From unitary dynamics to statistical mechanics in isolated quantum systems

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Thermodynamics of quantum systems: Measurement, engines, and control

KITP, Santa Barbara

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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
   - 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
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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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Recent 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)

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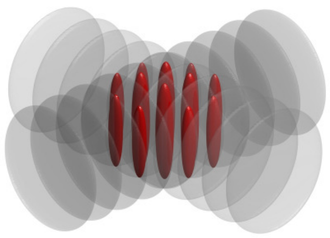
Experiment with ultracold bosons in one dimension



Effective 1D δ potential

M. Olshanii, PRL **81**, 938 (1998).

$$U_{1D}(x) = g_{1D}\delta(x)$$

Lieb-Liniger parameter

$$\gamma = \frac{mg_{1D}}{\hbar^2\rho}$$

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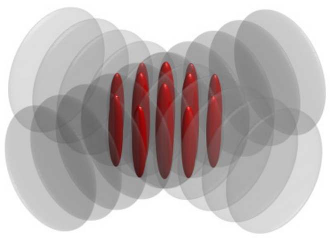

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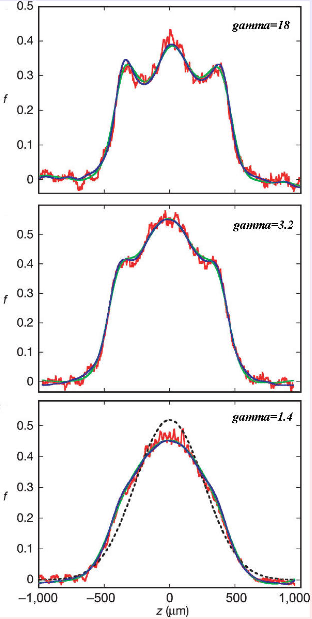
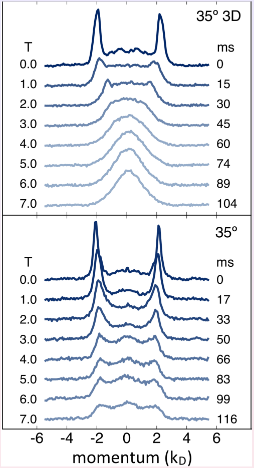
Observables (density and momentum distribution functions) equilibrated to nonthermal distributions

T. Kinoshita, T. Wenger, and D. S. Weiss, Nature **440**, 900 (2006).



Dipolar quantum Newton's cradle (dysprosium atoms)



Y. Tang, W. Kao, K.-Y. Li, S. Seo, K. Mallayya, MR, S. Gopalakrishnan, and B. L. Lev, Phys. Rev. X **8**, 021030 (2018).

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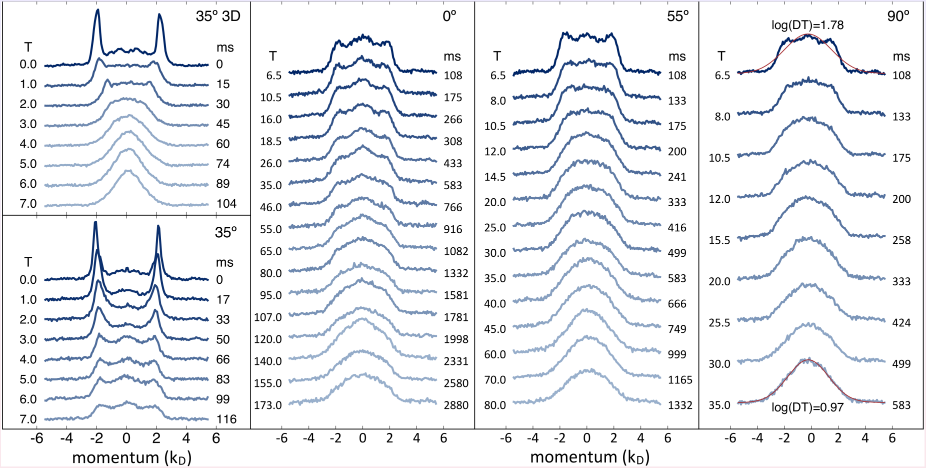

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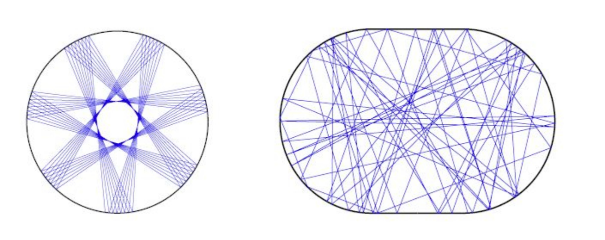
Classical chaos and integrability

