

**Quantum Mechanics
+ Open Systems
= Thermodynamics ?**

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Motivating Questions

more fundamental:

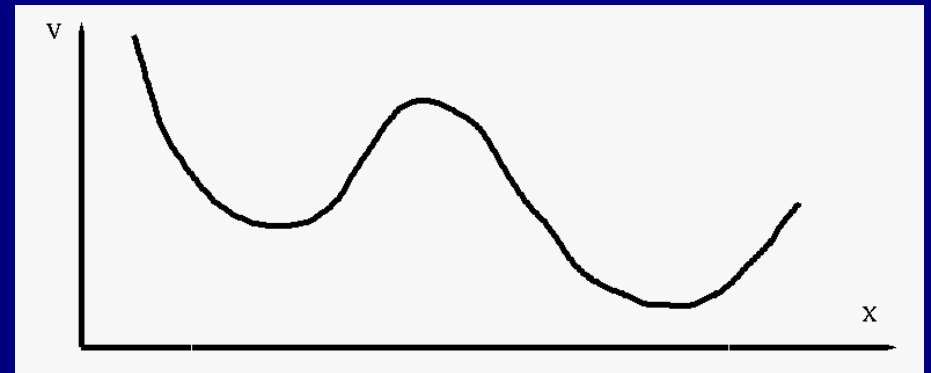
- understand the origin of thermodynamical behavior (2. law, Boltzmann distribution, etc.)
- understand the origin of classical behavior (decoherence)
- understand the origin of statistical dynamics, i.e. rate equations

$$\dot{P}_i = R_{ij}P_j \quad (\text{"master equations"})$$

more specific:

- understand the laser, laser cooling, etc.

- understand nuclear decay and chemical reactions



- understand the origin of typical transport equations

$$\dot{\rho} = \lambda \Delta \rho$$

“Fouriers Law: A challenge to theorists” (Bonetto et al., World Scientific)

Fundamental Law or Emergent Description?

Quantum Mechanics

$$i\hbar\frac{\partial}{\partial t}\Psi = \left(-\frac{\hbar^2}{2m}\Delta + V\right)\Psi$$

Classical Mechanics:

$$m\frac{d^2}{dt^2}\vec{x} = -\nabla V$$

Thermodynamics:

$$dU = TdS - pdV$$

$$\frac{dS}{dt} > 0$$

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→ “Heisenberg Cut” →

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Ergodicity



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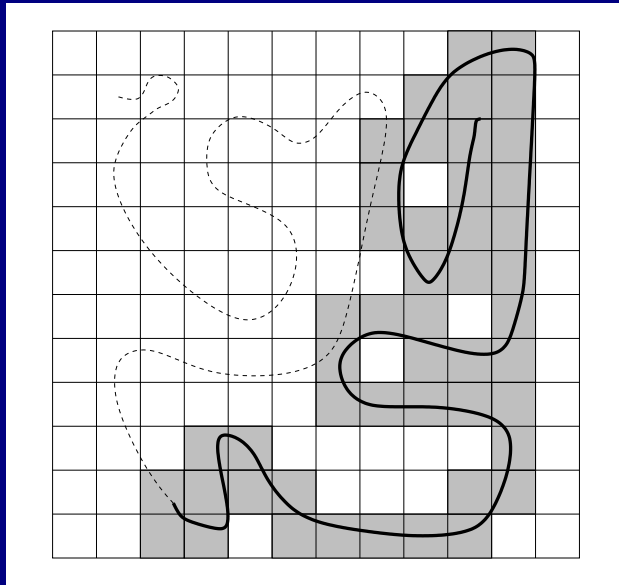
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Entropy Dynamics in Phase Space: The Second Law

