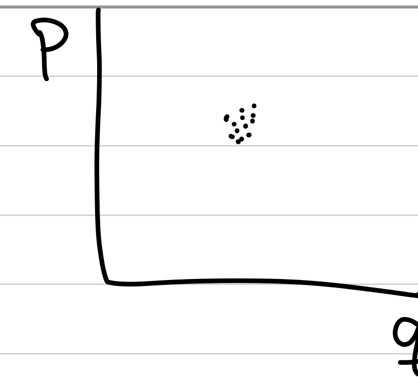
Liouville's eqn: $\dfrac{\partial \rho}{\partial t} = \{H, \rho\}$

$$= \sum_i \frac{\partial H}{\partial q_i}\frac{\partial \rho}{\partial p_i} - \frac{\partial \rho}{\partial q_i}\frac{\partial H}{\partial p_i}$$



1D

Single Particle system:

$$H = \frac{P^2}{2m} + V(X) \longrightarrow \frac{\partial \rho}{\partial t} = \frac{\partial V}{\partial X}\frac{\partial \rho}{\partial P} - \frac{\partial \rho}{\partial X}\frac{P}{m}$$

$P \longrightarrow y$

$$-\frac{\partial V}{\partial X} = F \Longrightarrow -\frac{\partial \rho}{\partial t} = F(X)\frac{\partial \rho}{\partial y} + \frac{y}{m}\frac{\partial \rho}{\partial X}$$

harmonic oscillator:

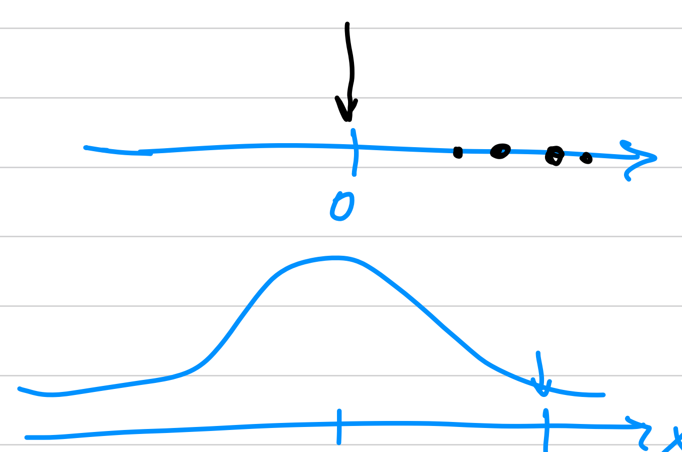
$$-\frac{\partial \rho}{\partial t} = -kX\frac{\partial \rho}{\partial y} + \frac{y}{m}\frac{\partial \rho}{\partial X} \qquad y = \sqrt{km}\,Y$$

$$-\frac{\partial \rho}{\partial t} = -\frac{k}{\sqrt{km}}X\frac{\partial \rho}{\partial Y} + \frac{\sqrt{km}}{m}Y\frac{\partial \rho}{\partial X}$$

$$= -\sqrt{\frac{k}{m}}\,X\frac{\partial \rho}{\partial Y} + \sqrt{k/m}\,Y\frac{\partial \rho}{\partial X} = \sqrt{\frac{k}{m}}\left(X\frac{\partial \rho}{\partial Y} - Y\frac{\partial \rho}{\partial X}\right)$$

