Thermal equilibration between two quantum systems

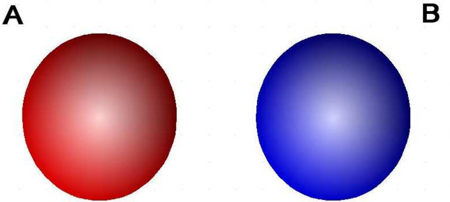
Peter Hänggi

University of Augsburg

with A. Ponomarev, and S. Denisov, arXiv:1004.2232

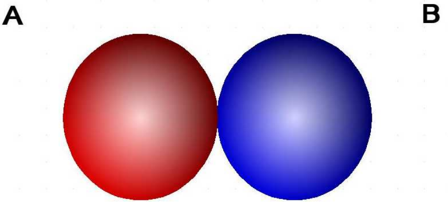
OUR SET-UP

(I)



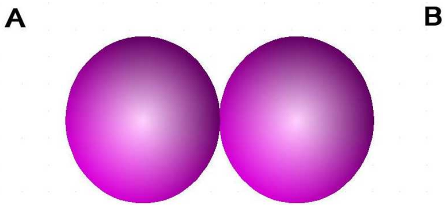
OUR SET-UP

(II)



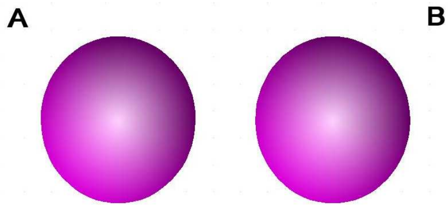
OUR SET-UP

(III)



OUR SET-UP

(IV)



Thermodynamics from the first principles

E. Schrödinger:
"The exchange of energy according to wave mechanics",
Annalen der Physik **83** (4), 956 (1927)

Microscopic derivation of thermodynamic behavior?

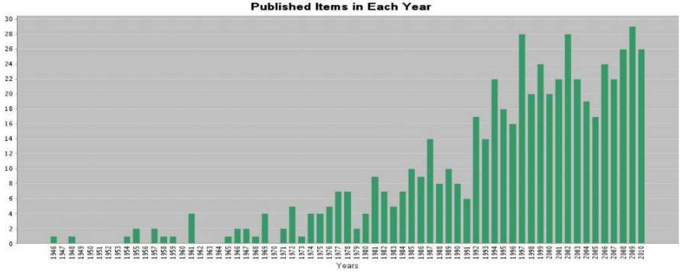
$$|\Psi_n\rangle = \sum_{n=1}^{N} e^{-i\epsilon_n t/\hbar} c_n |\psi_n\rangle$$

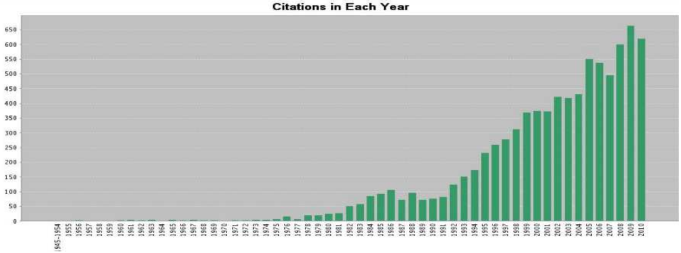
Time evolution of a quantum system is

- linear
- deterministic
- encoded in initial conditions via energy spectrum

Introduction: research timeline

Search with keywords (quantum + thermalization) in article titles





Introduction: irreversibility

ANNALEN DER PHYSIK

956

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DER GANZEN REIHE 388. BAND

1 9 2 7

3. *Energieaustausch nach der Wellenmechanik;*
von E. Schrödinger

1963 *Rep. Prog. Phys.* **26** 411

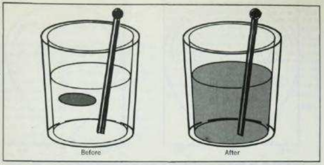
THE THEORY OF IRREVERSIBLE PROCESSES

By G. V. CHESTER†

Department of Mathematical Physics, The University, Birmingham

CONTENTS

PHYSICS TODAY / FEBRUARY 1973



Joel L. Lebowitz and Oliver Penrose

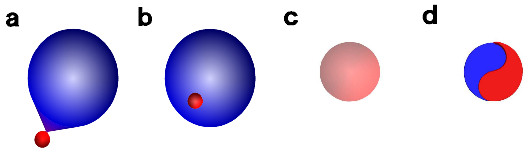
International Journal of Theoretical Physics, Vol. 2, No. 4 (1969), pp. 325–343