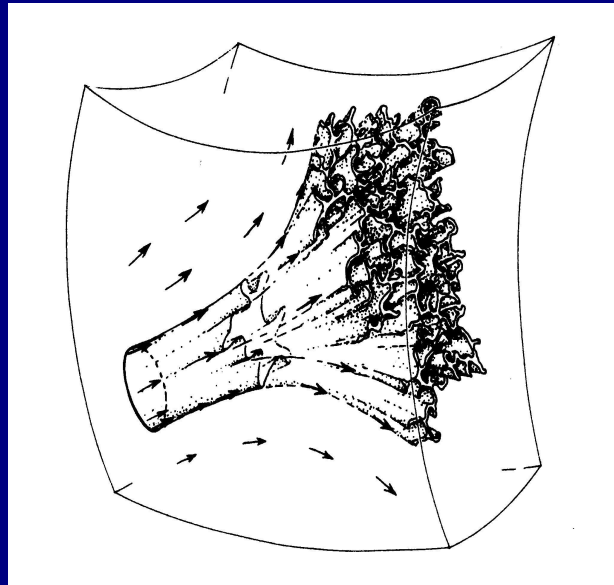
Boltzmann:



Problems:

- Ergodicity
- Cell Size
- Averaging Time

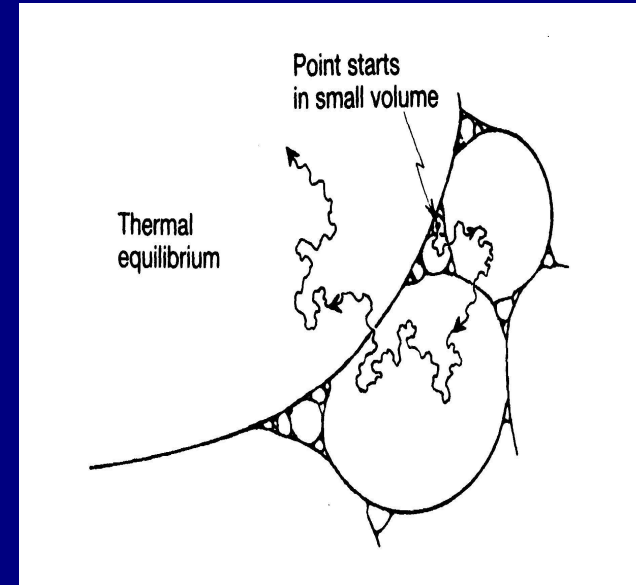
Gibbs:



Problems:

- Liouville's Law
- Mixing
- Cell Size

Ehrenfest:



Problems:

- Definition of Macroscopic Cells
- Phase Space Velocity

Movies

Film 1

Film 2

Film 3

Film 4

Open Quantum Systems

Model:

Small system \iff Big system. Typically: a lot of oscillators (phonons, photons, etc.)

e.g., Caldeira-Legett-model

$$\hat{H} = \underbrace{\frac{1}{2M}\hat{P}^2 + \hat{V}(\hat{X})}_{\hat{H}_S} + \underbrace{\sum_n \frac{1}{2}\hat{p}_n^2 + \omega_n \hat{x}_n^2}_{\hat{H}_E} + \underbrace{\hat{X} \sum_n f_n \hat{x}_n}_{\hat{V}}$$

Description:

State of the full system: density operator $\hat{\rho} = \sum_n P_n |\Psi_n\rangle\langle\Psi_n|$

State of the reduced system: $\hat{\rho}_S = \text{Tr}_E\{\hat{\rho}\}$

Open Quantum Systems

Projection operator techniques:

$$\mathcal{P}\hat{\rho} := \text{Tr}_E\{\hat{\rho}\} \otimes \hat{\rho}_E(T) \quad \mathcal{Q} = 1 - \mathcal{P}$$

$$\frac{d}{dt}\hat{\rho}(t) = -[\hat{V}(t), \hat{\rho}(t)] \quad \Rightarrow \quad \frac{d}{dt}\mathcal{P}\hat{\rho} = F_P(\mathcal{P}\hat{\rho}, \mathcal{Q}\hat{\rho}), \quad \frac{d}{dt}\mathcal{Q}\hat{\rho} = F_Q(\mathcal{P}\hat{\rho}, \mathcal{Q}\hat{\rho})$$