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



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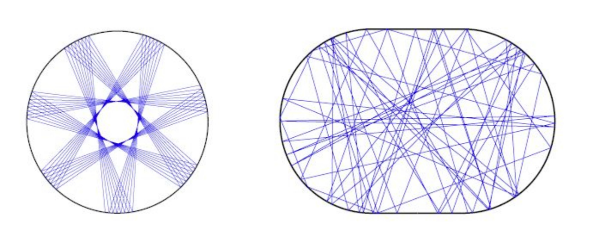

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$$\{I_\alpha, H\}=0,\quad \{I_\alpha, I_\beta\}=0,\quad \text{where}\quad \{f,g\}=\sum_{i=1,N}\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i}-\frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}.$$

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

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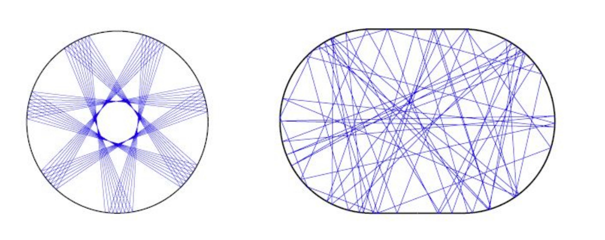

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- Chaos: exponential sensitivity of the trajectories to perturbations

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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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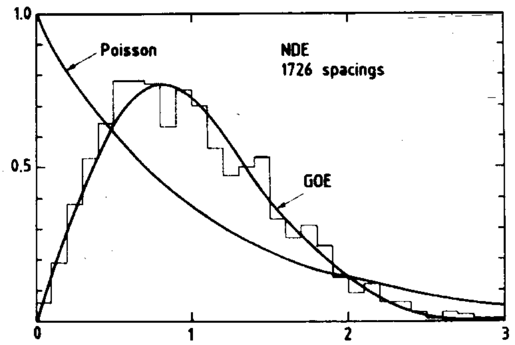
Distribution of level spacings for the “Nuclear Data Ensemble”



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

Semi-classical limit: Statistics of energy levels

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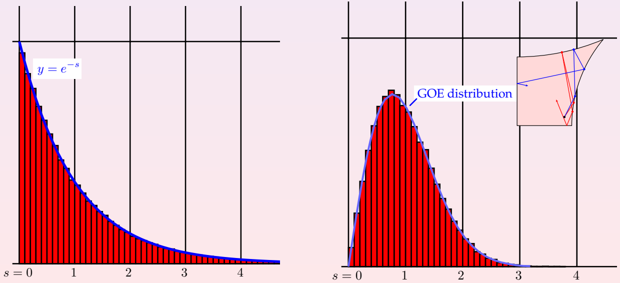
Distribution of level spacings: rectangular and chaotic cavities



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

Integrability to quantum chaos transition

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

$$\hat{H} = \sum_{i=1}^{L} \left\{ -t \left(\hat{f}_i^\dagger \hat{f}_{i+1} + \text{H.c.} \right) + V \hat{n}_i \hat{n}_{i+1} - t' \left(\hat{f}_i^\dagger \hat{f}_{i+2} + \text{H.c.} \right) + V' \hat{n}_i \hat{n}_{i+2} \right\}$$

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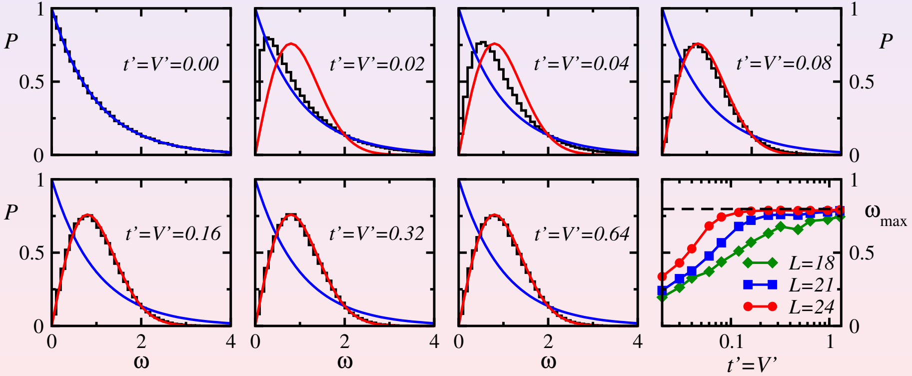
Level spacing distribution $(N_f = L/3)$



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 $\widehat{H}$

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

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

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

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

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

$$\overline{O(\tau)} = \lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau d\tau' \langle\Psi(\tau')|\hat{O}|\Psi(\tau')\rangle = \sum_\alpha |C_\alpha|^2 O_{\alpha\alpha} \equiv \langle\hat{O}\rangle_{\text{DE}},$$

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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 $t=0$

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

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:

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

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They are subextensive as in traditional ensembles in statistical mechanics.