$x = A\cos\omega t$

$\dot{x} = -A\omega\sin\omega t \longrightarrow P = -mA\omega\sin\omega t$



Equilibrium state: $\dfrac{\partial \rho}{\partial t} = 0$

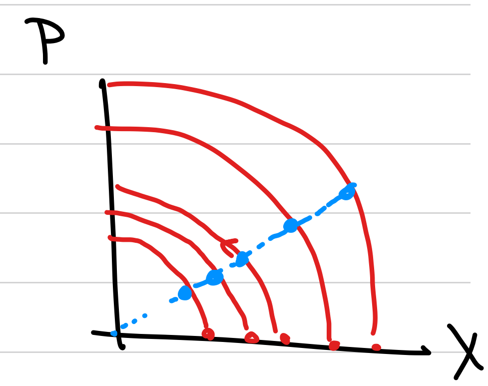
$$\left(\frac{\partial \rho}{\partial t}\right)_{P,X} = 0$$

$$\int \rho(X,P,t)\,dP$$

$$X\frac{\partial \rho}{\partial Y} = Y\frac{\partial \rho}{\partial X} \quad : \quad \rho(X,Y) = \rho(X^2+Y^2)$$

$$\frac{\partial \rho}{\partial Y} = \rho' \times 2Y$$

$$\frac{\partial \rho}{\partial X} = \rho' \times 2X$$



expectation Values: $A(q,p)$; $\rho \longleftrightarrow \underset{=}{f}$

$$\langle A \rangle = \int A(q,p)\, f(q,p,t)\, d^{3N}q\, d^{3N}p$$

$$\frac{d}{dt}\langle A \rangle = \int A(q,p) \frac{\partial f}{\partial t}\, dV \quad ; \quad \frac{\partial f}{\partial t} = \{H,f\} = \sum_i \frac{\partial H}{\partial q_i}\frac{\partial f}{\partial p_i} - \frac{\partial f}{\partial q_i}\frac{\partial H}{\partial p_i}$$

$$= \int A\{H,f\} = \sum_i \int A(q,p)\left(\frac{\partial H}{\partial q_i}\frac{\partial f}{\partial p_i} - \frac{\partial f}{\partial q_i}\frac{\partial H}{\partial p_i}\right) \underbrace{dV}$$

$$A\frac{\partial f}{\partial p_i} = \cancel{\frac{\partial}{\partial p_i}(Af)} - f\frac{\partial A}{\partial p_i} \qquad \frac{d}{dt}A = \cancel{\frac{\partial A}{\partial t}} + \{A,H\}$$

integration over p_i

$$\frac{d}{dt}\langle A \rangle = -\int f\{H,A\}\, dV = \int f \underbrace{\{A,H\}}_{\frac{dA}{dt}} dV$$

$$= \int f \frac{dA}{dt}\, dV = \left\langle \frac{dA}{dt} \right\rangle$$

$$\frac{d}{dt}\langle A \rangle = \left\langle \frac{dA}{dt} \right\rangle = \langle \{A,H\} \rangle$$

BBGKY : $f_1(\vec{r}_1,\vec{P}_1) = N\int \prod_{i=2}^{N} d^3\vec{r}_i\, d^3\vec{P}_i\; f(\vec{r}_1,\vec{r}_2,\dots,\vec{r}_N,\vec{P}_1,\vec{P}_2,\dots,\vec{P}_N)$

$n(\vec{r}_1,\vec{r}_2,\vec{r}_3,\dots)$

$$\int f_1(\vec{r},\vec{P})\, d^3\vec{r}\, d^3\vec{P} = N$$

- density : $n(\vec{r},t) = \int f_1(\vec{r},\vec{P},t)\, d^3\vec{P}$ — average Velocity : $\vec{u}(\vec{r},t) = \int d^3\vec{P}\, \frac{\vec{P}}{m} f_1(\vec{r},\vec{P},t)$

- Energy flux : $\vec{\mathcal{E}}(\vec{r},t) = \int d^3\vec{P}\, \frac{\vec{P}}{m} f_1(\vec{r},\vec{P},t)\, E(\vec{P})$

evolution of $f_1(\vec{r},t)$:

$$\frac{\partial}{\partial \vec{r}_i} = \frac{\partial}{\partial x_i}\hat{x}_i + \frac{\partial}{\partial y_i}\hat{y}_i + \frac{\partial}{\partial z_i}\hat{z}_i$$

