From unitary dynamics to statistical mechanics in isolated quantum systems

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L. D'Alessio, Y. Kafri, A. Polkovnikov, and MR, *From Quantum Chaos and Eigenstate Thermalization to Statistical Mechanics and Thermodynamics*, Adv. Phys. **65**, 239-362 (2016).

Outline

1. Motivation
   - A numerical experiment
   - Foundations of quantum statistical mechanics
   - Experiments with ultracold quantum gases
2. Quantum chaos and random matrix theory
   - Classical mechanics
   - Random matrix theory
3. Dynamics and thermalization
   - Quantum mechanics vs statistical mechanics
   - Dynamics
   - Thermalization
   - Eigenstate thermalization
4. Summary

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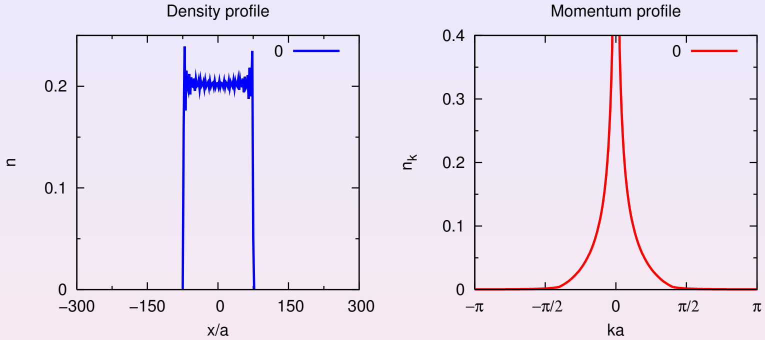

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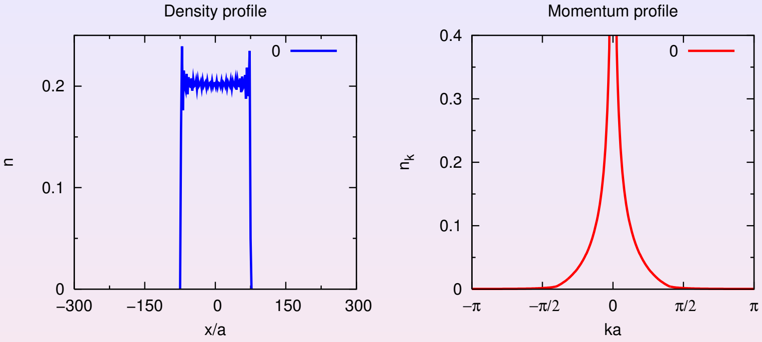

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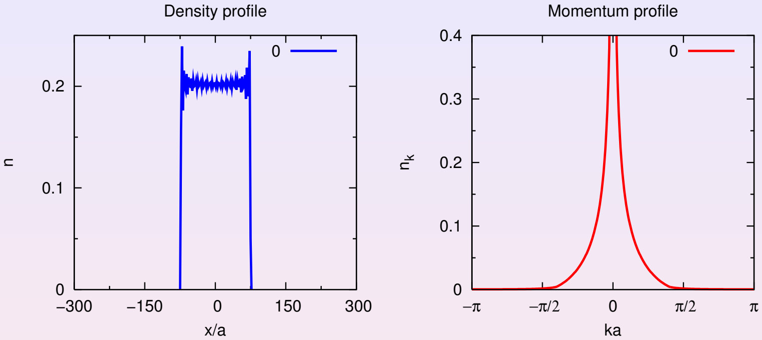

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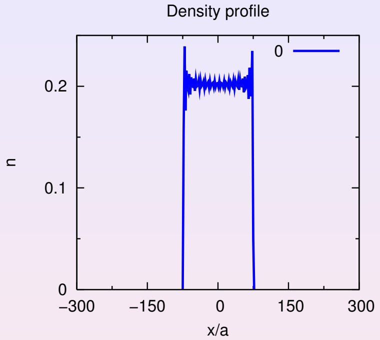

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- The expectation values of the observables become (almost) time independent. There is no need to couple the system to a bath to see equilibration!
- The density is nearly homogeneous. This is expected in thermal equilibrium!
- Is the momentum distribution after equilibration in "thermal" equilibrium?

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Foundations of quantum statistical mechanics

Quantum ergodicity: John von Neumann ‘29
(Proof of the ergodic theorem and the H-theorem in quantum mechanics)

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Some "more recent" related works (keywords)

Tasaki '98
(From Quantum Dynamics to the Canonical Distribution. . .)

Goldstein, Lebowitz, Tumulka, and Zanghi '06
(Canonical Typicality)

Popescu, Short, and A. Winter '06
(Entanglement and the foundation of statistical mechanics)

Goldstein, Lebowitz, Mastrodonato, Tumulka, and Zanghi '10
(Normal typicality and von Neumann's quantum ergodic theorem)

MR and Srednicki '12
(Alternatives to Eigenstate Thermalization)

P. Reimann '15
(Generalization of von Neumann's Approach to Thermalization)

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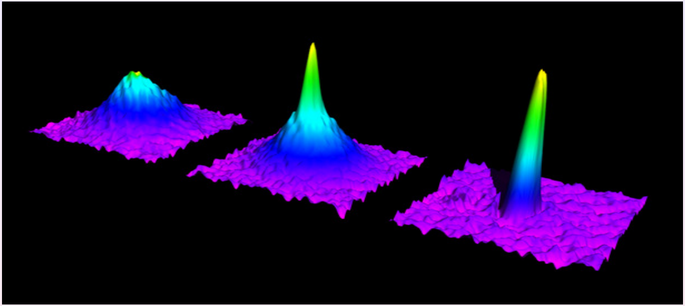
Bose-Einstein condensation

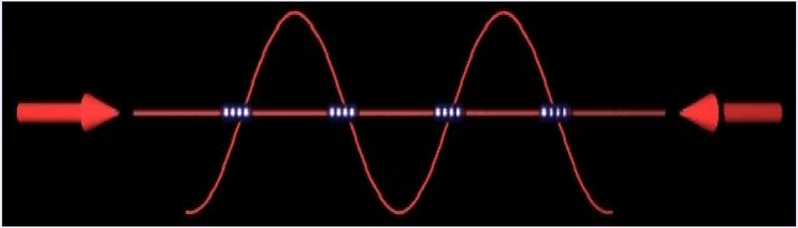
Eric A. Cornell, Wolfgang Ketterle, Carl E. Wieman (1995)
Nobel Prize in Physics 2001



