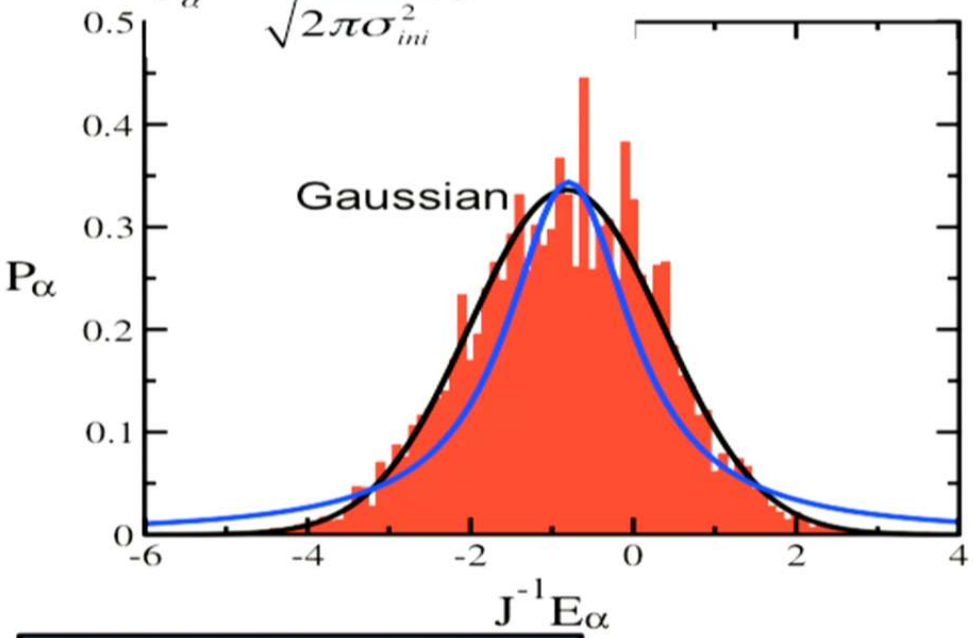
$$F(t) = \left| \sum_\alpha |C_\alpha^{ini}|^2 e^{-iE_\alpha t} \right|^2 = \left| \frac{1}{\sqrt{2\pi\sigma_{ini}^2}} \int_{-\infty}^{\infty} e^{-\frac{(E-E_{ini})^2}{2\sigma_{ini}^2}} e^{-iEt}\, dE \right|^2 = \exp(-\sigma_{ini}^2 t^2)$$

Perturbation increases Fidelity decays faster

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

$$\lambda = 1$$

$$P_\alpha = \frac{1}{\sqrt{2\pi\sigma_{ini}^2}} e^{-\frac{(E-E_{ini})^2}{2\sigma_{ini}^2}}$$



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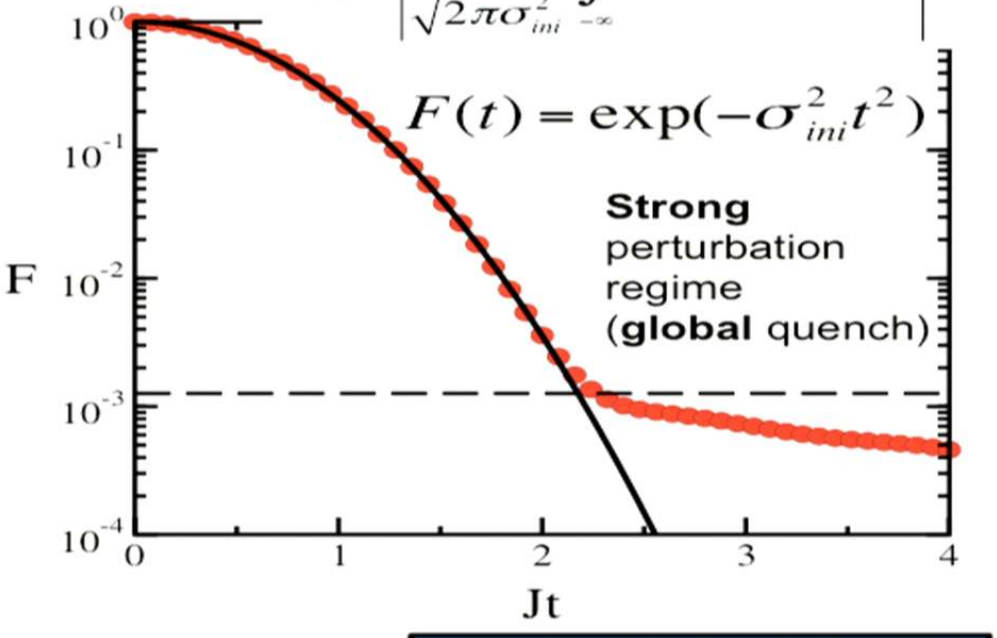


Néel state

$$H_{initial} = \sum_{n=1}^{L-1} S_n^z S_{n+1}^z$$

INITIAL STATES = site-basis

Néel state $\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$

$$\sigma_{ini}^2 = \sum_{\alpha} |C_\alpha|^2 (E_\alpha - E_{ini})^2$$

$$= \sum_{n \neq ini} \left| \langle n | H_{final} | ini \rangle \right|^2$$

$$\boxed{\sigma_{ini}^{Neel} = \frac{J}{2}\sqrt{L-1}}$$

FINAL HAMILTONIAN

$$H_{final} = H_{NN} + \lambda H_{NNN}$$

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

$$H_{NNN} = \left(J\sum_{n=1}^{L-2}(S_n^x S_{n+2}^x + S_n^y S_{n+2}^y) + J\Delta\sum_{n=1}^{L-2} S_n^z S_{n+2}^z \right)$$