$$\hat{\rho}(t=0) \stackrel{!}{=} \hat{\rho}_S \otimes \hat{\rho}_E(T) \quad \Rightarrow \text{to leading order in interaction strength and time} \Rightarrow$$

$$\frac{d}{dt}\hat{\rho}_S(t) = - \int_0^t \text{Tr}_E[\hat{V}(t), [\hat{V}(t'), \hat{\rho}_S(t') \otimes \hat{\rho}_E(T)]] dt' \quad \Rightarrow$$

Open Quantum Systems

$$\Rightarrow \frac{d}{dt} \hat{\rho}_S(t) = \int_0^t \mathcal{L}(t-t') \hat{\rho}_S(t') dt'$$

$$\mathcal{L}(t-t') \approx \mathcal{L} \times \text{Tr}_E \{ \hat{B}(t) \hat{B}(t') \hat{\rho}_E(T) \} \quad \text{“bath correlation functions”}$$

If decay of bath correlations short compared to relaxation dynamics of the considered system \Rightarrow “Markovian” \Rightarrow

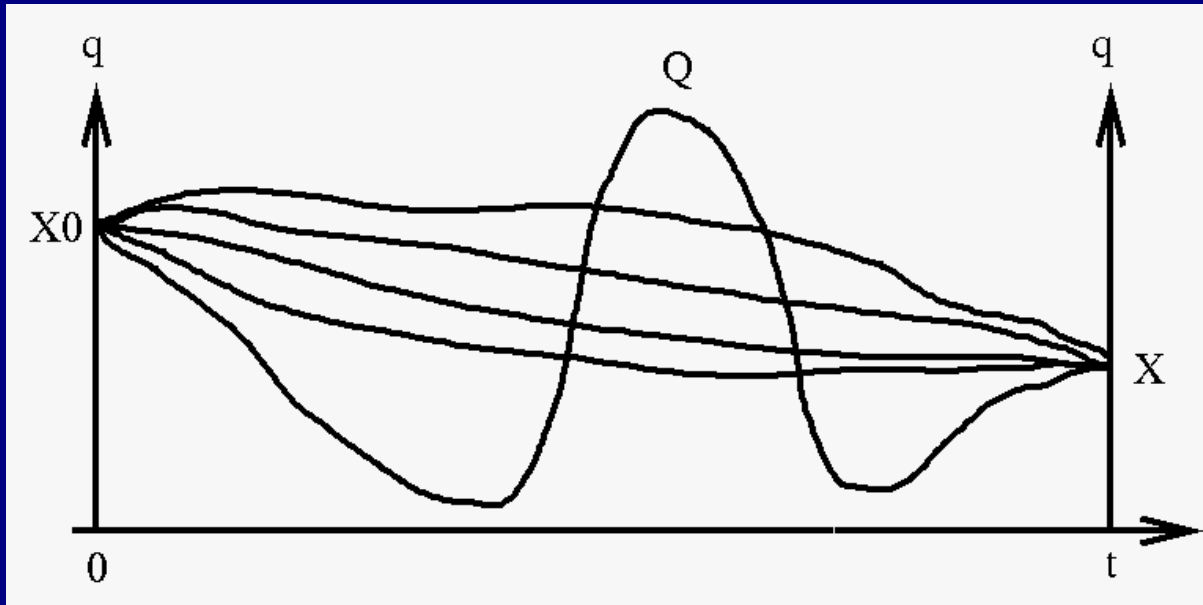
$$\frac{d}{dt} \hat{\rho}_S(t) = \mathcal{L} \hat{\rho}_S(t)$$

Quantum master equations

$$\frac{d\rho_{ii}}{dt} = \sum_j R_{ij} \rho_{jj} - \sum_l R_{li} \rho_{ii} \quad \text{“thermalization”} \quad \frac{d\rho_{ij}}{dt} = r_{ij} \rho_{ij} \quad \text{“decoherence”}$$

