Classical Hamiltonian system [tln45]

Consider an autonomous classical dynamical system with 3N degrees of freedom (e.g. N particles in a 3D box with reflecting walls). The dynamics is fully described by 6N independent variables, e.g. by a set of *canonical coordinates* $q_1, \ldots, q_{3N}; p_1, \ldots, p_{3N}$.

The time evolution of these coordinates is specified by a Hamiltonian function $H(q_1, \ldots, q_{3N}; p_1, \ldots, p_{3N})$ and determined by the canonical equations:

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}; \quad i = 1, \dots, 3N$$

The time evolution of an arbitrary dynamical variable $f(q_1, \ldots, q_{3N}; p_1, \ldots, p_{3N})$ is determined by *Hamilton's equation of motion*:

$$\frac{df}{dt} = \sum_{i=1}^{3N} \left(\frac{\partial f}{\partial q_i} \dot{q}_i + \frac{\partial f}{\partial p_i} \dot{p}_i \right) = \sum_{i=1}^{3N} \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right) \equiv \{f, H\}$$

Conserved quantity: $\frac{df}{dt} = 0 \iff \{f, H\} = 0.$ Energy conservation is guaranteed: $\frac{dH}{dt} = 0$ because $\{H, H\} = 0.$

The microstate of the system is specified by one point in the 6*N*-dimensional phase space (Γ -space): $\mathbf{X} \equiv (q_1, \ldots, q_{3N}; p_1, \ldots, p_{3N})$. As time evolves, this point traces a trajectory through Γ -space.

The conservation law $H(q_1, \ldots, q_{3N}; p_1, \ldots, p_{3N}) = \text{const}$ confines the motion of any phase point to a 6N - 1-dimensional hypersurface in Γ -space. Other conservation laws, provided they exist, will further reduce the dimensionality of the manifold to which phase-space trajectories are confined.

Note: Within the framework of kinetic theory, the microstate of the same system was described by N points in the 6D space spanned the position and velocity coordinates of a single particle, $(x, y, z; v_x, v_y, v_z)$.

Our knowledge of the instantaneous microstate of the system is expressed by a probability density $\rho(\mathbf{X}, t)$ in Γ -space.

Normalization:
$$\int_{\Gamma} d^{6N} X \rho(\mathbf{X}, t) = 1.$$

Instantaneous expectation value: $\langle f \rangle = \int_{\Gamma} d^{6N} X f(\mathbf{X}) \rho(\mathbf{X}, t).$

Maximum knowledge about microstate realized for $\rho(\mathbf{X}, 0) = \delta(\mathbf{X} - \mathbf{X}_0)$.