Entanglement and the Foundations of Statistical Mechanics

Thiago R. De Oliveira
partly in collaboration with P. Zanardi and S. Garnerone
Motivations

- Foundations of Statistical Mechanics
  - Static Properties
    - How to justify the use of ensembles averages
    - Why equal a priori probabilities
    - How about the Quantum setting?
Motivations

- **Foundations of Statistical Mechanics**
  - Static Properties
    - How to justify the use of ensembles averages
    - Wy equal a priori probabilities
    - How about the Quantum setting?
  - Dynamics
    - How equilibration occurs
    - Equilibration Times
Motivations

- **Foundations of Statistical Mechanics**
  - Static Properties
    - How to justify the use of ensembles averages
    - Why equal a priori probabilities
    - How about the Quantum setting?
  - Dynamics
    - How equilibration occurs
    - Equilibration Times

- **Practical Questions**
  - Easier way to obtain thermal averages?
  - New experiments with optical lattices
Disclaimer

- I will mainly review the “new” quantum information approach to these old questions
Disclaimer

- I will mainly review the “new” quantum information approach to these old questions
- I am not very familiar with all the previous literature
Disclaimer

- I will mainly review the “new” quantum information approach to these old questions
- I am not very familiar with all the previous literature
  - Hope to learn some old solutions
Typicality

- Macroscopic information $|\psi\rangle \in H_R$
- Two options
  - Assume
    $$\Omega = \frac{1}{d_R}$$
  - Look at the system
    $$\Omega_S = Tr_B[\Omega]$$
Typicality

- Macroscopi information $|\psi> \in \mathcal{H}_R$
- Two options
  - Assume $\Omega = \frac{1}{d_R}$
  - Look at the system
    $$\Omega_S = Tr_B[\Omega]$$
- $Pr(\psi)$ uniform: $\overline{\rho}_S = \Omega_S$
- Pick a random $|\psi>$ with $Pr(\psi)$
  - $\rho = |\psi><\psi|$
  - $\rho_S = Tr[|\psi><\psi|]$
Typicality

- Macroscopic information \(|\psi\rangle \in \mathcal{H}_R\)
- Two options
  - Assume \(\Omega = \frac{1}{d_R}\)
  - Look at the system
    \[ \Omega_S = \text{Tr}_B[\Omega] \]
  - \(\text{Pr(}\psi)\) uniform: \(\rho_S = \Omega_S\)
  - What is the difference?
    \[ D_1 = \|\rho_S - \bar{\rho}_S\|_1 \quad \text{ou} \quad \text{Tr}[O\rho_S] - \text{Tr}[O\bar{\rho}_S] \]
Concentrations of measure

- Function $f: V^n \rightarrow \mathbb{C}$
- If $f$ does not oscillate much it is almost constant for $n \gg 1$

\[
\text{Prob}\left\{ |f - \bar{f}| \geq \epsilon \right\} \leq k_1 \exp(-k_2 \epsilon^2 n / \eta^2)
\]

\[
\eta \equiv \sup_{U_1 \neq U_2} \frac{|f(U_1) - f(U_2)|}{\|U_1 - U_2\|_2}
\]
Entanglement and the foundations of statistical mechanics

SANDU POPESCU¹,², ANTHONY J. SHORT¹* AND ANDREAS WINTER³

¹H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK
²Hewlett-Packard Laboratories, Stoke Gifford, Bristol BS12 6QZ, UK
³Department of Mathematics, University of Bristol, University Walk, Bristol BS8 1TW, UK
*e-mail: tony.short@bristol.ac.uk

\[
\overline{D_1} \leq \sqrt{\frac{d_S^2}{d_B}} \quad \text{Prob} \left[ D_1 \geq \epsilon + \sqrt{\frac{d_S}{d_B}} \right] \leq 2e^{-Cd_B\epsilon^2}
\]

- Typically \( \rho_\Sigma \approx \Omega_\Sigma \)
  - Principle of apparently equal \( a \ a \ priori \) probabilities
  - Entanglement is the responsible for the local ignorance
Canonical Typicality

Abstract

Download: PDF (76 kB)   Export: BibTeX or EndNote (RIS)

