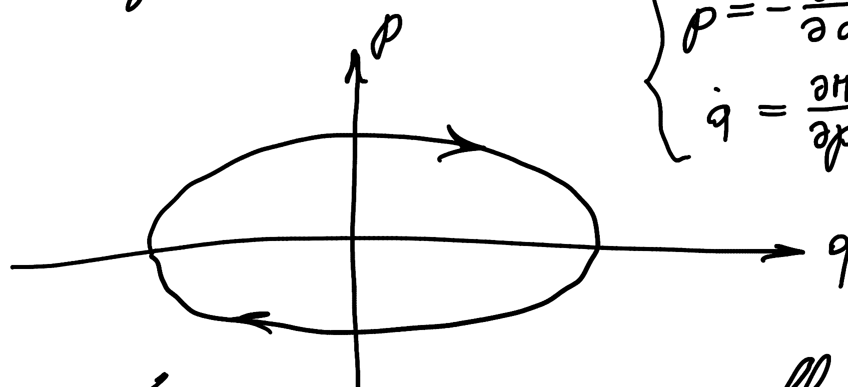
Concept of thermalisation. Liouville's theorem

We've learnt of the concept of phase space. For a closed system, motion occurs along deterministic trajectories in phase space

$$\begin{cases} \dot{p} = -\dfrac{\partial H}{\partial q} \\ \dot{q} = \dfrac{\partial H}{\partial p} \end{cases}$$



Phase trajectory of an oscillator

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

If the system is connected to an environment, it may „forget" its state after some time T_{relax}.

<u>Equilibrium</u> = the state of the system is independent of how the system came there

Environment = thermostat = bath = the environment which brings the system to equilibrium

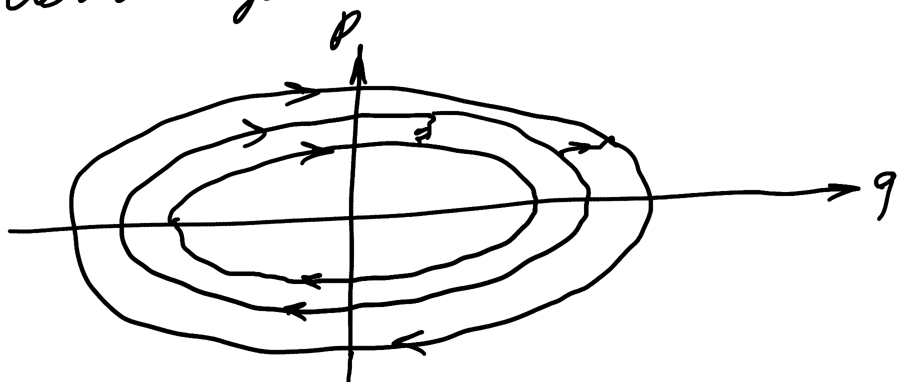
Example

Example

$$H = \underbrace{\frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}}_{H_{osc.}} + \underbrace{q\xi}_{V_{coupling}} + \underbrace{H_{bath}(\xi, P_\xi)}_{\text{Hamiltonian of the bath}}$$

For a weak coupling, the system will come to equilibrium on a long time T_{relax}.

At times $t \ll T_{relax}$ the system still obeys the equations of motion of a closed system



Coupling to the environment makes the system ergodic = makes the trajectories dense in phase space

Let's find how the density evolves

Liouville's theorem

Instead of time average, one may think about ensembe averages. Then ρ is the density of systems in phase space ensembe averages. Then ρ is the density of systems in phase space.

$$\frac{\partial \rho}{\partial t} + div\,(\rho \vec{v}) = 0 \quad \text{(For isolated systems)}$$

here $div\,(\rho \vec{v}) = \sum_{i=1}^{f} \left(\frac{\partial}{\partial q_i}(\rho \dot{q}_i) + \frac{\partial}{\partial p_i}(\rho \dot{p}_i) \right)$

$$\left.\begin{array}{l} \dfrac{\partial \rho}{\partial t} + \dfrac{\partial(\rho \dot{\vec{q}})}{\partial \vec{q}} + \dfrac{\partial(\rho \dot{\vec{q}})}{\partial \vec{p}} = 0 \\ \rho \dfrac{\partial \dot{\vec{q}}}{\partial \vec{q}} + \rho \dfrac{\partial \dot{\vec{q}}}{\partial \vec{p}} = \rho \dfrac{\partial^2 H}{\partial \vec{q}\, \partial \vec{p}} - \rho \dfrac{\partial^2 H}{\partial \vec{q}\, \partial \vec{p}} = 0 \end{array}\right\} \rightarrow$$

$$\rightarrow \frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial \vec{q}} \dot{\vec{q}} + \frac{\partial \rho}{\partial \vec{p}} \dot{\vec{p}} = 0$$

In an isolated system the destribution function is constant along phase trajectories