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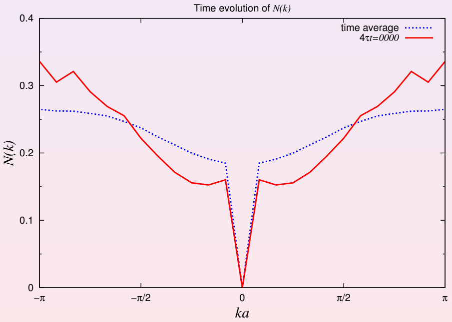
Nonequilibrium dynamics in 1D (density-density structure factor)



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

$N_b = 8$ hard-core bosons

$N = 24$ lattice sites

Fix $t' = V'$ and "quench"
$t_{\text{ini}} = 0.5, V_{\text{ini}} = 2$
$\rightarrow t_{\text{fin}} = 1, V_{\text{fin}} = 1$

Integrated results for $L = 24$, $N_b = 8$

Relative difference

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

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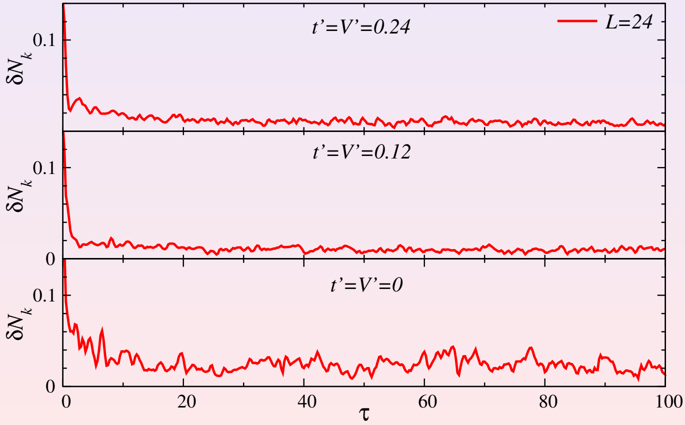

Scaling of the integrated results with system size

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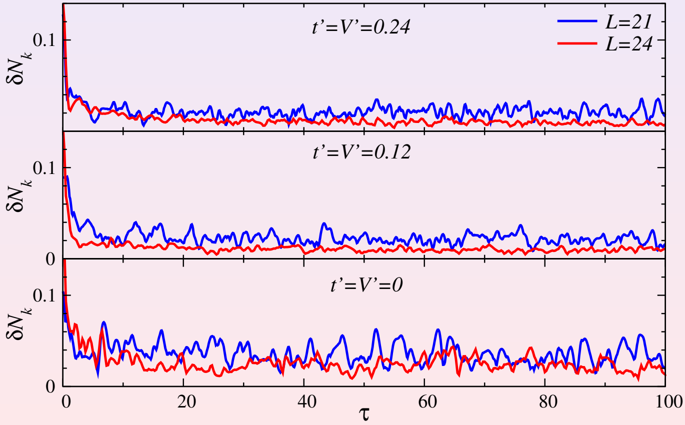

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Statistical description after relaxation (nonintegrable)

Canonical calculation

$$O_{\mathsf{CE}} = \mathrm{Tr}\left\{\hat{O}\hat{\rho}_{\mathsf{CE}}\right\}$$

$$\hat{\rho}_{\mathsf{CE}} = Z_{\mathsf{CE}}^{-1}\exp\left(-\hat{H}/k_B T\right)$$

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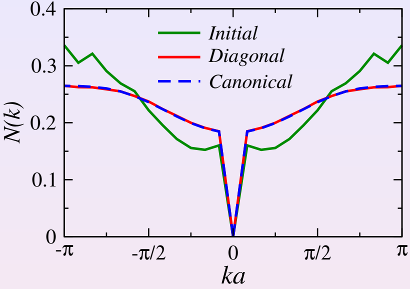
Structure factor



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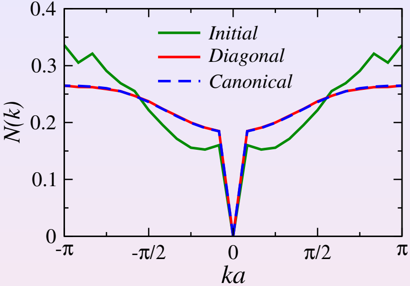
Microcanonical calculation

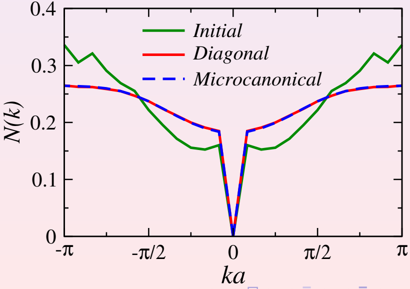
$$O_{\text{ME}} = \frac{1}{N_{\text{states}}}\sum_{\alpha}\langle\Psi_\alpha|\hat{O}|\Psi_\alpha\rangle$$