$$f_1(\vec{r},\vec{p}) := N \int \prod_{i=2}^{N} d^3\vec{r}_i\, d^3\vec{p}_i\; f(\vec{r}_1,\vec{r}_2,\dots,\vec{r}_N,\vec{p}_1,\vec{p}_2,\dots,\vec{p}_N)$$

$$\frac{\partial f_1}{\partial t} = N \int \prod_{i=2}^{N} d^3\vec{r}_i\, d^3\vec{p}_i \;\frac{\partial f}{\partial t} = N \int \prod_{i=2}^{N} d^3\vec{r}_i\, d^3\vec{p}_i\; \{H,f\}$$

$$H = \frac{1}{2m}\sum_i p_i^2 + \sum_i V(\vec{r}_i) + \sum_{i<j} U(\vec{r}_i-\vec{r}_j) \; ; \; \{A,B\} = \sum_i \frac{\partial A}{\partial \vec{r}_i}\cdot\frac{\partial B}{\partial \vec{p}_i} - \frac{\partial B}{\partial \vec{r}_i}\cdot\frac{\partial A}{\partial \vec{p}_i}$$

$$\frac{\partial f_1}{\partial t} = N \int \prod_{i=2}^{N} d^3\vec{r}_i\, d^3\vec{p}_i \left(\frac{1}{2m}\sum_i \underbrace{\{p_i^2,f\}}_{-2\vec{p}_i\cdot\frac{\partial f}{\partial \vec{r}_i}} + \sum_i \underbrace{\{V(\vec{r}_i),f\}}_{\frac{\partial V(\vec{r}_i)}{\partial \vec{r}_i}\cdot\frac{\partial f}{\partial \vec{p}_i}} + \sum_{k<j} \underbrace{\{U(\vec{r}_k-\vec{r}_j),f\}}_{\sum_i \frac{\partial U(\vec{r}_k-\vec{r}_j)}{\partial \vec{r}_i}\cdot\frac{\partial f}{\partial \vec{p}_i}} \right)$$

$$\frac{\partial f_1}{\partial t} = N \int \prod_{i=2}^{N} d^3\vec{r}_i\, d^3\vec{p}_i \sum_i \left(-\frac{\vec{p}_i}{m}\cdot\frac{\partial f}{\partial \vec{r}_i} + \frac{\partial V}{\partial \vec{r}_i}\cdot\frac{\partial f}{\partial \vec{p}_i} + \sum_{k<j}\frac{\partial U}{\partial \vec{r}_i}\cdot\frac{\partial f}{\partial \vec{p}_i} \right)$$

$$\frac{\partial f_1}{\partial t} = N \int \prod_{i=2}^{N} d^3\vec{r}_i\, d^3\vec{p}_i \left(\frac{\vec{p}_1}{m}\cdot\frac{\partial f}{\partial \vec{r}_1} + \frac{\partial V}{\partial \vec{r}_1}\cdot\frac{\partial f}{\partial \vec{p}_1} + \sum_{k<j}\frac{\partial U}{\partial \vec{r}_1}\cdot\frac{\partial f}{\partial \vec{p}_1} \right)$$

$$N\int \prod_{i=2}^{N} d^3\vec{r}_i\, d^3\vec{p}_i\; \frac{\vec{p}_1}{m}\cdot\frac{\partial f}{\partial \vec{r}_1} = \frac{\vec{p}_1}{m}\cdot\frac{\partial}{\partial \vec{r}_1}\left(N\int \prod_{i=2}^{N} d^3\vec{r}_i\, d^3\vec{p}_i\; f \right)$$
$$= \frac{\vec{p}_1}{m}\cdot\frac{\partial f_1}{\partial \vec{r}_1}$$

$$\boxed{H_1 = \frac{p_1^2}{2m} + V(\vec{r}_1)}$$

$$\frac{\partial f_1}{\partial t} = \{H_1,f_1\} + N\int \prod_{i=2}^{N} d^3\vec{r}_i\, d^3\vec{p}_i \sum_{k=2}^{N} \frac{\partial U(\vec{r}_1-\vec{r}_k)}{\partial \vec{r}_1}\,\frac{\partial f}{\partial \vec{p}_1}$$