Sheldon Goldstein\textsuperscript{1,*}, Joel L. Lebowitz\textsuperscript{1,†}, Roderich Tumulka\textsuperscript{2,‡}, and Nino Zanghì\textsuperscript{3,§}

\textsuperscript{1}Departments of Mathematics and Physics, Hill Center, Rutgers, The State University of New Jersey, 110 Frelinghuysen Road, Piscataway, New Jersey 08854-8019, USA
\textsuperscript{2}Mathematisches Institut, Eberhard-Karls-Universität, Auf der Morgenstelle 10, 72076 Tübingen, Germany
\textsuperscript{3}Dipartimento di Fisica dell’Università di Genova and INFN sezione di Genova, Via Dodecaneso 33, 16146 Genova, Italy

Received 4 November 2005; published 8 February 2006

It is well known that a system $S$ weakly coupled to a heat bath $B$ is described by the canonical ensemble when the composite $S+B$ is described by the microcanonical ensemble corresponding to a suitable energy shell. This is true for both classical distributions on the phase space and quantum density matrices. Here we show that a much stronger statement holds for quantum systems. Even if the state of the composite corresponds to a single wave function rather than a mixture, the reduced density matrix of the system is canonical subspace corresponding ensemble. This clarifies, e
Typicality for Generalized Microcanonical Ensembles

Abstract

For a macroscopic, isolated quantum system in an unknown pure state, the expectation value of any given observable is shown to hardly deviate from the ensemble average with extremely high probability under generic equilibrium and nonequilibrium conditions. Special care is devoted to the uncontrollable microscopic details of the system state. For a subsystem weakly coupled to a large heat bath, the canonical ensemble is recovered under much more general and realistic assumptions than those implicit in the usual microcanonical description of the composite system at equilibrium.
Summary

- Typicality may help to understand the use of ensemble averages
  - Ignorance about the system is objective and unavoidable due to entanglement
- Type of ergodic argument
Problems

- Nature does not explore the whole Hilbert Space

- Dynamics
  - Equilibration
  - Independence from details of the initial condition
  - Eq. state has to be in the Boltzamann form
Quantum mechanical evolution towards thermal equilibrium

Abstract

Received 2 February 2009; published 4 June 2009

The circumstances under which a system reaches thermal equilibrium, and how to derive this from basic dynamical laws, has been a major question from the very beginning of thermodynamics and statistical mechanics. Despite considerable progress, it remains an open problem. Motivated by this issue, we address the more general question of equilibration. We prove, with virtually full generality, that reaching equilibrium is a universal property of quantum systems: almost any subsystem in interaction with a large enough bath will reach an equilibrium state and remain close to it for almost all times. We also prove several general results about other aspects of thermalization besides equilibration, for example, that the equilibrium state does not depend on the detailed microstate of the bath.

Foundation of Statistical Mechanics under Experimentally Realistic Conditions

Peter Reimann
Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

Received 19 September 2008; published 7 November 2008

We demonstrate the equilibration of isolated macroscopic quantum systems, prepared in nonequilibrium mixed states with a significant population of many energy levels, and observed by instruments with a reasonably bound working range compared to the resolution limit. Both properties are satisfied under many, if not all, experimentally realistic conditions. At equilibrium, the predictions and limitations of statistical mechanics are recovered.
Dynamical Typicality

\[ |\psi_0\rangle = \sum c_n |E_n\rangle \]

\[ |\psi(t)\rangle = \sum c_n e^{-iHt} |E_n\rangle \]

\[ \langle A(t) \rangle \text{thermalizes?} \]

\[ \bar{\rho} = \lim_{T \to \infty} \frac{1}{T} \int \rho(t) \, dt = \sum |c_n|^2 |E_n\rangle \langle E_n| \]

\[ (A(t) - \bar{A})^2 \leq \| A \| \text{Tr} [\bar{\rho}^2] \]
Dynamical Typicality

\[ (A(t) - \overline{A})^2 \leq \|A\| \text{Tr} [\overline{\rho^2}] \]

- A (t) thermalizes if
  - A is a sum of local operators
  - There are non-degenerated gaps
  - Initial state is distributed over many eigenstates