On the Nature of Theories of Irreversible Processes

TA-YOU WU

Statistical Physics Laboratory, Department of Physics,
State University of New York, at Buffalo, New York

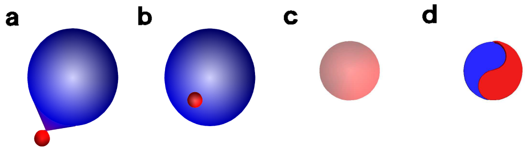
Prehistory and recent developments



a | System (A) weakly coupled to huge finite environment (B)

- Canonical thermalization of A
  - Idea: Schrödinger, Annalen der Physik **83** (4), 956 (1927)
    Worked out in:
    Bocchieri & Loinger, Phys. Rev. **114**, 948 (1959)
  - (A+B) as a sum of specific pure states:
    H. Tasaki, PRL **80**, 1373 (1998)
  - General pure state of (A+B):
    Goldstein et al , PRL **96**, 050403 (2006)

Prehistory and recent developments



b | System as a part of "Universe"

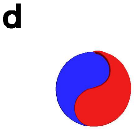
For entire system in a pure state the subsystem bears

- Canonical typicality
  Popescu et al, Nature Physics **2**, 754 (2006)

c | Single isolated quantum system

- Microcanonical thermalization after quench
  Rigol et al, Nature **432**, 854 (2008)

Our model setup



d | Finite subsystems on equal footing: $H \equiv H_{\mathrm{A}} = H_{\mathrm{B}}$

$$H_{\mathrm{tot}}^{\lambda} = H_{\mathrm{A}} \otimes \mathbf{1}_{\mathrm{B}} + \mathbf{1}_{\mathrm{A}} \otimes H_{\mathrm{B}} + \lambda H_{\mathrm{int}}$$

- Subsystems: different initial temperatures, T_{A} and T_{B}
- in Gibbs states, i.e. $\varrho^{\mathrm{A,B}}(0) \propto \sum_n e^{-\epsilon_n/k_B T_{\mathrm{A,B}}} |n\rangle\langle n|$, or in pure "typical" states, i.e. $\varrho^{\mathrm{A,B}}(0) = |\psi\rangle\langle\psi|$ with $|\psi\rangle \propto \sum_n e^{i\theta_n} e^{-\epsilon_n/2k_B T_{\mathrm{A,B}}} |n\rangle$.
- The entire system: $\varrho^{\mathrm{tot}}(0) = \varrho^{\mathrm{A}}(0) \otimes \varrho^{\mathrm{B}}(0)$

Central questions

What is the equilibrium population of subsystem energy levels?

$$p_j^{\mathrm{A,B}}(t > \tau_{\mathrm{eq}}) = \mathrm{Tr}_{\mathrm{B,A}}\left[\varrho^{\mathrm{tot}}(t)\mathbf{P}_j^{\mathrm{A,B}}\right]$$

where projectors: $\mathbf{P}_j^{\mathrm{A}} = |j\rangle\langle j| \otimes \mathbf{1}_{\mathrm{B}}$, and $\mathbf{P}_j^{\mathrm{B}} = \mathbf{1}_{\mathrm{A}} \otimes |j\rangle\langle j|$.

How do the populations evolve towards equilibrium distribution?

- Intermediate states, time scales, and etc.
- Where equilibration (irreversibility) in isolated quantum system comes from?

Time evolution

Density matrix

$$\varrho^{\mathrm{tot}}(t) = \mathbf{U}(t)\varrho^{\mathrm{tot}}(0)\mathbf{U}(t)^{\dagger}$$

Evolution operator

In the basis $|\psi_n^{\lambda=0}\rangle = |\psi_{kj}^{\lambda=0}\rangle \equiv |k\rangle_{\mathrm{A}} \otimes |j\rangle_{\mathrm{B}}$:

$$U_{n,n'}(t) = \sum_{n''} e^{-iE_{n''}^{\lambda}t/\hbar}\Lambda_{n'',n}^{*}\Lambda_{n'',n'}$$

Transformation matrix:

$$|\psi_n^{\lambda}\rangle = \sum_{n'} \Lambda_{n,n'}|\psi_{n'}^{\lambda=0}\rangle$$

Superweak coupling: $\lambda\{H_{\rm int}\} < \{\Delta E^{\lambda=0}\}$

Two-fold degenerate levels with: $k \neq j$

$$E^0_{kj} = \epsilon_k + \epsilon_j = \epsilon_j + \epsilon_k = E^0_{jk}$$

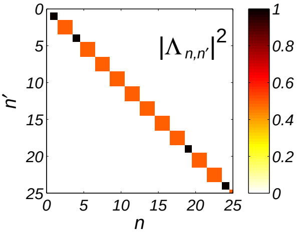
$$|\psi^\lambda_{kj}\rangle = \frac{1}{\sqrt{2}}\left(|\psi^0_{kj}\rangle + \chi_{kj}|\psi^0_{jk}\right)$$

where $\chi_{kj} = \mathrm{sgn}(k - j)$ – sign function.

