From unitary dynamics to statistical mechanics in isolated quantum systems

Marcos Rigol

Department of Physics
The Pennsylvania State University

599. WEH-Seminar:
Isolated Quantum Many-Body Systems out of Equilibrium
Bad Honnef, Germany

L. D'Alessio, Y. Kafri, A. Polkovnikov, and MR, *From Quantum Chaos and Eigenstate Thermalization to Statistical Mechanics and Thermodynamics*, arXiv:1509.06411.

Alejandro Muramatsu (Buenos Aires, 1951 - Stuttgart, 2015)

Alejandro Muramatsu (Buenos Aires, 1951 - Stuttgart, 2015)

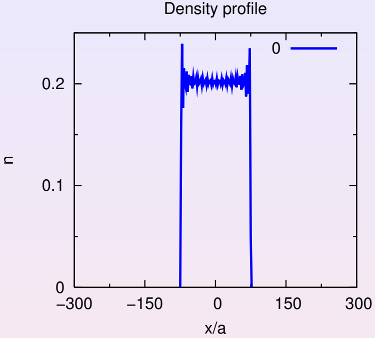
- Strongly correlated systems. QFT, QMC, DMRG
- High-Tc superconductivity. 3-Band Hubbard model. t-J Model
- Ultracold atoms in optical lattices
- Dynamics after quantum quenches. t-DMRG
- Spin liquids in Hubbard-like models

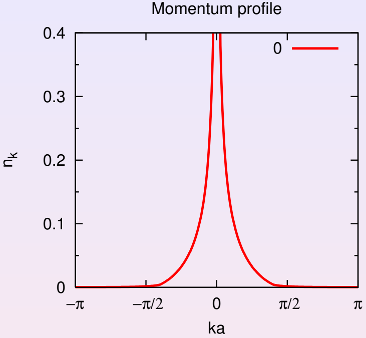
Outline

Outline

1. Motivation
   - Foundations of Quantum Statistical Mechanics
   - Experiments with Ultracold Gases
2. Quantum Chaos and Random Matrix Theory
   - Classical and Quantum Chaos
   - Random Matrix Theory
3. Dynamics and Thermalization of Isolated Quantum Systems
   - Quantum Quenches and Thermalization
   - Dynamics
   - Thermalization
   - Eigenstate Thermalization
4. Quantum Quenches in the Thermodynamic Limit
   - Numerical Linked Cluster Expansions
   - Quenches in the t-V-t'-V' chain
   - Quenches in the XXZ chain
   - Summary

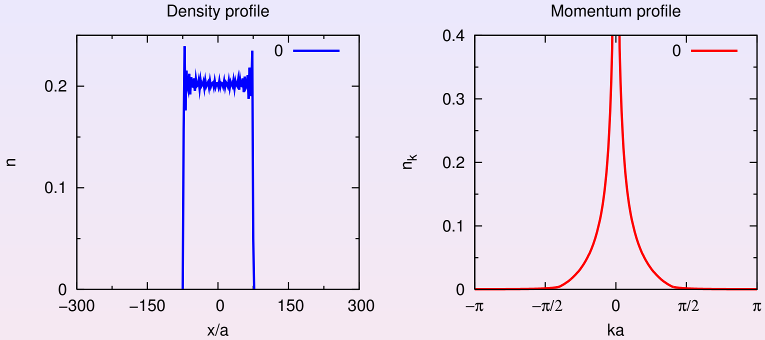
Numerical experiment





MR, V. Dunjko, V. Yurovsky, and M. Olshanii, PRL **98**, 050405 (2007).

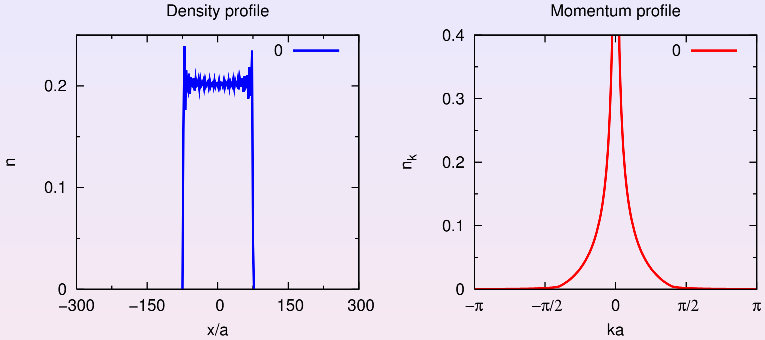
Numerical experiment



MR, V. Dunjko, V. Yurovsky, and M. Olshanii, PRL **98**, 050405 (2007).

- The expectation values of the observables become (almost) time independent. (No need to couple the system to a bath to see relaxation.)

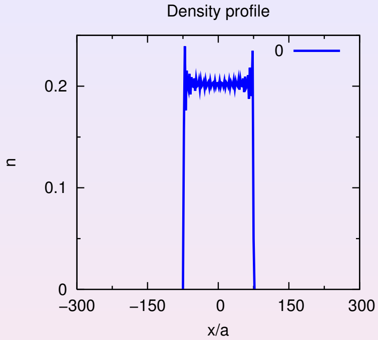
Numerical experiment

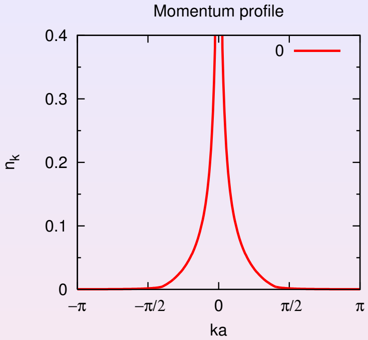


MR, V. Dunjko, V. Yurovsky, and M. Olshanii, PRL **98**, 050405 (2007).

- The expectation values of the observables become (almost) time independent. (No need to couple the system to a bath to see relaxation.)
- The density is nearly homogeneous. (Expected in thermal equilibrium.)

Numerical experiment

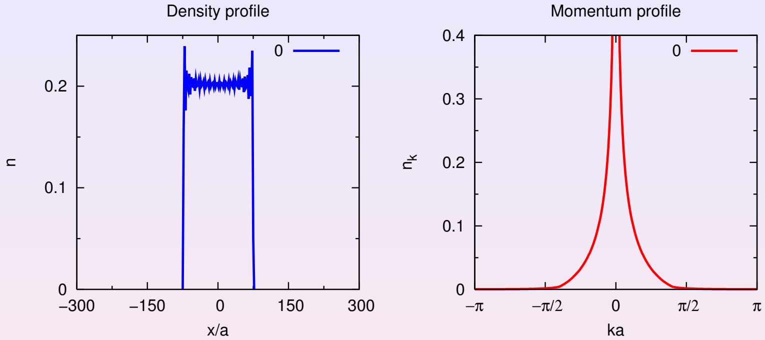




MR, V. Dunjko, V. Yurovsky, and M. Olshanii, PRL **98**, 050405 (2007).

- The expectation values of the observables become (almost) time independent. (No need to couple the system to a bath to see relaxation.)
- The density is nearly homogeneous. (Expected in thermal equilibrium.)
- Is the momentum distribution function the one in thermal equilibrium?

Numerical experiment



MR, V. Dunjko, V. Yurovsky, and M. Olshanii, PRL **98**, 050405 (2007).

- The expectation values of the observables become (almost) time independent. (No need to couple the system to a bath to see relaxation.)
- The density is nearly homogeneous. (Expected in thermal equilibrium.)
- Is the momentum distribution function the one in thermal equilibrium?
- Do we need to couple the system to a bath for the latter to occur?

Foundations of quantum statistical mechanics

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

Foundations of quantum statistical mechanics

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

Recent works and 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)

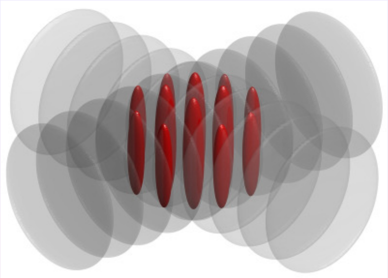
Goldstein, Lebowitz, Mastrodonato, Tumulka, and Zanghi '10
(Normal typicality and von Neumann's quantum ergodic theorem)

MR and Srednicki '12
(Alternatives to Eigenstate Thermalization)

Outline

1. Motivation
   - Foundations of Quantum Statistical Mechanics
   - Experiments with Ultracold Gases
2. Quantum Chaos and Random Matrix Theory
   - Classical and Quantum Chaos
   - Random Matrix Theory
3. Dynamics and Thermalization of Isolated Quantum Systems
   - Quantum Quenches and Thermalization
   - Dynamics
   - Thermalization
   - Eigenstate Thermalization
4. Quantum Quenches in the Thermodynamic Limit
   - Numerical Linked Cluster Expansions
   - Quenches in the t-V-t'-V' chain
   - Quenches in the XXZ chain
   - Summary

Experiments with ultracold gases in 1D



Effective one-dimensional δ potential

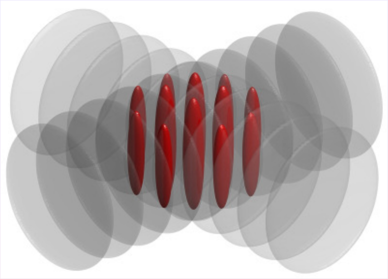
M. Olshanii, PRL **81**, 938 (1998).

