Physical nature of equilibrium stationary states

I. System with no interaction w/ environment: an isolated system confined in finite space, w/ no gain/loss of energy, obeying classical mechanics

Total energy $E = H(\vec{q}, \vec{p})$ is conserved

$\uparrow$ (3N coordin. all particle positions)
$\uparrow$ (all particle momenta (3N coordinates))
$[N$ particles volume $\checkmark]$
\[ E = H(\dot{x}, \dot{p}) \] is a surface of \((6N-1)\)-dim.

\[ 6N\text{-dim. phase space of all } (\vec{q}, \vec{p}) = \dot{X} \]

Divide up surface into area elements \(d^N x\), \(6N-1\)

\[ p_n(t) \leftrightarrow \rho(\vec{q}, \vec{p}) d^N x \]

Focus:
- prob. density
- in phase space

Note new notation, to not conflict with \(N = \) particle number.
Liouville aside:

\[ \frac{\partial}{\partial t} \rho(q, p) = \left[ \mathcal{H}, \rho \right] + \Gamma \]

- pure classical
- interaction w/ environment

no environment: \( \Gamma \to 0 \)

in this case: \( \rho^s(q, p) = S(E - \mathcal{H}(q, p)) \)

is a stationary distribution

\[ \left[ \mathcal{H}, \rho \right] = \frac{\partial \mathcal{H}}{\partial q} \frac{\partial \rho}{\partial p} - \frac{\partial \mathcal{H}}{\partial p} \frac{\partial \rho}{\partial q} = 0 \]

for discrete, this would correspond to

\[ p_n^s = \text{constant for given } E \]

\[ \sum_n p_n^s = 1 \Rightarrow p_n^s = \left[ \Theta(E) \right]^{-1} \]

microcanonical ensemble
Harmonic oscillator example:

\[ E = \frac{p^2}{2m} + \frac{kq^2}{2} \]

divide surface into

\[ \Theta(E) = 60 \text{ states} \]

(like seconds on a clock)

prepare a microcanonical ensemble of initial conditions: mixed ensemble

\[ p_n(0) = \frac{1}{\Theta(E)} \]

prepare \[ p_n(t) = \frac{1}{\Theta(E)} \]

Thus \[ p_n^s = \frac{1}{\Theta(E)} \]

is a stationary distribution.

prepare a pure ensemble with all systems in state 1

\[ p_n(0) = \delta_{n,1} \]

\[ p_n(t) = \delta_{n,m(t)} \quad m(t+\tau) = m(t) \]
\[ P_n(t) \] for pure ensemble never relaxes to equilibrium stationary distribution \( P_{n}^{s} \).

SHO visits all states as \( t \to \infty \), but \( p_{n}(t) \neq P_{n}^{s} \) as \( t \to \infty \).
Another example: \( N = 2 \) non-interacting (ideal gas)
prepare two states with same \( E \)

\[
\begin{align*}
A & : \\
E_1 &= 4 \times 10^{-21} \text{J} \\
E_2 &= 1 \times 10^{-21} \text{J} \\
E &= E_1 + E_2 = 5 \times 10^{-21} \text{J}
\end{align*}
\]

\[
\begin{align*}
B & : \\
E_1 &= E_2 = 2.5 \times 10^{-21} \text{J} \\
E &= 5 \times 10^{-21} \text{J}
\end{align*}
\]

\[
\text{time evolution}
\]

\[
\begin{align*}
A' & : \\
E_1 &= 4, \ E_2 = 1 \\
E &= 5
\end{align*}
\]

\[
\begin{align*}
B' & : \\
E_1 &= E_2 = 2.5 \\
E &= 5
\end{align*}
\]

Individual particle energies are also constants of motion.

State A will never visit state B as \( t \to \infty \).

Ideal gas is non-ergodic!!

Arnold-KAM: (1954-1963) Kolmogorov-Moser theory indicates this non-ergodicity could persist even for weak interparticle interactions.

1970: Yakov Sinai makes mathematical breakthrough (Abel prize, 2014)

\( \Rightarrow \) shows two hard disks on 2D square w/ periodic boundary conditions are ergodic! (and mixing)

hard disk \( \Rightarrow \) strong interaction (infinite repulsion on overl
Through 2003, ergodicity has almost been proven for $N \geq 2$ d-dim spheres in d-dim's.

Key aspect to ergodicity/mixing $\Rightarrow$ chaotic trajectories, exhibited by the Sinai billiard.

A pinch of chaos is a necessary ingredient in allowing a system at constant energy to relax to equilibrium.

Good recipe: many, strongly interacting particles, with $E$ being only constant of motion.

To summarize: our fundamental assumption for a system at constant $E$ (isolated):

$n = 1, \ldots, \Theta(E)$

labels states

$p_n(t) \xrightarrow{t \to \infty} p^s = \frac{1}{\Theta(E)}$

for any $p_n(t)$.