Non-degenerate levels: $k = j$

$$E^0_{kj} = \epsilon_k + \epsilon_j = 2\epsilon_k$$

$$|\Psi^\lambda_{kk}\rangle = |\Psi^0_{kk}\rangle$$



Superweak coupling: $\lambda\{H_{\rm int}\} < \{\Delta E^{\lambda=0}\}$

Exact result

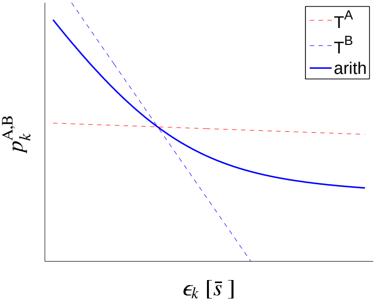
$$p_k^{\rm A}(t) = \frac{1}{2}\left[p_k^{\rm A}(0) + p_k^{\rm B}(0)\right] + \frac{1}{2}\sum_j X_{kj}^{\rm A} \cos\left(\omega_{kj}^{\lambda} t\right),$$

where $X_{kj}^{\rm A} = p_k^{\rm A}(0)p_j^{\rm B}(0) - p_j^{\rm A}(0)p_k^{\rm B}(0)$, $\omega_{kj}^{\lambda} = (E_{kj}^{\lambda} - E_{jk}^{\lambda})/\hbar$.

Equilibration to arithmetic mean

$$p_k^{\rm A}(t > \tau_{\rm eq}) \approx \frac{1}{2}\left[p_k^{\rm A}(0) + p_k^{\rm B}(0)\right],$$

estimation for the equilibration time: $\tau_{\rm eq} \approx 2\pi/{\rm RMSD}(\omega_{jk}^{\lambda})$.



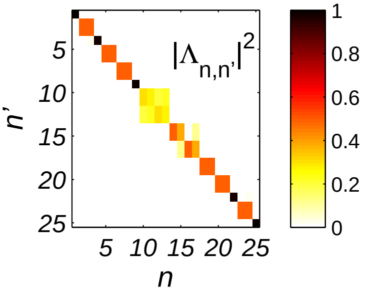
Weak coupling: $\{\Delta E\} < \lambda\{H^{\rm int}\}$ and $\lambda\Delta_{H^{\rm int}} \ll \Delta_{H_S}$

Generalization to $\Lambda_{n,n'}$ having different $2n \times 2n$ blocks

$$E^0_{kj} = \epsilon_k + \epsilon_j = \epsilon_j + \epsilon_k = E^0_{jk}$$

$$|\psi^\lambda_{kj}\rangle = \sum_{\{k'j'\}_{kj}} c_{k'j'} \left(|\psi^0_{k',j'}\rangle + \chi_{k,j}|\psi^0_{j',k'}\rangle\right) \; (c_{k'j'} = c_{j'k'})$$

where $\chi_{kj} = \mathrm{sgn}(k-j)$ – sign function.



Equilibration to thermal state?

$$p^{\rm A}_k(t > \tau_{\rm eq}) \approx \frac{1}{2}\left[p^{\rm A}_k(0) + p^{\rm B}_k(0)\right] + \Delta^{\rm A}_k$$

corrections $\Delta^{\rm A}_k$ due to blocks of size $2n > 2$.

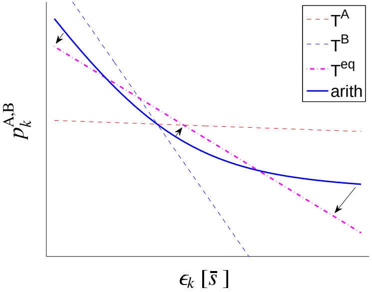
Weak coupling: $\{\Delta E\} < \lambda\{H^{\rm int}\}$ and $\lambda\Delta_{H^{\rm int}} \ll \Delta_{H_S}$

Generalization to $\Lambda_{n,n'}$ having different $2n \times 2n$ blocks

$$E^0_{kj} = \epsilon_k + \epsilon_j = \epsilon_j + \epsilon_k = E^0_{jk}$$

$$|\psi^\lambda_{kj}\rangle = \sum_{\{k'j'\}_{kj}} c_{k'j'} \left(|\psi^0_{k',j'}\rangle + \chi_{k,j} |\psi^0_{j',k'}\rangle \right) \; (c_{k'j'} = c_{j'k'})$$

where $\chi_{kj} = \mathrm{sgn}(k-j)$ – sign function.

