Title: Equilibration of Complex Quantum Systems in the Thermodynamic and Macroscopic Limits

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Abstract: There has been some significant recent progress on the long-standing problem of identifying the conditions under which equilibrium statistical mechanics can arise from an exact quantum mechanical treatment of the dynamics. I will give an overview of this progress, describing in particular how random matrix models and the associated concentration of measure phenomena imply that equilibration is generic even for the closed system evolution of pure quantum states. I will then discuss the relevance of these models to clarifying the conditions for quantum-classical correspondence of few-body chaotic systems. In particular, I will show that the Newtonian description of the dynamics of chaotic macroscopic bodies, remarkably, does not emerge from the underlying quantum mechanical description. These results suggest, under reasonable assumptions, that pure quantum states require a statistical interpretation.

Equilibration of Complex Quantum Systems

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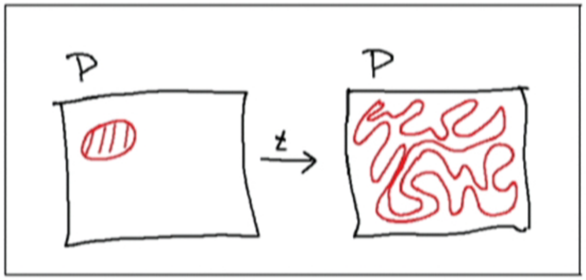
Equilibration: Background and Motivation

- An old and fundamental problem: how do generic properties of equilibrium statistical mechanics emerge from the underlying reversible mechanical theory, eg,
  - Justify the fundamental statistical postulate
  - Derivation of the 2nd Law
  - Derivation of the Gibbs state for systems in thermal equilibrium
- Basic idea of equilibration: values of physically accessible observables approach, and remain very close to, equilibrium values that:
  - (i) depend only on the energy, and
  - (ii) are independent of the details of the initial state.
- Both conceptual and practical aspects of this problem:
  - Under what *minimal conditions* and *on what time-scales* do physical systems equilibrate?

Classical Equilibration: Background

- For classical systems, recall Boltzman's idea of "ergodicity": a trajectory spends equal times in areas of equal measure.
  - Boltzman idea requires a notion of time-averaged measurements.
  - Ergodic hypothesis allows for substituting time-averages with phase space averages.
- But Gibbs requires mixing behaviour of phase space densities - *a stronger requirement* - for equilibration.



- Intrinsic chaos/mixing properties of dynamics now accepted as central to the answer of how and when systems equilibrate. ***
- Gibbs point of view only part of a "full explanation" - it does not account for individual measurements on individual systems.

Quantum Equilibration: Motivation

- For quantum systems, the necessary assumptions and conditions for equilibration are far less clear.
- In the quantum setting, modelling the ideas of *Boltzman and Gibbs* depends upon the *ontic v epistemic* interpretation of pure quantum states!!
- Is a dynamical **pure** quantum state analogous to an individual system's trajectory (ontic view) or to a time-evolving statistical ensemble (epistemic view)?
  - Under the **ontic** view, we *should* consider time-averages to reproduce Boltzman's approach.
  - Under the **ontic** view, we *should* construct mixtures of quantum states to reproduce Gibbs approach.
  - Under the **epistemic** view, we *should* see phenomena analogous to Gibbs' mixing condition directly in the dynamics of pure quantum states!

Equilibration of Complex Quantum Systems

Let's consider two important classes of "complex quantum systems":

- Many-body systems in the thermodynamics limit $n \gg 1$.
  - For n subsystems, each with Hilbert space $\mathbb{C}^{d_s}$, the full Hilbert space for the composite system is $(\mathbb{C}^{d_s})^{\otimes n}$
  - Typically restrict to an energy band $[E, E + \Delta E]$
  - Dynamics is then restricted to the subspace $\mathcal{H} = \mathbb{C}^D \subseteq (\mathbb{C}^{d_s})^{\otimes n}$
  - Here $D \gg 1$ even though ΔE is small.
- Few-body "quantum chaotic" systems in the macroscopic limit
  - "Quantum chaotic" means: quantum system whose classical counterpart is chaotic.
  - For action scale S: macroscopic limit is $\hbar/S \to 0$ or just "$\hbar \to 0$"
  - Dynamics occur in a Hilbert space $\mathcal{H} = \mathbb{C}^D$ for which $D \gg 1$.