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

where

$$g_{1D} = \frac{2\hbar a_s \omega_\perp}{1 - C a_s \sqrt{\frac{m\omega_\perp}{2\hbar}}}$$

Experiments with ultracold gases in 1D



Girardeau '60, Lieb and Liniger '63

T. Kinoshita, T. Wenger, and D. S. Weiss, Science **305**, 1125 (2004).

T. Kinoshita, T. Wenger, and D. S. Weiss, Phys. Rev. Lett. **95**, 190406 (2005).

$\gamma_{\text{eff}} = \frac{m g_{1D}}{\hbar^2 \rho}$

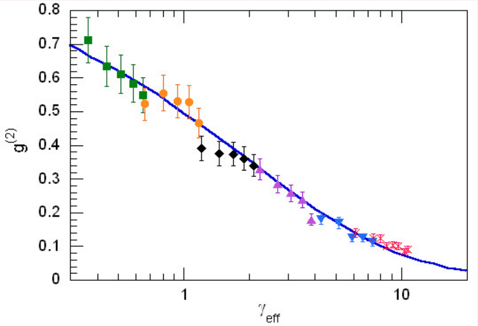
Effective one-dimensional δ potential

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

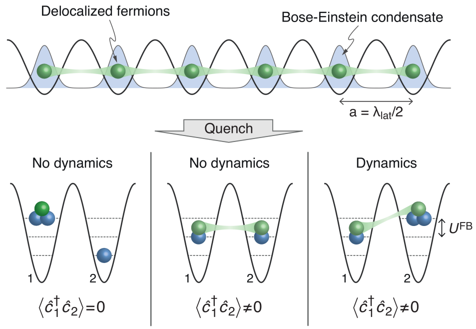
$$U_{1D}(x) = g_{1D}\delta(x)$$

where

$$g_{1D} = \frac{2\hbar a_s \omega_\perp}{1 - C a_s \sqrt{\frac{m\omega_\perp}{2\hbar}}}$$

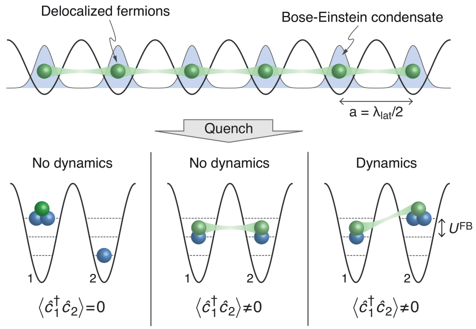


Coherence after quenches in Bose-Fermi mixtures



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

Coherence after quenches in Bose-Fermi mixtures

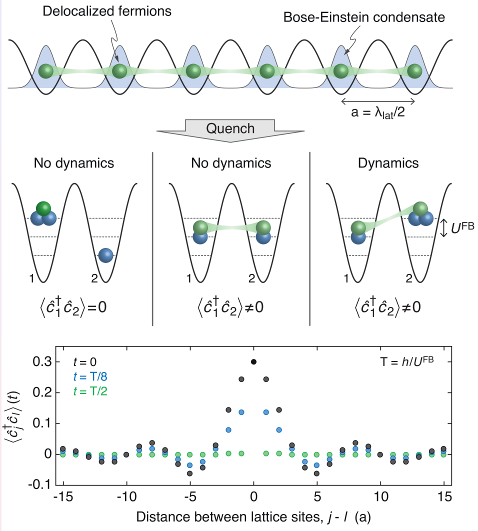


$$\langle \hat{c}^\dagger_{j\neq 0}\hat{c}_0\rangle(t) = \frac{n_F \sin[\pi n_F j] e^{2n_B[\cos(U^{\rm FB}t/\hbar)-1]}}{j},$$

n_F and n_B are the fermion and boson fillings.

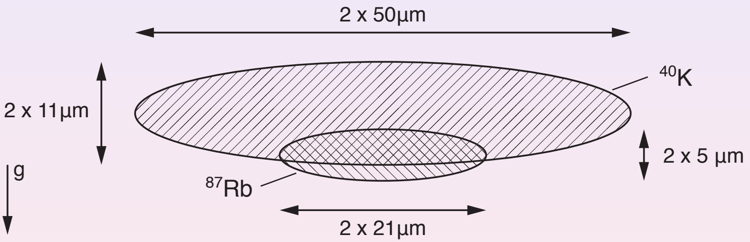
S. Will, D. Iyer, and MR
Nat. Commun. **6**, 6009 (2015).

Coherence after quenches in Bose-Fermi mixtures

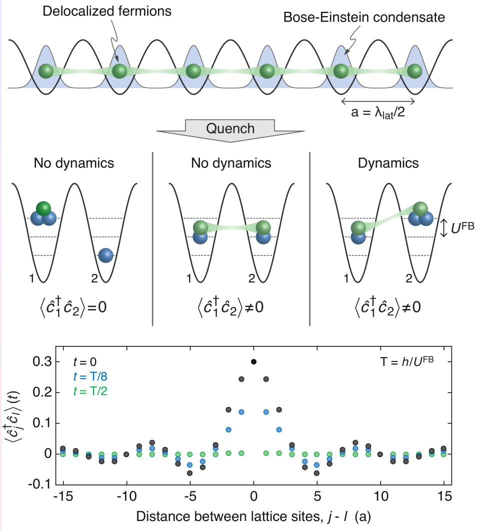


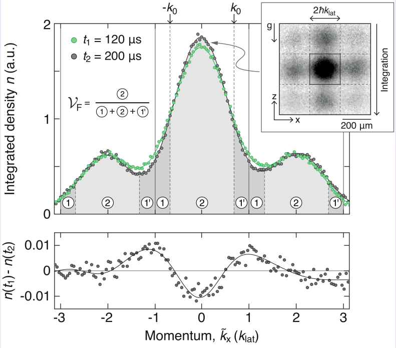
S. Will, D. Iyer, and MR
Nat. Commun. **6**, 6009 (2015).

Coherence after quenches in Bose-Fermi mixtures



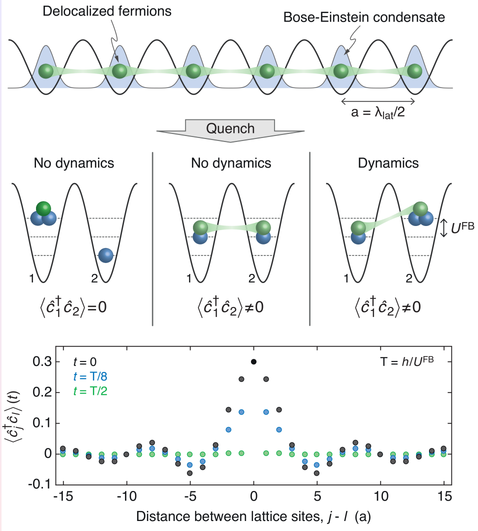
Coherence after quenches in Bose-Fermi mixtures

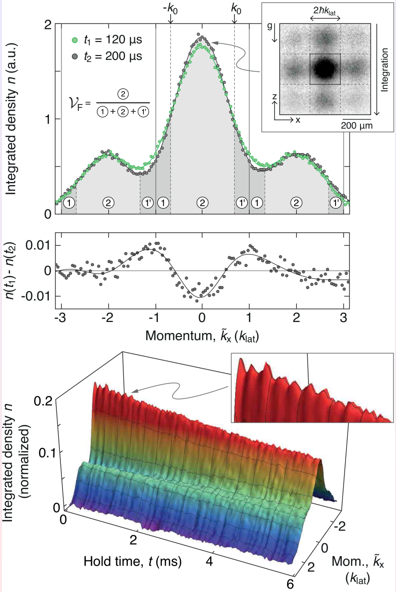




S. Will, D. Iyer, and MR
Nat. Commun. **6**, 6009 (2015).

Coherence after quenches in Bose-Fermi mixtures



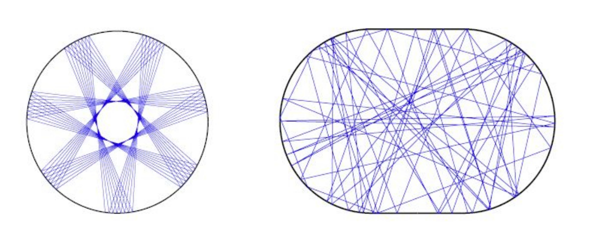


S. Will, D. Iyer, and MR
Nat. Commun. **6**, 6009 (2015).

Outline

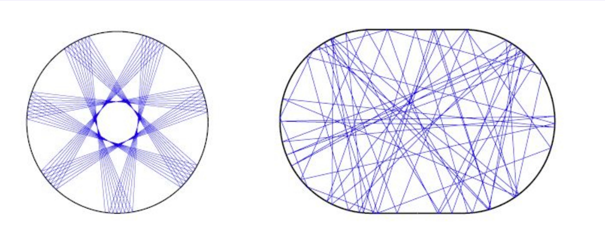
Classical Chaos and Integrability

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



Classical Chaos and Integrability

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

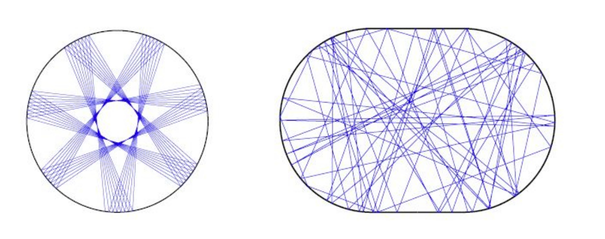


- A Hamiltonian $H(\mathbf{p},\mathbf{q})$, with $\mathbf{q}=(q_1,\cdots,q_N)$ and $\mathbf{p}=(p_1,\cdots,p_N)$, is said to be integrable if there are N functionally independent constants of the motion $\mathbf{I}=(I_1,\cdots,I_N)$ in involution:

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

Classical Chaos and Integrability

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



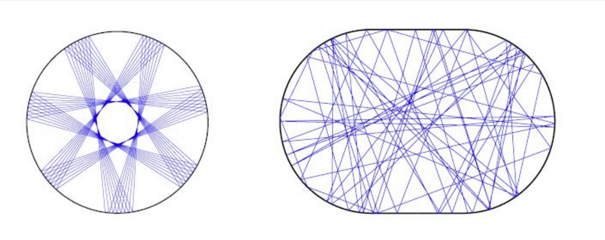
- A Hamiltonian $H(\mathbf{p},\mathbf{q})$, with $\mathbf{q}=(q_1,\cdots,q_N)$ and $\mathbf{p}=(p_1,\cdots,p_N)$, is said to be integrable if there are N functionally independent constants of the motion $\mathbf{I}=(I_1,\cdots,I_N)$ in involution:

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

- Liouville's integrability theorem: There is a canonical transformation $(\mathbf{p},\mathbf{q})\rightarrow(\mathbf{I},\mathbf{\Theta})$ (action-angle variables) so that:
  $H(\mathbf{p},\mathbf{q})=H(\mathbf{I})\rightarrow I_\alpha(t)=I_\alpha^0=\text{const}$ and $\Theta_\alpha(t)=\Omega_\alpha t+\Theta_\alpha(0)$

Classical Chaos and Integrability

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



- 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: There is a canonical transformation $(\mathbf{p},\mathbf{q})\to(\mathbf{I},\mathbf{\Theta})$ (action-angle variables) so that:
  $H(\mathbf{p},\mathbf{q})=H(\mathbf{I})\to I_\alpha(t)=I_\alpha^0=\text{const}$ and $\Theta_\alpha(t)=\Omega_\alpha t+\Theta_\alpha(0)$

- Chaos: exponential sensitivity of the trajectories to perturbations

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.)

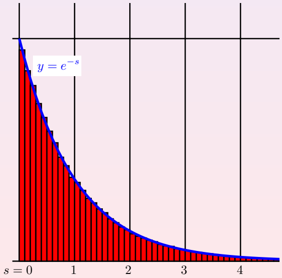
Semi-Classical Limit: Statistics of Energy Levels

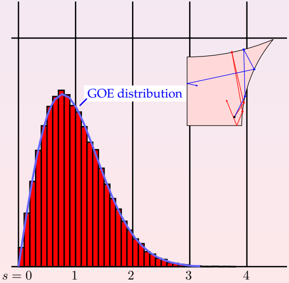
- Berry-Tabor conjecture (1977): The statistics of level spacings of quantum systems whose classical counterpart is integrable is described by a Poisson distribution. (Energy eigenvalues behave like a sequence of independent random variables.)
- Bohigas, Giannoni, and Schmit (1984): At high energies, the statistics of level spacings of a particle in a Sinai billiard is described by a Wigner-Dyson distribution. This was conjecture to apply to quantum systems that have a classically chaotic counterpart (violated in singular cases).

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.)
- Bohigas, Giannoni, and Schmit (1984): At high energies, the statistics of level spacings of a particle in a Sinai billiard is described by a Wigner-Dyson distribution. This was conjecture to apply to quantum systems that have a classically chaotic counterpart (violated in singular cases).

Distribution of level spacings: rectangular and chaotic cavities





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

Outline

1. Motivation
   - Foundations of Quantum Statistical Mechanics
   - Experiments with Ultracold Gases
2. Quantum Chaos and Random Matrix Theory
   - Classical and Quantum Chaos
   - Random Matrix Theory
3. Dynamics and Thermalization of Isolated Quantum Systems
   - Quantum Quenches and Thermalization
   - Dynamics
   - Thermalization
   - Eigenstate Thermalization
4. Quantum Quenches in the Thermodynamic Limit
   - Numerical Linked Cluster Expansions
   - Quenches in the t-V-t'-V' chain
   - Quenches in the XXZ chain
   - Summary

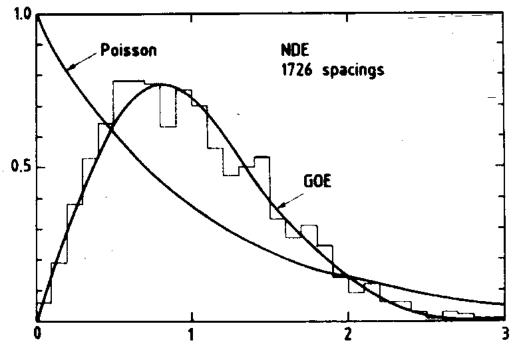
Random Matrix Theory

- 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.

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.

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

$$\begin{bmatrix} \varepsilon_1 & \frac{V}{\sqrt{2}} \\ \frac{V^*}{\sqrt{2}} & \varepsilon_2 \end{bmatrix}, \qquad E_{1,2} = \frac{\varepsilon_1 + \varepsilon_2}{2} \pm \frac{1}{2}\sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 2|V|^2}.$$

Distribution of level spacings $P(\omega)$

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

$$\begin{bmatrix} \varepsilon_1 & \frac{V}{\sqrt{2}} \\ \frac{V^*}{\sqrt{2}} & \varepsilon_2 \end{bmatrix}, \qquad E_{1,2} = \frac{\varepsilon_1 + \varepsilon_2}{2} \pm \frac{1}{2}\sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 2|V|^2}.$$

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.

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

Distribution of level spacings $P(\omega)$

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

$$\begin{bmatrix} \varepsilon_1 & \frac{V}{\sqrt{2}} \\ \frac{V^*}{\sqrt{2}} & \varepsilon_2 \end{bmatrix}, \qquad E_{1,2} = \frac{\varepsilon_1 + \varepsilon_2}{2} \pm \frac{1}{2}\sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 2|V|^2}.$$

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.

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

Calculating the integrals (change of variables plus cylindrical coordinates)

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

Distribution of level spacings $P(\omega)$

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

$$\begin{bmatrix} \varepsilon_1 & \frac{V}{\sqrt{2}} \\ \frac{V^*}{\sqrt{2}} & \varepsilon_2 \end{bmatrix}, \qquad E_{1,2} = \frac{\varepsilon_1 + \varepsilon_2}{2} \pm \frac{1}{2}\sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 2|V|^2}.$$

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.

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

Calculating the integrals (change of variables plus cylindrical coordinates)

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

Wigner Surmise (Wigner-Dyson distribution)

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

Outline

1. Motivation
   - Foundations of Quantum Statistical Mechanics
   - Experiments with Ultracold Gases
2. Quantum Chaos and Random Matrix Theory
   - Classical and Quantum Chaos
   - Random Matrix Theory
3. Dynamics and Thermalization of Isolated Quantum Systems
   - Quantum Quenches and Thermalization
   - Dynamics
   - Thermalization
   - Eigenstate Thermalization
4. Quantum Quenches in the Thermodynamic Limit
   - Numerical Linked Cluster Expansions
   - Quenches in the t-V-t'-V' chain
   - Quenches in the XXZ chain
   - Summary

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:

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

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:

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

What is it that we call thermalization?

$$\overline{O(t)} = O(E) = O(T) = O(T,\mu).$$

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:

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

What is it that we call thermalization?

$$\overline{O(t)} = O(E) = O(T) = O(T,\mu).$$

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 $\hat{\rho}_{\text{DE}} \equiv \sum_\alpha |C_\alpha|^2|\alpha\rangle\langle\alpha|$)

$$\overline{O(t)} = \lim_{t\to\infty} \frac{1}{t}\int_0^t dt' \langle\Psi(t')|\hat{O}|\Psi(t')\rangle = \sum_\alpha |C_\alpha|^2 O_{\alpha\alpha} \equiv \langle\hat{O}\rangle_{\text{DE}},$$

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

Width of the energy density after a sudden quench

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).

Width of the energy density after a sudden quench

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

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

The width of the energy density after a quench, ΔE, is then

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

or

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

where N is the total number of lattice sites.

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

Width of the energy density after a sudden quench

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

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

The width of the energy density after a quench, ΔE, is then

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

or

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

where N is the total number of lattice sites.
Since $E \propto N$, then the ratio

$$\frac{\Delta E}{E} \overset{N\to\infty}{\propto} \frac{1}{\sqrt{N}},$$

so, as in traditional ensembles, it vanishes in the thermodynamic limit.