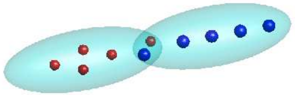


Equilibration to thermal state

$$p_k^{\rm A}(t > \tau_{\rm eq}) \approx \frac{1}{2}\left[p_k^{\rm A}(0) + p_k^{\rm B}(0)\right] + \Delta_k^{\rm A}$$

corrections $\Delta_k^{\rm A}$ drag $p_k^{\rm A,B}(t)$ towards canonical distribution

Exact numerical calculations for two different models

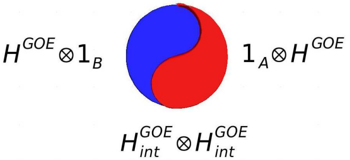


1. Cold atoms in two traps

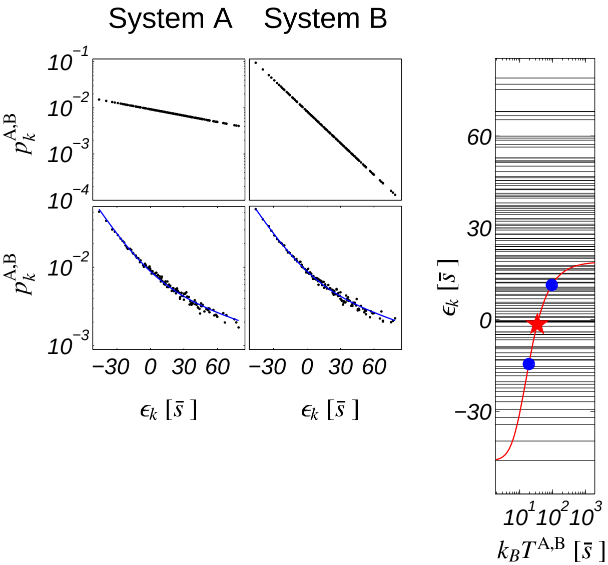
- 2 x Bose-Hubbard Hamiltonian, $N = 5$ (Hilbert space size 15876)
- Contact coupling, $n_{j_A = L} \otimes n_{j_B = 1}$

2. Random matrix model

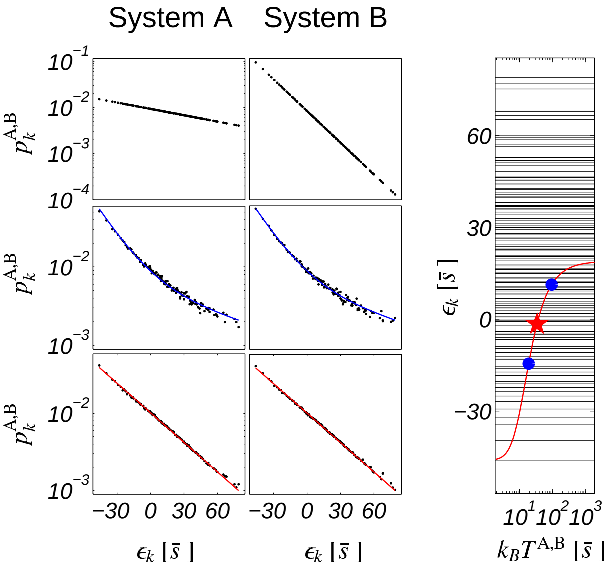
- 2 x Random matrix (RM) GOE Hamiltonian, $\mathcal{N} = 192$ (Hilbert space size 36864)
- $A \leftrightarrow B$ invariant RM GOE coupling term, $H_{\text{int}}^{GOE} \otimes H_{\text{int}}^{GOE}$