Dynamical Problem under Consideration

- Let $\rho(0) = |\psi(0)\rangle\langle\psi(0)|$ be an initial pure state.
- Let $U(t) = \exp(-iHt)$ be a unitary describing the isolated, reversible dynamics of the system under Hamiltonian H.
- Consider some random *maximally fine-grained global observable* A acting on $\mathcal{H}$.
  - Take A to be non-degenerate with spectral decomposition $A = \sum_{k=1}^{D} a_k \hat{P}_k$.
  - Each of the eigenspaces $\hat{P}_k$ are rank-one projectors.
  - The eigenvalues a_k are just labels that don't really matter.
- The fundamental dynamical quantity is the time-dependent probability of outcome k of the observable A,

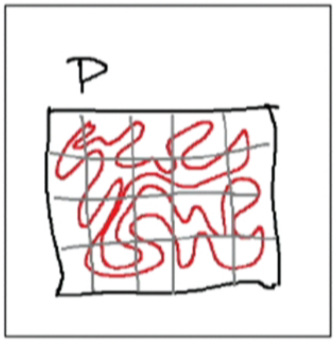
$$Pr(k|\psi(0), U(t)) = Tr\left[\hat{P}_k U(t)\rho(0)U(t)^\dagger\right].$$

Types of Equilibration

- **Microcanonical equilibration** of an isolated system: one expects relevant (macro) dynamical variables to equilibrate to their microcanonical values
  - Quantum microcanonical state is $\rho_{mc} = \mathbb{1}/D$ on the D-dimensional Hilbert space typically associated with an energy interval.
- **Thermal equilibration** of a subsystem: assuming weak coupling to a reservoir - the reduced state should equilibrate to the canonical ensemble (Gibbs state).
  - Interesting recent progress on this problem: Lloyd (1988), Popescu et al (2006):Linden et al (2009): Riera et al (2011), Brandao et al (2011), Masanes et al (2011), Vinayak and Znidaric (2011).
- Here we are primarily interested in the problem of microcanonical equilibration.
- What is the classical analog (classical limit) for this problem?

Equilibration to *Classical* Microcanonical Measure

- Classical microcanonical state: uniform measure on the energy shell (or the *accessible* phase space $\mathcal{P}$).
- Classically this is a **more fundamental problem** - the *fundamental statistical postulate* implies the canonical (thermal) state for small subsystems.
- Of course, microcanonical equilibration can not occur *exactly* for closed classical systems.



- Symplectic classical flow preserves volumes, so can only have microcanonical equilibration wrt a coarse-grained observable as $t \to \infty$.

Microcanonical Equilibration for Quantum Observables

Microcanonical equilibration can not occur *exactly* also for isolated quantum systems.

- In quantum setting, unitary evolution preserves purity, so one can never reach $\rho_{mc} = \mathbb{1}/D$ from any other initial state.
- So, we consider equilibration wrt to maximal observables on the Hilbert space $\mathbb{C}^D$:

For finite-dimensional quantum systems, all quantum observables have an "intrinsic" discretization due to discrete spectrum!

- This is great: unlike the classical case, there's no fundamental requirement for coarse-graining!

Specification of the Problem

- Working in the eigenbasis of A, we can write $U(t) = CF(t)C^\dagger$
- For definiteness, take an initial state which is an eigenstate of the observable A, namely $\rho(0) = \hat{P}_i = |a_i\rangle\langle a_i|$.
- Our dynamical quantity of interest is

$$Pr(k|i, C, F(t)) = Tr\left[\hat{P}_k CF(t)C^\dagger \hat{P}_i CF(t)^\dagger C^\dagger\right].$$

- Starting from the localized state $\hat{P}_i$, does $Pr(k|i, C, F(t)$ approach the microcanonical value $Pr(k|\rho_{mc}) = 1/D$, on a time-scale t_{eq} and remain *effectively indistinguishable* from it for almost all $t > t_{eq}$?
- **Definition:** If the above property holds, for some H and some finite t_{eq}, we say that H **equilibrates** wrt to A.

C is the matrix that diagonalizes

U in the basis of A.