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

Outline

Integrability to Quantum Chaos Transition

Spinless fermions (hard-core bosons) in one dimension

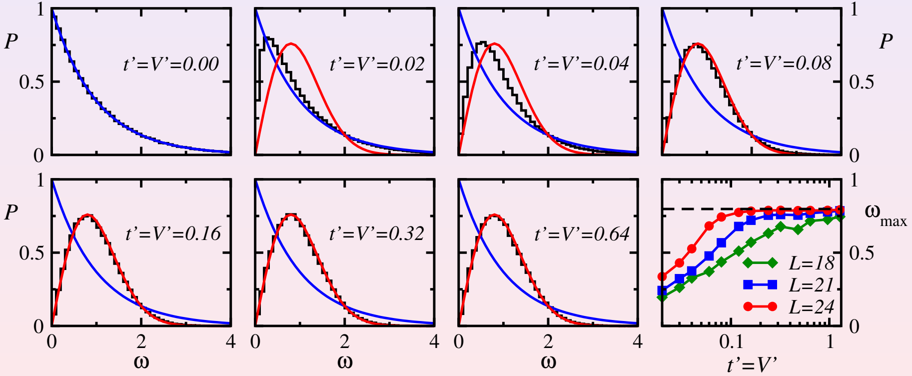
$$\hat{H} = \sum_{i=1}^{L} \left\{ -t \left(\hat{f}_i^\dagger \hat{f}_{i+1} + \text{H.c.} \right) + V \hat{n}_i \hat{n}_{i+1} - t' \left(\hat{f}_i^\dagger \hat{f}_{i+2} + \text{H.c.} \right) + V' \hat{n}_i \hat{n}_{i+2} \right\}$$

Integrability to Quantum Chaos Transition

Spinless fermions (hard-core bosons) in one dimension

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

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



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

Relaxation dynamics after a quantum quench

Hard-core bosons in one dimension

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

Relaxation dynamics after a quantum quench

Hard-core bosons in one dimension

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

"One can rewrite

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

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

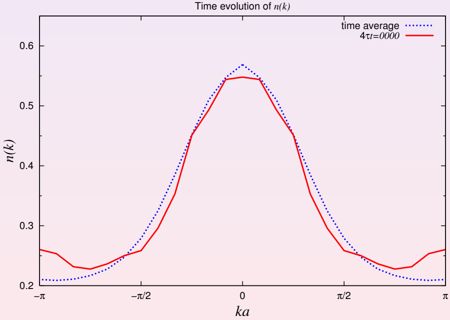
$$\overline{O(t)} = \lim_{t\to\infty} \frac{1}{t} \int_0^t dt' \langle \Psi(t') | \hat{O} | \Psi(t') \rangle = \sum_\alpha |C_\alpha|^2 O_{\alpha\alpha} \equiv \langle \hat{O} \rangle_{\text{DE}},$$

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

Hard-core bosons in one dimension

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

Nonequilibrium dynamics in 1D



$N_b = 8$ hard-core bosons

$N = 24$ lattice sites

Hilbert space: 735,471
Largest k-sector: 30,667

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

Initial state in the $k = 0$ sector.

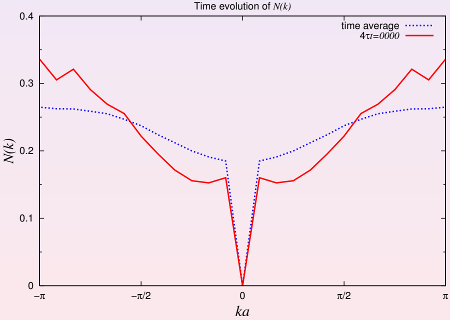
MR, PRL **103**, 100403 (2009); PRA **80**, 053607 (2009).

Relaxation dynamics after a quantum quench

Hard-core bosons in one dimension

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

Nonequilibrium dynamics in 1D



$N_b = 8$ hard-core bosons

$N = 24$ lattice sites

Hilbert space: 735,471
Largest k-sector: 30,667

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

Initial state in the $k = 0$ sector.

MR, PRL **103**, 100403 (2009); PRA **80**, 053607 (2009).

Time evolution results for $L = 24$, $N_b = 8$

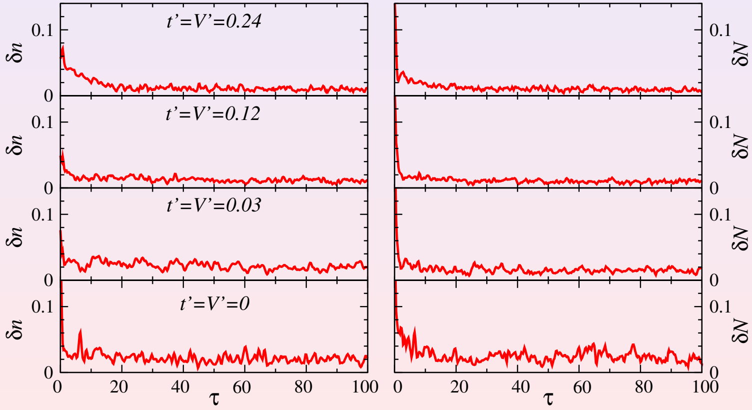
Compute the relative differences

$$\delta n(\tau) = \frac{\sum_k |n(k,\tau) - n_{\rm DE}(k)|}{\sum_k n_{\rm DE}(k)} \quad \text{and} \quad \delta N(\tau) = \frac{\sum_k |N(k,\tau) - N_{\rm DE}(k)|}{\sum_k N_{\rm DE}(k)}$$

Time evolution results for $L = 24$, $N_b = 8$

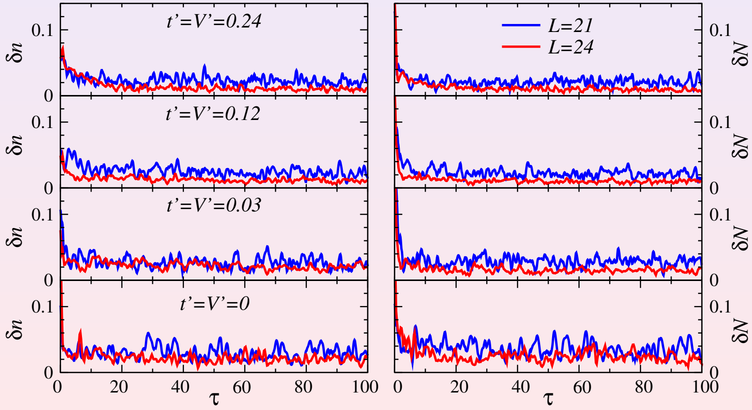
Compute the relative differences

$$\delta n(\tau) = \frac{\sum_k |n(k,\tau) - n_{\rm DE}(k)|}{\sum_k n_{\rm DE}(k)} \quad \text{and} \quad \delta N(\tau) = \frac{\sum_k |N(k,\tau) - N_{\rm DE}(k)|}{\sum_k N_{\rm DE}(k)}$$



Compute the relative differences

$$\delta n(\tau) = \frac{\sum_k |n(k,\tau) - n_{\mathrm{DE}}(k)|}{\sum_k n_{\mathrm{DE}}(k)} \quad \text{and} \quad \delta N(\tau) = \frac{\sum_k |N(k,\tau) - N_{\mathrm{DE}}(k)|}{\sum_k N_{\mathrm{DE}}(k)}$$



Outline

Statistical description after relaxation (nonintegrable)

Canonical calculation

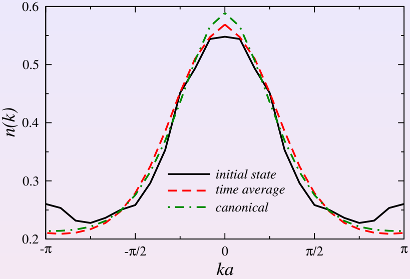
$$O_{\mathrm{CE}} = \mathrm{Tr}\left\{\hat{O}\hat{\rho}_{\mathrm{CE}}\right\}$$

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

$$Z_{\mathrm{CE}} = \mathrm{Tr}\left\{\exp\left(-\hat{H}/k_B T\right)\right\}$$

$$E = \mathrm{Tr}\left\{\hat{H}\hat{\rho}_{\mathrm{CE}}\right\} \qquad T = 3.0$$

Momentum distribution



Statistical description after relaxation (nonintegrable)

Canonical calculation

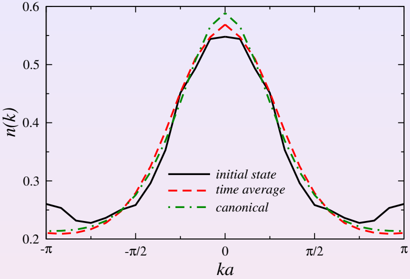
$$O_{\mathsf{CE}} = \mathrm{Tr}\left\{\hat{O}\hat{\rho}_{\mathsf{CE}}\right\}$$