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

N_{states} : # of states in the window

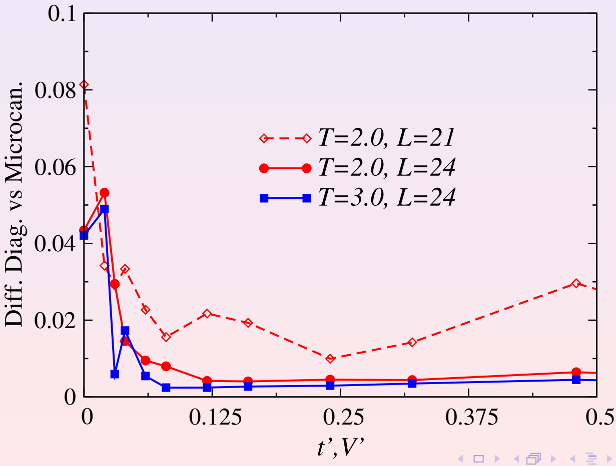
Structure factor





Relative difference

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



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   - Thermalization
   - Eigenstate thermalization
4. Summary

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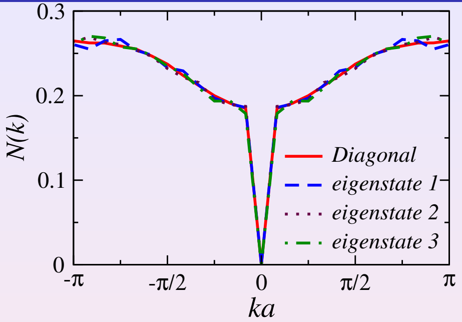
Eigenstate thermalization hypothesis (ETH): diagonal part
[Deutsch, PRA **43** 2046 (1991); Srednicki, PRE **50**, 888 (1994);
MR, Dunjko, and Olshanii, Nature **452**, 854 (2008).]

> 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 ($t' = V' = 0.24$)

Structure factor

Eigenstates with energies closest to E



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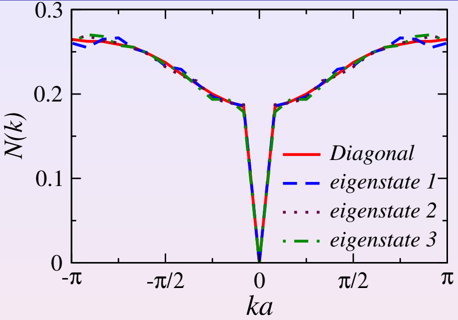
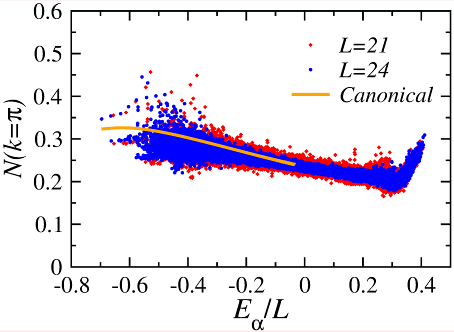




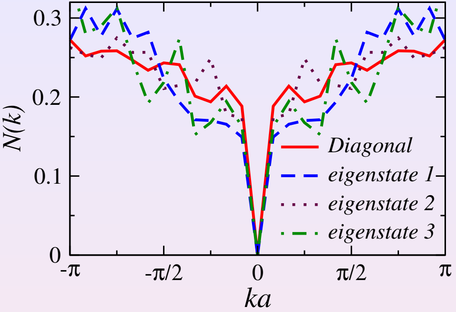
$N(k=\pi)$ vs eigenstate energy

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

Breakdown of ETH at integrability ($t' = V' = 0$)

Structure factor

Eigenstates with energies closest to E



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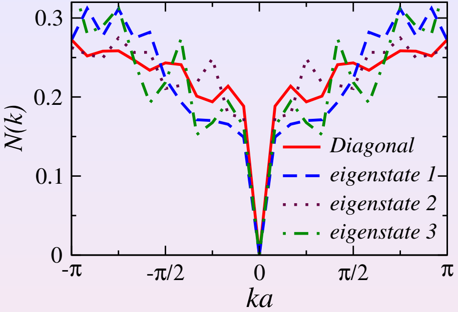
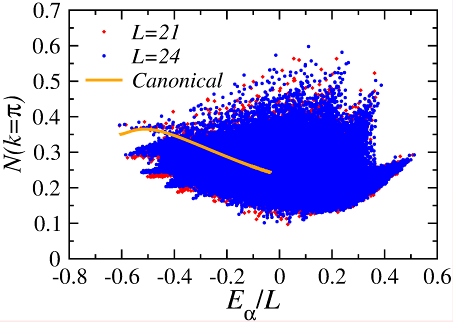