Open Quantum Systems

Feynmann-Vernon-(Weiss)-technique: based on path integrals of the action:



$$L(\dot{q}, q) := T - V$$

$$\int_Q L(\dot{q}, q) dt := S(Q, X, X_0)$$

Feynman path integral approach:

$$\Psi(X, t) = \int dX_0 \underbrace{\int dQ \exp\{-iS(Q, X, X_0)\}}_{G(X, X_0, t)} \Psi(X_0, 0), \quad G(X, X_0, t) : \text{“propagator”}$$

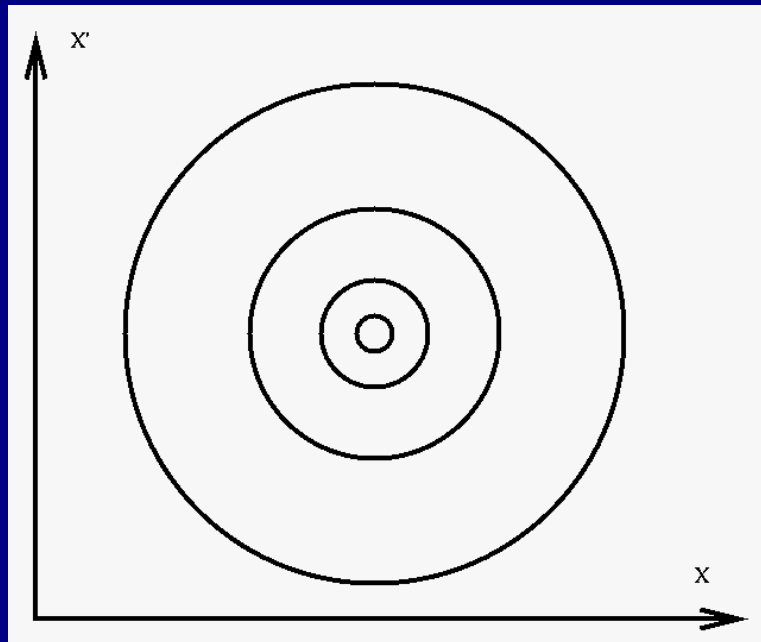
($G(X, X_0, t)$ may be computed analytically for a harmonic oscillator)

Open Quantum Systems

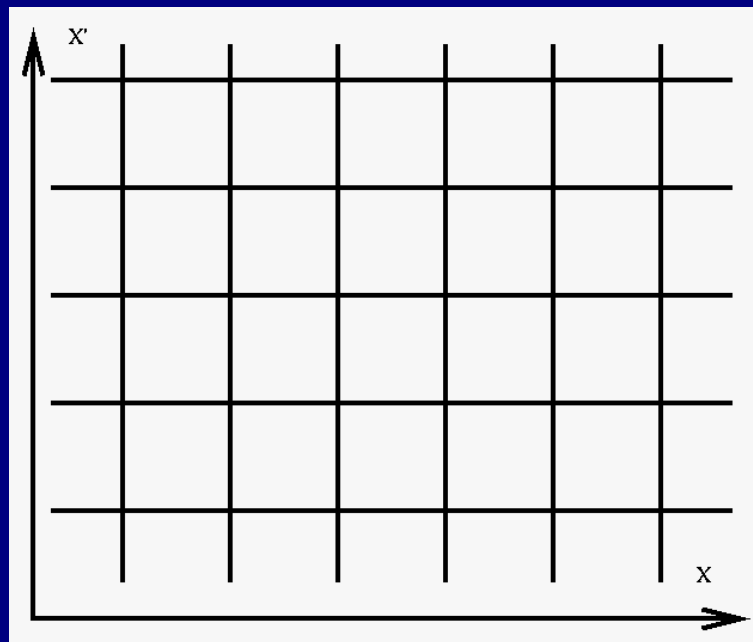
Description via density matrix in “X-representation” $\rho(X, X')$, e.g., for some pure state:

$$\Psi(X) \propto \exp\left\{\frac{X^2}{\Delta^2 X}\right\} \exp\{-iP_0 X\}, \quad \rho(X, X') = \Psi(X)\Psi^*(X')$$