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

$$Z_{\mathsf{CE}} = \mathrm{Tr}\left\{\exp\left(-\hat{H}/k_B T\right)\right\}$$

$$E = \mathrm{Tr}\left\{\hat{H}\hat{\rho}_{\mathsf{CE}}\right\} \qquad T = 3.0$$

Momentum distribution

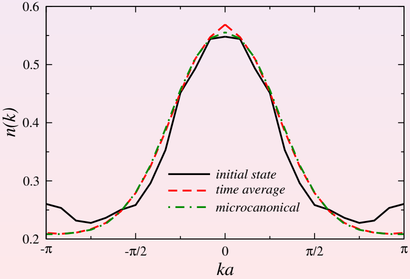


Microcanonical calculation

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

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

N_{states} : # of states in the window



Thermalization and the lack thereof at integrability

Compute the relative differences

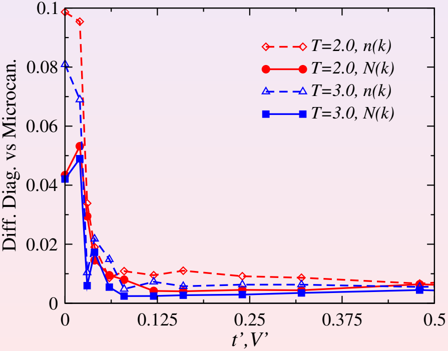
$$\frac{\sum_k |n_{\mathsf{DE}}(k) - n_{\mathsf{ME}}(k)|}{\sum_k n_{\mathsf{DE}}(k)} \quad \text{and} \quad \frac{\sum_k |N_{\mathsf{DE}}(k) - N_{\mathsf{ME}}(k)|}{\sum_k N_{\mathsf{DE}}(k)}$$

Thermalization and the lack thereof at integrability

Compute the relative differences

$$\frac{\sum_k |n_{\mathsf{DE}}(k) - n_{\mathsf{ME}}(k)|}{\sum_k n_{\mathsf{DE}}(k)} \quad \text{and} \quad \frac{\sum_k |N_{\mathsf{DE}}(k) - N_{\mathsf{ME}}(k)|}{\sum_k N_{\mathsf{DE}}(k)}$$

$L = 24,\ N_b = 8$

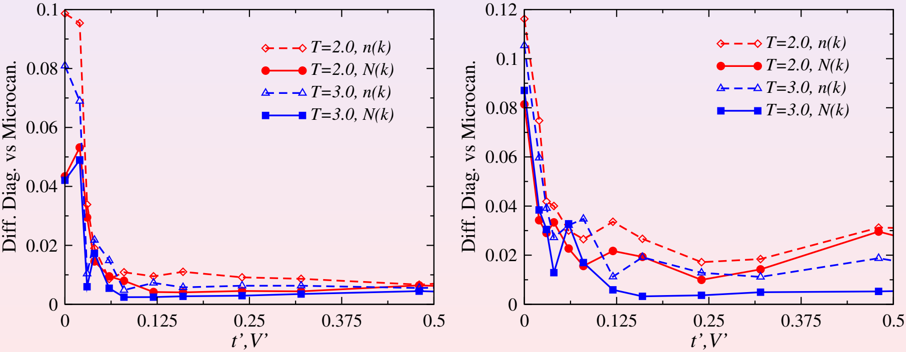


Thermalization and the lack thereof at integrability

Compute the relative differences

$$\frac{\sum_k |n_{\mathsf{DE}}(k) - n_{\mathsf{ME}}(k)|}{\sum_k n_{\mathsf{DE}}(k)} \quad \text{and} \quad \frac{\sum_k |N_{\mathsf{DE}}(k) - N_{\mathsf{ME}}(k)|}{\sum_k N_{\mathsf{DE}}(k)}$$

$L = 24,\ N_b = 8$ $\qquad$ $L = 21,\ N_b = 7$



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

Eigenstate Thermalization

Paradox?

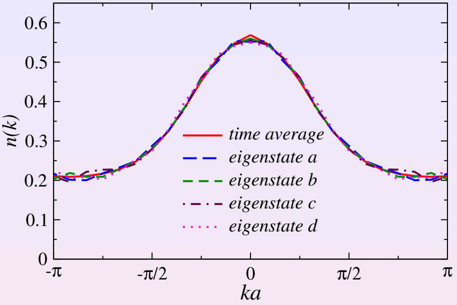
$$\sum_{\alpha} |C_\alpha|^2 O_{\alpha\alpha} = \frac{1}{N_{E,\Delta E}} \sum_{|E-E_\alpha|<\Delta E} O_{\alpha\alpha}$$

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

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:
>
> $$\langle\alpha|\widehat{O}|\alpha\rangle = O_{\text{ME}}(E_\alpha)$$

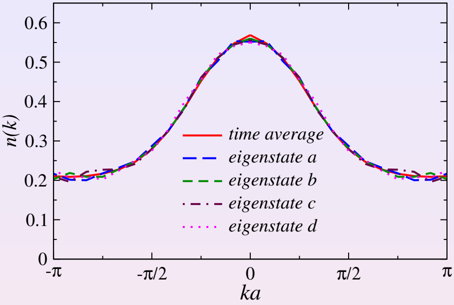
ETH – far away from integrability ($t' = V' = 0.24$)



Momentum distribution

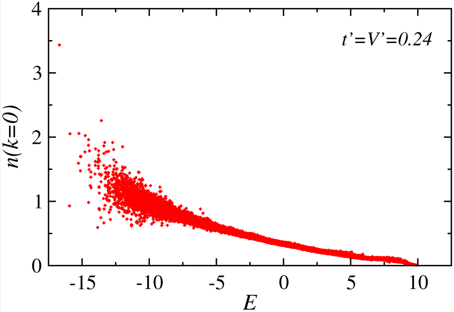
Eigenstates $a - d$ are the ones with energies closest to E

ETH – far away from integrability ($t' = V' = 0.24$)



Momentum distribution

Eigenstates $a - d$ are the ones with energies closest to E



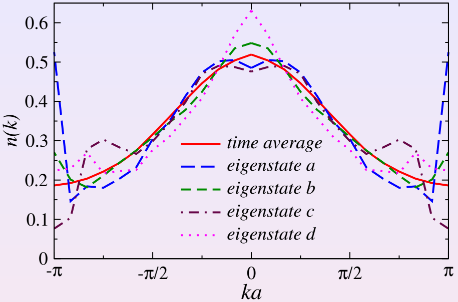
$n(k_x = 0)$ vs energy

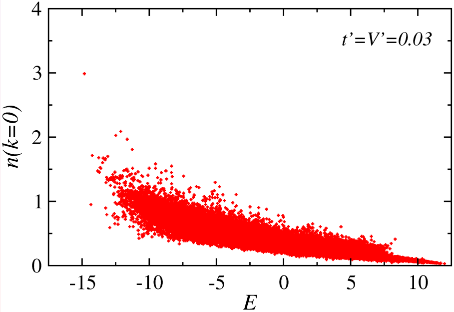
There is no eigenstate thermalization at the edges of the spectrum (there is no quantum chaos either)

Breakdown of ETH $\longrightarrow$ integrability ($t' = V' = 0.03$)

Momentum distribution

Eigenstates $a - d$ are the ones with energies closest to E





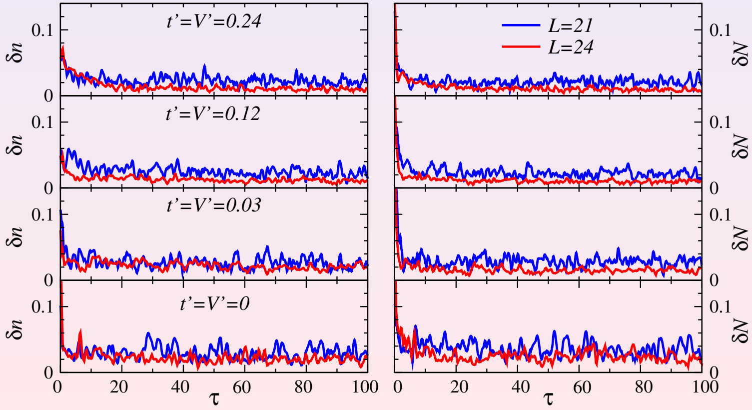
$n(k_x = 0)$ vs energy

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

Time evolution and scaling with system size

Compute the relative differences

$$\delta n(\tau) = \frac{\sum_k |n(k,\tau) - n_{\mathrm{DE}}(k)|}{\sum_k n_{\mathrm{DE}}(k)} \quad \text{and} \quad \delta N(\tau) = \frac{\sum_k |N(k,\tau) - N_{\mathrm{DE}}(k)|}{\sum_k N_{\mathrm{DE}}(k)}$$



Time fluctuations

Are they small because of dephasing?

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

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

Time fluctuations

Are they small because of dephasing?

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

$$\sim \frac{\sqrt{N_{\text{states}}^2}}{N_{\text{states}}} O_{\alpha\beta}^{\text{typical}} \sim O_{\alpha\beta}^{\text{typical}}$$

Time average of $O(t)$

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

$$\sim \sum_\alpha \frac{1}{N_{\text{states}}} O_{\alpha\alpha} \sim O_{\alpha\alpha}^{\text{typical}}$$

Time fluctuations

Are they small because of dephasing?

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

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

Time average of $O(t)$

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

$$\sim \sum_\alpha \frac{1}{N_{\text{states}}} O_{\alpha\alpha} \sim O^{\text{typical}}_{\alpha\alpha}$$

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

Time fluctuations

Are they small because of dephasing?