$\Delta = 1, \lambda = 0$ ▲

$\Delta = 0.5, \lambda = 0$ ▼

$\Delta = 1, \lambda = 0.4$ ×

$\Delta = 1, \lambda = 1$ ●

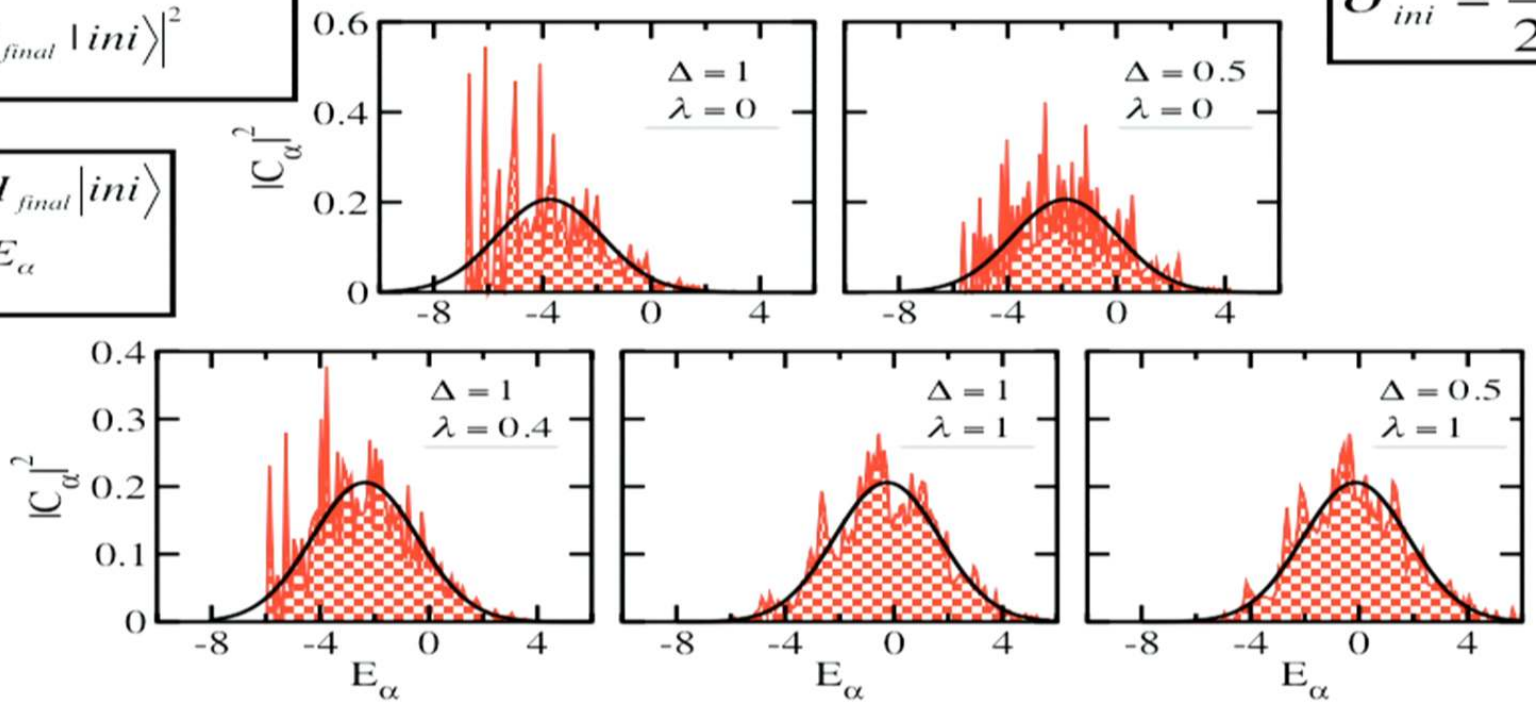
$\Delta = 0.5, \lambda = 1$ ■

Néel state: energy distribution

$$\sigma^2_{ini} = \sum_{\alpha} |C_\alpha|^2 (E_\alpha - E_{ini})^2 = \sum_{n \neq ini} \left| \langle n | H_{final} | ini \rangle \right|^2$$

$$E_{ini} = \langle ini | H_{final} | ini \rangle = \sum_{\alpha} |C_\alpha|^2 E_\alpha$$

$$\sigma^{Neel}_{ini} = \frac{J}{2}\sqrt{L-1}$$



Dynamics of few-body observables

Simple general picture when $[O, H_I] = 0$ H_I defines the initial state

$$\langle O(t)\rangle = \langle ini \mid e^{iH_F t} O e^{-iH_F t} \mid ini\rangle = \sum_{n,m} \langle ini \mid e^{iH_F t} \mid m\rangle\langle m \mid O \mid n\rangle\langle n \mid e^{-iH_F t} \mid ini\rangle$$

$$= F(t)O(0) + \sum_{n \neq ini} \langle n \mid O \mid n\rangle \left|\langle n \mid e^{-iH_F t} \mid ini\rangle\right|^2$$

Short-time dynamics:

$$\langle O(t)\rangle = (1 - \sigma_{ini}^2 t^2) O(0) + t^2 \sum_{n \neq ini} \langle n \mid O \mid n\rangle \left|\langle n \mid H_F \mid ini\rangle\right|^2$$

Observables show a very similar short-time dynamics for H_F leading to comparable σ_{ini} and off-diagonal elements.

Lea F. Santos, Yeshiva University

Torres & LFS PRA (2014)

Torres, Manan, LFS NJP (2014)

Perimeter Institute, 2014

Dynamics of few-body observables

$$[O, H_I] = 0 \Rightarrow \langle O(t)\rangle = (1-\sigma_{ini}^2 t^2)O(0) + t^2 \sum_{n\neq ini} \langle n|O|n\rangle \left|\langle n|H_F|ini\rangle\right|^2$$

Observables show a very similar short-time dynamics for H_F leading to comparable σ_{ini} and off-diagonal elements.

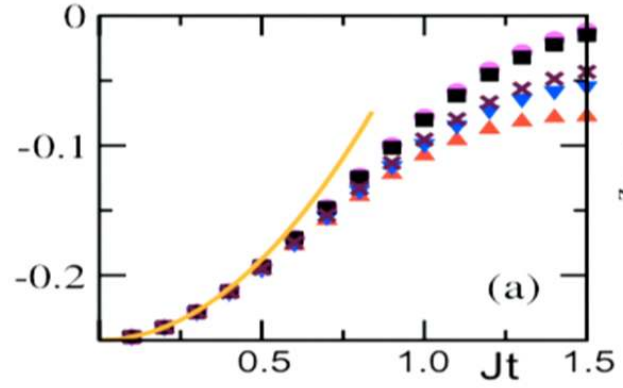
The particularities of the observables become irrelevant and Hamiltonians with very different properties can give equivalent outcomes.