$|\rho(X, X')|$



phase of $\rho(X, X')$



Open Quantum Systems

Evolution of the density matrix:

$$\rho(X, X', t) = \int G(X, X_0, t) G^*(X', X'_0, t) \rho(X_0, X'_0, 0) dX_0 dX'_0$$

This generalizes directly to the full system: $X \rightarrow X, x_n$

\Rightarrow Integrate out all the bath variables \Rightarrow Bath-effect may be expressed as a “weight” for the considered system’s (double) path:

$$W(Q, Q') = \exp\{\Phi_{deco} + i\Phi_{therm}\}$$

Feynman-Vernon influence functionals:

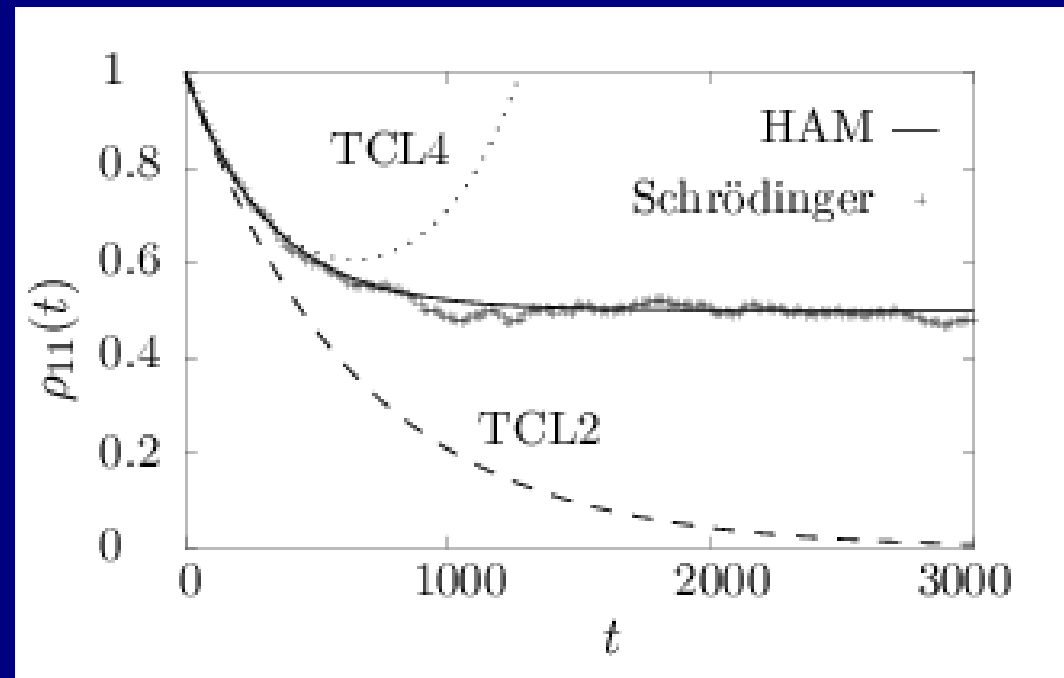
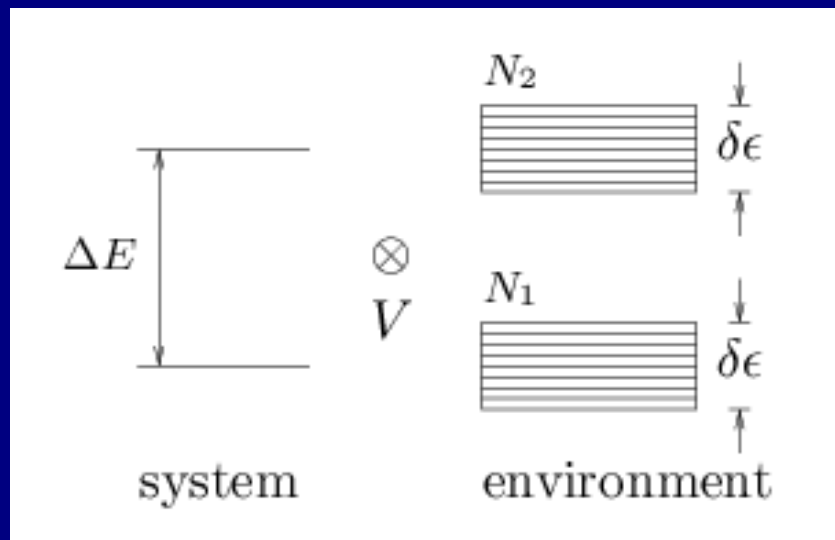
$$\Phi_{deco} \approx -D \int (q - q')^2 dt \quad \Phi_{therm} \approx \eta \int (q - q') \frac{d}{dt} (q + q') dt$$