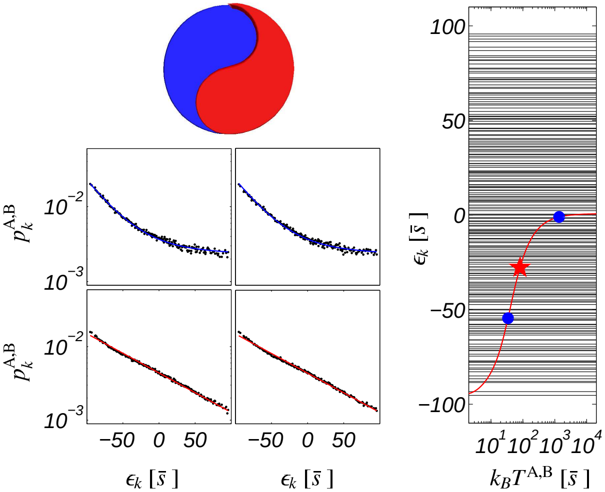
Arithmetic equilibration (cold atoms)



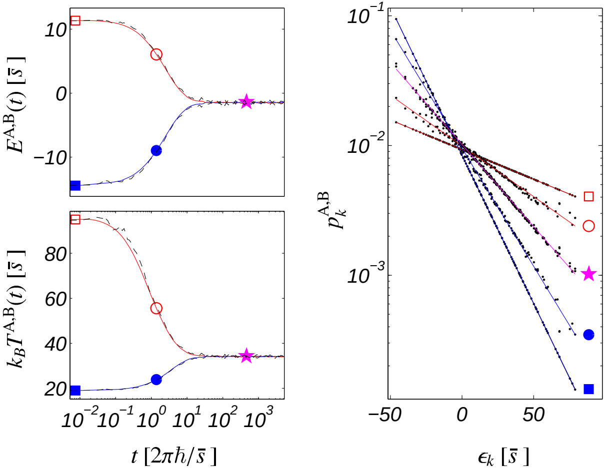
Arithmetic vs. Thermal equilibration (cold atoms)



Arithmetic vs. Thermal equilibration (RM model)

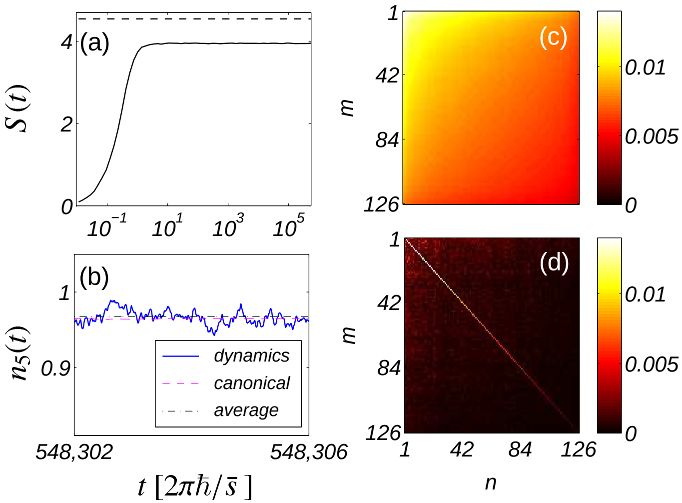


Quasistatic equilibration (cold atoms)



Evolution of initially pure (dashed lines) and Gibbs (solid lines) states.

Typicality and growth of entanglement entropy



Evolution of initially pure state.

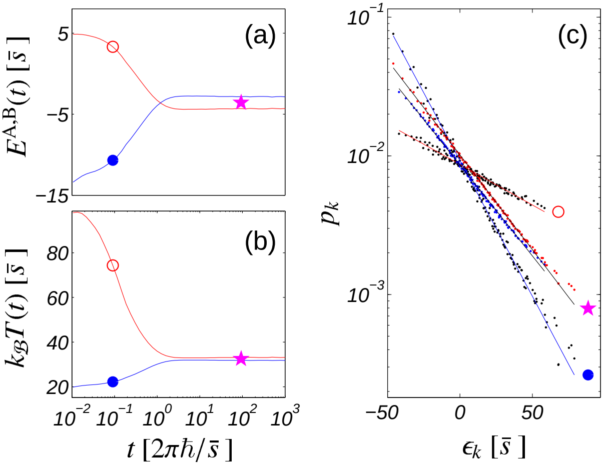
Summary

- Non-equilibrium thermodynamic process in an isolated quantum system in a pure state
- Quasistatic thermal equilibration: assignment of temperature at any instant of time
- Irreversibility: development of quantum correlations
- “Dynamical typicality” of thermodynamic evolution

A. V. Ponomarev, S. Denisov, P. Hänggi, arXiv:1004.2232

Thank You!

Arithmetic vs. Thermal equilibration (cold atoms)



Non-identical systems in contact

($L_A = N_A = 5$ and $L_B = 6$, $N_B = 4$).