- Thermal state depends on the initial
- Equilibration time \( \sim \frac{1}{\text{gap}} \)
Probing the relaxation towards equilibrium in an isolated strongly correlated one-dimensional Bose gas

S. Trotzky$^{1,2,3}$*, Y-A. Chen$^{1,2,3}$, A. Flesch$^{4}$*, L. P. McCulloch$^{5}$, U. Schollwöck$^{1,6}$, J. Eisert$^{6,7,8}$
and I. Bloch$^{1,2,3}$
Dynamical Typicality

- There is “local” equilibration for
  - Hamiltonians with not a lot of degenerated gaps
  - Most of the initial states
- Source of equilibration is entanglement
- Ergodic Theorem?
- But
  - Equilibration state depend on the initial state
  - Equilibration time scales $\exp(N)$
    - Similar to quantum recurrence time
Showing results 1 through 1 (of 1 total) for au:von_Neumann

1. arXiv:1003.2133 [pdf, ps, other]
   Title: Proof of the Ergodic Theorem and the H-Theorem in Quantum Mechanics
   Authors: John von Neumann
Beweis des Ergodensatzes und des \( H \)-Theorems in der neuen Mechanik.


(Eingegangen am 10. Mai 1929.)

Es wird gezeigt, wie der scheinbare Widerspruch zwischen dem makroskopischen Ansatz des Phasenraumes und dem Bestehen von Unbestimmtheitsrelationen aufzulösen ist. Danach werden die hauptsächlichsten Begriffsbildungen der statistischen Mechanik quantenmechanisch umgedeutet, der Ergodensatz und das \( H \)-Theorem formuliert und (ohne „Unordnungsannahmen“) bewiesen. Es folgt eine Diskussion des physikalischen Sinnes der ihren Gültigkeitsbereich festlegenden mathematischen Bedingungen.
Summary

- Typicality may help to understand the use of ensemble averages
  - Ignorance about the system is objective and unavoidable due to entanglement
- Dynamic thermalization may also originate on entanglement
- New approach?
  - von Neumann, Boltzmann
- Time scale?
- Which observables equilibrate?
- Eigenstate Thermalization hypotheses
Problems

• Nature does not explore the whole Hilbert Space

• Typicality for a set of “physical” states
  – Not unique choice
Matriz Product States (MPS)

\[ |\psi\rangle = \text{tr}[A_{i_1}^{[1]} A_{i_2}^{[2]} \ldots A_{i_N}^{[N]}]|i_1 i_2 \ldots i_N\rangle \]

- \(A_k\) is matrix of dimension \(\chi \times \chi: d^N \Rightarrow N \times d \times \chi^2\)
- \(\chi\) is the fundamental parameter
- DMRG is a variational method in the MPS set
- Good approximation for 1D local hamiltonians with gap
- Obey the area law for entanglement
- Can describe any state for \(\chi \sim d^N\)
Tipicalidade para MPS

- Observable in L sites: $\hat{O}$

$$-Pr\left[|O - \bar{O}| \geq \epsilon \right] c_1 \exp\left[-c_2 \epsilon^2 \frac{\chi(N)}{N^2}\right]$$

- Bound is exponential in N
  - $\chi$ has to scale poly(N)
Resultados Numéricos

- Partículas de Spin $\frac{1}{2}$
  - $\hat{O} = S_x$
  - Variance

Figure 5: (a) The variance of the expectation value of $\sigma_x$ ($L = 1$) increasing the size of the system and for fixed but different values of $\chi = 2, 4, 6, 8, 12, 20, 50, 100$, and 180 (from top to bottom). (b) The variance of the expectation value of $\sigma_x$ ($L = 1$) for increasing system size when the MPS dimension increases linearly with the number of particles in the bath: $\chi = N - L$. 