Outline of Results and their Implications

Proof that equilibration wrt A occurs for *almost all* Hamiltonians H:

- First we show that
  - (i) $\mathbb{E}\{Pr(k|i, C, F(t))\} \simeq O(1/D)$
  - (ii) $\mathbb{V}\{Pr(k|i, C, F(t))\} \simeq O(1/D^2)$

  hold for all t after some t_{eq}, where the averages are taken wrt a natural measure on the space of Hamiltonians.
- Then argue that the size of fluctuations implied by (ii) is strong enough to conclude that the predictions for pure quantum states are **indistinguishable** in practice from those of the quantum (and classical!) microcanonical states.

Outline of Results and their Implications

- While this shows that equilibration is generic, it is a mathematical result about equilibration for "typical" Hamiltonians drawn from a random matrix ensemble (RMT model).
  - For example, it could be that actual physical systems are not representative of "typical" Hamiltonians from the ensemble.
- Motivate the physical relevance of RMT typicality by reviewing some of the successes of RMT and clarifying the kinds of physical properties which RMT is known to predict reliably.
- The physical relevance of the RMT model will also be supported with numerical evidence for:
  - (a) an ensemble of random 2-local Hamiltonians, showing that typical members of this ensemble also satisfy the equilibration conditions (i) and (ii); and
  - (b) an individual dynamical model that equilibrates (due to chaos) and demonstrate it too satisfies conditions (i) and (ii).

Outline of Results and their Implications

- The proof of (i) and (ii) suggests a minimal condition on the complexity of a system's eigenvectors which leads to a nice relationship between the equilibration time and the spectral form factor.
- Also, we have a condition of sufficient complexity based on the statistics of an individual system's eigenvector components.
- Finally I will discuss the dramatic implications of these results:
  - (a) debunk the myth that the emergence of classicallity requires decoherence,
  - (b) argue for the absence of a proper Newtonian limit for quantum mechanics (eg Hyperion),
  - (c) present arguments for a statistical interpretation of the quantum state.

RMT Model: GUE

- We take H uniformly at random from the Gaussian Unitary Ensemble, the unique RMT ensemble which satisfies:
  - (1) invariance of the distribution $P(H)dH$ under any unitary transformation $H \to UHU^\dagger$,
  - (2) the joint distribution over all elements of H is a product of distributions over each element of H.
- This implies the probability distribution of H for GUE:

$$P(H) = c_1 e^{-\frac{1}{2\sigma^2} Tr[H^2]},$$

w.r.t the Lebesgue measure on the matrix elements of H.

- For GUE, the ensemble of diagonalizing matrices C are distributed according to Haar measure on $U(D)$.

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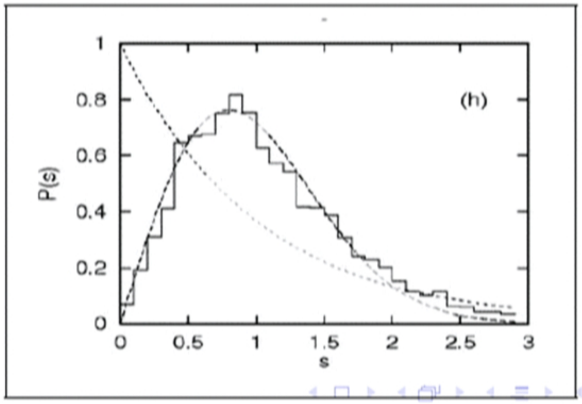
RMT models for physical systems

RMT models (GUE, GOE etc) proposed by Wigner as model of level structure of heavy nuclei

- Now widely used as models for other *many-body* complex systems, eg quantum transport in mesoscopic structures.
- RMT models also widely successful for modeling *few-body* systems from "quantum chaos"
  - Random matrix conjecture of Bohigas, Giannoni, and Schmit (1984) now often taken to define quantum chaos.
- Eg, RMT predicts accurately short-range "level repulsion", eg level-spacing distribution P(s).