Néel state

$\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$

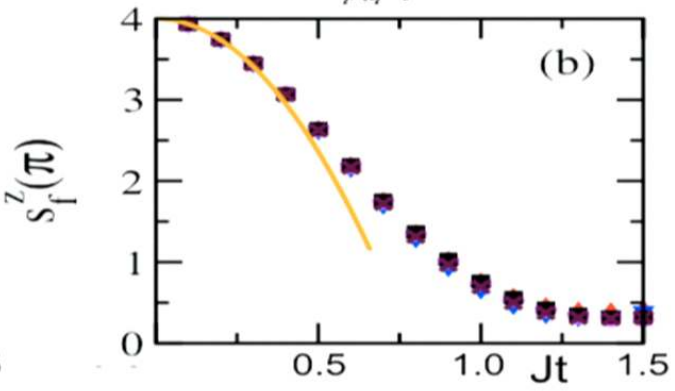
$$\sigma_{ini} = \frac{J}{2}\sqrt{L-1}$$

$$C^z_{L/2,L/2+1} = S^z_{L/2} S^z_{L/2+1}$$



Torres & LFS PRA (2014)

$$s^z_f(k) = \frac{1}{L}\sum_{p,q=1}^{L} e^{ik(p-q)} S^z_p S^z_q$$



Torres, Manan, LFS NJP (2014)

$\Delta = 1, \lambda = 0$

$\Delta = 0.5, \lambda = 0$

$\Delta = 1, \lambda = 0.4$

$\Delta = 1, \lambda = 1$

$\Delta = 0.5, \lambda = 1$

$L = 16, S^z = 0$

Equilibration

Quantum system $H\,|\psi_\alpha\rangle = E_\alpha\,|\psi_\alpha\rangle$

Initial state: $|\Psi(0)\rangle = \sum_\alpha C_\alpha\,|\psi_\alpha\rangle$

Quantum system:
linear time evolution
discrete spectrum

Time evolution of a generic observable:

$$O_{\alpha\beta} = \langle\psi_\alpha\,|\,O\,|\,\psi_\beta\rangle$$

$$\langle O(t)\rangle = \langle\Psi(t)\,|\,O\,|\,\Psi(t)\rangle = \sum_\alpha |\,C_\alpha\,|^2\,O_{\alpha\alpha} + \sum_{\alpha\neq\beta} C_\alpha^* C_\beta e^{i(E_\alpha - E_\beta)t} O_{\alpha\beta}$$

Infinite time average: (generic system with nondegenerate and incommensurate spectrum)

$$\overline{\langle O(t)\rangle} = \lim_{t\to\infty}\frac{1}{t}\int_0^t O(\tau)\,d\tau = \sum_\alpha |\,C_\alpha\,|^2\,O_{\alpha\alpha} = O_{diag}$$ (diagonal ensemble)

Closer look at integrable and chaotic systems

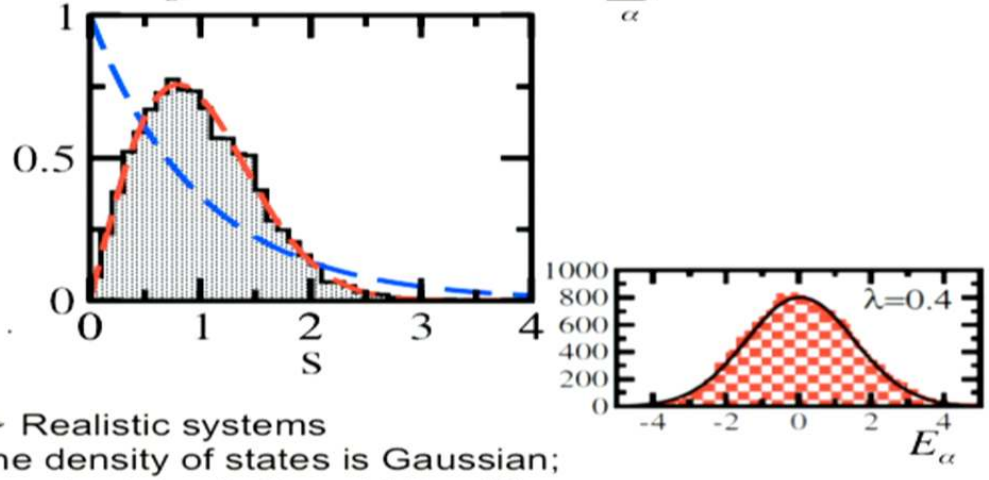
Temporal fluctuations of O after relaxation: σ_O

System size: L

Srednicki, JPA **32** 1163 (1999)

Fully chaotic systems

$$\sigma_O \propto e^{-L} \qquad |\Psi(t)\rangle = \sum_\alpha C_\alpha e^{-iE_\alpha t} |\psi_\alpha\rangle$$



➢ Realistic systems
the density of states is Gaussian;
➢ only states in the middle of the spectrum may become chaotic;

Time fluctuations vs L

Integrable isotropic $H_{NN} = J\sum_{n=1}^{L-1}(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + S_n^z S_{n+1}^z) \rightarrow \Delta = 1$