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

$$\sim \frac{\sqrt{N_{\text{states}}^2}}{N_{\text{states}}} O_{\alpha\beta}^{\text{typical}} \sim O_{\alpha\beta}^{\text{typical}}$$

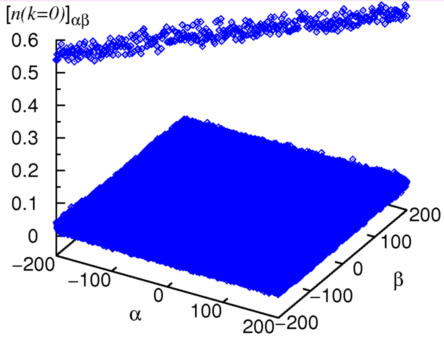
Time average of $O(t)$

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

$$\sim \sum_\alpha \frac{1}{N_{\text{states}}} O_{\alpha\alpha} \sim O_{\alpha\alpha}^{\text{typical}}$$

Dephasing is not enough.

One needs $O_{\alpha\beta}^{\text{typical}} \ll O_{\alpha\alpha}^{\text{typical}}$



Eigenstate thermalization hypothesis

Eigenstate thermalization hypothesis

M. Srednicki, J. Phys. A **32**, 1163 (1999).

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

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.

Eigenstate thermalization hypothesis

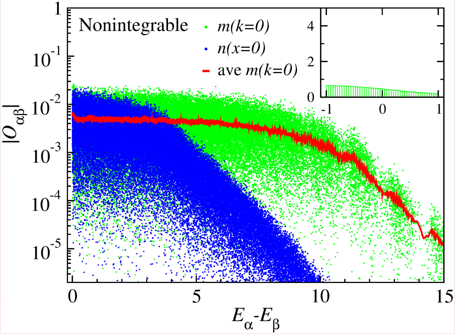
Eigenstate thermalization hypothesis

M. Srednicki, J. Phys. A **32**, 1163 (1999).

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

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.

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).

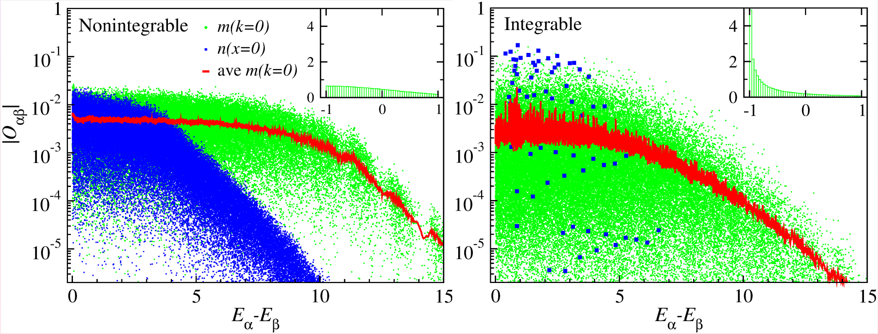
Eigenstate thermalization hypothesis

M. Srednicki, J. Phys. A **32**, 1163 (1999).

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

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.

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

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

This means that (to leading order):

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

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

This means that (to leading order):

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

With more work one can show that:

$$\overline{O_{\alpha\alpha}^2} - \overline{O_{\alpha\alpha}}^2 = \overline{|O_{\alpha\beta}|^2} = \frac{1}{\mathcal{D}^2} \sum_i O_i^2 \equiv \frac{1}{\mathcal{D}} \overline{O^2}.$$

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

This means that (to leading order):

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

With more work one can show that:

$$\overline{O_{\alpha\alpha}^2} - \overline{O_{\alpha\alpha}}^2 = \overline{|O_{\alpha\beta}|^2} = \frac{1}{\mathcal{D}^2}\sum_i O_i^2 \equiv \frac{1}{\mathcal{D}}\overline{O^2}.$$

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).

Outline

Linked-Cluster expansions (thermal equilibrium)

Extensive observables $\hat{\mathcal{O}}$ per lattice site ($\mathcal{O}$) in the thermodynamic limit

$$\mathcal{O} = \sum_c L(c) \times W_{\mathcal{O}}(c)$$

where $L(c)$ is the number of embeddings of cluster c

Linked-Cluster expansions (thermal equilibrium)

Extensive observables $\hat{\mathcal{O}}$ per lattice site ($\mathcal{O}$) in the thermodynamic limit

$$\mathcal{O} = \sum_c L(c) \times W_{\mathcal{O}}(c)$$

where $L(c)$ is the number of embeddings of cluster c and $W_{\mathcal{O}}(c)$ is the weight of observable $\mathcal{O}$ in cluster c

$$W_{\mathcal{O}}(c) = \mathcal{O}(c) - \sum_{s \subset c} W_{\mathcal{O}}(s).$$

$\mathcal{O}(c)$ is the result for $\mathcal{O}$ in cluster c

$$\begin{aligned}
\mathcal{O}(c) &= \mathrm{Tr}\left\{\hat{\mathcal{O}}\,\hat{\rho}_c^{\mathsf{GC}}\right\}, \\
\hat{\rho}_c^{\mathsf{GC}} &= \frac{1}{Z_c^{\mathsf{GC}}} \exp^{-\left(\hat{H}_c - \mu \hat{N}_c\right)/k_B T} \\
Z_c^{\mathsf{GC}} &= \mathrm{Tr}\left\{\exp^{-\left(\hat{H}_c - \mu \hat{N}_c\right)/k_B T}\right\}
\end{aligned}$$

and the s sum runs over all subclusters of c.

Numerical linked-cluster expansions

- In HTEs $\mathcal{O}(c)$ is expanded in powers of β and only a finite number of terms is retained

Numerical linked-cluster expansions

- In HTEs $\mathcal{O}(c)$ is expanded in powers of β and only a finite number of terms is retained
- In numerical linked cluster expansions (NLCEs) an exact diagonalization of the cluster is used to calculate $\mathcal{O}(c)$ at any temperature
  (Spins models in the square, triangular, and kagome lattices)
  MR, T. Bryant, and R. R. P. Singh, PRL **97**, 187202 (2006).
  MR, T. Bryant, and R. R. P. Singh, PRE **75**, 061118 (2007).

  (t-J model in the square lattice)
  MR, T. Bryant, and R. R. P. Singh, PRE **75**, 061119 (2007).

Numerical linked-cluster expansions

- In HTEs $\mathcal{O}(c)$ is expanded in powers of β and only a finite number of terms is retained
- In numerical linked cluster expansions (NLCEs) an exact diagonalization of the cluster is used to calculate $\mathcal{O}(c)$ at any temperature
  (Spins models in the square, triangular, and kagome lattices)
  MR, T. Bryant, and R. R. P. Singh, PRL **97**, 187202 (2006).
  MR, T. Bryant, and R. R. P. Singh, PRE **75**, 061118 (2007).

  (t-J model in the square lattice)
  MR, T. Bryant, and R. R. P. Singh, PRE **75**, 061119 (2007).
- Zero temperature NLCEs
  (pinwheel distorted kagome lattice, material $Rb_2Cu_3SnF_{12}$)
  E. Khatami, R. R. P. Singh, and MR, PRB **84**, 224411 (2011).

Numerical linked-cluster expansions

- In HTEs $\mathcal{O}(c)$ is expanded in powers of β and only a finite number of terms is retained
- In numerical linked cluster expansions (NLCEs) an exact diagonalization of the cluster is used to calculate $\mathcal{O}(c)$ at any temperature
  (Spins models in the square, triangular, and kagome lattices)
  MR, T. Bryant, and R. R. P. Singh, PRL **97**, 187202 (2006).
  MR, T. Bryant, and R. R. P. Singh, PRE **75**, 061118 (2007).

  (t-J model in the square lattice)
  MR, T. Bryant, and R. R. P. Singh, PRE **75**, 061119 (2007).
- Zero temperature NLCEs
  (pinwheel distorted kagome lattice, material $Rb_2Cu_3SnF_{12}$)
  E. Khatami, R. R. P. Singh, and MR, PRB **84**, 224411 (2011).
- Bipartite entanglement entropy of quantum models
  (two-dimensional transverse field Ising model)
  A. B. Kallin, K. Hyatt, R. R. P. Singh, and R. G. Melko, PRL **110**, 135702 (2013).

Numerical linked-cluster expansions

- In HTEs $\mathcal{O}(c)$ is expanded in powers of β and only a finite number of terms is retained
- In numerical linked cluster expansions (NLCEs) an exact diagonalization of the cluster is used to calculate $\mathcal{O}(c)$ at any temperature
  (Spins models in the square, triangular, and kagome lattices)
  MR, T. Bryant, and R. R. P. Singh, PRL **97**, 187202 (2006).
  MR, T. Bryant, and R. R. P. Singh, PRE **75**, 061118 (2007).