RMT models: relevance and limitations

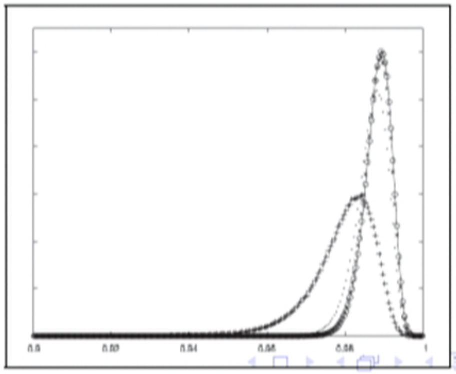
- For GUE/GOE etc, the eigenvectors are an orthogonal set of random quantum states.
  - For chaotic quantum systems, numerical evidence that energy eigenstates also look like "random states" in the basis of typical observables - Zyzckowski (1990), Kus and Zyzckowski (1991), Haake (1991), Emerson et al (unpublished).
- There is growing evidence that the complexity and randomness of eigenvectors of GUE is generic for short sequences of random interactions, viz random circuits, Emerson et al (2003), Brandao et al (unpublished).
- However, RMT is not a good model of long-range level structure and shape of level density of physical systems!

RMT models and Concentration of Measure

Crucial concept for modeling individual systems by ensemble average: concentration of measure!

- Why do, eg energy level spacings, for an individual system match those of an RMT ensemble average?
- The energy level spacing for "almost all" elements of the ensemble are narrowly concentrated about the ensemble mean.
- This is an extremely generic phenomena for GUE, Haar-measure on $U(D)$, Fubini-Study measure on $\mathbb{C}^D$, etc.

- Eg, distribution of entanglement for random quantum states for $n = 10$ qubits.



Main Theorem: Equilibration for GUE

- There exists a finite time $t_{eq}(D)$, such that for all $t > t_{eq}(D)$, the mean and variance over GUE satisfy:

$$\text{(i)}\ \ \mathbb{E}\{Pr(k|i, U(t))\} = \frac{\delta_{ik} + 1}{D + 1} + O(D^{-2})$$

$$\text{(ii)}\ \ \mathbb{V}\Big\{Pr(k|i, U(t))\Big\} = \frac{2\delta_{ik} + 1}{D^2} + O(D^{-3})$$

- **Key point:** the probabilities converge to a uniform distribution as $D \to \infty$ because, *remarkably*, pure state fluctuations become vanishingly small in this limit!!
- By Chebyshev inequality, for individual U drawn from the ensemble, the probability that $Pr(k|i, t)$ deviates by $O(1)$ from the maximally mixed state (mc state) is less than $O(1/D^2)$.
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Dynamical pure states indistinguishable from mixed states

- For these fluctiaitons, we expect at least $O(D^{1/4})$ trials required to distinguish pure state fluctuations from the mc state.
- **Key Point:** Without imposing any coarse-graining on the measurements, and without assuming mixed states, it follows that pure quantum states are indistinguishable from the completely mixed state assuming only realistic conditions:
  - (i) One can not prepare and measure the system $O(D^{1/4})$ times.
  - (ii) One can not classically compute the details of the dynamical state (because it is in an inaccessibly large Hilbert space). ***
  - (iii) One can not perform entangling measurements across multiple/joint copies of the physical system.

Time-scale of equilibration for GUE

- From the GUE spectrum we get

$$t_{eq}(D,\sigma) = O\left(\frac{1}{D^{1/6}\sigma}\right).$$

- Here σ is the free parameter in GUE - set by energy scale of underlying physical model.
- Masanes et al (2011), and Visnayak and Znidaric (2011) examine GUE models to estimate time-scale of subsystem equilibration.
- Surgeon General's Warning: In general the GUE model for the spectrum is NOT faithful for modeling large-scale energy variations and hence short-time behaviours of physical systems!

Time-scale of equilibration for GUE

- By averaging only over Haar-measure on eigenvectors, one obtains a general relation connecting the spectral form factor $\mu(t) := Tr[U(t)] = Tr[F(t)]$ to the time-dependence of the observable:

$$\mathbb{E}_C\{Pr(k|i, C, F(t))\} := \int_{\mathbb{U}(D)} Tr\left[\hat{P}_k CF(t)C^\dagger \hat{P}_i CF(t)^\dagger C^\dagger\right]\mu_H(dC)$$

$$= \frac{D - \frac{1}{D}|\mu(t)|^2 + \delta_{ik}\left(|\mu(t)|^2 - 1\right)}{D^2 - 1},$$

- So if the spectral form factor can be approximated or measured (eg, efficiently with the DQC1 model of quantum computation), then one can infer the equilibration time-scale; similar result in Brandao et al (2011).