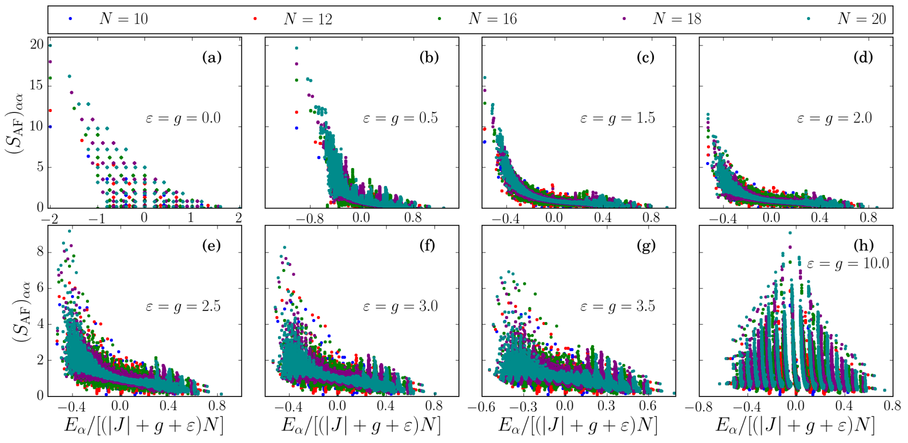


$N(k = \pi)$ vs eigenstate energy

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

Eigenstate thermalization in the 2D AF-TFIM

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



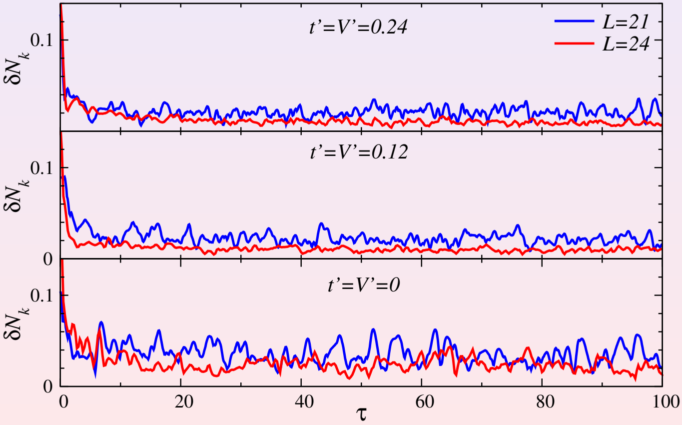
R. Mondaini, K. R. Fratus, M. Srednicki, and MR, PRE **93**, 032104 (2016).

Santos & MR'10, Khatami *et al.*'13, Sorg *et al.*'14, Kim *et al.*'14, Beugeling *et al.*'14'15, Steinigeweg *et al.*'14'15, Luitz'16, Luitz & Bar Lev'16...

Smallness of the time fluctuations

Relative difference

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



Time fluctuations

Are they small because of dephasing?

$$O(t) - \overline{O(t)} = \sum_{\substack{\alpha,\beta \\ \alpha\neq\beta}} C^\star_\alpha C_\beta e^{i(E_\alpha - E_\beta)t} O_{\alpha\beta} \sim \sum_{\substack{\alpha,\beta \\ \alpha\neq\beta}} \frac{e^{i(E_\alpha - E_\beta)t}}{N_{\text{states}}} O_{\alpha\beta}$$

$$\sim \frac{\sqrt{N^2_{\text{states}}}}{N_{\text{states}}} O^{\text{typical}}_{\alpha\beta} \sim O^{\text{typical}}_{\alpha\beta}$$

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Time average of $O(t)$

$$\overline{O(t)} = \sum_\alpha |C_\alpha|^2 O_{\alpha\alpha}$$

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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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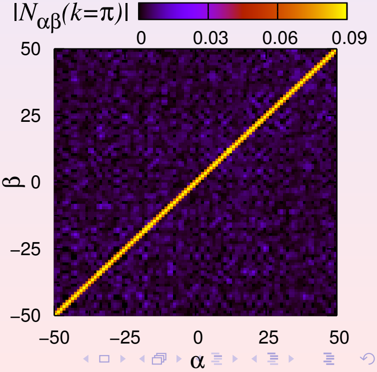

MR, PRA **80**, 053607 (2009).

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.