Experimental systems

- Temperatures between 1nK and 100μK
- Maximum densities 10^{11} to 10^{15} atoms per cm^3
- Gas with 1000 to 10^8 neutral alkali atoms

Optical lattices and lattice models



Jaksch *et al.* ’98

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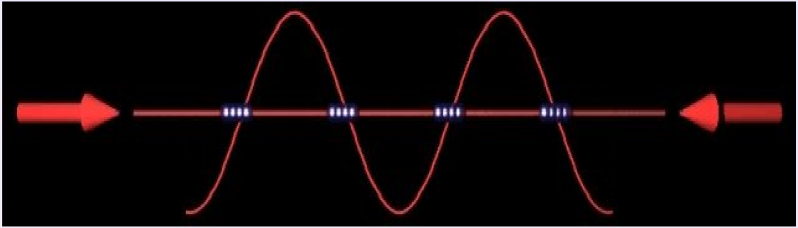

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Bose-Hubbard model

$$\hat{H} = -J \sum_{\langle ij \rangle} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1).$$

Fermi-Hubbard model

$$H = -J \sum_{\substack{\langle ij \rangle \\ \sigma=\uparrow,\downarrow}} \left(\hat{f}_{i\sigma}^\dagger \hat{f}_{j\sigma} + \hat{f}_{j\sigma}^\dagger \hat{f}_{i\sigma} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}.$$

Quenches in one-dimensional superlattices

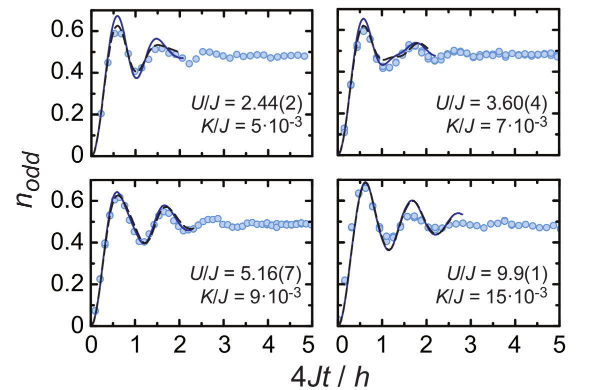
Quantum dynamics from a 1D superlattice

Trotzky *et al.*,
Nature Phys. **8**, 325 (2012).

Initial state $|01010\ldots1010\rangle$

Unitary dynamics under the "Bose-Hubbard" Hamiltonian

Experimental results (○) vs exact t-DMRG calculations (lines) without free parameters



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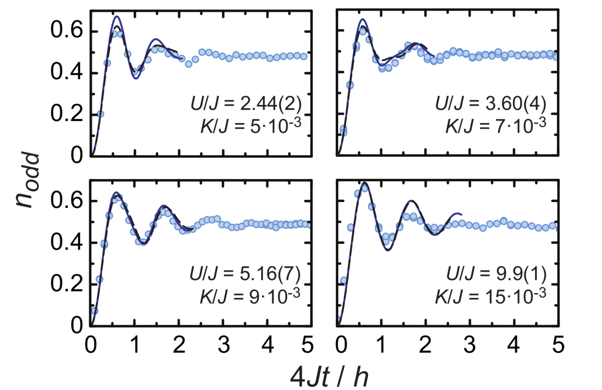
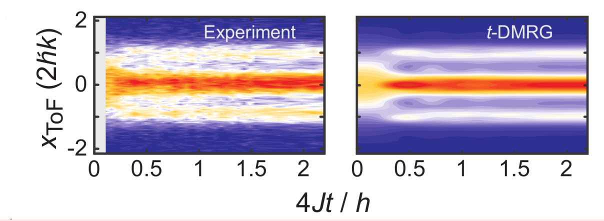
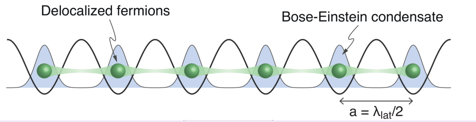




local observables (top)
vs
nonlocal observables (bottom)

Slow equilibration in quenches in Bose-Fermi mixtures



S. Will, D. Iyer, and MR,
Nat. Commun. **6**, 6009 (2015).

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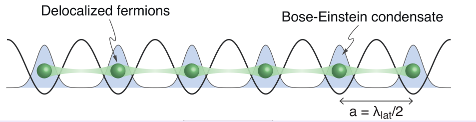

$$\langle \hat{c}^{\dagger}_{j\neq 0}\hat{c}_0\rangle(t) = \frac{n_F \sin[\pi n_F j] e^{2n_B[\cos(U^{\mathrm{FB}}t/\hbar)-1]}}{j},$$

n_F and n_B are the fermion and boson fillings.

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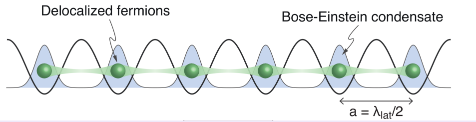

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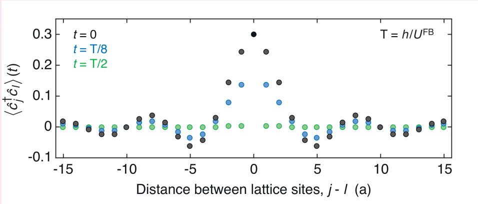

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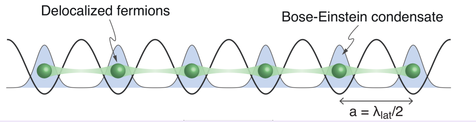

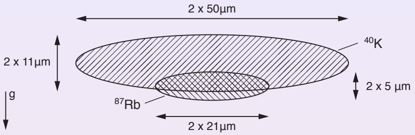

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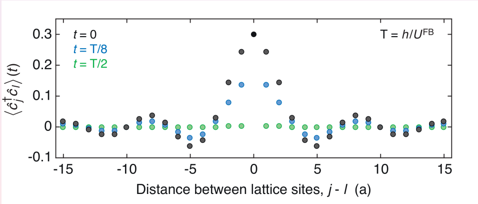