Sufficient Conditions for Equilibration

- The GUE has Haar-random eigenvectors - which is a strong assumption.
  - Can we clarify the minimal sufficient conditions on the degree of randomness of the eigenvectors?
- A sufficient condition on the ensemble which implies (i) and (ii) is that the diagonalizing matrices form a *unitary 4-design* (Dankert et al, 2006/2009).
- In particular we only need the mean and variance of eigenvector components of the ensemble to satisfy
  - (i) $\mathbb{E}\{|C_{i,j}|^2|C_{k,j}|^2\} \simeq O(1/D^2)$
  - (ii) $\mathbb{V}\{|C_{i,j}|^2|C_{k,j}|^2\} \simeq O(1/D^4)$
- Sightly weaker condition than Brandao et al (2011) and Masanes et al (2011) found in the context of subsystem equilibration for GUE models.

Numerical evidence for random 2-local Hamiltonian models

- It's interesting to examine whether these minimal complexity assumptions hold in a more physically realistic ensemble of Hamiltonians.
- We consider the ensemble of random 2-local Hamiltonians of n-qubits:

$$H = \sum_{j=1}^{n} \sum_{p=\{X,Y,Z\}} a_{j,p}\sigma_j^p + \sum_{j=1}^{n} \sum_{k \neq j} \sum_{p,q=\{X,Y,Z\}} a_{j,k,p,q}\sigma_j^p \sigma_k^q$$

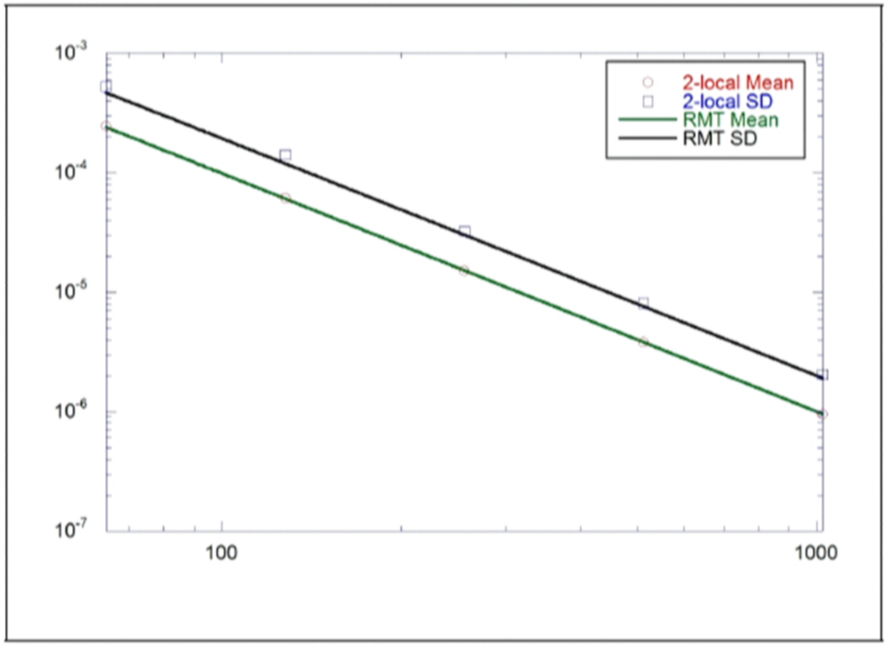
  where the coefficients a are chosen randomly from the Gaussian distribution $\mathcal{N}(0, 1)$.
- We also examine the time-scale of equilibration as n increases, where $D = 2^n$.

