THERMAL EQUILIBRIUM: (in) Quantum non-integrable and classical integrable systems

(i.e., an attempt to learn something without machines)

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Summary

1) Thermal equilibrium in quantum mechanics: problems

2) Hamiltonian as a Random Matrix: Quantum Chaos

3) Bohigas-Giannoni-Schmit's conjecture

4) The Eigenstate Thermalization Hypothesis (too much?)

5) An overlooked result: Von Neumann's 'Quantum Ergodic Theorem'

6) Thermal equilibrium in a classical integrable system: Toda

7) A final remark: do we really care about integrability?

8) The BGV's conjecture

9) Conclusion

THIS PRESENTATION IN ONE SLIDE

Theorem:
ONLY **VON NEUMANN** REALLY UNDERSTOOD QUANTUM MECHANICS
Proof: **Trivial**

‘Proof of the Ergodic Theorem and the H-Theorem in Quantum Mechanics’
arXiv:1003.2133 **(2010)**

Translated from
‘Beweis des Ergodensatzes und des H-Theorems in der neuen Mechanik’.
Zeitschrift für Physik **57** **(1929)**.

‘Long-Time behaviour of Macroscopic Quantum Systems’
S. Goldstein, Joel L. Lebowitz. R. Tumulka, N. Zanghì, *arXiv:1003.2129* **(2010)**

QUANTUM MICROCANONICAL ENSEMBLE

Quantum Mechanics $|\psi\rangle \in \mathcal{H}$ (Hilbert Space)

Hamiltonian: a self-adjoint operator $\hat{H} : \mathcal{H} \longrightarrow \mathcal{H}$ $\quad i\hbar \frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle$

Complete set of eigenstates: $\hat{H}\ |\alpha\rangle = \varepsilon_\alpha\ |\alpha\rangle$

$$|\psi\rangle = \sum_{\varepsilon_\alpha \in \mathrm{Sp}(\hat{H})} c_\alpha\ |\alpha > \qquad c_\alpha = \langle\alpha|\psi\rangle$$

Energy of the system: $\langle\psi|\hat{H}|\psi\rangle = E$

Energy shell: $\mathcal{I}_E = [E - \delta E,\ E + \delta E]$ $\quad E \ll \delta E \ll 1$ $\quad \begin{cases} E \sim N \\ \delta E \sim \sqrt{N} \end{cases}$

Microcanonical Density Matrix $\quad \hat{\rho}_E = \frac{1}{\mathcal{N}_E} \sum_{\{\alpha\ |\ \varepsilon_\alpha \in\ \mathcal{I}_E\}} |\alpha\rangle\ \langle\alpha|$

QUANTUM MICROCANONICAL ENSEMBLE

Microcanonical Density Matrix
$$\hat{\rho}_E = \frac{1}{\mathcal{N}_E} \sum_{\{\alpha \,\mid\, \varepsilon_\alpha \in \mathcal{I}_E\}} |\alpha\rangle \langle\alpha|$$

Microcanonical Expectation
$$\langle \hat{O} \rangle_E = \mathrm{Tr}[\ \hat{\rho}_E \hat{O}\ ]$$

$$\langle \hat{O} \rangle_E = \frac{1}{\mathcal{N}_E} \sum_{\{\alpha \,\mid\, \varepsilon_\alpha \in \mathcal{I}_E\}} \langle\alpha|\hat{O}|\alpha\rangle = \overline{O}(E) + \mathcal{O}(\sqrt{N})$$

QUESTION:
CAN THE MICROCANONICAL AVERAGE BE REPLACED WITH THE TIME AVERAGE?

QUANTUM THERMAL EQUILIBRIUM

$|\psi_I\rangle = \text{initial state} \qquad |\psi_I\rangle \in \mathcal{H} \qquad \dim(\mathcal{H}) = \mathcal{D}$

$$\langle \hat{O}(t) \rangle = \langle \psi_I | \; e^{i\hat{H}t/\hbar} \; \hat{O} \; e^{-i\hat{H}t/\hbar} \; | \psi_I \rangle$$

$$\frac{1}{T} \int_0^T dt \; \langle \hat{O}(t) \rangle = \langle \hat{O} \rangle_E$$

For which time T it is reasonably true?

$$\langle \hat{O}(t) \rangle = \sum_{\alpha,\beta} \; \langle \psi_I | e^{i\hat{H}t/\hbar} | \alpha \rangle \; \langle \alpha | \hat{O} | \beta \rangle \; \langle \beta | e^{-i\hat{H}t/\hbar} | \psi_I \rangle$$

$$\langle \hat{O}(t) \rangle = \sum_{\alpha,\beta} \; e^{i(E_\alpha - E_\beta)t/\hbar} \; c_\alpha^* c_\beta \; O_{\alpha\beta}$$

QUANTUM THERMAL EQUILIBRIUM

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For which time T it is reasonably true?

$$\langle \hat{O}(t)\rangle = \sum_{\alpha\in \mathrm{Sp}(\hat{H})} |c_\alpha|^2\ O_{\alpha\alpha} + \sum_{\alpha\neq\beta} e^{i(E_\alpha - E_\beta)t/\hbar}\ c_\alpha^* c_\beta\ O_{\alpha\beta}$$

1) At which time *T* ?
(decoherence)

$$\frac{1}{T}\int_0^T \sum_{\alpha\neq\beta} e^{i(E_\alpha - E_\beta)t/\hbar}\ c_\alpha^* c_\beta\ O_{\alpha\beta} = 0$$

2) How is it possible to have ?