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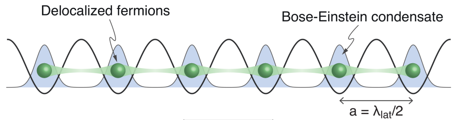

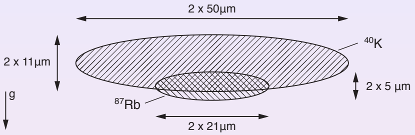

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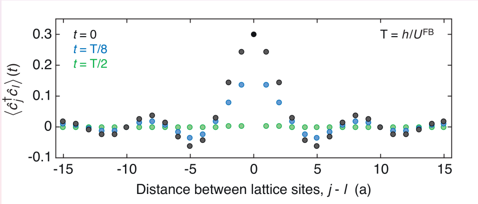

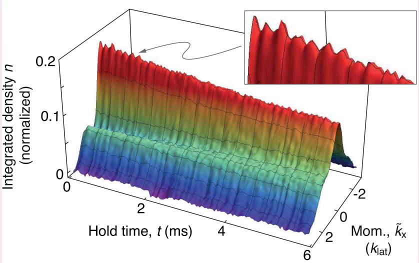

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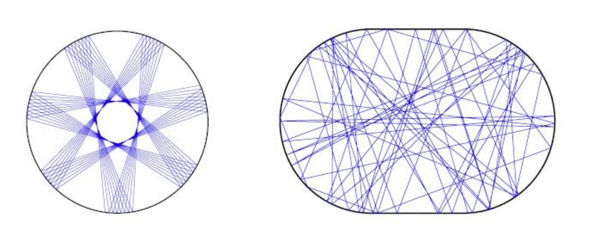
Outline

Classical chaos and integrability

Particle trajectories in a circular cavity and a Bunimovich stadium (scholarpedia)



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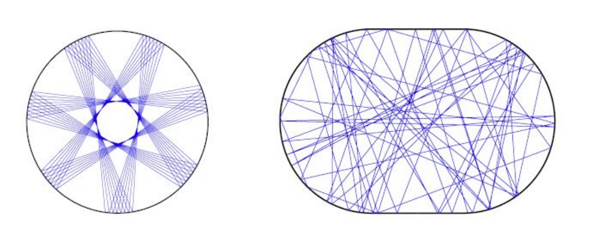

- A Hamiltonian $H(\mathbf{p},\mathbf{q})$, with $\mathbf{q}=(q_1,\cdots,q_N)$ and $\mathbf{p}=(p_1,\cdots,p_N)$, is said to be integrable if there are N functionally independent constants of the motion $\mathbf{I}=(I_1,\cdots,I_N)$ in involution:

$$\{I_\alpha, H\}=0, \quad \{I_\alpha, I_\beta\}=0, \quad \text{where} \quad \{f,g\}=\sum_{i=1,N}\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i}-\frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}.$$

Liouville's integrability theorem: $(\mathbf{p},\mathbf{q})\to(\mathbf{I},\mathbf{\Theta})$, so that $H(\mathbf{p},\mathbf{q})\to H(\mathbf{I})$.

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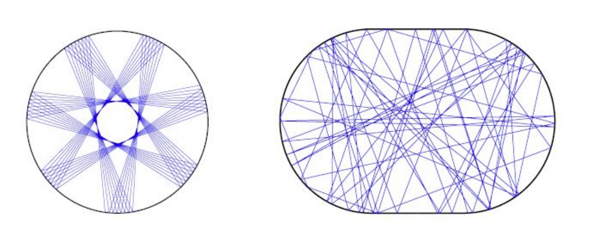

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- Chaos: exponential sensitivity of the trajectories to perturbations

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Random matrix theory

- Wigner (1955) & Dyson (1962): Statistical properties of the spectra of complex quantum systems (in a narrow energy window) can be predicted from the statistical properties of the spectra of random matrices (with the appropriate symmetries). It was used with great success to understand the spectra of complex nuclei.

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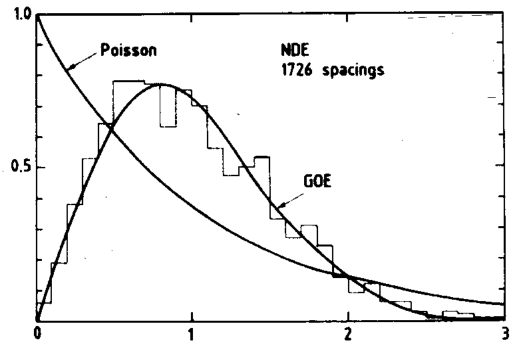
Distribution of level spacings for the "Nuclear Data Ensemble"



T. Guhr *et al.*, Physics Reports **299**, 189 (1998).

Distribution of level spacings $P(\omega)$

$P(\omega)$ can be understood using 2×2 matrices

$$\left[\begin{array}{cc} \varepsilon_1 & \frac{V}{\sqrt{2}} \\ \frac{V^*}{\sqrt{2}} & \varepsilon_2 \end{array} \right], \qquad E_{1,2} = \frac{\varepsilon_1 + \varepsilon_2}{2} \pm \frac{1}{2}\sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 2|V|^2}.$$

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For systems that are invariant under time reversal, $\hat{H}$ can be written as a real matrix. Draw ε_1, ε_2, and V from a Gaussian distribution with zero mean and variance σ.

$$\begin{aligned} P(\omega \equiv E_1 - E_2) &= \frac{1}{(2\pi)^{3/2}\sigma^3} \int d\varepsilon_1 \int d\varepsilon_2 \int dV\, \delta\left(\sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 2V^2} - \omega\right) \\ &\quad \times \exp\left(-\frac{\varepsilon_1^2 + \varepsilon_2^2 + V^2}{2\sigma^2}\right). \end{aligned}$$

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Calculating the integrals (change of variables plus cylindrical coordinates)

$$P(\omega) = \frac{\omega}{2\sigma^2} \exp\left[-\frac{\omega^2}{4\sigma^2}\right]$$

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Wigner Surmise (Wigner-Dyson distribution)

$P(\omega) = A_\beta\, \omega^\beta\, \exp[-B_\beta \omega^2]$, where $\beta = 1$ (GOE) and $\beta = 2$ (GUE)

Semi-classical limit: Statistics of energy levels

- Berry-Tabor conjecture (1977): The statistics of level spacings of quantum systems whose classical counterpart is integrable is described by a Poisson distribution. (Energy eigenvalues behave like a sequence of independent random variables.)