Sufficent Complexity of eigenvectors for random 2-local Hamiltonian models

- Mean and variance of the (2,2)-products,

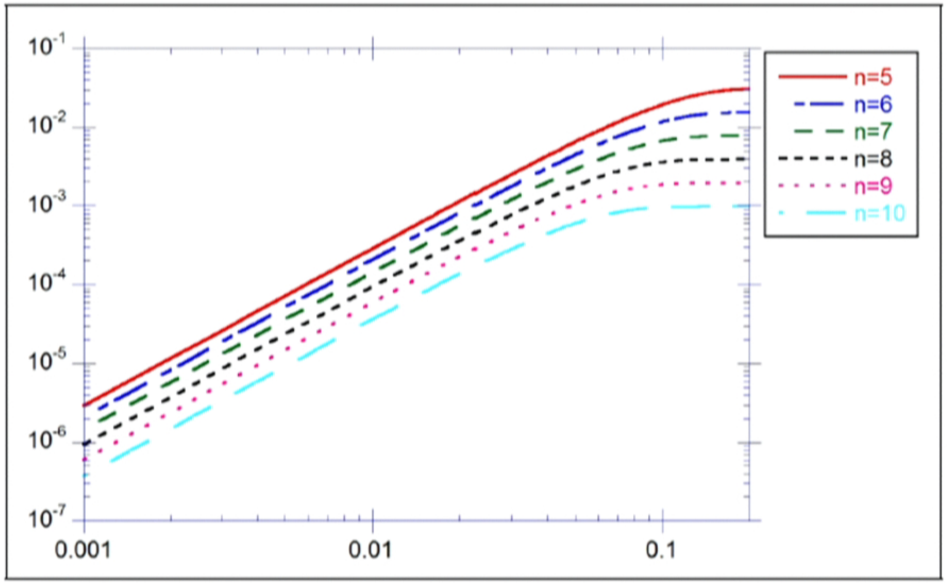
$$|C_{i,j}|^2|C_{k,j}|^2$$

of eigenvector components vs D.



Dynamical Equilibration of Probabilities for random 2-local Hamiltonian models

- Average $Pr(k|i)$ vs time for $k \neq i$
- Equilibration time-scale $t_{eq} \sim \sqrt{n}/||\mathrm{H}||$



What about Individual Physical Systems?

A physical system is *not* (**!**) drawn from a random ensemble.

- When will an individual physical model exhibit equilibration?
- Consider the following decomposition (suggested by P. Hayden):

$$Pr(k| \quad |a_i\rangle, C, F(t)) = \sum_l \exp(-i\theta_l(t)) \sum_{m,n \in z^{-1}(\theta_l \pm (\Delta\theta)/2)} C_{k,m}\overline{C}_{i,m}C_{i,n}\overline{C}_{k,n}.$$

  where $z(m, n) = \exp(-i(\phi_m - \phi_n)t)$, and we've discretized z into D bins centered on $\theta_l = 2\pi l/D$, each of width $\Delta\theta = 2\pi/D$.
- One can show that, for t large enough that the distribution of phases is uniform on the unit circle, then

$$Pr(k|i) \simeq)(1/D)$$

  provided that the **mean** and **second moment** of the products $C_{km}C_{im}C^*_{in}C^*_{kn}$ are Haar-distributed ***.

From Ensembles to Individual Systems

Let's look at whether an *individual dynamical system*, in particular a few-body model with classically chaotic counterpart, can exhibit equilibration for dynamical pure states.

- Quantum kicked top:

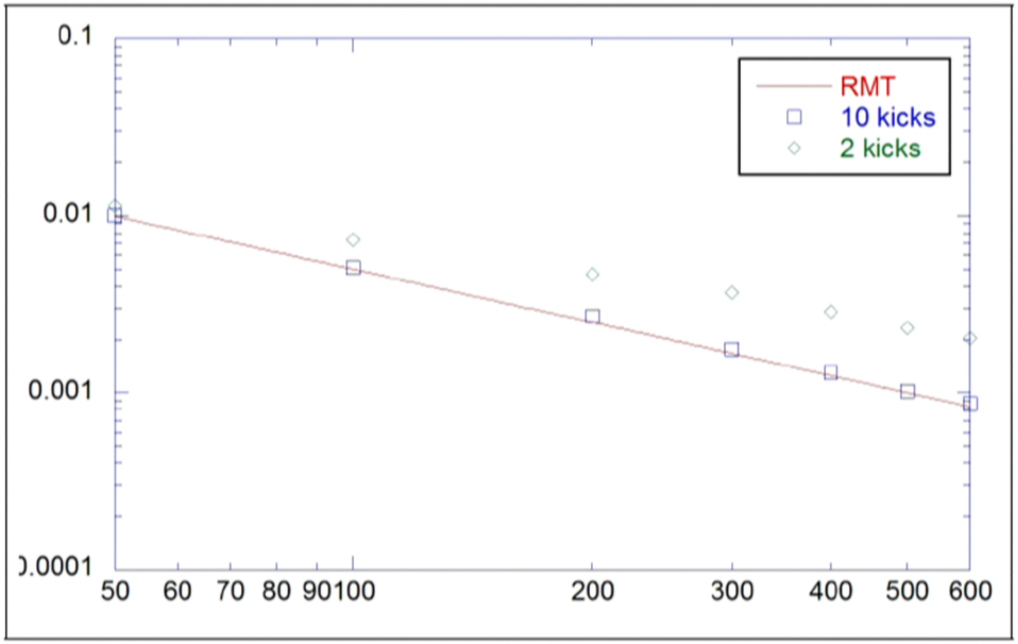
$$\begin{aligned} U \; = \; & \exp(-i\tau_3 J_z^2/(2j+1) - i\alpha_3 J_z) \\ & \exp(-i\tau_2 J_y^2/(2j+1) - i\alpha_2 J_y) \exp(-i\tau_1 J_x^2/(2j+1) - i\alpha_1 J_x) \end{aligned}$$