$$\sum_{\alpha\in \mathrm{Sp}(\hat{H})} |c_\alpha|^2\ O_{\alpha\alpha} = \frac{1}{\mathcal{N}_E} \sum_{\{\alpha\ |\ \varepsilon_\alpha \in\ \mathcal{I}_E\}} \hat{O}_{\alpha\alpha}$$

QUANTUM THERMAL EQUILIBRIUM

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Many degrees of freedom → Exponentially small level spacing

$\Delta E_{\alpha\beta} \sim \exp(-N)$ → **Decoherence in times exceeding age of the universe!**

QUANTUM THERMAL EQUILIBRIUM:
Hypothesis on the matrix elements

$$\langle \hat{O}(t) \rangle = \sum_{\alpha \in \mathrm{Sp}(\hat{H})} |c_\alpha|^2 \; O_{\alpha\alpha} + \sum_{\alpha \neq \beta} e^{i(E_\alpha - E_\beta)t/\hbar} \; c_\alpha^* c_\beta \; O_{\alpha\beta}$$

Diagonal elements are 'almost identical' and equal to equilibrium expectation

$$\langle \hat{O} \rangle_E \sum_{\alpha \in \mathrm{Sp}(\hat{H})} |c_\alpha|^2 = \langle \hat{O} \rangle_E$$

Off-diagonal elements are almost negligible

Decoherence needed for just a few levels, much shorter times

TWO PROPOSALS

1) HAMILTONIAN = RANDOM MATRIX

2) EIGENSTATE THERMALIZATION HYPOTHESIS

RANDOM MATRIX THEORY

$$\hat{H} : \mathcal{H} \longrightarrow \mathcal{H} \qquad \dim(\mathcal{H}) = \mathcal{D}$$

$$\hat{H}_{\alpha\beta} = \mathcal{D} \times \mathcal{D} \ \text{ symmetric matrix}$$

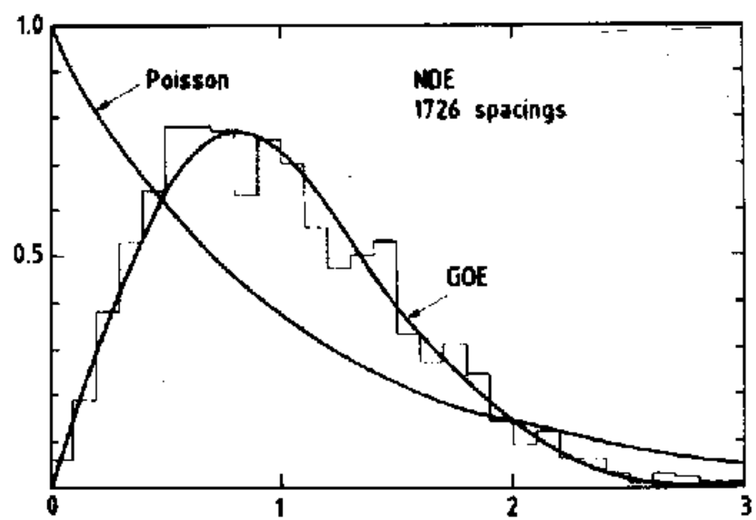
Gaussian Orthogonal Ensemble (time-reversal, no magnetic field)

Probability distribution
of levels spacings
$\Delta E = \omega$

$$P(\omega) \ \propto \ \omega \ \exp\left(-A \ \frac{\omega^2}{2} \right)$$

Wigner-Dyson

Nearest neighbour energy spacings for the 'Nuclear Data Ensemble'



RANDOM MATRIX THEORY

Question:
What is really the point of random matrices concerning the 'quantum ergodicity' problem?

Answer:
Their eigenvectors are **'random vectors'**

$$\hat{H}|\alpha\rangle = \varepsilon_\alpha |\alpha\rangle$$

$$\overline{\langle\alpha|\hat{O}|\beta\rangle} = \overline{\hat{O}}_{\alpha\beta} \approx \overline{O}\ \delta_{\alpha\beta} + \sqrt{\mathcal{D}}\ \eta_{\alpha\beta}$$

$\eta_{nm} =$ Random Gaussian variate, zero mean, unit variance

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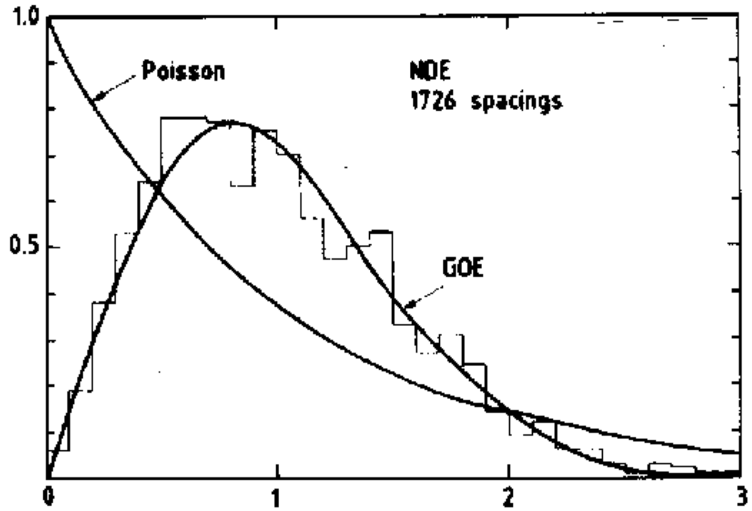

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Identical diagonal elements | **Small off-diagonal elements**

$$\langle\hat{O}(t)\rangle = \sum_{\alpha\in\mathrm{Sp}(\hat{H})} |c_\alpha|^2\ O_{\alpha\alpha} + \sum_{\alpha\neq\beta} e^{i(E_\alpha - E_\beta)t/\hbar}\ c^*_\alpha c_\beta\ O_{\alpha\beta}$$