Typicality for MPS

- Typicality can also arise for a physically accessible smaller set of states
- But our ensemble does not have any specific physical property
  - Infinity temperature thermal state
  - How to restrict to MPS with some given energy
Thermal Pure States

- One does not need a strictly uniform distribution for the microcanonical
- Use the power method to change the ensemble
  - Thermal pure quantum states at finite temperature, Sho Sugira and Arika Shimizu PRL 108, 240401 (2012)
  - $\mathbb{I} - \left( \frac{H - E}{\sigma} \right)^2$
Thermal Pure States

- After $K \gg 1$ interactions

\[
|\psi\rangle\langle\psi|^k = A^k |\psi\rangle\langle\psi| A^k \sim A^{2k}
\]

\[
A^{2k} \overset{k \gg 1}{\longrightarrow} \sum_{|\frac{E_i - E}{\sigma}| \ll 1} \left[ 1 - \left(\frac{E_i - E}{\sigma}\right)^2 \right] |E_i\rangle\langle E_i|
\]

\[
\sim \sum_{|\frac{E_i - E}{\sigma}| \ll 1} \exp\left[-2k \left(\frac{E_i - E}{\sigma}\right)^2 \right] |E_i\rangle\langle E_i|
\]
Thermal Pure MPS

- XXX spin chain in external magnetic field

*Figure:* Magnetization for the Heisenberg chain with external field for different values of $E$ and $N = 50$ and $\chi = 16$
Thermal Pure MPS

- See also
  - Minimally entangled typical quantum states at finite temperature, Steven R. White PRL 102, 190601 (2009)
Conclusions

- Tipicality may help to better understand the foundations of statistical mechanics
- May also be of practical use to simulate thermal states
- Still open questions
  - Time scale
  - Physical properties responsible for the equilibration: integrability versus caos?
- Not really a new approach
  - But mathematically more well founded
Thermal Equilibrium of a Macroscopic Quantum System in a Pure State

Sheldon Goldstein,1,* David A. Huse,2,† Joel L. Lebowitz,3,‡ and Roderich Tumulka4,§

1Department of Mathematics, Rutgers University, Hill Center, 110 Frelinghuysen Road, Piscataway, New Jersey 08854-8019, USA
2Department of Physics, Princeton University, Jadwin Hall, Washington Road, Princeton, New Jersey 08544-0708, USA
3Departments of Mathematics and Physics, Rutgers University, Hill Center, 110 Frelinghuysen Road, Piscataway, New Jersey 08854-8019, USA
4Department of Mathematics, Rutgers University, Hill Center, 110 Frelinghuysen Road, Piscataway, New Jersey 08854-8019, USA

(Received 7 July 2015; published 4 September 2015)

We consider the notion of thermal equilibrium for an individual closed macroscopic quantum system in a pure state, i.e., described by a wave function. The macroscopic properties in thermal equilibrium of such a system, determined by its wave function, must be the same as those obtained from thermodynamics, e.g., spatial uniformity of temperature and chemical potential. When this is true we say that the system is in macroscopic thermal equilibrium (MATE). Such a system may, however, not be in microscopic thermal equilibrium (MITE). The latter requires that the reduced density matrices of small subsystems be close to those obtained from the microcanonical, equivalently the canonical, ensemble for the whole system. The distinction between MITE and MATE is particularly relevant for systems with many-body localization for which the energy eigenfunctions fail to be in MITE while necessarily most of them, but not all, are in MATE. We note, however, that for generic macroscopic systems, including those with MBL, most wave functions in an energy shell are in both MATE and MITE. For a classical macroscopic system, MATE holds for most phase points on the energy surface, but MITE fails to hold for any phase point.
Conclusions

BOLTZMANN’S ENTROPY AND TIME’S ARROW

Given that microscopic physical laws are reversible, why do all macroscopic events have a preferred time direction? Boltzmann’s thoughts on this question have withstood the test of time.

Joel L. Lebowitz

PHYSICS TODAY  SEPTEMBER 1993

Typical vs averaged behavior

I conclude by emphasizing again that having results for typical microstates rather than averages is not just a mathematical nicety but is at the heart of understanding the microscopic origin of observed macroscopic behavior. We neither have nor do we need ensembles when we carry out observations like those in figure 2. What we do need and can expect to have is typical behavior. Ensembles are merely mathematical tools, useful for computing typical behavior as long as the dispersion in the quantities of interest is sufficiently small.