  where $\vec{J}$ is an angular momentum operator satisfying the usual commutation relations.

- Here the macroscopic limit corresponds to a sequence of irrep's of this model with increasing j, where $D = 2j + 1$.
- We consider a choice of parameters where the classical model is fully chaotic.

Dynamical Equilibration of Quantum Kicked Top

- Mean and variance of $Pr(k|i)$ vs system size j
- Results for both $t < t_{eq}$ and $t > t_{eq}$... Wow!



Dynamical Equilibration of Quantum Kicked Top

- In particular, for initially localized pure quantum states, observables equilibrate on a time-scale

$$t_{eq} \simeq \lambda^{-1} \log(D),$$

  with equilibrium fluctuations for $t > t_{eq}$ that decrease precisely as per the RMT scaling of Haar-random states!!
- See Emerson and Ballentine (2001) for another numerical model showing this RMT same scaling. ***
- The RMT analysis presented earlier supports the idea that numerical results for these dynamical models are in fact typical !!
- In this and other models, as D increases the pure state dynamics converge to the predictions of the associated 11classical" model...
  - but we get the predictions of Liouville dynamics rather than the Newtonian dynamics!

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Hyperion

Hyperion is a potato shaped satellite of Saturn with a chaotic tumble and positive Lyapunov exponent.

- Berry and Zurek have argued that according to quantum chaos, an initially localized pure state of Hyperion will spread out over macroscopic dimensions on the time-scale $t \simeq 20$ years!!
- In order to deal with this (interpretational) embarrasment, Berry and Zurek invoke the ubiquitous effects of decoherence in order to wash away any possibility of “macro-coherence”, which is somehow an affront to direct observation...

Hyperion

- Macro-coherence of complex dynamics is in fact almost impossible to detect
  - ... without access to extraordinary computational resources or extraordinary experimental control of the system in question.
- Moreover, with or without decoherence, quantum mechanics does not offer an ontological story for Hyperion's time-dependent properties over physical time-scales.
- To get such a story, we need to supplement pure quantum states with some ontology.

Summary

- For complex systems, pure quantum states generically equilibrate in the same qualitative and quantitive manner that Liouville (statistical) densities do.
- The sufficient conditions for this equilibration are that
  - (i) the Hamiltonian eigenvector components meet some limited randomness condition (4-design condition) in the basis of the observable, and
  - (ii) the spectrum and gaps satisfy some reasonable conditions, such as sufficient non-degeracy.
- These results are motivated
  - (i) Analytically using RMT arguments.
  - (ii) Numerically for more physically realistic ensembles and model dynamical systems.

Summary

- Emergent classicality under physically realistic set of conditions without decoherence!
  - The classical statistical description of an individual system emerges for pure quantum states (states of maximal knowledge) without adding decoherence or coarse-graining of measurements.
- On the other hand, it appears that the Newtonian theory of macroscopic dynamics does not emerge from the quantum description!
  - So some additional beables must be specified to recover the Newtonian description ;-)
  - Or simply abandon the belief that the moon of Hyperion is there when no is looking ;-(.
- None of these results are surprising, in fact they are even expected, under a statistical/epistemic interpretation of pure states. See Emerson, quant-ph/0211035 for more details!