Basically what we needed to have … $T^{-1}\int_0^T dt\ \langle\hat{O}(t)\rangle\ \approx\ \langle\hat{O}\rangle_E$

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η_{nm} = Random Gaussian variate, zero mean, unit variance

PROBLEM:

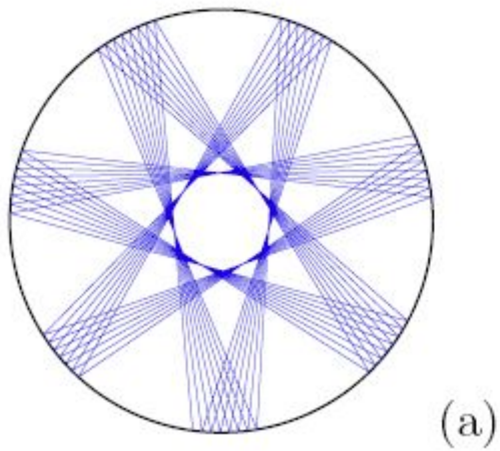
In the random matrix ensemble there is no dependence on specific energy (temperature) … a good assumption in the infinite temperature limit (very high energies)

SOLUTION: Eigenstate Thermalization Hypothesis

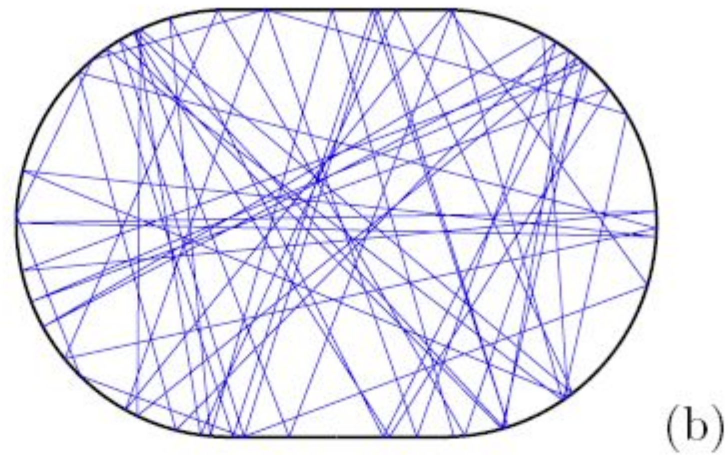
Basically what we needed to have … $$T^{-1}\int_0^T dt\ \langle\hat{O}(t)\rangle \approx \langle\hat{O}\rangle_E$$

SMALL DETOUR: RMT and QUANTUM CHAOS

CLASSICAL

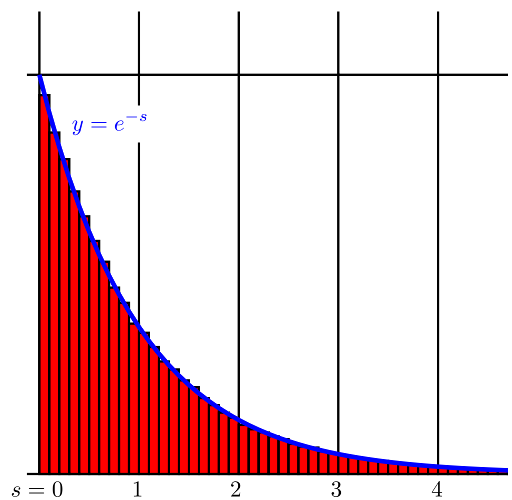


Integrable

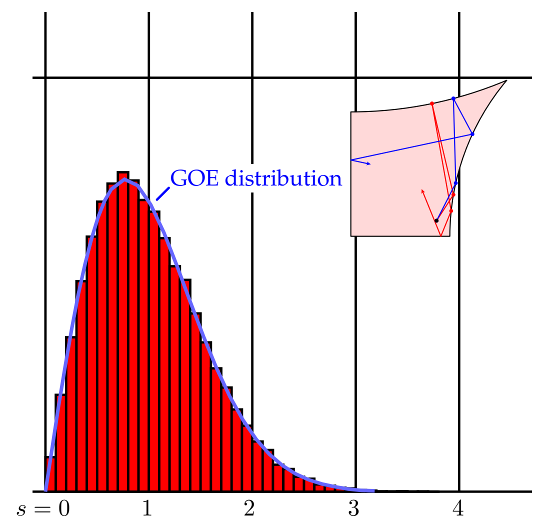


Chaotic billiard

QUANTUM (level spacing)

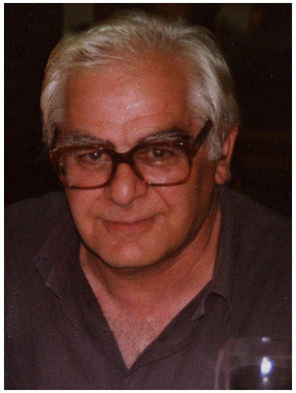


Poisson

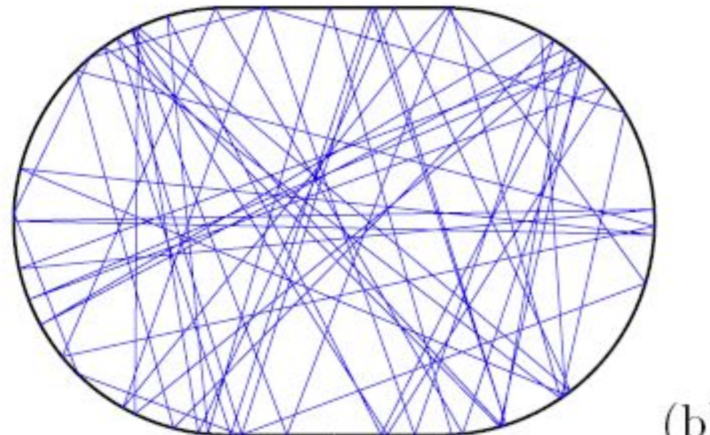


Wigner-Dyson

SMALL DETOUR: RMT and QUANTUM CHAOS



Oriol Bohigas
(Dec 1937- Oct 2013)

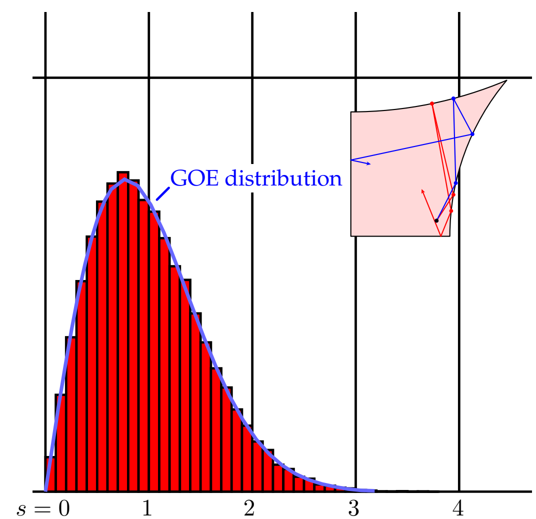


Chaotic billiard

'Characterization of Chaotic Quantum Spectra and Universality of Level Fluctuations Law', O. Bohigas, M. Giannoni, C. Schmit, *Phys. Rev. Lett.* **52** (1984)

Fact:
Quantum particle in an infinite potential well shaped as a Sinai billiard has level spacing statistics, at high energies, which follows **Wigner-Dyson** distribution.

Conjecture (BGS):
Quantum systems whose classical counterpart is chaotic are characterized by Random Matrix Theory



Wigner-Dyson

SMALL DETOUR: RMT and QUANTUM CHAOS

Logical framework
(attention: the sequence of arrows cannot be reversed)

1) Classical Chaotic System

↓

2) Promote them to quantum systems

↓

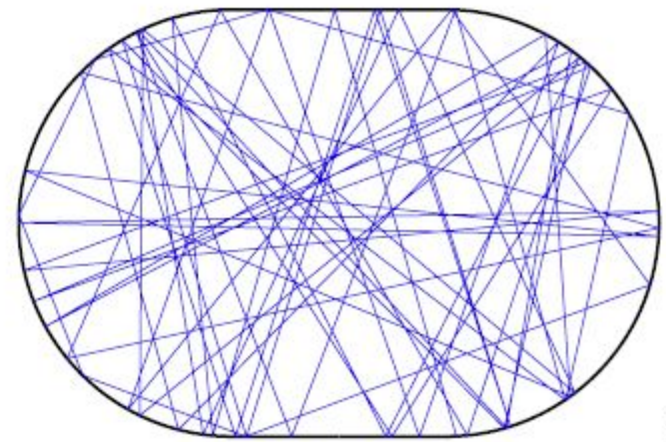
3) High energy (semiclassical) limit: Wigner-Dyson statistics

↓

4) Random Matrix Theory

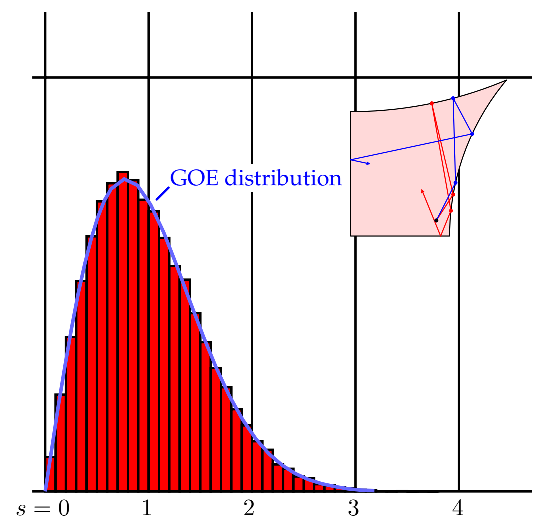
↓

5) Quantum Ergodicity



(b)

Chaotic billiard



Wigner-Dyson

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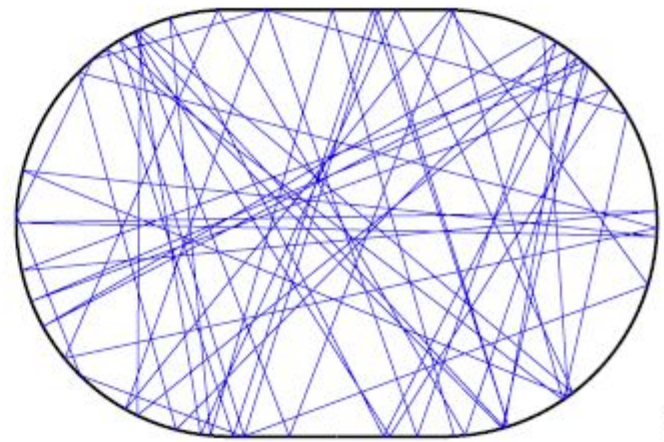

(b)

Chaotic billiard

Dominant Way of Thinking

Classical Chaotic System

↓ ↑

Quantum Ergodicity

That is way Von Neumann ‘quantum ergodic theorem’ was overlooked: ***no distinction between chaotic and integral systems***

CHAOTIC EIGENSTATES

Random structureless vectors in any basis $\hat{H}|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle$

$$\langle n|\alpha\rangle = \psi_n(\alpha) \qquad \overline{\psi_n^*(\alpha)\psi_m(\beta)} = \frac{1}{\mathcal{D}}\delta_{\alpha\beta}\delta_{mn}$$

Chaoticity in **classical** mechanics:
small shifts in **initial conditions** produce **trajectories** totally uncorrelated

Chaoticity in **quantum** mechanics:
small shifts in **energy** produce **eigenvectors** totally uncorrelated

Measure of eigenvector chaoticity: **information entropy**

Choose randomly two eigenvalues

$$\varepsilon_\alpha \neq \varepsilon_\beta$$

$$S = -\sum_\beta |\psi_\beta(\alpha)|^2 \log|\psi_\beta(\alpha)|^2$$

$$S_{GOE} = \log(0.48\ \mathcal{D}) + \mathcal{O}(1/\mathcal{D})$$

ENTROPY DOES NOT INCREASE IN QUANTUM SYSTEMS: FALSE

Classical Hamiltonian mechanics: microcanonical probability distribution is conserved due to Liouviulle theorem. So does entropy.

$$\left.\begin{aligned} &S = -\int d^N q d^N p \; \rho(q,p) \log[\rho(q,p)] \\ &\rho(q,p) = \rho(\mathcal{H}(q,p)) \Longrightarrow \dot{\rho} = \{\mathcal{H}, \rho\} = 0 \end{aligned}\right\} \longrightarrow \dot{S} = 0$$

But if you chose a marginalized probability you are not limited by Liouville theorem

$$\rho_A(\mathbf{q}_A, \mathbf{p}_A) = \mathrm{Tr}_{\mathbf{q}_B, \mathbf{p}_B}[\rho(q,p)] \qquad \dot{S}(\rho_A) > 0$$

THE SAME IS TRUE FOR QUANTUM SYSTEMS

$$\hat{\rho}_A = \mathrm{Tr}_B[\hat{\rho}_E] \qquad S_{\mathrm{ent}} = -\mathrm{Tr}[\hat{\rho}_A \log(\hat{\rho}_A)]$$

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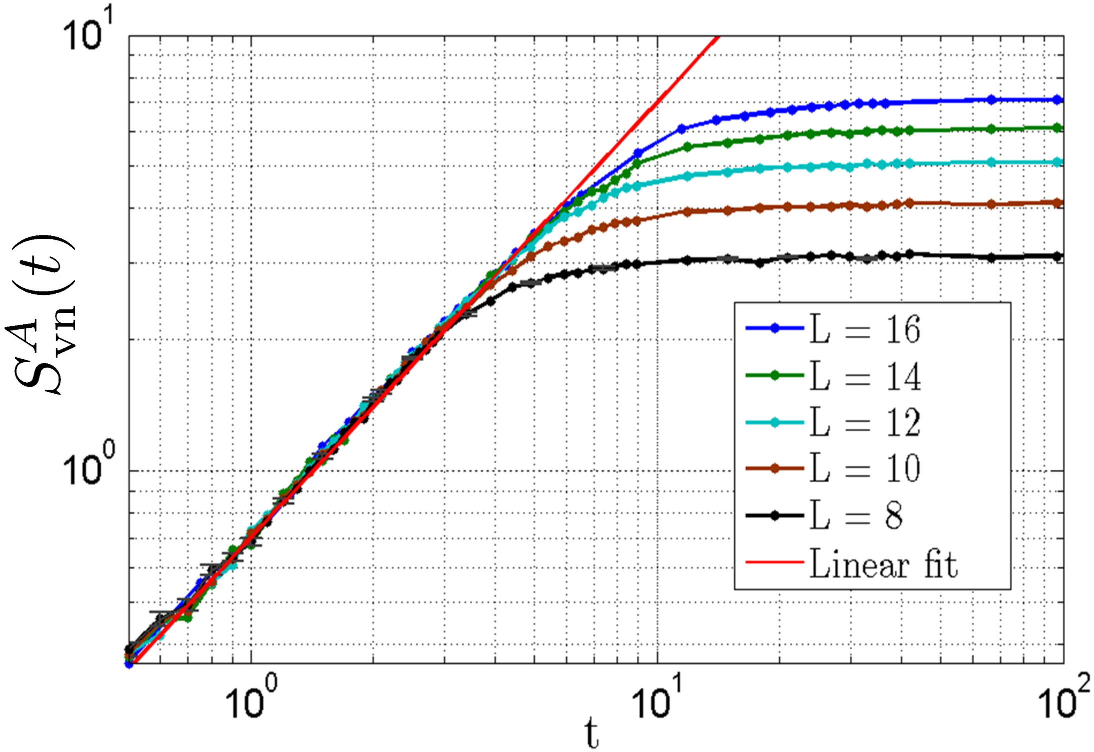

Half spins have been traced out

THE SAME IS TRUE FOR QUANTUM SYSTEMS

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$$S_{\mathrm{ent}} = -\mathrm{Tr}[\hat{\rho}_A \log(\hat{\rho}_A)]$$

Von Neumann (entanglement) entropy

EIGENSTATE THERMALIZATION HYPOTHESIS (ETH)

$$\frac{1}{T}\int_0^T dt\ \langle\hat{O}(t)\rangle = \langle\hat{O}\rangle_E$$

For which time T it is reasonably true?

$$\langle\hat{O}(t)\rangle = \sum_{\alpha\in\mathrm{Sp}(\hat{H})} |c_\alpha|^2\ O_{\alpha\alpha} + \sum_{\alpha\neq\beta} e^{i(E_\alpha-E_\beta)t/\hbar}\ c^*_\alpha c_\beta\ O_{\alpha\beta}$$

Make them EQUAL

Make them SMALL

Ansatz for **observables matrix elements** in the basis of Hamiltonian eigenstates

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

$\overline{E} = (E_\alpha + E_\beta)/2$ $\qquad$ $S(E) = \text{entropy}$

$\omega = E_\beta - E_\alpha$ $\qquad$ $\overline{\eta}_{\alpha\beta} = 0 \quad \overline{\eta^2}_{\alpha\beta} = 1$

EIGENSTATE THERMALIZATION HYPOTHESIS (ETH)

$$\frac{1}{T}\int_0^T dt\ \langle\hat{O}(t)\rangle = \langle\hat{O}\rangle_E$$

For which time T it is reasonably true?