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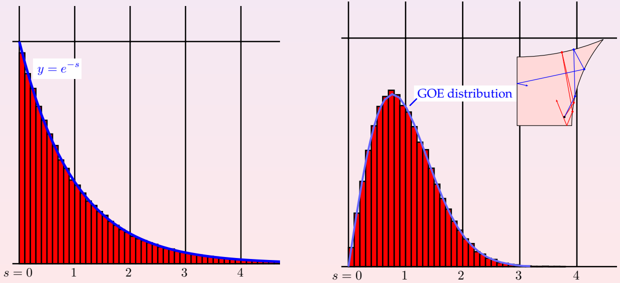
Distribution of level spacings: rectangular and chaotic cavities



Z. Rudnik, Notices AMS **55**, 32 (2008).

Lattice models with no classical counterpart

Spinless fermions (hard-core bosons, spin-1/2) in one dimension

$$\hat{H} = \sum_{i=1}^{L} \left\{ -J \left(\hat{f}_i^\dagger \hat{f}_{i+1} + \text{H.c.} \right) + V \hat{n}_i \hat{n}_{i+1} - J' \left(\hat{f}_i^\dagger \hat{f}_{i+2} + \text{H.c.} \right) + V' \hat{n}_i \hat{n}_{i+2} \right\}$$

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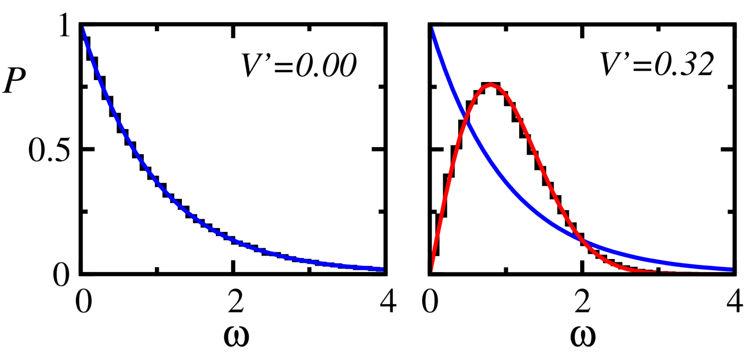
Level spacing distribution $(N_f = L/3,\ J = V = 1,\ J' = V')$



L. Santos and MR, PRE **81**, 036206 (2010); PRE **82**, 031130 (2010).

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Exact results from quantum mechanics

If the initial state is not an eigenstate of $\widehat{H}$

$$|\psi_{\rm ini}\rangle \neq |\alpha\rangle \quad \text{where} \quad \widehat{H}|\alpha\rangle = E_\alpha|\alpha\rangle \quad \text{and} \quad E = \langle\psi_{\rm ini}|\widehat{H}|\psi_{\rm ini}\rangle,$$

then observables $\hat{O}$ evolve in time:

$$O(t) \equiv \langle\psi(t)|\widehat{O}|\psi(t)\rangle \quad \text{where} \quad |\psi(t)\rangle = e^{-i\widehat{H}t}|\psi_{\rm ini}\rangle.$$

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One can rewrite

$$O(t) = \sum_{\alpha,\beta} C^\star_\alpha C_\beta e^{i(E_\alpha - E_\beta)t} O_{\alpha\beta} \quad \text{using} \quad |\psi_{\text{ini}}\rangle = \sum_\alpha C_\alpha|\alpha\rangle.$$

Taking the infinite time average (diagonal ensemble $\hat{\rho}_{\text{DE}} \equiv \sum_\alpha |C_\alpha|^2|\alpha\rangle\langle\alpha|$)

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which depends on the initial conditions through $C_\alpha = \langle\alpha|\psi_{\text{ini}}\rangle$.

Energy fluctuations after a sudden quench (locality)

Initial state $|\psi_{\text{ini}}\rangle = \sum_\alpha C_\alpha |\alpha\rangle$ is an eigenstate of $\widehat{H}_{\text{ini}}$. At $t = 0$

$$\widehat{H}_{\text{ini}} \to \widehat{H} = \widehat{H}_{\text{ini}} + \widehat{W} \qquad \text{with} \quad \widehat{W} = \sum_j \hat{w}(j) \quad \text{and} \quad \widehat{H}|\alpha\rangle = E_\alpha|\alpha\rangle.$$

MR, V. Dunjko, and M. Olshanii, Nature **452**, 854 (2008).

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The energy fluctuations after a quench, ΔE, are:

$$\Delta E = \sqrt{\sum_\alpha E_\alpha^2 |C_\alpha|^2 - (\sum_\alpha E_\alpha |C_\alpha|^2)^2} = \sqrt{\langle \psi_{\text{ini}}|\widehat{W}^2|\psi_{\text{ini}}\rangle - \langle \psi_{\text{ini}}|\widehat{W}|\psi_{\text{ini}}\rangle^2},$$

from which it follows that:

$$\Delta E = \sqrt{\sum_{j_1, j_2} \left[\langle \psi_{\text{ini}}|\hat{w}(j_1)\hat{w}(j_2)|\psi_{\text{ini}}\rangle - \langle \psi_{\text{ini}}|\hat{w}(j_1)|\psi_{\text{ini}}\rangle\langle \psi_{\text{ini}}|\hat{w}(j_2)|\psi_{\text{ini}}\rangle\right]} \overset{N\to\infty}{\propto} \sqrt{N},$$

where N is the total number of lattice sites.

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They are subextensive as in traditional ensembles in statistical mechanics.

MR, V. Dunjko, and M. Olshanii, Nature **452**, 854 (2008).

Outline

Numerical experiments in one dimension

Hard-core bosons ($\hat{b}_i^2 = \hat{b}_i^{\dagger 2} = 0$) in one-dimension

$$\hat{H} = \sum_{i=1}^{L} \left\{ -J \left(\hat{b}_i^\dagger \hat{b}_{i+1} + \text{H.c.} \right) + V \hat{n}_i \hat{n}_{i+1} - J' \left(\hat{b}_i^\dagger \hat{b}_{i+2} + \text{H.c.} \right) + V' \hat{n}_i \hat{n}_{i+2} \right\}$$

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"One can rewrite

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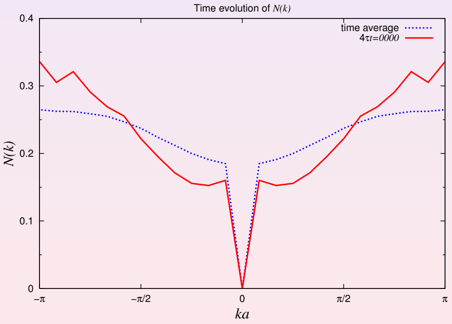
Nonequilibrium dynamics in 1D (density-density structure factor)



MR, PRL **103**, 100403 (2009).

$$\hat{N}(k) = \frac{1}{L} \sum_{j,l} e^{-ik(j-l)} \hat{n}_j \hat{n}_l$$

$N_b = 8$ hard-core bosons

$N = 24$ lattice sites

Fix $J' = V'$ and "quench"
$J_{\text{ini}} = 0.5, V_{\text{ini}} = 2$
$\rightarrow J_{\text{fin}} = 1, V_{\text{fin}} = 1$

Outline

Statistical description after equilibration

Microcanonical calculation

$$O_{\mathsf{ME}} = \frac{1}{N_{\text{states}}} \sum_{\alpha} \langle \Psi_\alpha | \hat{O} | \Psi_\alpha \rangle$$

with $E - \Delta E < E_\alpha < E + \Delta E$

N_{states} : # of states in the window

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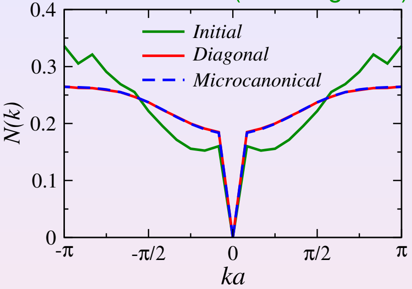

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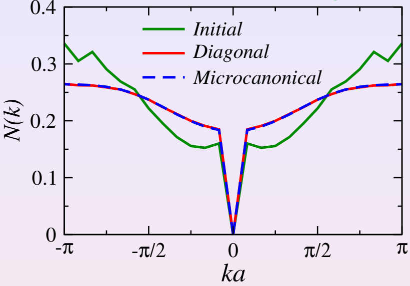

Relative difference
(at fixed $e = E/L$ or T)

$$\frac{\sum_k |N_{\text{DE}}(k) - N_{\text{ME}}(k)|}{\sum_k N_{\text{DE}}(k)}$$

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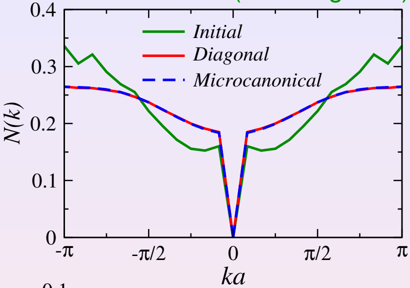

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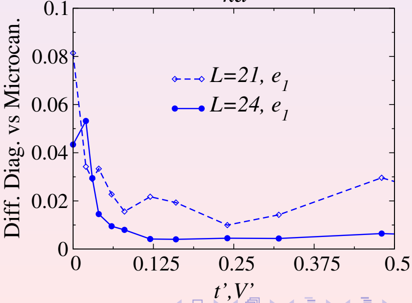

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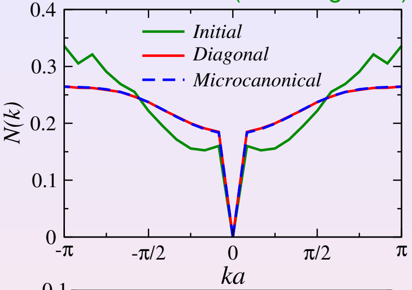

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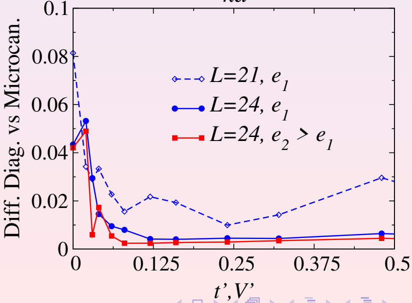

Outline

Eigenstate thermalization

Paradox?

$$\sum_{\alpha} |C_\alpha|^2 O_{\alpha\alpha} = \frac{1}{N_{E,\Delta E}} \sum_{|E-E_\alpha|<\Delta E} O_{\alpha\alpha}$$

Left hand side: Depends on the initial conditions through $C_\alpha = \langle \alpha | \psi_{\text{ini}} \rangle$
Right hand side: Depends only on the energy

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Left hand side: Depends on the initial conditions through $C_\alpha = \langle\alpha|\psi_{\text{ini}}\rangle$
Right hand side: Depends only on the energy

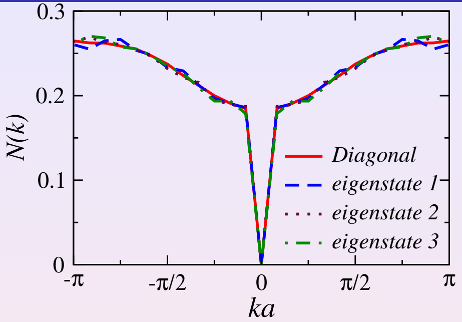
Eigenstate thermalization hypothesis (ETH): diagonal part
[Deutsch, PRA **43** 2046 (1991); Srednicki, PRE **50**, 888 (1994);
MR, Dunjko, and Olshanii, Nature **452**, 854 (2008).]

> The expectation value $\langle\alpha|\widehat{O}|\alpha\rangle$ of a few-body observable $\widehat{O}$ in an eigenstate of the Hamiltonian $|\alpha\rangle$, with energy E_α, of a large interacting many-body system equals the thermal average of $\widehat{O}$ at the mean energy E_α:
>
> $$\langle\alpha|\widehat{O}|\alpha\rangle = O_{\text{ME}}(E_\alpha)$$

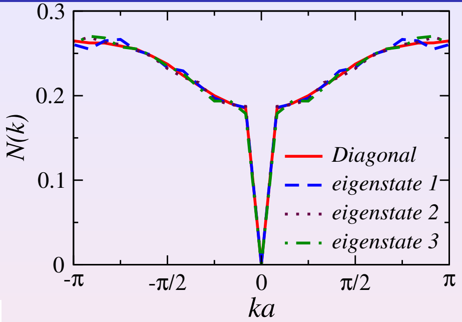
ETH – away from integrability ($J' = V' = 0.24$)

Structure factor

Eigenstates with energies closest to E



ETH – away from integrability ($J' = V' = 0.24$)



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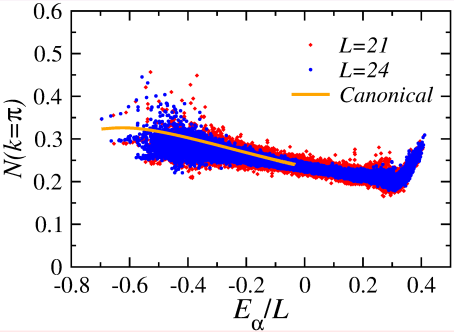
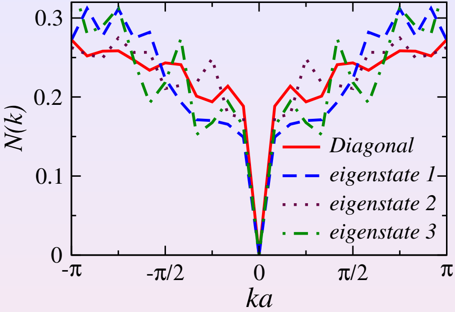


$N(k = \pi)$ vs eigenstate energy

There is no eigenstate thermalization at the edges of the spectrum (there is no quantum chaos either)

Breakdown of ETH at integrability ($J' = V' = 0$)



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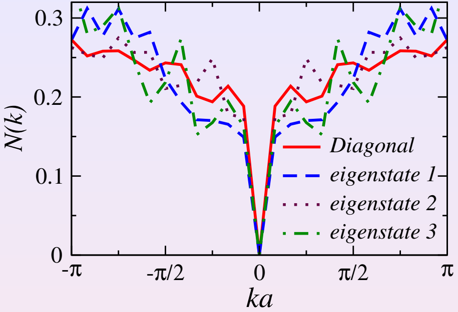

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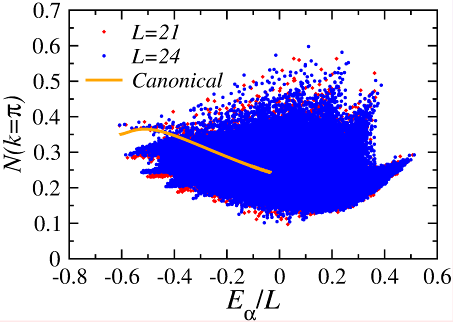
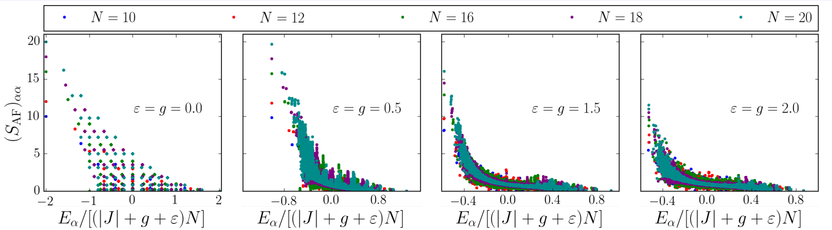


$N(k = \pi)$ vs eigenstate energy

In finite systems, eigenstate thermalization breaks down close to integrable points (there is no quantum chaos either). Quantum KAM?

Eigenstate thermalization, other models/observables

$$\hat{H} = J \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \hat{\sigma}^z_{\mathbf{i}} \hat{\sigma}^z_{\mathbf{j}} + g \sum_{\mathbf{i}} \hat{\sigma}^x_{\mathbf{i}} + \varepsilon \sum_{\mathbf{i}} \hat{\sigma}^z_{\mathbf{i}}, \qquad \hat{S}_{\text{AF}} = \frac{1}{N} \sum_{\mathbf{i},\mathbf{j}} (-1)^{\theta_{\mathbf{ij}}} \hat{\sigma}^z_{\mathbf{i}} \hat{\sigma}^z_{\mathbf{j}}$$



R. Mondaini, K. R. Fratus, M. Srednicki, and MR, PRE **93**, 032104 (2016).

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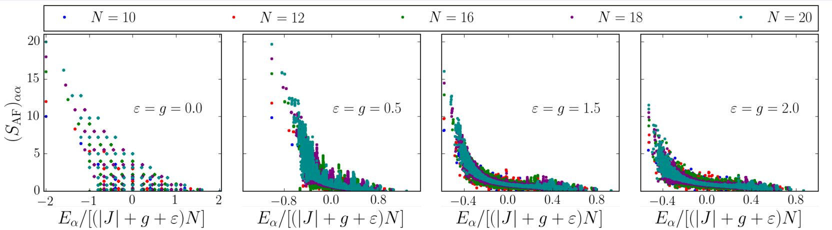

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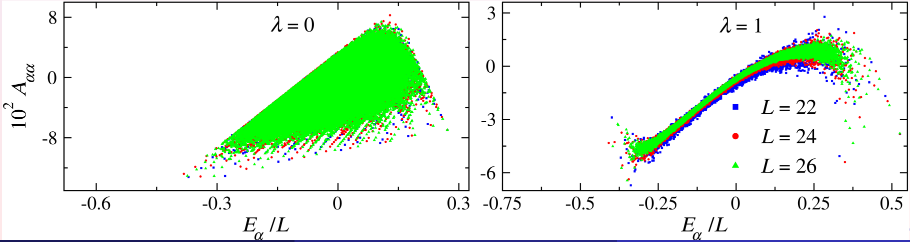
1D model, local observable: $\hat{A} = \frac{1}{L}\sum_{i=1}^{L} \hat{S}^z_i \hat{S}^z_{i+1}$, T. LeBlond *et al.*, PRE **100**, 062134 (2019).



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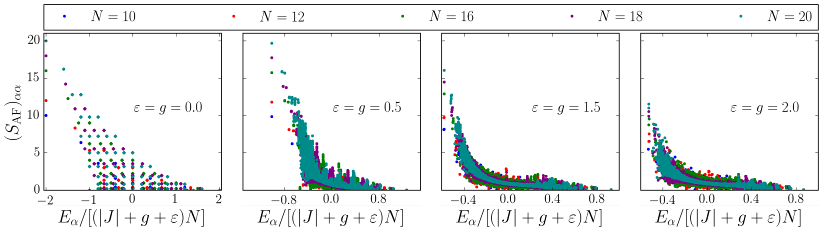

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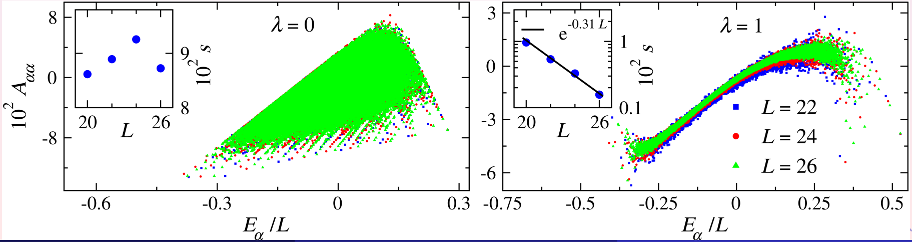

Time fluctuations

Relative difference

$$\delta N(\tau) = \frac{\sum_k |N(k,\tau) - N_{\mathrm{DE}}(k)|}{\sum_k N_{\mathrm{DE}}(k)}$$

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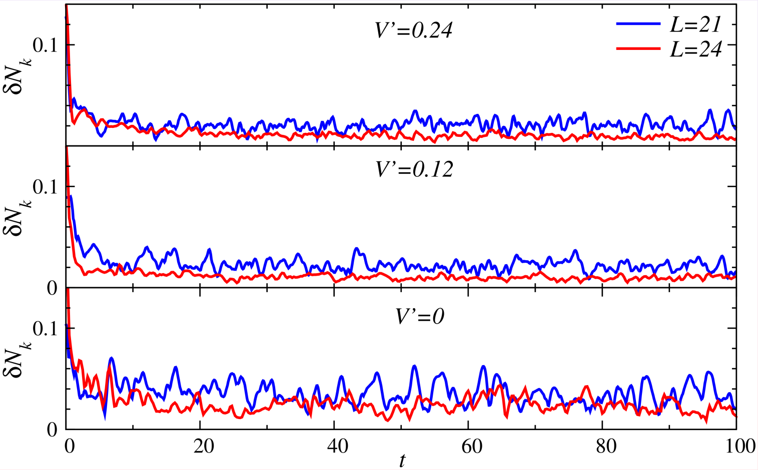

Time fluctuations

Will they always be small because of dephasing?

$$\sigma_O^2 \equiv \lim_{t_0\to\infty} \frac{1}{t_0}\int_0^{t_0} dt\, [O(t)]^2 - (\overline{O})^2 = \sum_{\alpha,\beta\neq\alpha} |C_\alpha|^2 |C_\beta|^2 |O_{\alpha\beta}|^2$$

$$\sim |O_{\alpha\beta}^{\text{typical}}|^2 \sum_{\alpha,\beta} |C_\alpha|^2 |C_\beta|^2 = |O_{\alpha\beta}^{\text{typical}}|^2$$

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Time average of $O(t)$

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Dephasing is not enough.
One needs $|O_{\alpha\beta}^{\text{typical}}| \ll |O_{\alpha\alpha}^{\text{typical}}|$

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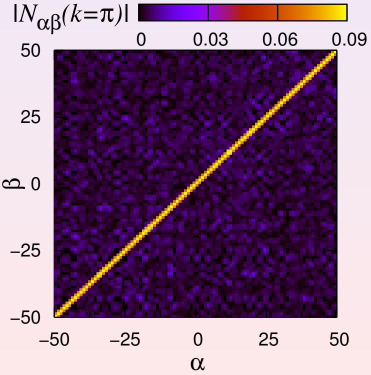

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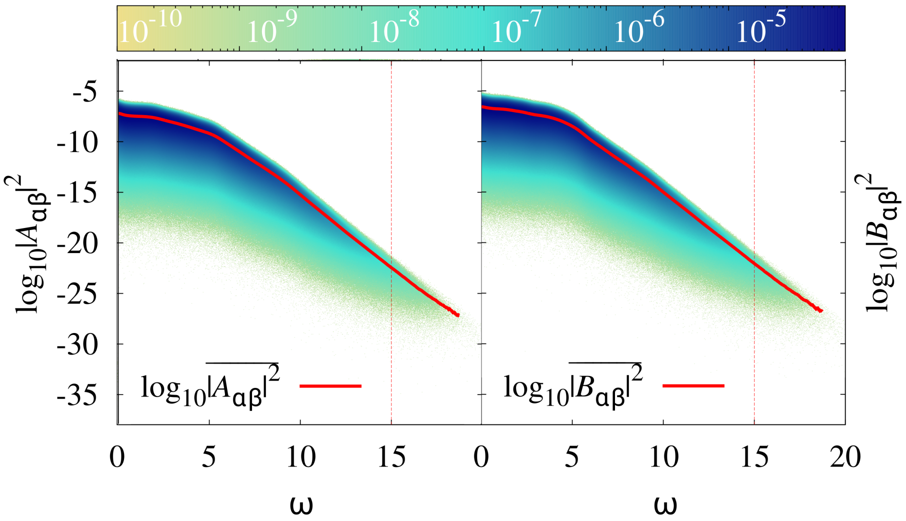
MR, PRA **80**, 053607 (2009).

Eigenstate thermalization hypothesis

Off-diagonal ETH: Results vs $\omega = E_\alpha - E_\beta$, at constant $E = (E_\alpha + E_\beta)/2$



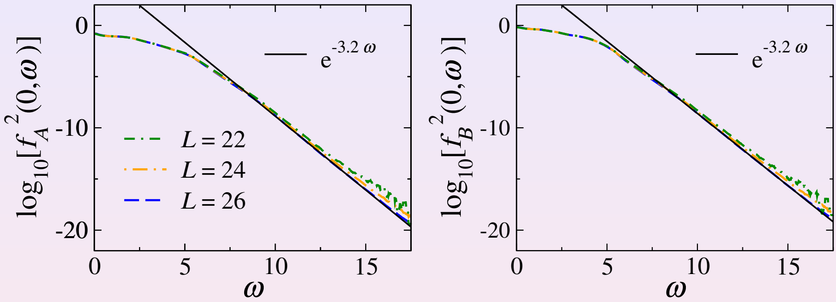
T. LeBlond, K. Mallayya, L. Vidmar, and MR, PRE **100**, 062134 (2019).

T. LeBlond and MR, PRE **102**, 062113 (2020).

Eigenstate thermalization hypothesis

Off-diagonal ETH:

Smooth size-independent function: $|f_O(\bar{E} \simeq 0, \omega)|^2 = LD\,\overline{|O_{\alpha\beta}|^2}$



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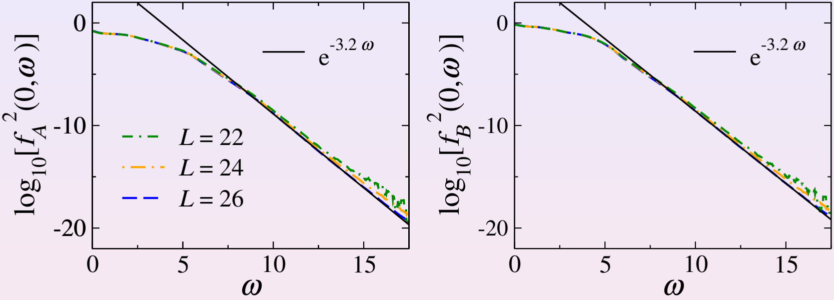

T. LeBlond, K. Mallayya, L. Vidmar, and MR, PRE **100**, 062134 (2019).

Eigenstate thermalization hypothesis

M. Srednicki, J. Phys. A **32**, 1163 (1999); L. D'Alessio *et al.*, Adv. Phys. **65**, 239 (2016).

$$O_{\alpha\beta} = O(E)\delta_{\alpha\beta} + e^{-S(E)/2} f_O(E,\omega) R_{\alpha\beta}$$

where $E \equiv (E_\alpha + E_\beta)/2$, $\omega \equiv E_\alpha - E_\beta$, $S(E)$ is the thermodynamic entropy at energy E, and $R_{\alpha\beta}$ is a random number with zero mean and unit variance.

Matrix elements of Hermitian operators within RMT

Let $\hat{O} = \sum_i O_i |i\rangle\langle i|$, where $\hat{O}|i\rangle = O_i|i\rangle$,

$$O_{\alpha\beta} \equiv \langle\alpha|\hat{O}|\beta\rangle = \sum_i O_i \langle\alpha|i\rangle\langle i|\beta\rangle = \sum_i O_i (\psi_i^\alpha)^* \psi_i^\beta$$

$|\alpha\rangle$ and $|\beta\rangle$ are eigenstates of a random matrix. Averaging over $|\alpha\rangle$ and $|\beta\rangle$ (random orthogonal unit vectors in arbitrary bases): $\overline{(\psi_i^\alpha)^*(\psi_i^\beta)} = \frac{1}{\mathcal{D}}\delta_{\alpha\beta}$.

Matrix elements of Hermitian operators within RMT

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Combining these results one can write

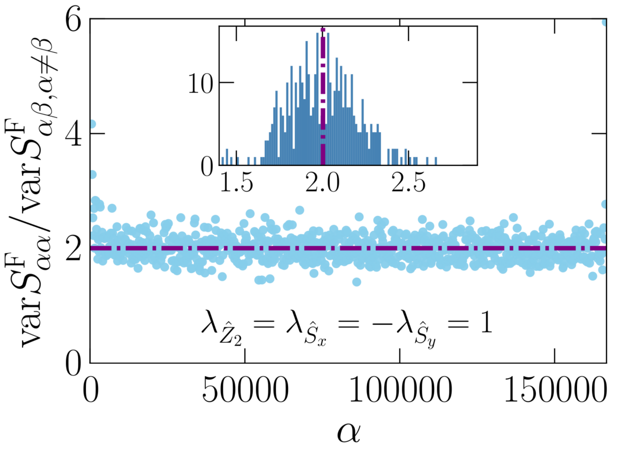
$$O_{\alpha\beta} \approx \bar{O}\delta_{\alpha\beta} + \sqrt{\frac{\overline{O^2}}{\mathcal{D}}} R_{\alpha\beta},$$

where $R_{\alpha\beta}$ is a random variable (real for GOE and complex for GUE).

Ratio of variances in the 2D F-TFIM

Hamiltonian: $\hat{H} = -J \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \hat{\sigma}^z_{\mathbf{i}} \hat{\sigma}^z_{\mathbf{j}} + g \sum_{\mathbf{i}} \hat{\sigma}^x_{\mathbf{i}}.$

Ratio of variances for the ferromagnetic structure factor



R. Mondaini and MR, PRE **96**, 012157 (2017).

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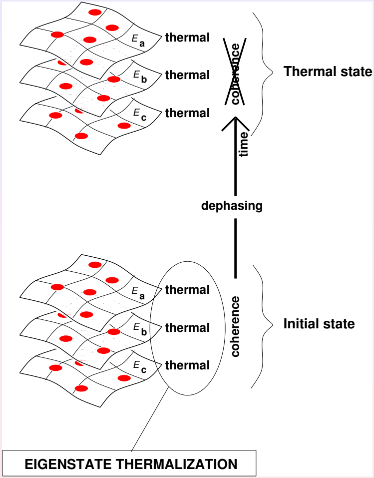

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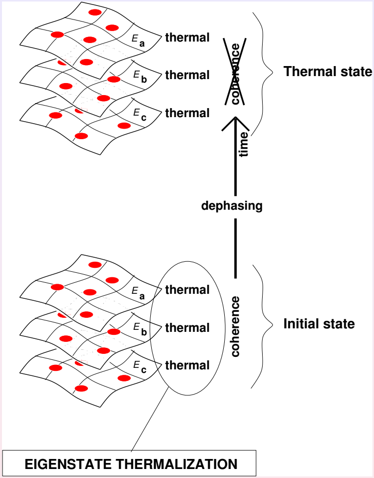
L. Vidmar and MR, J. Stat. Mech. 064007 (2016).



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