Separable Hamiltonians & the role of interaction in ergodicity

Let's consider a separable Hamiltonian written in its "natural" variables say $p_m\ q_m$

$$H = \sum_1^N {}_m H_m(p_m, q_m)$$

$$\dot{q}_K = \frac{\partial H}{\partial p_K} = \frac{\partial H_K}{\partial p_K}$$

Separable system

$$\dot{p}_K = -\frac{\partial H}{\partial q_K} = -\frac{\partial H_K}{\partial q_K}$$

Therefore each separate $H_m(p_m(t), q_m(t)) = H_m(p_m(0), q_m(0))$

Since $\{H, H_m\} = 0$ each H_m is a constant of motion -

This fact precludes equipartition and stricta sensu ergodicity the phase space is separated in N disconnected sections

The Micro Canonical distribution

$$\rho(p_1 \ldots p_N\, q_1 \ldots q_N) \propto \delta(E-H) = \delta(E - \Sigma_n H_n)$$

is instead replaced by the product

$$\rho = \Pi_n \rho_n(q_n\, p_n) \qquad \rho_n(q_n\, p_n) \propto \delta\left(E_n - H_n(p_n q_n)\right)$$

of independent distribution.

For a analytical example let's consider N independent harmonic oscillators

$$H = \sum_1^N{}_n \frac{\bar{p}_n^2}{2m_n} + \frac{1}{2} m_n \omega_n^2 \bar{q}_n^2$$

we have the explicit solution for any of them

$$\begin{cases} q_n^\alpha = A_n^\alpha \cos(\omega_n t + \varphi_n^\alpha) \\ p_n^\alpha = -m_n A_n^\alpha \omega_n \sin(\omega_n t + \varphi_n^\alpha) \end{cases} \qquad \begin{matrix} \alpha = 1,3 \\ n = 1,N \end{matrix}$$

the energy is

$$E_n = \sum_1^3{}_\alpha \frac{(p_n^\alpha)^2}{2m_n} + \frac{1}{2} m_n \omega_n^2 (q_n^\alpha)^2$$

$$= \sum_1^3{}_\alpha \frac{m_n^{\cancel{2}} \omega_n^2 A_n^{\alpha 2}}{2\cancel{m_n}} \sin^2(\ldots) + \frac{1}{2} m_n \omega_n^2 A_n^{\alpha 2} \cos^2(\ldots)$$

$$= \sum_1^3{}_\alpha \frac{1}{2} m_n A_n^{\alpha\, 2} \omega_n^2$$

$$E_m = \frac{1}{2} m_m \omega_m^2 \sum_\alpha (A_m^\alpha)^2$$

Averaging over the surface of constant energy E_n is equivalent to average over uncorrelated random φ_m^α

And we have that despite each mode do ~~not~~ undergoes thermalization the

$$\frac{1}{T}\int_0^T dt\, f_n(p_m(t), q_m(t)) =$$

$$= \int_0^{2\pi} \prod_{\alpha=1}^{3} \frac{d\varphi_m^\alpha}{2\pi} f_n(-A_m^\alpha \omega_m m_m \sin(\varphi_m^\alpha)_{\alpha=1,3}, A_m^\alpha \cos(\varphi_m^\alpha)_{\alpha=1,3})$$

Because for a single 1-d Harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2$$

$$\begin{cases} p = -m\omega A \sin(\omega t + \varphi) \\ q = A\cos(\omega t + \varphi) \end{cases} \qquad A = \sqrt{\frac{2E}{m\omega^2}}$$

$$\frac{1}{T}\int_0^T dt\, f(p(t), q(t)) =$$

$$= \frac{1}{T}\int_0^T dt\, f(-m\omega A \underbrace{\sin(\omega t+\varphi)}_{\text{periodic}}, A \underbrace{\cos(\omega t+\varphi)}_{\text{periodic}})$$

for a single function of a periodic functio

$$\frac{1}{T}\int_0^T dt\, f(\sin(\omega t+\varphi)) = \frac{1}{\omega T}\int_0^{\omega T+\varphi} d\tilde{\varphi}\, f(\sin(\tilde{\varphi}))$$

now let T a certain # of periods $\tau = \frac{2\pi}{\omega}$

$$T = M\tau$$

$$\omega T = \omega M \tau = M 2\pi$$

$$\overline{(f)}_T = \frac{1}{M2\pi}\int_0^{M2\pi+\varphi} d\tilde{\varphi}\, f(\sin(\tilde{\varphi})) =$$

$$= \frac{1}{M2\pi}\int_0^{M2\pi} d\tilde{\varphi}\, f(\sin(\tilde{\varphi})) + \int_{M2\pi}^{M2\pi+\varphi} d\tilde{\varphi}\, f(\sin(\tilde{\varphi}))\frac{1}{M2\pi}$$

as $M \to \infty$ $\longrightarrow 0$

$$\overline{(f)}_T = \frac{1}{M2\pi}\int_0^{M2\pi} d\tilde{\varphi}\, f(\sin(\tilde{\varphi})) = \frac{1}{2\pi}\int_0^{2\pi} d\tilde{\varphi}\, f(\sin(\tilde{\varphi}))$$

therefore the time average

$$\overline{\left[f(\sin(\omega t+\varphi))\right]}_T \to \int_0^{2\pi} \frac{d\tilde{\varphi}}{2\pi} f(\sin(\tilde{\varphi}))$$

↑
Uniformly distributed phase

But average over uniformly distributed phase is exactly average over the surface of constant energy to this extent a single harmonic oscillator is ergodic

<u>However does not equipartite the energy</u>

Therefore equipartition theorem is no longer valid and each oscillator DO NOT THERMALIZE

$$E = \sum_{1}^{N} {}_n E_n$$

but

$$\overline{(E_n)}_T = E_n(t=0) \text{ is conserved} \neq \frac{E}{N}$$

equipartition in isolated system!

for equipartition to hold and thermalization to occur a certain interaction btw oscillator should exists such that at equilibrium (d=1)

$$E = N\left(\underbrace{\frac{1}{2}k_BT + \frac{1}{2}k_BT}_{\text{Energy of one oscillator}}\right) = N E^{(1)}$$

- Interaction is necessary <u>to</u> equilibrium
- Weak interactions could be neglected for calculations of quantities <u>at</u> equilibrium