ETH: good *ansatz* for the matrix elements, inspired (more or less) by what learned in the framework of Random Matrix Theory, let me say **'Quantum ergodicity driven by quantum chaos'.**

IS THIS REALLY THE WHOLE STORY?

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

AREN'T WE ASKING A TOO MUCH STRONG PROPERTY?

ISN'T PERHAPS THERMALIZATION A MORE GENERAL PROPERTY?

VON NEUMANN QUANTUM ERGODIC THEOREM

1) Consider an Energy Shell $\mathcal{I}_E = [E - \delta E,\ E + \delta E]$

$\mathcal{H} =$ Hilbert space of all eigenvectors such that

$$\hat{H}|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle \quad \text{with} \quad \varepsilon_\alpha \in \mathcal{I}_E$$

$$\dim(\mathcal{H}) = \mathcal{D}$$

2) So far so good: now consider a family of
'Macroscopic Observables which can be measured simultaneously'

$$\mathcal{H} = \bigoplus_\nu \mathcal{H}_\nu \qquad P_\nu = \text{projector} \qquad d_\nu = \dim(\mathcal{H}_\nu) \qquad \sum_\nu d_\nu = \mathcal{D}$$

Any wavefunction with unit norm defines a probability of macrostates

$$\psi \in \mathcal{H} \qquad ||\psi||^2 = 1 \longrightarrow ||P_\nu \psi||^2 = \langle\psi|P_\nu|\psi\rangle$$

VON NEUMANN QUANTUM ERGODIC THEOREM

3) Microcanonical density matrix defines a probability of macrostates

$$\rho_E = \frac{1}{\mathcal{D}} \sum_{\alpha|\varepsilon_\alpha \in \mathcal{I}_E} |\alpha\rangle\langle\alpha| \qquad \mathrm{Tr}[\rho_E P_\nu] = \frac{d_\nu}{\mathcal{D}}$$

Does the time-evolution of a generic macroscopic observable leads to microcanonical equilibrium?

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THEOREM (see Goldstein, Lebowitz, Tumulka, Zanghì, arXiv:1003.2129)

Under certain general conditions on the choice of the Hamiltonian $\mathcal{H}$ and the orthogonal decomposition of the Hilbert space $\mathcal{H} = \bigoplus_\nu \mathcal{H}_\nu$ one has that for **every wavefunction** $\psi_0 \in \mathcal{H}$ with $||\psi|| = 1$ the property **(QE)** holds for most of the time.

QUITE REMARKABLY (VON NEUMANN'S GUILT):
NOTHING IS SAID OR CLAIMED ABOUT THE INTEGRABILITY/CHAOTICITY OF THE SYSTEM

AN ‘INTERNATIONAL’ COLLABORATION

DECIDED TO CARRY ON AN INVESTIGATION

Baldovin

Gradenigo

Vulpiani

DO WE REALLY NEAD CHAOS TO HAVE THERMAL EQUILIBRIUM?

THERMAL EQUILIBRIUM IN AN INTEGRABLE SYSTEM

TODA Lattice

$$\mathcal{H}(q,p) = \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i=1}^{N} V(q_{i+1} - q_i) \qquad V(x) = e^{-x} - 1 + x$$

- Classical integrable system with Hamiltonian dynamics

$$\mathcal{I}_k(q,p) : \mathbb{R}^{2N} \to \mathbb{R} \quad \text{with} \quad k = 1, \ldots, N \quad \text{such that} \quad \{\mathcal{I}_k, \mathcal{I}_l\} = \delta_{kl}$$

THE SYSTEM IS INTEGRABLE

The Liouville-Arnol'd theorem guarantees the existence of Action-Angle canonical variables such that the Hamilton equations are trivial:

$$I_i(q,p) \qquad \dot{I}_i(q,p) = 0$$

$$\phi_i(q,p) \qquad \dot{\phi}_i(q,p) = \omega_i \qquad \phi_i(t) = \phi_i(0) + \omega_i t$$

Coherence between angles is preserved **at all times** (in perfect analogy to quantum)

All Lyapunov exponents are zero: **NO CHAOS!** … but …

THE ANTI-FPU EXPERIMENT

Fermi-Pasta-Ulam

- Non-integrable system

- Weakly non-linear regime (low energies)

- Non-equilibrium initial condition on the variables which 'almost diagonalize' the Hamiltonian

Anti Fermi-Pasta-Ulam

- Integrable system

- Highly non-linear regime (high energies)

- Non-equilibrium initial condition on the **wrong** variables, those which do not diagonalize the Hamiltonian