  (t-J model in the square lattice)
  MR, T. Bryant, and R. R. P. Singh, PRE **75**, 061119 (2007).
- Zero temperature NLCEs
  (pinwheel distorted kagome lattice, material $Rb_2Cu_3SnF_{12}$)
  E. Khatami, R. R. P. Singh, and MR, PRB **84**, 224411 (2011).
- Bipartite entanglement entropy of quantum models
  (two-dimensional transverse field Ising model)
  A. B. Kallin, K. Hyatt, R. R. P. Singh, and R. G. Melko, PRL **110**, 135702 (2013).
- Disordered systems
  (spin-1/2 models with binary disorder in 2D)
  B. Tang, D. Iyer and MR, PRB **91**, 174413 (2015).

Finite size effects (finite temperature)

- In unordered phases, not all ensemble calculations of finite systems approach the thermodynamic limit the same way

  There is a *preferred ensemble* (the grand canonical ensemble) and *preferred boundary conditions* (periodic boundary conditions, so that the system is translationally invariant) for which finite-size effects are exponentially small in the system size. All others exhibit power-law convergence with system size.

D. Iyer, M. Srednicki, and MR, Phys. Rev. E **91**, 062142 (2015).

Finite size effects (finite temperature)

- In unordered phases, not all ensemble calculations of finite systems approach the thermodynamic limit the same way

  There is a *preferred ensemble* (the grand canonical ensemble) and *preferred boundary conditions* (periodic boundary conditions, so that the system is translationally invariant) for which finite-size effects are exponentially small in the system size. All others exhibit power-law convergence with system size.

- NLCEs convergence is also exponential, but a faster one!

D. Iyer, M. Srednicki, and MR, Phys. Rev. E **91**, 062142 (2015).

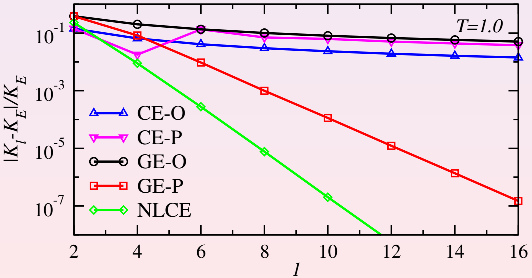
Finite size effects (finite temperature)

- In unordered phases, not all ensemble calculations of finite systems approach the thermodynamic limit the same way

  There is a *preferred ensemble* (the grand canonical ensemble) and *preferred boundary conditions* (periodic boundary conditions, so that the system is translationally invariant) for which finite-size effects are exponentially small in the system size. All others exhibit power-law convergence with system size.

- NLCEs convergence is also exponential, but a faster one!

Kinetic energy in the t-V model



D. Iyer, M. Srednicki, and MR, Phys. Rev. E **91**, 062142 (2015).

NLCEs for quantum quenches

The initial state is in thermal equilibrium in contact with a reservoir

$$\hat{\rho}_c^I = \frac{\sum_a e^{-(E_a^c - \mu_I N_a^c)/T_I} |a_c\rangle\langle a_c|}{Z_c^I}, \quad \text{where} \quad Z_c^I = \sum_a e^{-(E_a^c - \mu^I N_a^c)/T_I},$$

$|a_c\rangle$ (E_a^c) are the eigenstates (eigenvalues) of the initial Hamiltonian $\hat{H}_c^I$ in c.

MR, PRL **112**, 170601 (2014).

NLCEs for quantum quenches

The initial state is in thermal equilibrium in contact with a reservoir

$$\hat{\rho}_c^I = \frac{\sum_a e^{-(E_a^c - \mu_I N_a^c)/T_I} |a_c\rangle\langle a_c|}{Z_c^I}, \quad \text{where} \quad Z_c^I = \sum_a e^{-(E_a^c - \mu^I N_a^c)/T_I},$$

$|a_c\rangle$ (E_a^c) are the eigenstates (eigenvalues) of the initial Hamiltonian $\hat{H}_c^I$ in c.

At the time of the quench $\hat{H}_c^I \to \hat{H}_c$, the system is detached from the reservoir. Writing the eigenstates of $\hat{H}_c^I$ in terms of the eigenstates of $\hat{H}_c$

$$\hat{\rho}_c^{\text{DE}} \equiv \lim_{t'\to\infty} \frac{1}{t'} \int_0^{t'} dt\, \hat{\rho}(t) = \sum_\alpha W_\alpha^c\, |\alpha_c\rangle\langle\alpha_c|$$

where

$$W_\alpha^c = \frac{\sum_a e^{-(E_a^c - \mu_I N_a^c)/T_I} |\langle\alpha_c|a_c\rangle|^2}{Z_c^I},$$

$|\alpha_c\rangle$ (ε_α^c) are the eigenstates (eigenvalues) of the final Hamiltonian $\hat{H}_c$ in c.

MR, PRL **112**, 170601 (2014).

NLCEs for quantum quenches

The initial state is in thermal equilibrium in contact with a reservoir

$$\hat{\rho}_c^I = \frac{\sum_a e^{-(E_a^c - \mu_I N_a^c)/T_I} |a_c\rangle\langle a_c|}{Z_c^I}, \quad \text{where} \quad Z_c^I = \sum_a e^{-(E_a^c - \mu^I N_a^c)/T_I},$$

$|a_c\rangle$ (E_a^c) are the eigenstates (eigenvalues) of the initial Hamiltonian $\hat{H}_c^I$ in c.

At the time of the quench $\hat{H}_c^I \rightarrow \hat{H}_c$, the system is detached from the reservoir. Writing the eigenstates of $\hat{H}_c^I$ in terms of the eigenstates of $\hat{H}_c$

$$\hat{\rho}_c^{\text{DE}} \equiv \lim_{t' \rightarrow \infty} \frac{1}{t'} \int_0^{t'} dt\, \hat{\rho}(t) = \sum_\alpha W_\alpha^c\, |\alpha_c\rangle\langle\alpha_c|$$

where

$$W_\alpha^c = \frac{\sum_a e^{-(E_a^c - \mu_I N_a^c)/T_I} |\langle\alpha_c|a_c\rangle|^2}{Z_c^I},$$

$|\alpha_c\rangle$ (ε_α^c) are the eigenstates (eigenvalues) of the final Hamiltonian $\hat{H}_c$ in c.

Using $\hat{\rho}_c^{\text{DE}}$ in the calculation of $\mathcal{O}(c)$, NLCEs allow one to compute observables in the DE in the thermodynamic limit.

MR, PRL **112**, 170601 (2014).

Outline

Models and quenches

Hard-core bosons in 1D lattices at half filling ($\mu_I = 0$)

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

Quench: T_I, $t_I = 0.5$, $V_I = 1.5$, $t'_I = V'_I = 0 \to t = V = 1.0$, $t' = V'$

Models and quenches

Hard-core bosons in 1D lattices at half filling ($\mu_I = 0$)

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

Quench: T_I, $t_I = 0.5$, $V_I = 1.5$, $t'_I = V'_I = 0 \rightarrow t = V = 1.0$, $t' = V'$

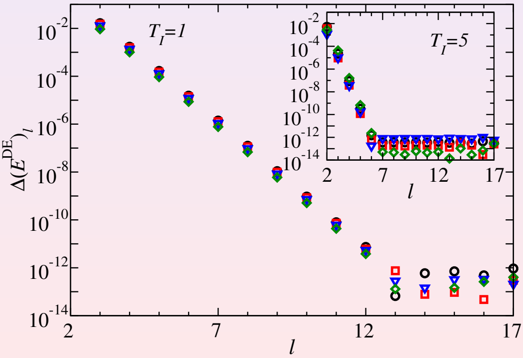
NLCE with maximally connected clusters ($l = 18$ sites)

Energy: $E^{\text{DE}} = \text{Tr}[\hat{H}\hat{\rho}^{\text{DE}}]$

Convergence:

$$\Delta(\mathcal{O}^{\text{DE}})_l = \frac{|\mathcal{O}_l^{\text{DE}} - \mathcal{O}_{18}^{\text{DE}}|}{|\mathcal{O}_{18}^{\text{DE}}|}$$

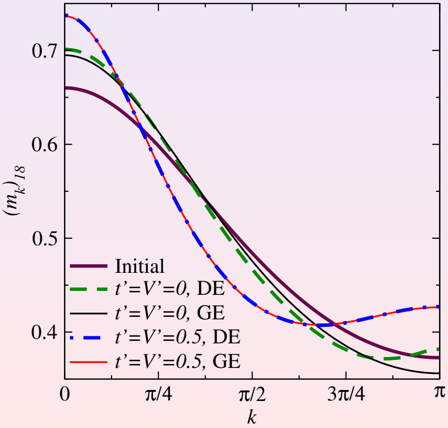
Convergence of E^{DE} with l



Few-body experimental observables in the DE

Momentum distribution

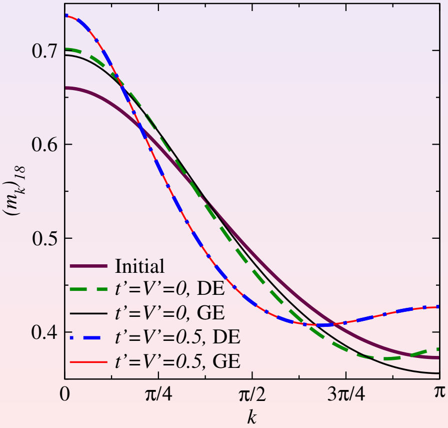
$$\hat{m}_k = \frac{1}{L} \sum_{jj'} e^{ik(j-j')} \hat{\rho}_{jj'}$$