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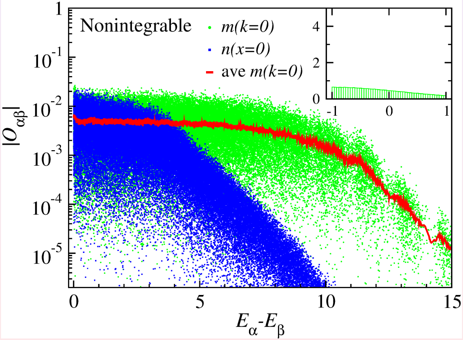
Off-diagonal matrix elements [histogram of $(|O_{\alpha\beta}| - |O_{\alpha\beta}|_{\text{ave}})/|O_{\alpha\beta}|_{\text{ave}}$]



E. Khatami, G. Pupillo, M. Srednicki, and MR, PRL **111**, 050403 (2013).

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): $\overline{(\psi_i^\alpha)^*(\psi_i^\beta)} = \frac{1}{\mathcal{D}}\delta_{\alpha\beta}$.

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This means that (to leading order):

$$\overline{O_{\alpha\alpha}} = \frac{1}{\mathcal{D}} \sum_i O_i \equiv \bar{O}, \quad \text{while} \quad \overline{O_{\alpha\beta}} = 0 \quad \text{for} \quad \alpha \neq \beta.$$

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One can further show that ($\eta = 2$ for GOE and $\eta = 1$ for GUE):

$$\overline{O_{\alpha\alpha}^2} - \overline{O_{\alpha\alpha}}^2 = \eta\overline{|O_{\alpha\beta}|^2} = \frac{\eta}{\mathcal{D}^2} \sum_i O_i^2 \equiv \frac{\eta}{\mathcal{D}}\overline{O^2}.$$

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Combining these results one can write

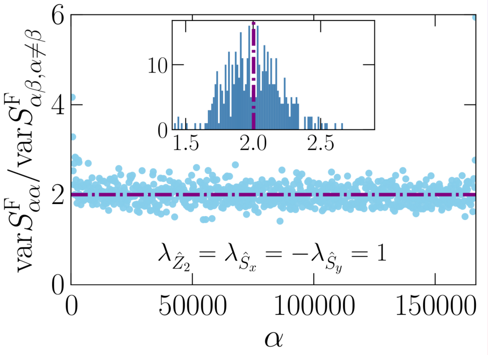
$$O_{\alpha\beta} \approx \bar{O}\delta_{\alpha\beta} + \sqrt{\frac{\overline{O^2}}{\mathcal{D}}} R_{\alpha\beta},$$

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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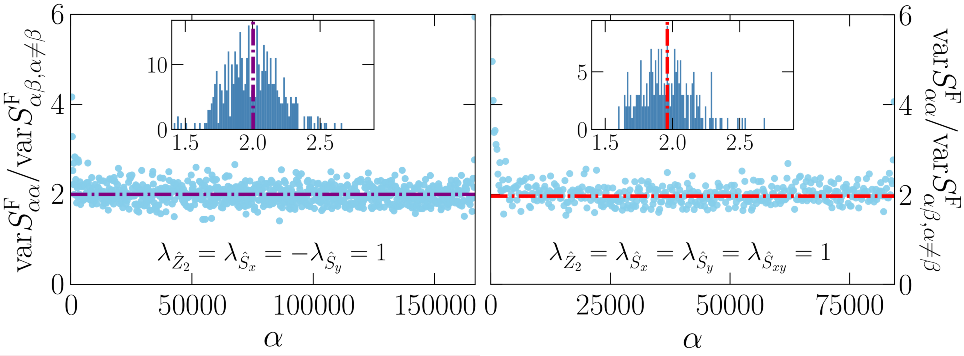

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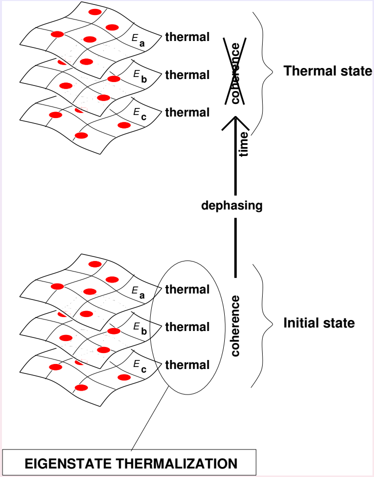

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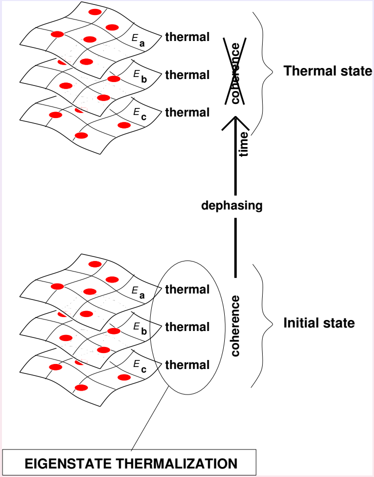