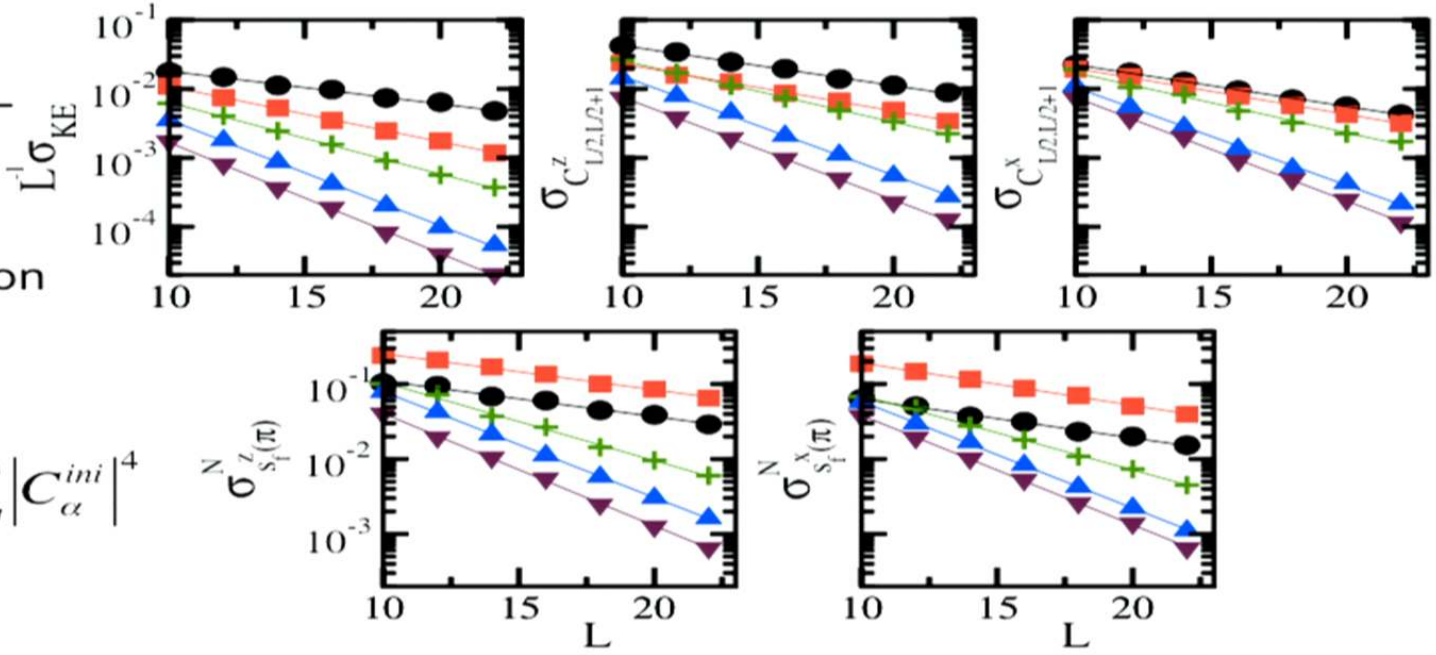
Exponential decay with L

$$\sigma_O \propto e^{-\kappa L}$$

Exponent depends on the level of delocalization of the initial state

$$\sigma_O \leq (O_{\max} - O_{\min})\sum_{\alpha}\left|C_{\alpha}^{ini}\right|^4$$

Reimann, PRL **108** (2008);
Phys. Scr. **86** (2012)
Short, NJP **13**, (2011)
Short, Farrelly, NJP **14** (2012)



Zangara et al,
PRE **88**, 032913 (2013)

L/2 up spins

von Neumann (1929)

Peres (1984)
Jensen & Shankar (1985)

90's
Flambaum, Izrailev, Zelevinsky

Srednicki, Deutsch

THERMALIZATION

Kinoshita, Wenger, and Weiss,
Nature **440**, 900 (2006)

Kollath et al
PRL **98**, 180601 (2007)

Rigol, Dunjko, Olshanii,
Nature **452**, 854 (2008)

Lea F. Santos, Yeshiva University

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Thermalization

Infinite time average: $\overline{\langle O(t)\rangle} = \sum_{\alpha} |C_\alpha|^2 O_{\alpha\alpha} = O_{diag}$

Eigenstate Expectation Value: $\boxed{O_{\alpha\alpha} = \langle \psi_\alpha | O | \psi_\alpha \rangle}$

Will the system thermalize?
Will the predictions from the **infinite time average** coincide with the predictions of the **microcanonical** ensemble?

$$O_{diag} \equiv \sum_{\alpha} |C_\alpha|^2 O_{\alpha\alpha} \overset{=?}{\longleftrightarrow} O_{micro} \equiv \frac{1}{N_{E_0,\Delta E}} \sum_{\substack{\alpha \\ |E_0 - E_\alpha| < \Delta E}} O_{\alpha\alpha}$$

depends on the initial conditions — depends only on the energy

Thermalization

Infinite time average: $\overline{\langle O(t)\rangle} = \sum_{\alpha} |C_\alpha|^2 O_{\alpha\alpha} = O_{diag}$

Eigenstate Expectation Value: $O_{\alpha\alpha} = \langle \psi_\alpha | O | \psi_\alpha \rangle$

Will the system thermalize?
Will the predictions from the **diagonal ensemble** coincide with the predictions of the **microcanonical** ensemble?

$$O_{diag} \equiv \sum_{\alpha} |C_\alpha|^2 O_{\alpha\alpha} \overset{=?}{\longleftrightarrow} O_{micro} \equiv \frac{1}{N_{E_0,\Delta E}} \sum_{\substack{\alpha \\ |E_0 - E_\alpha| < \Delta E}} O_{\alpha\alpha}$$

depends on the initial conditions — depends only on the energy

Equation holds for all initial states that are narrow in energy when…

ETH: the expectation values $O_{\alpha\alpha}$ of few-body observables do not fluctuate for eigenstates close in energy

Zelevinsky, Flambaum, Izrailev
Casati, Borgonovi

Onset of chaos is associated with the onset of **chaotic eigenstates**

LFS & M. Rigol
PRE **81** 036206 (2010)
PRE **82** 031130 (2010)
M. Rigol and LFS
PRA **82** 011604(R) (2010)

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

Structure of the eigenstates

Delocalization Measure

Inverse Participation Ratio

$$\psi^{(\alpha)} = \sum_{i=1}^{D} c_i^{(\alpha)} \phi_i \Rightarrow \boxed{IPR^{(\alpha)} \equiv \frac{1}{\sum_{i=1}^{D} | c_i^{(\alpha)} |^4}}$$

IPR – small localization

$IPR \sim \dim/3$ maximum delocalization
chaotic states - GOE

Shannon entropy $S = -\sum_{i=1}^{D} | c_i^{(\alpha)} |^2 \ln | c_i^{(\alpha)} |^2$
(information)

Hardcore bosons in 1D: (clean, periodic)