Φ_{deco} “diagonalizes” $\rho(X, X')$

Φ_{therm} “flattens” $\rho(X, X')$

Open Quantum Systems

Breakdown of the standard approaches:

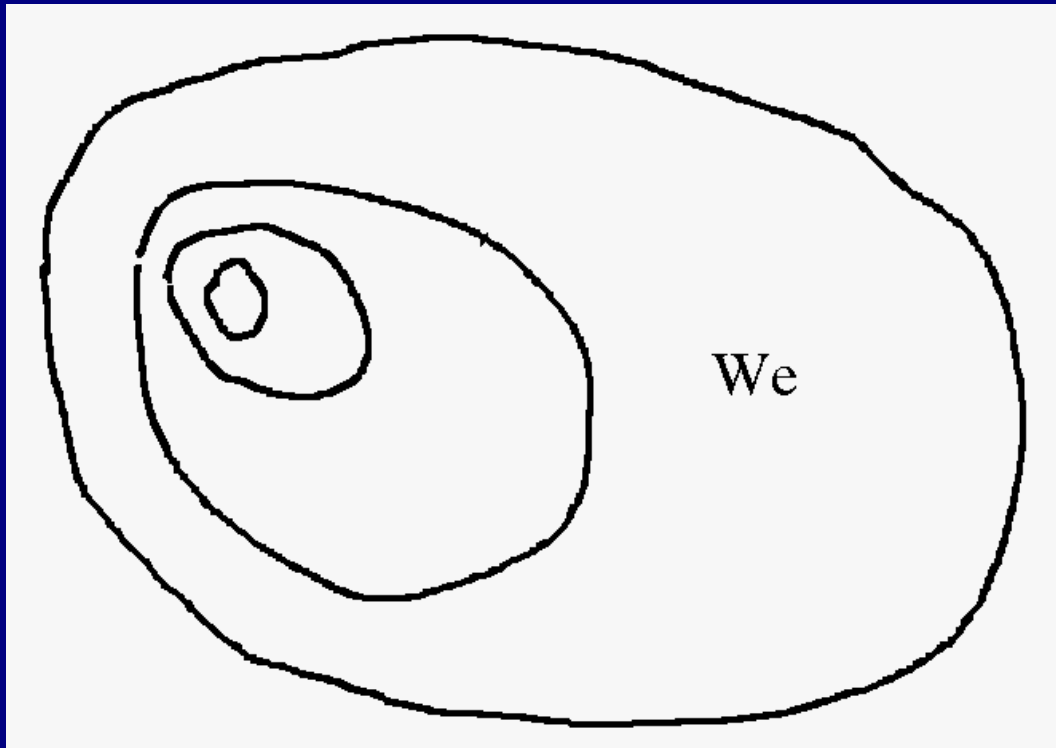


Feynman-Vernon: not applicable

Standard projection operator technique: does not converge

Hilbert space Average Method

Obseables generate “landscapes” in Hilbert space



$$[[W_e]] = \frac{N_1}{N_1 + N_2}$$

$$[[W_g]] = \frac{N_2}{N_1 + N_2}$$

$$[[S]] \approx S_{max}$$

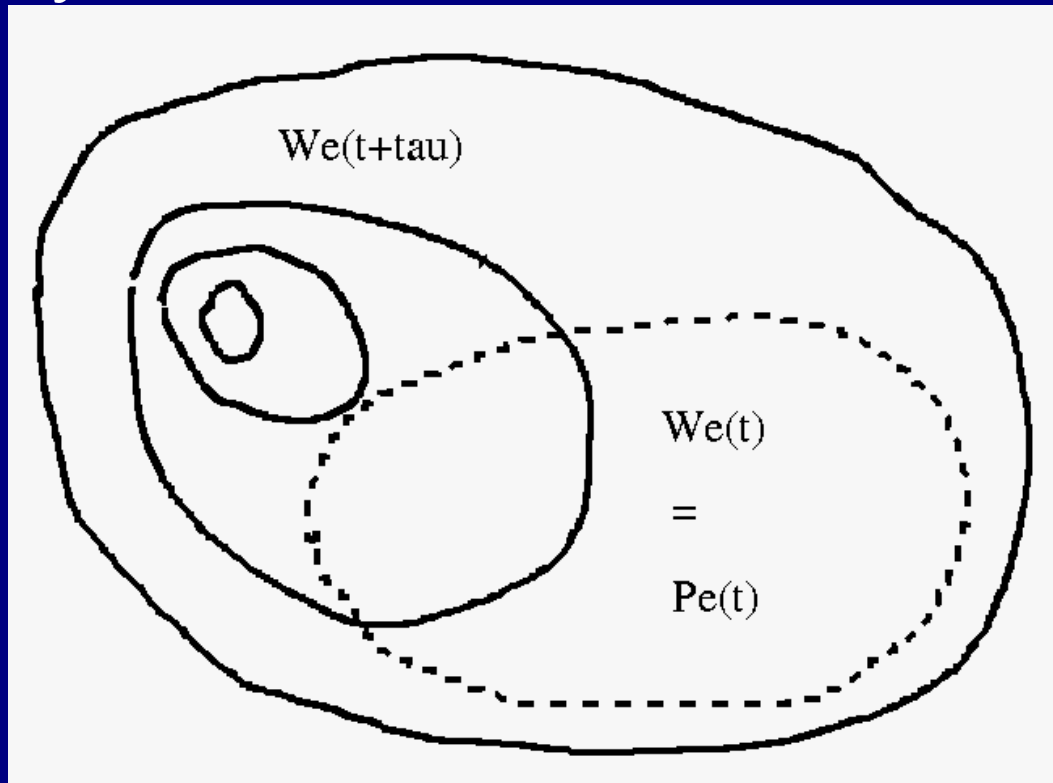
crucial guess: $W_e(t) \approx [[W_e]],$ $W_g(t) \approx [[W_g]],$ $S(t) \approx [[S]]$

Only valid if the landscapes are flat.

This principle allows for an explanation of the canonical equilibrium state

Hilbert space Average Method

Dynamics:



$$\begin{aligned} & \llbracket W'_e(t + \tau) \rrbracket_{\{W'_e(t) = P'_e(t)\}} \\ & \approx P'_e(t) - \tau R P'_e(t) \end{aligned}$$

replace actual values by
Hilbert space averages
(guess):

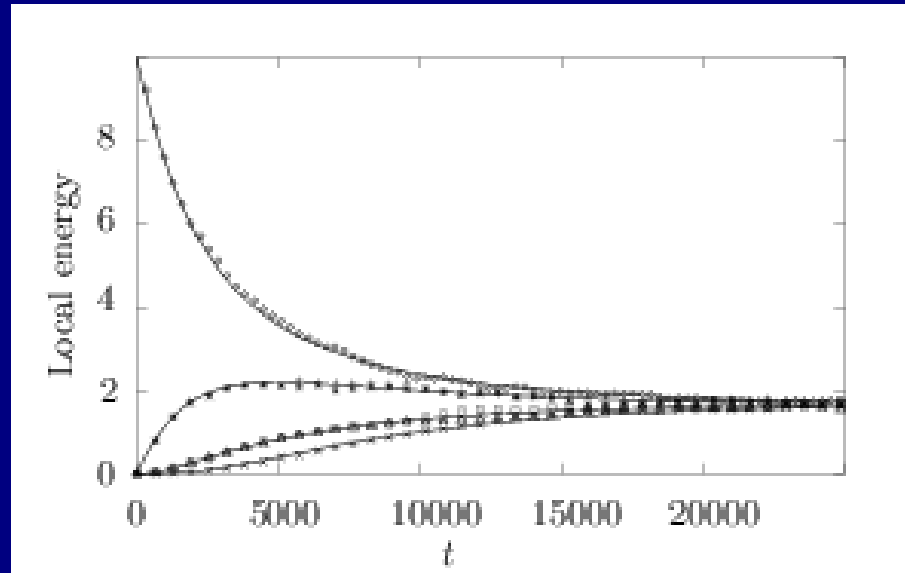
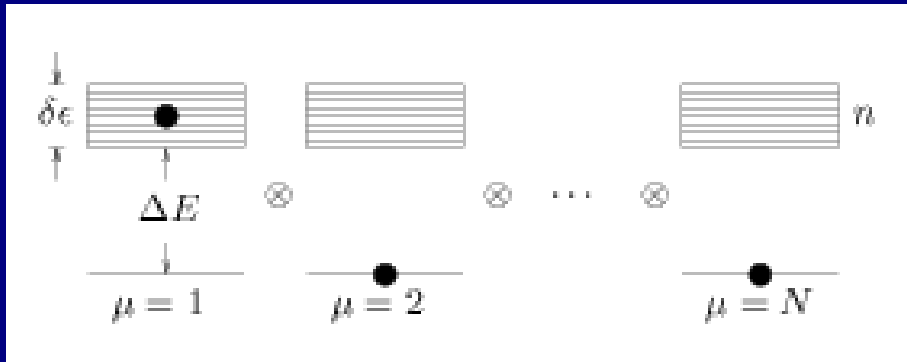
$$P'_e(t + \tau) \rightarrow \llbracket W'_e(t + \tau) \rrbracket_{\{W'_e(t) = P'_e(t)\}}$$

this allows for iteration

$$\frac{1}{\tau} \{P'_e(t + \tau) - P'_e(t)\} = -R P'_e(t) \quad \tau \rightarrow 0, \quad \Rightarrow \quad \dot{P}'_e = -R P'_e$$

Hilbert space Average Method

Energy diffusion, Fourier's law:



$$\frac{1}{\tau} (\langle [E_n(t + \tau)] \rangle_{\{E_\mu(t) = h_\mu(t)\}} - h_\mu(t)) = \lambda \{ (h_{\mu+1} - h_\mu) - (h_\mu - h_{\mu-1}) \}$$

$$\dot{h}_\mu = \lambda \{ (h_{\mu+1} - h_\mu) - (h_\mu - h_{\mu-1}) \}$$

$$\dot{\rho}(x, t) = \lambda \Delta \rho(x, t)$$

HAM explains the occurrence of diffusive transport.

The End

“Wenn man keinen Schimmer hat, worum es im zweiten thermodynamischen Hauptsatz geht, [...], dann wird niemand daraus auf mangelnde Bildung schließen.”

D. Schwanitz in : **Bildung**

Kapitel: Was man nicht wissen sollte.

Thank you for your attention!