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- Vanja Dunjko (U Mass Boston)
- Yariv Kafri (Technion)
- Ehsan Khatami (San Jose State U)
- Rubem Mondaini (CSRC, Beijing)
- Maxim Olshanii (U Mass Boston)
- Anatoli Polkovnikov (Boston U)
- Guido Pupillo (U Strasbourg)
- Lea F. Santos (Yeshiva U)
- Mark Srednicki (UC Santa Barbara)

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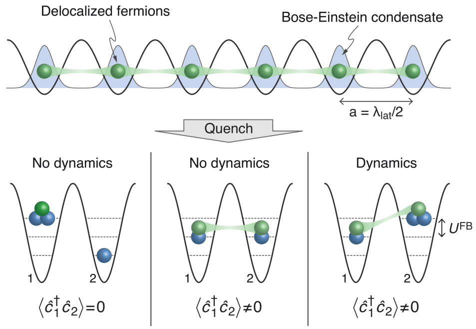
Coherence after quenches in Bose-Fermi mixtures



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

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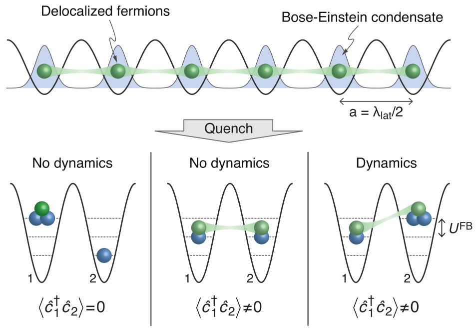

$$\langle \hat{c}^\dagger_{j\neq 0} \hat{c}_0 \rangle (t) = \frac{n_F \sin[\pi n_F j] e^{2 n_B [\cos(U^{\rm FB} t/\hbar) - 1]}}{j},$$

n_F and n_B are the fermion and boson fillings.

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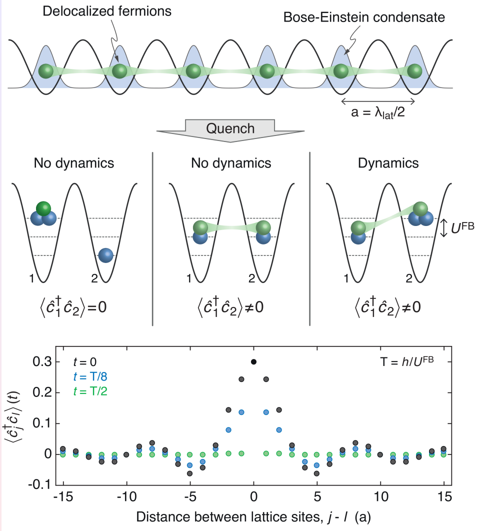

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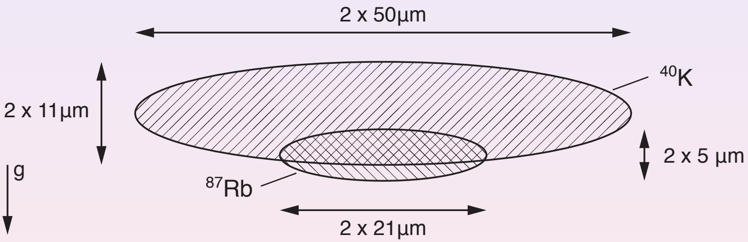

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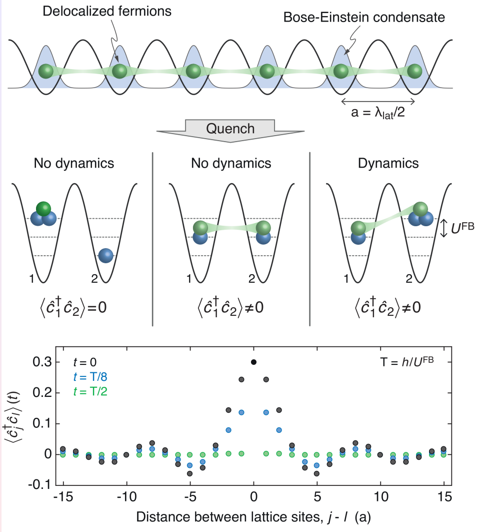

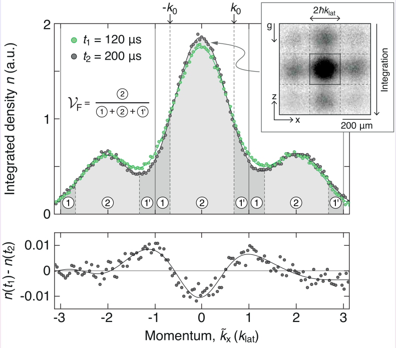

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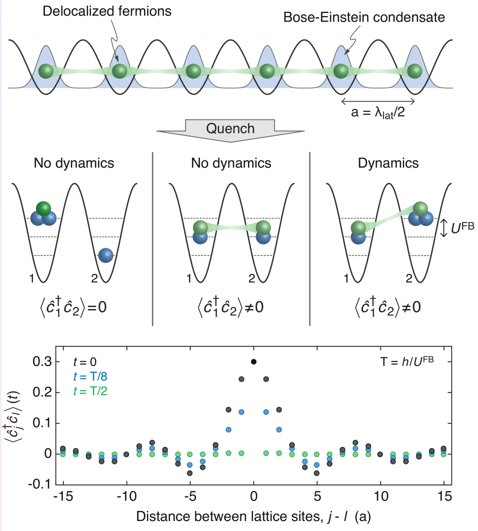