QUENCH: from NN model to NN + t' NNN model

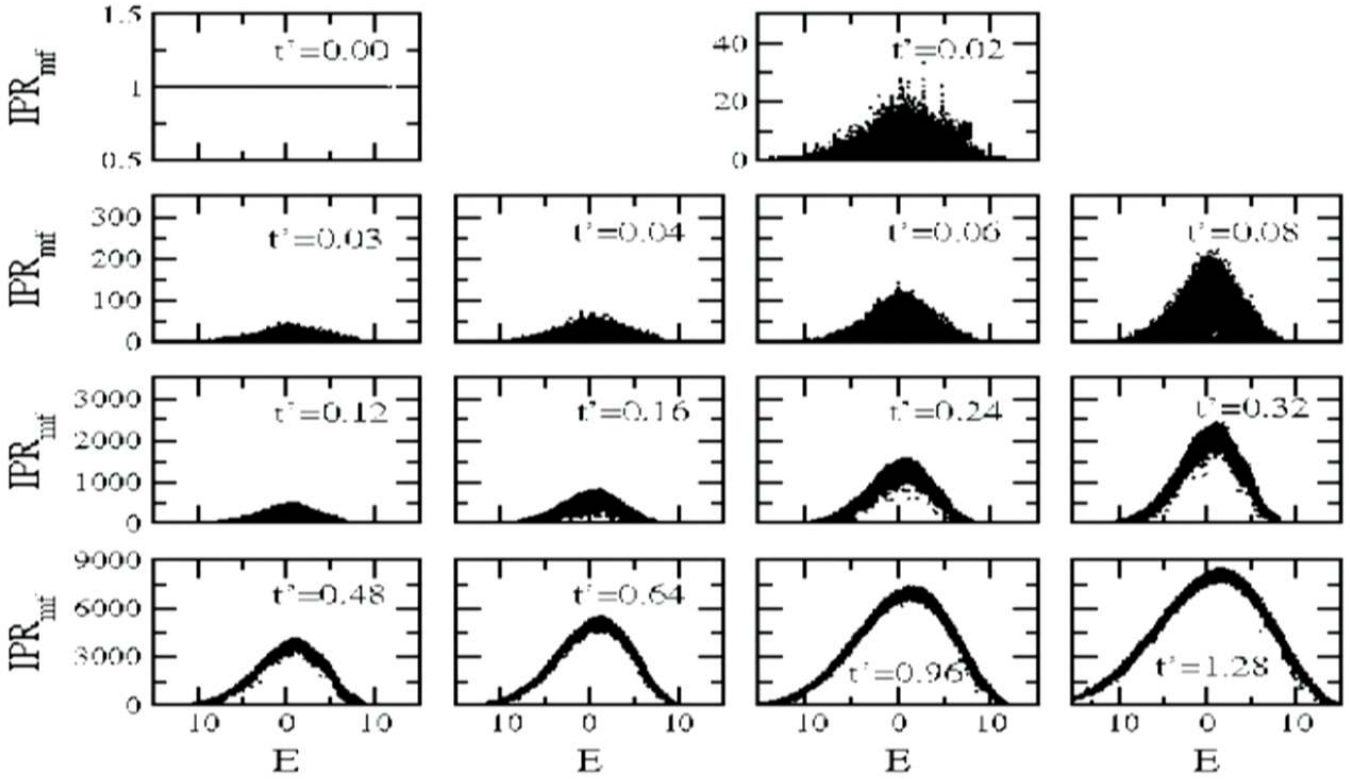
$$H = \sum_{i=1}^{L} \left[-t\left(b_i^+ b_{i+1} + h.c.\right) + V\left(n_i^b - \frac{1}{2}\right)\left(n_{i+1}^b - \frac{1}{2}\right) - t'\left(b_i^+ b_{i+2} + h.c.\right) + V'\left(n_i^b - \frac{1}{2}\right)\left(n_{i+2}^b - \frac{1}{2}\right) \right]$$

$$n_i^b = b_i^+ b_{i+1}$$

$\boxed{t' = V'}$

Mean-field basis: eigenstates of integrable system ($t'=V'=0$)
separates regular from chaotic behavior

Bosons: eigenstates



$t = V = 1$
$t' = V'$

L=24, 8 particles, k=2
dim=30624

Fluctuations
increase close to integrable point

ETH breaks down

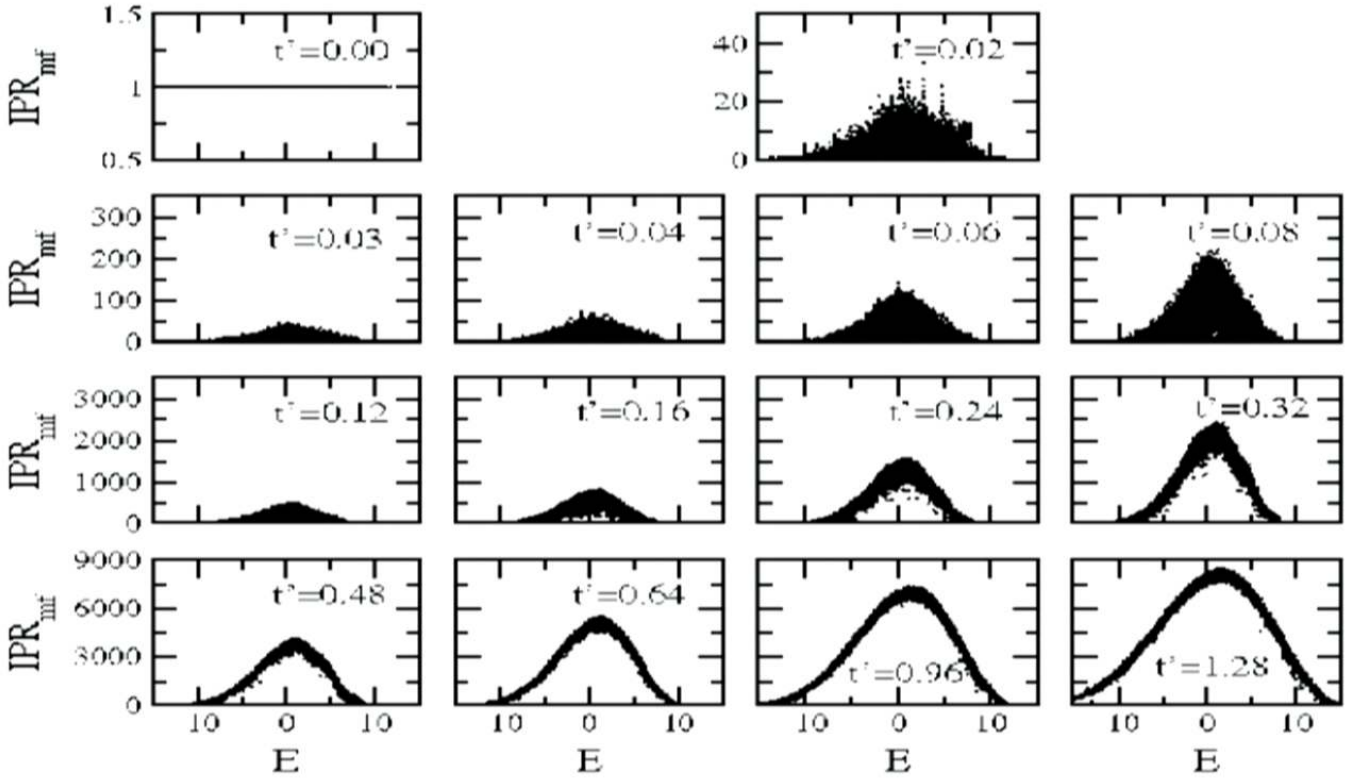
Chaotic region:
IPR is a smooth function of E

Middle of spectrum

$$IPR_{mf} \rightarrow IPR_{GOE}$$

LFS & M. Rigol
PRE **81** 036206 (2010)
PRE **82** 031130 (2010)
M. Rigol and LFS
PRA **82** 011604(R) (2010)

Bosons: eigenstates



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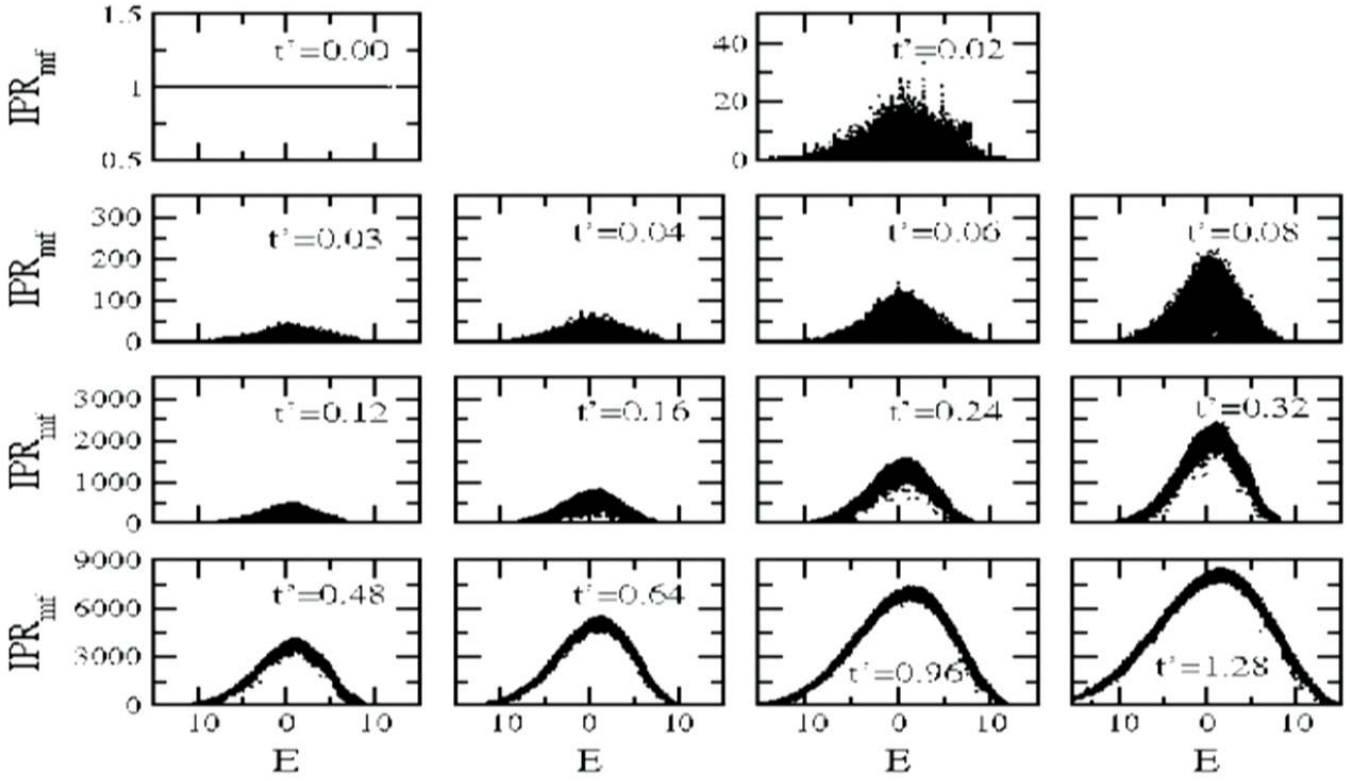

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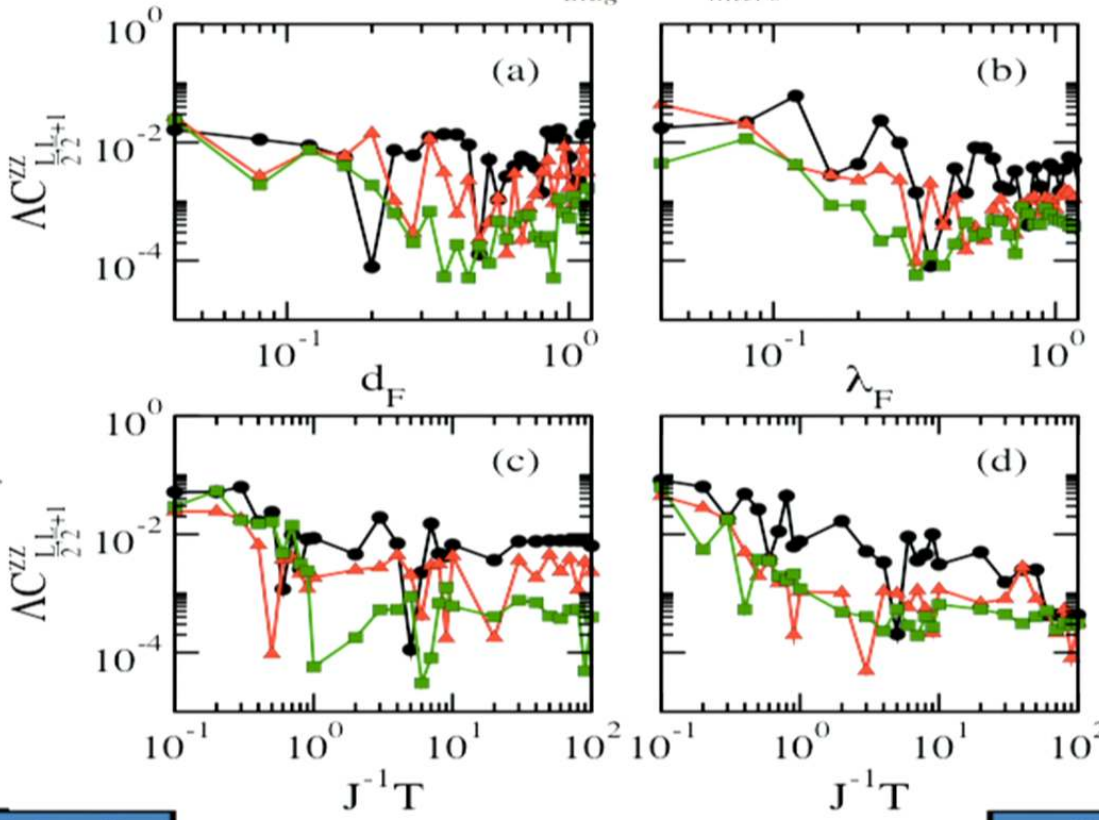
LFS & M. Rigol
PRE **81** 036206 (2010)
PRE **82** 031130 (2010)
M. Rigol and LFS
PRA **82** 011604(R) (2010)

Thermalization: local and nonlocal quenches

$$\Lambda C^{zz} = | C^{zz}_{diag} - C^{zz}_{micro} |$$

Quench:
XXZ to
Chaotic
Impurity
Model



Quench:
XXZ to
Chaotic
NNN
Model

L=12
L=15
L=18

$$E_{ini} = \frac{1}{Z}\sum_{\alpha} E_{\alpha} e^{-E_{\alpha}/T}$$

$\Delta = 0.48, \lambda = 0.44$
$d = 0.9, T = 7J$
1/3 up

He & Rigol
PRA **85**, 063609 (2012)
PRA **87**, 043615 (2013)

Torres & LFS
PRE (2013);
PRE (2014)

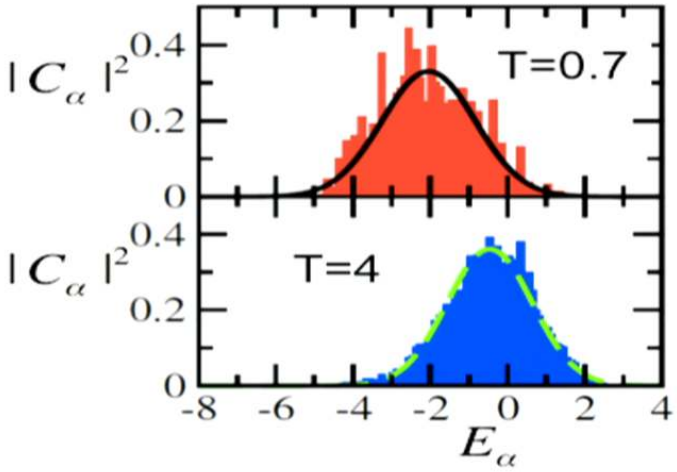
Quench: chaos to integrable

$XXZ_{nn} + \lambda XXZ_{nnn} \rightarrow XXZ_{nn}$ $\quad \Delta = 0.5, \lambda = 1 \rightarrow \Delta = 0.5, \lambda = 0$

Quench: chaotic $H_{initial}$ to interacting integrable H_{final}

$$\delta O = \left| O_{diag} - O_{micro} \right|$$

$$E_{ini} = \frac{1}{Z} \sum_{\alpha} E_{\alpha} e^{-E_{\alpha}/T}$$



Chaotic state
fills the energy shell

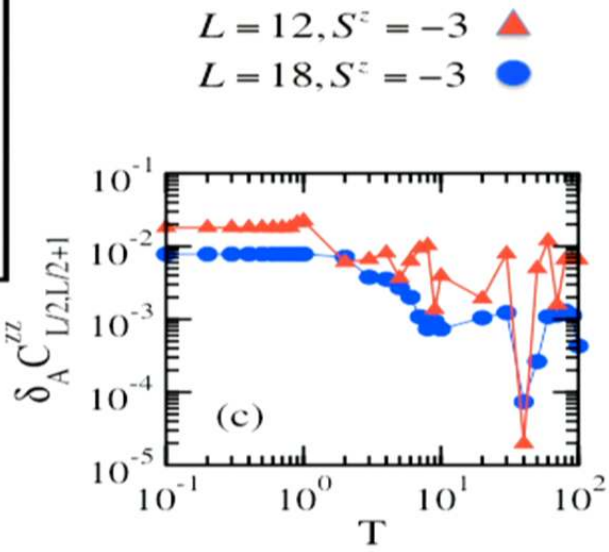
$$O_{diag} \equiv \sum_{\alpha} |C_{\alpha}|^2 O_{\alpha\alpha}$$