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Some Final Thoughts

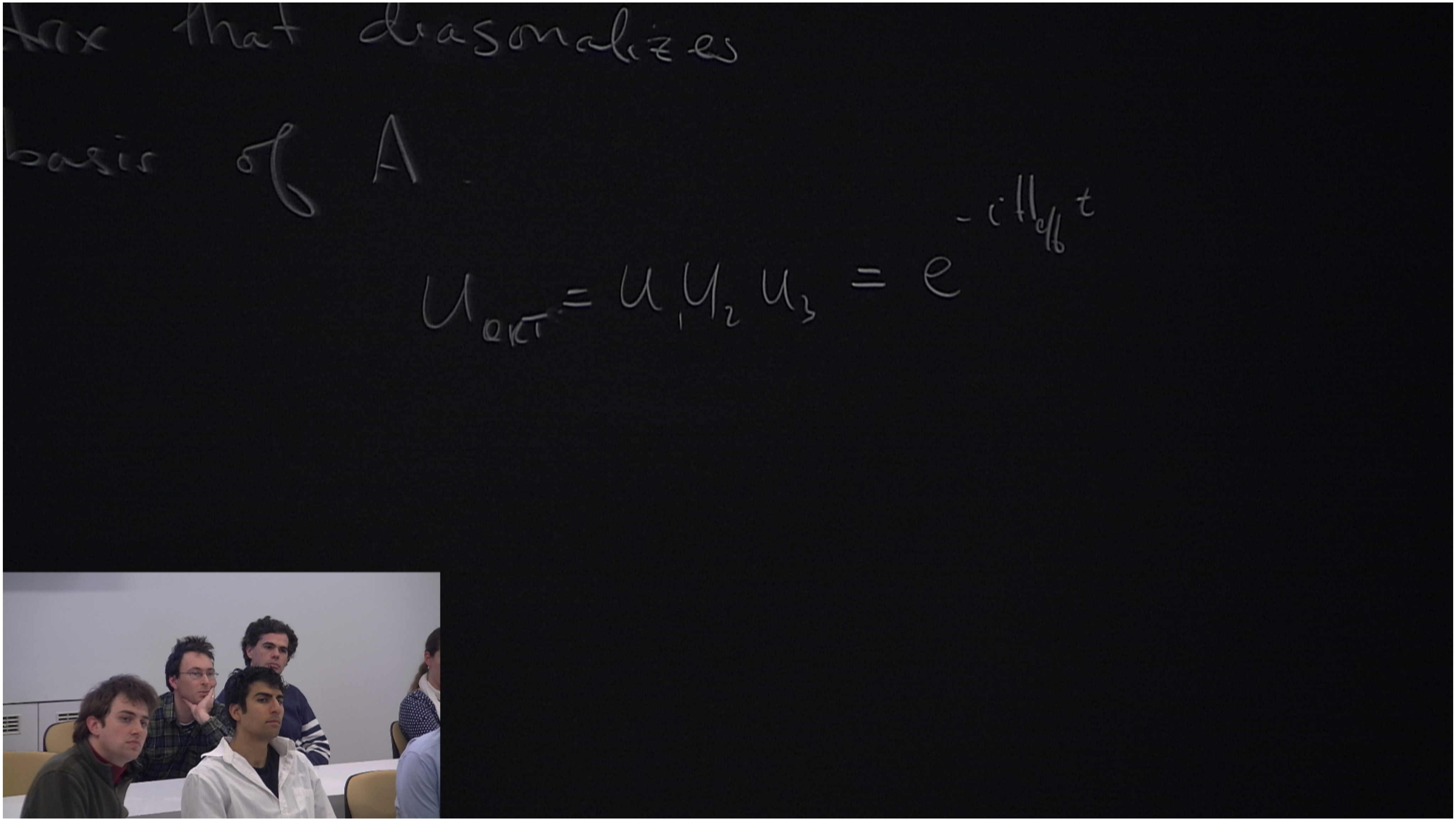
R. Feynman (1965)

"I think that I can safely say that nobody understands quantum mechanics."

On a more speculative note:

- What is the classical limit of quantum gravity?
- Can these results help clarify the more general, non-Newtonian, states that may be expected in the non-relativistic and macroscopic limit of a theory of quantum gravity?
- Emergent properties may not be those of Newtonian propeties/trajectories, but can instead be highly delocalized, and still enirely classical, *statistical* states.

Thank you for your attention!


that diagonalizes
basis of A.
U_ext = U_1 U_2 U_3 = e^{-iH_eff t}