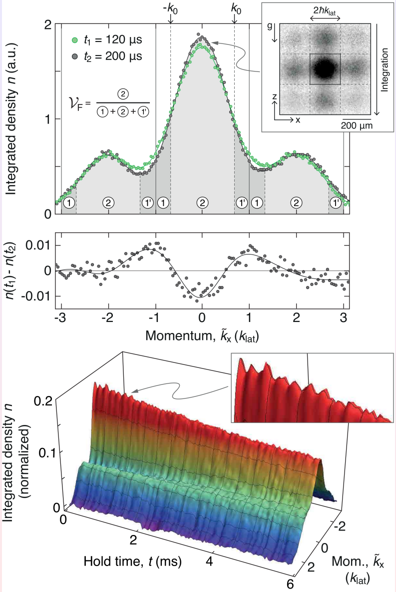

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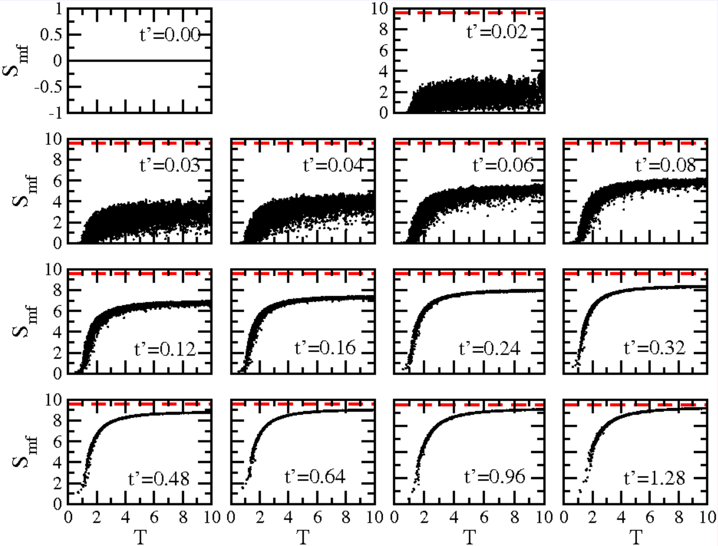
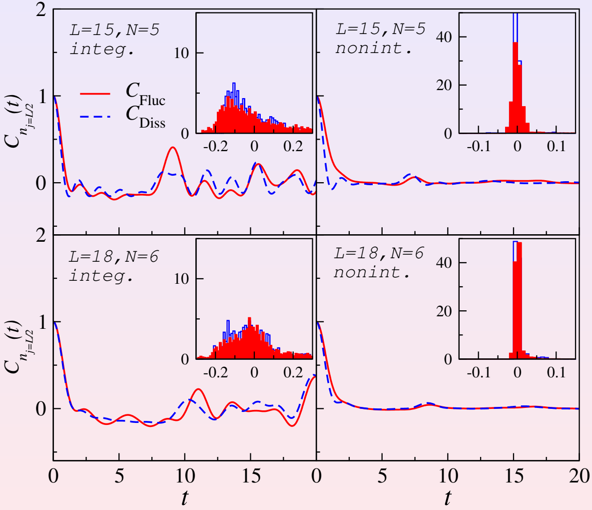
Information entropy ($S_j = -\sum_{k=1}^{D} |c_j^k|^2 \ln |c_j^k|^2$)



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

Fluctuation-dissipation theorem (dipolar bosons)

Occupation in the center of the trap ($n_{j=L/2}$)



Hamiltonian

$$\hat{H} = -J \sum_{j=1}^{L-1} \left(\hat{b}_j^\dagger \hat{b}_{j+1} + \text{H.c.} \right) + V \sum_{j<l} \frac{\hat{n}_j \hat{n}_l}{|j-l|^3} + g \sum_j x_j^2 \, \hat{n}_j$$

magnetic atoms, polar molecules

Relaxation dynamics

$$O(t) = C(t) O(t=0)$$

where

$$C(t) = \frac{\overline{O(t+t')O(t')}}{\overline{(O(t'))^2}}$$

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

E. Khatami, G. Pupillo, M. Srednicki, and MR, PRL **111**, 050403 (2013).