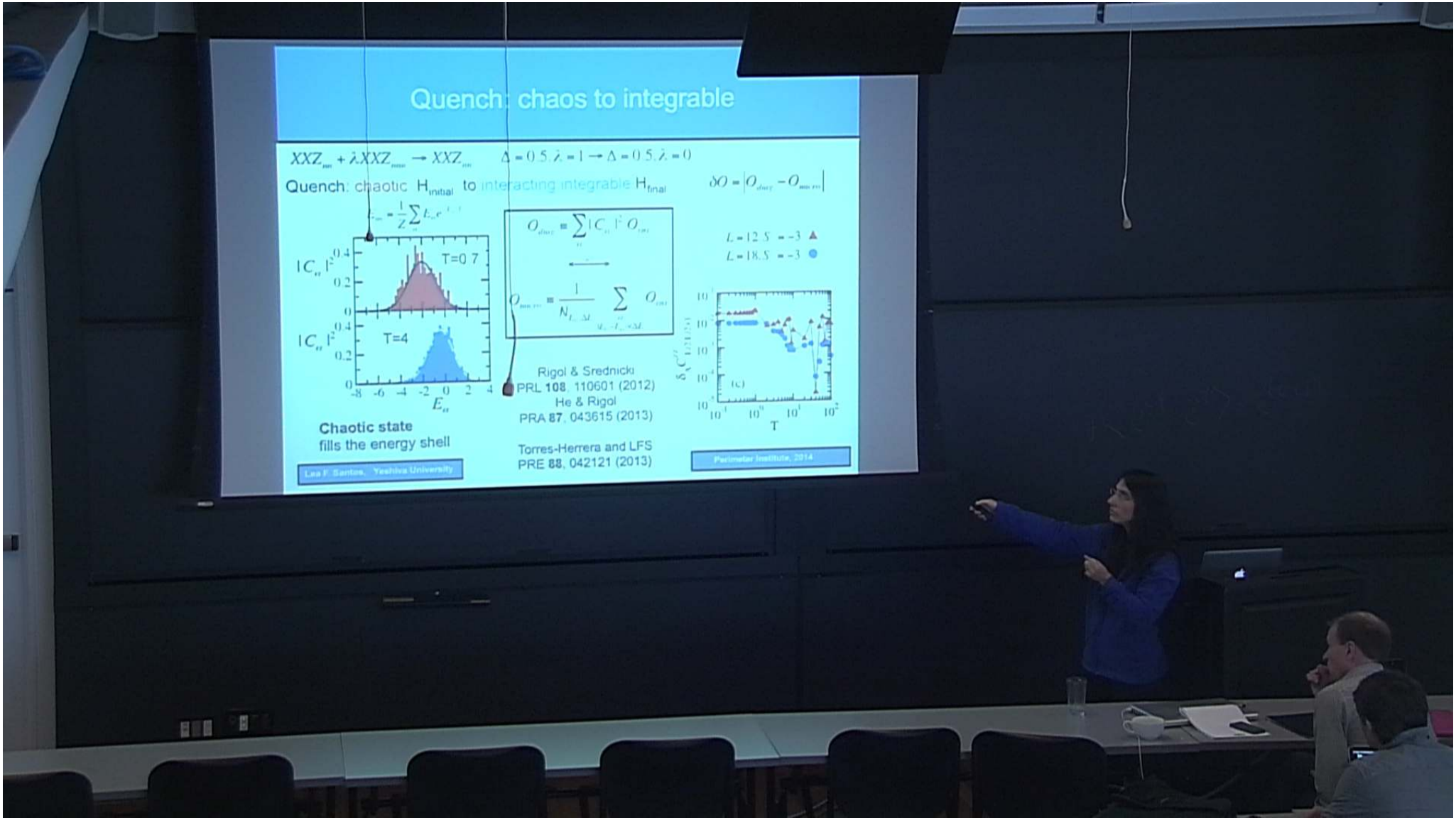
$$\overset{=?}{\longleftrightarrow}$$

$$O_{micro} \equiv \frac{1}{N_{E_0, \Delta E}} \sum_{\substack{\alpha \\ |E_0 - E_\alpha| < \Delta E}} O_{\alpha\alpha}$$

Rigol & Srednicki
PRL **108**, 110601 (2012)
He & Rigol
PRA **87**, 043615 (2013)

Torres-Herrera and LFS
PRE **88**, 042121 (2013)




Quench: chaos to integrable
Quench: chaotic H_initial to interacting integrable H_final
T=0.7
T=4
Chaotic state
fills the energy shell
Rigol & Srednicki
PRL 108, 110601 (2012)
He & Rigol
PRA 87, 043615 (2013)
Torres-Herrera and LFS
PRE 88, 042121 (2013)
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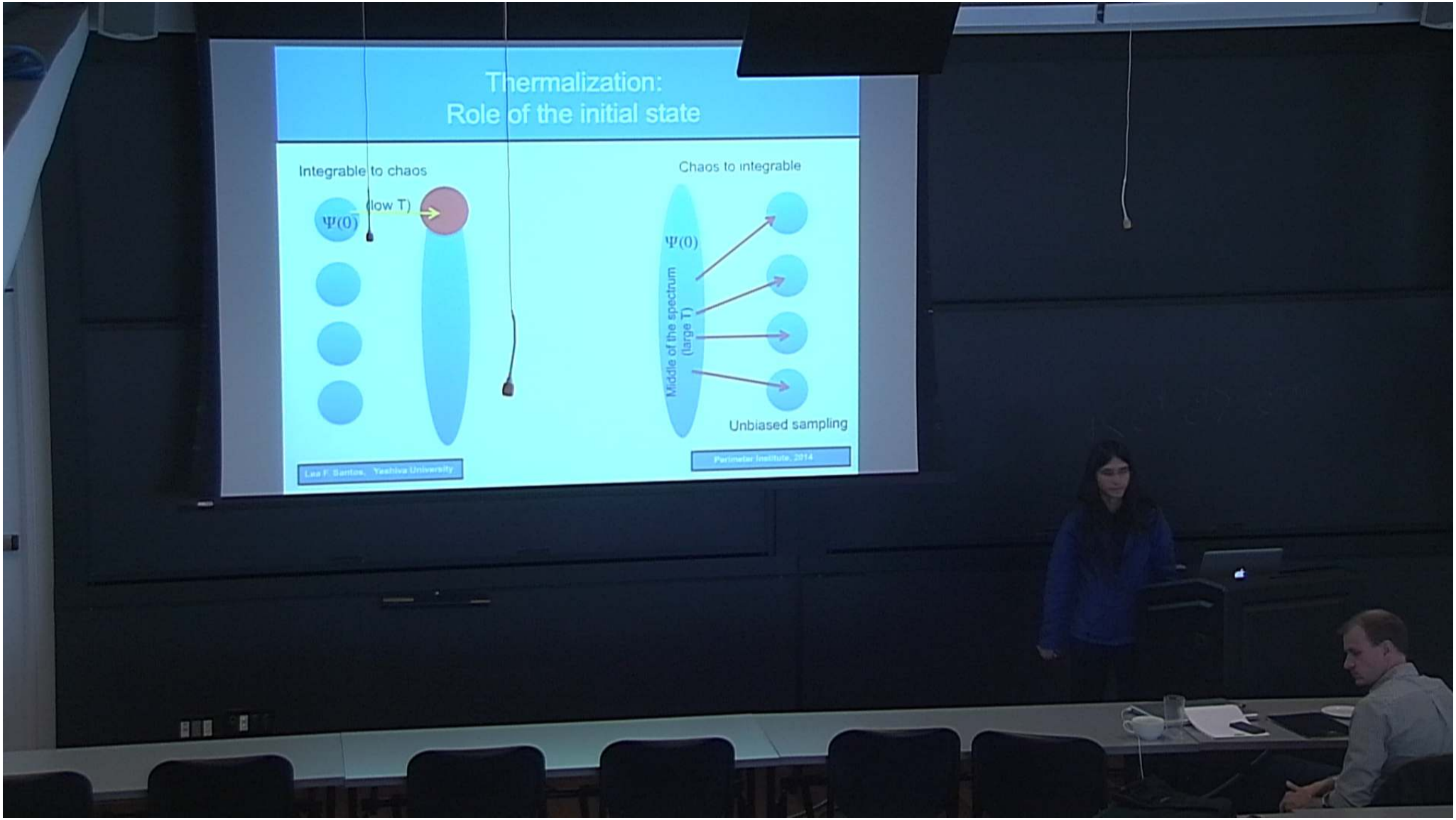
Thermalization:
Role of the initial state
Integrable to chaos
(low T)
$\Psi(0)$
Chaos to integrable
$\Psi(0)$
Middle of the spectrum
(large T)
Unbiased sampling
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