FOURIER MODES

$$\mathcal{Q}(k) = \sqrt{\frac{2}{N+1}} \sum_{i=1}^{N} q_i \ \sin\left(\frac{ik\pi}{N+1}\right)$$

$$\mathcal{P}(k) = \dots$$

INITAL CONDITION

$$k = 1: \quad \omega_k^2 \mathcal{Q}^2(k) = \mathcal{P}^2(k) = cN$$

$$k \neq 1: \quad \omega_k^2 \mathcal{Q}^2(k) = \mathcal{P}^2(k) = 0$$

THE ANTI-FPU EXPERIMENT

$$\mathcal{H}(\mathcal{Q},\mathcal{P}) = \frac{1}{2}\sum_{k=1}^{N} \mathcal{P}^2(k) + \omega_k^2 \mathcal{Q}^2(k) +$$

$$+\sum_{n=3}^{\infty} \frac{1}{n!} \sum_{k_1,\dots,k_n} \omega_{k_1}\cdots\omega_{k_n}\; \mathcal{Q}(k_1)\cdots\mathcal{Q}(k_n)\; \delta_{k_1,-(k_2+\cdots+k_p)}$$

Higly Non-Linear in Fourier modes

Anti Fermi-Pasta-Ulam

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- Non-equilibrium initial condition on the **wrong** variables, those which do not diagonalize the Hamiltonian

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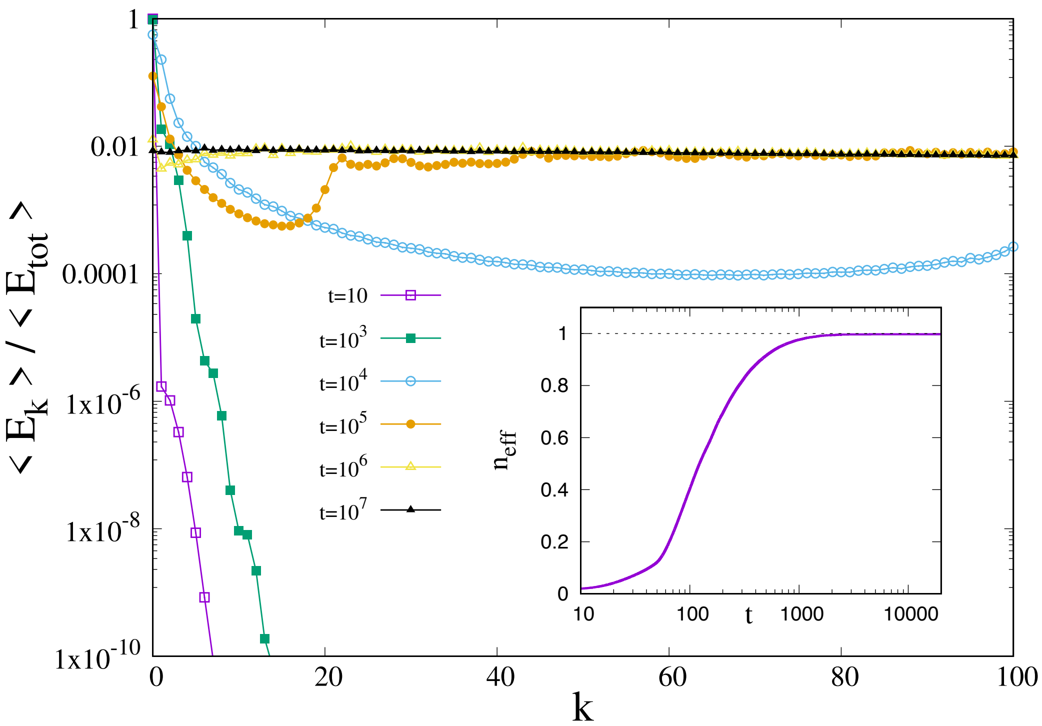
THE ANTI-FPU EXPERIMENT: RESULTS



$$n_{eff} = 1 \quad \text{Equipartition}$$

$$n_{eff} = 1/N \quad \text{Localization}$$

$$n_{eff} = \frac{\exp(S_{sp})}{N}$$

$$S_{sp} = -\sum_{k=1}^{N} u_k \log(u_k)$$

$$u_k = \langle E_k \rangle / \langle E_{tot} \rangle$$

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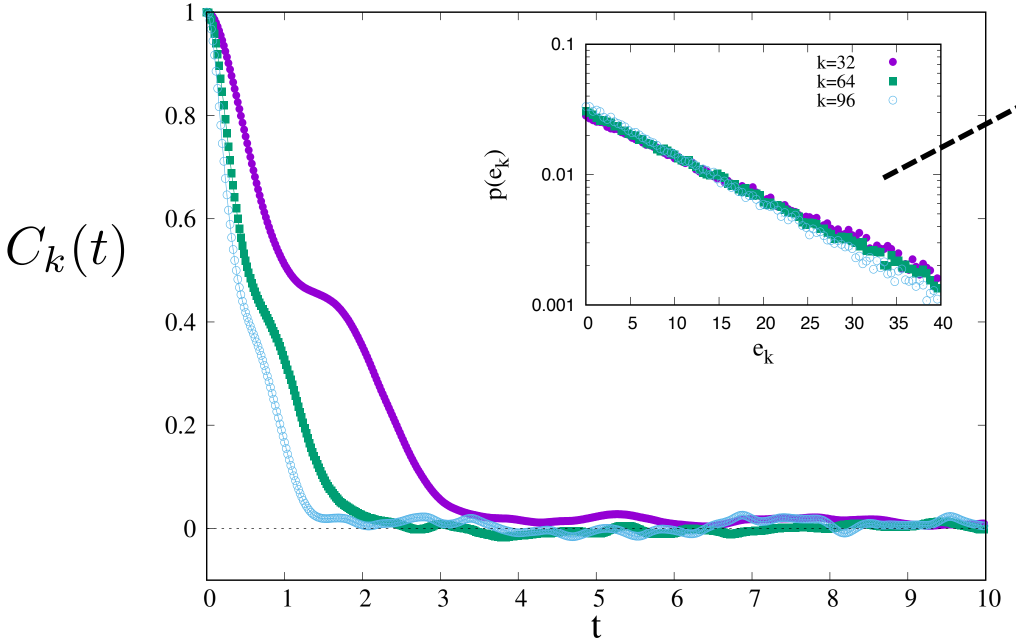
$$k = 1: \quad \omega_k^2 \mathcal{Q}^2(k) = \mathcal{P}^2(k) = cN$$

$$k \neq 1: \quad \omega_k^2 \mathcal{Q}^2(k) = \mathcal{P}^2(k) = 0$$

THE ANTI-FPU EXPERIMENT: EQUILIBRIUM

$$C_k(t) = \langle E_k(t) E_k(0) \rangle - \langle E_k \rangle^2$$



Oh! It looks like …

$$p(E_k) \sim \exp(-\beta E_k)$$

FOURIER MODES

$$\mathcal{Q}(k) = \sqrt{\frac{2}{N+1}} \sum_{i=1}^{N} q_i \ \sin\left(\frac{ik\pi}{N+1}\right)$$

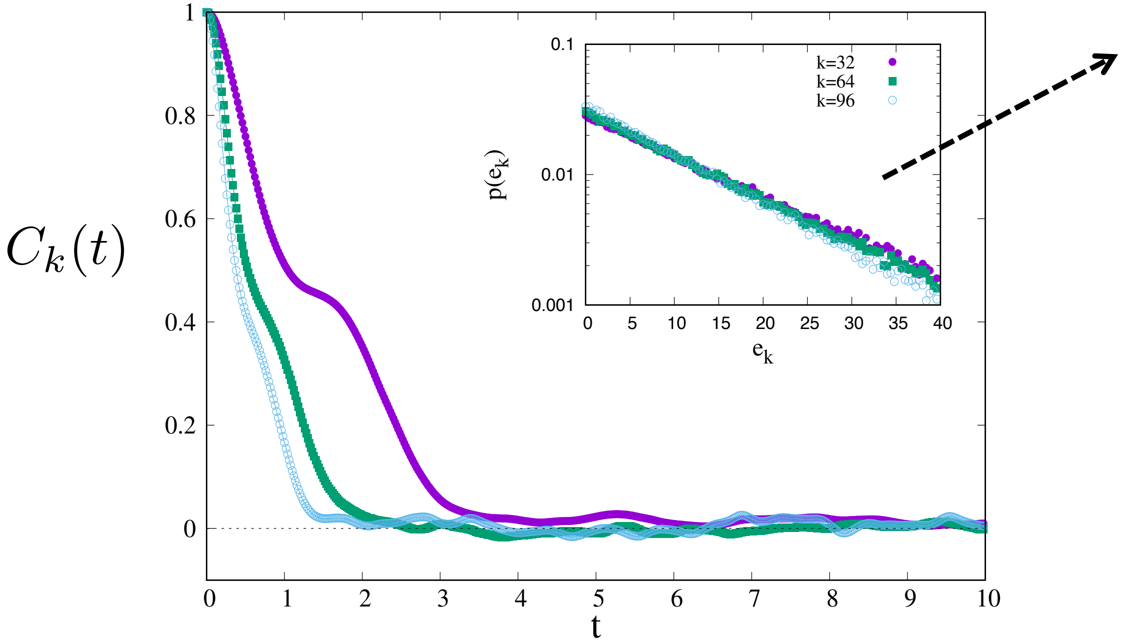
$$\mathcal{P}(k) = \ldots$$

EQUILIBRIUM INITAL CONDITION

$$\forall \ k : \quad \omega_k^2 \mathcal{Q}^2(k) = \mathcal{P}^2(k) = 1$$

THE ANTI-FPU EXPERIMENT: EQUILIBRIUM

$$C_k(t) = \langle E_k(t) E_k(0) \rangle - \langle E_k \rangle^2$$



Oh! It looks like …

$$p(E_k) \sim \exp(-\beta E_k)$$

Our integrable system:

- Relax to equipartition
- Decorrelates
- Has a Boltzmann distribution

OF COURSE … YOU HAVE TO LOOK AT THE WRONG CANONICAL VARIABLES

BGV Conjecture (Baldovin-Gradenigo-Vulpiani)

Whether or not a classical Hamiltonian system has reached thermal equilibrium cannot be said in general, BUT it is a statement relative to the choice of canonical variables

Footnote: The Hamiltonian dynamics (symplectic structure of the manifold) is general with respect to the choice of coordinates (it does not depend on them). This means that, even for an integrable system, there are infinitely many choices of canonical variables for which the Hamiltonian is non-diagonal.
For such coordinates equilibrium can be expected.

Von Neumann (quantum): ***'equilibrium' make sense with respect to a given choice of observables, irrespectively to integrability***

TODA (classica integrable): ***'equilibrium' make sense with respect to a given choice of variables, irrespectively to integrability***

BGV Conjecture (Baldovin-Gradenigo-Vulpiani)

Whether or not a classical Hamiltonian system has reached thermal equilibrium cannot be said in general, BUT it is a statement relative to the choice of canonical variables

Maybe we are wrong …
but at least we agree with him!

Von Neumann (quantum): ***'equilibrium' make sense with respect to a given choice of observables, irrespectively to integrability***

TODA (classical integrable): ***'equilibrium' make sense with respect to a given choice of variables, irrespectively to integrability***

THANKS FOR YOUR ATTENTION

'...any non-trivial idea is in a certain sense correct. ***The garbage of the past often becomes the treasure of the present (and vice-versa)'***

Alexander Polyakov

Footnote: 'vice-versa' = the trasure of the present becomes the garbage of the future