$$\boxed{\frac{\partial f_1}{\partial t} = \{H_1,f_1\} + \left(\frac{\partial f_1}{\partial t}\right)_{coll.}}$$

$$\left(\frac{\partial f_1}{\partial t}\right)_{coll.} = N\int \prod_{i=2}^{N} d^3\vec{r}_i\, d^3\vec{p}_i \sum_{k=2}^{N} \frac{\partial U(\vec{r}_1-\vec{r}_k)}{\partial \vec{r}_1} \frac{\partial f}{\partial \vec{p}_1}$$

$$= N(N-1)\int \prod_{i=2}^{N} d^3\vec{r}_i\, d^3\vec{p}_i \frac{\partial U(\vec{r}-\vec{r}_2)}{\partial \vec{r}_1}\cdot\frac{\partial f}{\partial \vec{p}_1}$$

$$= N(N-1)\int d^3\vec{r}_2\, d^3\vec{p}_2 \frac{\partial U(\vec{r}_1-\vec{r}_2)}{\partial \vec{r}_1}\cdot\frac{\partial}{\partial \vec{p}_1}\left(\int \prod_{i=3}^{N} d^3\vec{r}_i\, d^3\vec{p}_i\, f\right)$$

$$f_1(\vec{r}_1,\vec{p}_1) := N\int \prod_{i=2}^{N} d^3\vec{r}_i\, d^3\vec{p}_i\, f(\vec{r}_1,\vec{r}_2,\dots,\vec{p}_1,\vec{p}_2,\dots)$$

$$f_2(\vec{r}_1,\vec{r}_2,\vec{p}_1,\vec{p}_2) := N(N-1)\int \prod_{i=3}^{N} d^3\vec{r}_i\, d^3\vec{p}_i\, f(\vec{r}_1,\vec{r}_2,\dots,\vec{p}_1,\vec{p}_2,\dots)$$

$$\boxed{\left(\frac{\partial f_1}{\partial t}\right)_{coll.} = \int d^3\vec{r}_2\, d^3\vec{p}_2 \frac{\partial U(\vec{r}_1-\vec{r}_2)}{\partial \vec{r}_1}\cdot\frac{\partial f_2}{\partial \vec{p}_1}}$$

$$\boxed{\frac{\partial f_1}{\partial t} = \{H_1, f_1\} + \left(\frac{\partial f_1}{\partial t}\right)_{coll.}} \qquad \boxed{H_1 = \frac{p_1^2}{2m} + V(\vec{r}_1)}$$

Bogoliubov – Born – Green – Kirkwood – Yvon

BBGKY hierarchy :

$$f_n(\vec{r}_1,\vec{r}_2,\dots,\vec{r}_n,\vec{p}_1,\vec{p}_2,\dots,\vec{p}_n) := \frac{N!}{(N-n)!}\int \prod_{i=n+1}^{N} d^3\vec{r}_i\, d^3\vec{p}_i\, f(\vec{r}_1,\vec{r}_2,\dots,\vec{r}_N,\vec{p}_1,\vec{p}_2,\dots,\vec{p}_N)$$

$$\frac{\partial f_n}{\partial t} = \{H_n, f_n\} + \sum_{i=1}^{n}\int d^3\vec{r}_{n+1}\, d^3\vec{p}_{n+1} \frac{\partial U(\vec{r}_i-\vec{r}_{n+1})}{\partial \vec{r}_i}\cdot\frac{\partial f_{n+1}}{\partial \vec{p}_i}$$

$$H_n = \sum_{i=1}^{n}\left(\frac{p_i^2}{2m} + V(\vec{r}_i)\right) + \sum_{i<j\le n} U(\vec{r}_i-\vec{r}_j)$$