Few-body experimental observables in the DE

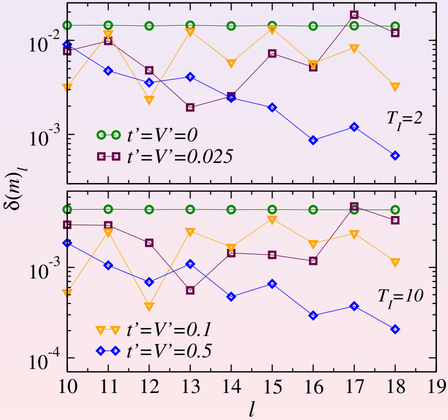
Momentum distribution

$$\hat{m}_k = \frac{1}{L}\sum_{jj'} e^{ik(j-j')}\hat{\rho}_{jj'}$$



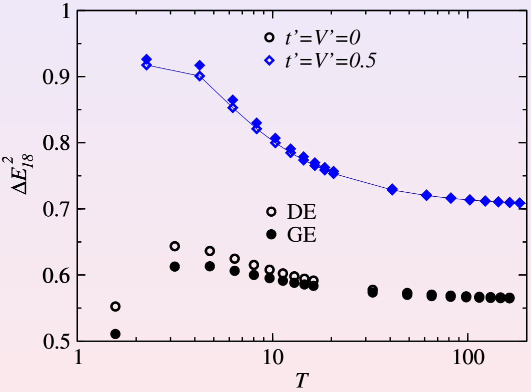
Differences between DE and GE

$$\delta(m)_l = \frac{\sum_k |(m_k)_l^{\mathrm{DE}} - (m_k)_{18}^{\mathrm{GE}}|}{\sum_k (m_k)_{18}^{\mathrm{GE}}}$$



Energy variance

$$\Delta E^2 = \frac{1}{L}(\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2)$$

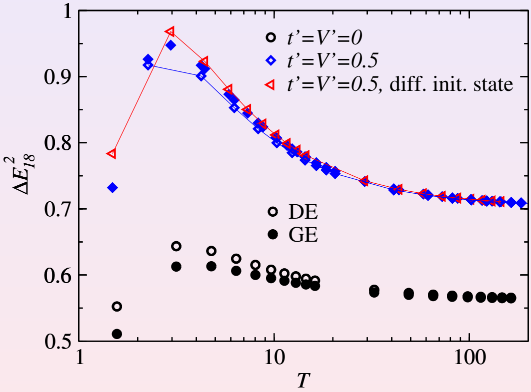


The dispersion of the energy (and of the particle number) in the DE depends on the initial state independently of whether the system is integrable or not.

Energy variance

Energy variance

$$\Delta E^2 = \frac{1}{L}(\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2)$$



The dispersion of the energy (and of the particle number) in the DE depends on the initial state independently of whether the system is integrable or not.

Outline

Failure of GGE based on known conserved quantities

XXZ (integrable) Hamiltonian

$$\hat{H} = J\left(\sum_i \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z\right)$$

Quench starting from the Neel state to different values of $\Delta \geq 1$

Saddle point solution differs from GGE based on known conserved quantities:

B. Wouters, J. De Nardis, M. Brockmann, D. Fioretto, MR, and J.-S. Caux,
PRL **113**, 117202 (2014).

B. Pozsgay, M. Mestyán, M. A. Werner, M. Kormos, G. Zaránd, and G. Takács,
PRL **113**, 117203 (2014).

Failure of GGE based on known conserved quantities

XXZ (integrable) Hamiltonian

$$\hat{H} = J \left(\sum_i \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z \right)$$

Quench starting from the Neel state to different values of $\Delta \geq 1$

Saddle point solution differs from GGE based on known conserved quantities:

B. Wouters, J. De Nardis, M. Brockmann, D. Fioretto, MR, and J.-S. Caux, PRL **113**, 117202 (2014).

B. Pozsgay, M. Mestyán, M. A. Werner, M. Kormos, G. Zaránd, and G. Takács, PRL **113**, 117203 (2014).

Can we use NLCEs for ground states (pure states)?

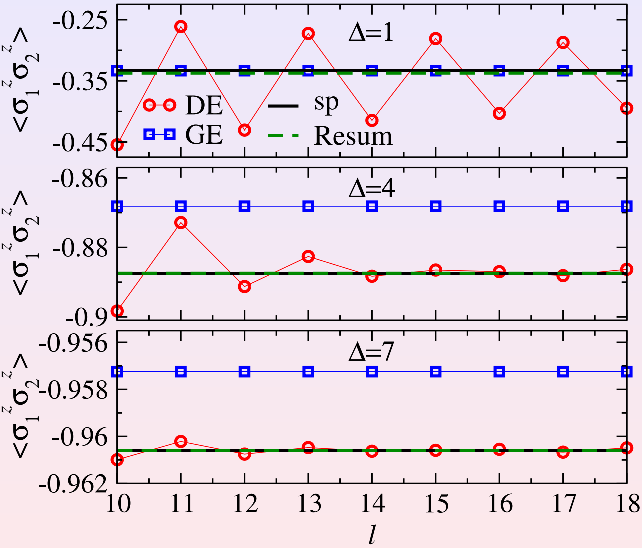
Using the parity symmetry of the clusters:

$$|a_c^e\rangle = \frac{1}{\sqrt{2}}(|\ldots\uparrow\downarrow\uparrow\downarrow\ldots\rangle + |\ldots\downarrow\uparrow\downarrow\uparrow\ldots\rangle)$$

$$|a_c^o\rangle = \frac{1}{\sqrt{2}}(|\ldots\uparrow\downarrow\uparrow\downarrow\ldots\rangle - |\ldots\downarrow\uparrow\downarrow\uparrow\ldots\rangle)$$

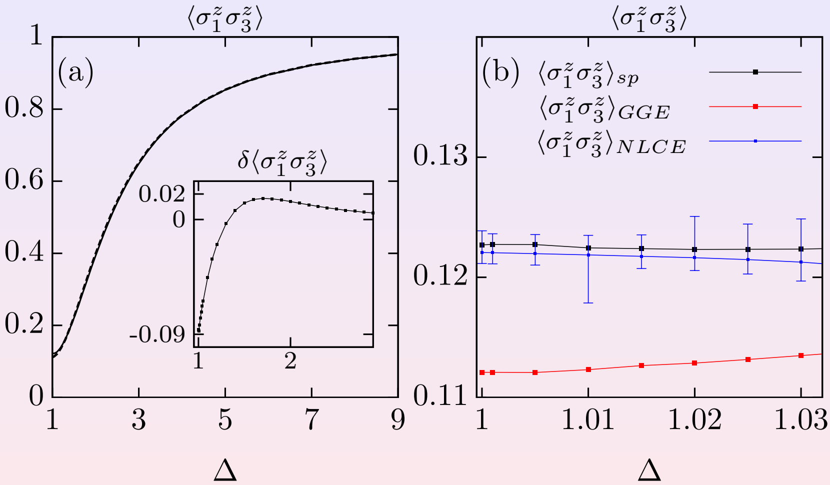
$$W_\alpha^{c,e/o} = |\langle \alpha_c^{e/o} | a_c^{e/o} \rangle|^2$$

Results for spin-spin correlations



MR, PRE **90**, 031301(R) (2014).

Saddle point, GGE, and NLCE



$$\delta\langle\sigma_1^z\sigma_3^z\rangle = \langle\sigma_1^z\sigma_3^z\rangle_{\text{GGE}}/\langle\sigma_1^z\sigma_3^z\rangle_{\text{sp}} - 1$$

B. Wouters *et al.*, PRL **113**, 117202 (2014).

Outline

Conclusions

- NLCE results support the expectation that, in the thermodynamic limit, few-body observables thermalize in nonintegrable systems while they do not thermalize in integrable systems. Time scale for thermalization as one approaches the integrable point?
- Quantum quenches in the integrable XXZ chain revealed the existence of unknown (extensive/local) conserved quantities. *They have already been found: PRL* **115***, 120601 & 157201 (2015).* New things to be learned about integrable systems!
- NLCEs provide a general framework to study the diagonal ensemble in lattice systems after a quantum quench in the thermodynamic limit.
- The grand canonical ensemble in translationally invariant systems *is special* (exponentially small finite size effects vs power law for other ensembles/boundaries). NLCEs also converge exponentially, but faster!

Collaborators

- M. Brockmann (ITP Amsterdam)
- J.-S. Caux (ITP Amsterdam)
- Luca D'Alessio (Exa Corporation)
- Jacopo De Nardis (ITP Amsterdam)
- Vanja Dunjko (U Mass Boston)
- Davide Fioretto (ITP Amsterdam)
- Deepak Iyer (Bucknell U)
- Yariv Kafri (Technion)
- Ehsan Khatami (San Jose State)
- Maxim Olshanii (U Mass Boston)
- Anatoli Polkovnikov (Boston U)
- Guido Pupillo (U Strasbourg)
- Lea F. Santos (Yeshiva)
- Mark Srednicki (UC Santa Barbara)
- Sebastian Will (MIT)
- Bram Wouters (ITP Amsterdam)

Supported by: