Dilute gas of N non-interacting particles

$$H = \underbrace{\sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \mathcal{U}(\vec{q}_i)}_{\equiv H_1,\ \text{non interacting dynamics}} + \underbrace{\frac{1}{2}\sum_{i\neq j} V(\vec{q}_i - \vec{q}_j)}_{\text{interactions}}$$

$$H_1 = \sum_{i=1}^{N} h_1(\vec{p}_i, \vec{q}_i)$$

Liouville's equation

$$\boxed{\partial_t \rho + \{\rho, H_1\} = \sum_{i=1}^{N}\left[\frac{\partial \rho}{\partial \vec{p}_i} \cdot \sum_{k\neq i} \frac{\partial V(\vec{q}_i - \vec{q}_k)}{\partial \vec{q}_i}\right]} \qquad (LE)$$

2.1.3) One-body density

$$\Rightarrow N_V(t) = \left\langle \int_V \sum_{i=1}^{N} \delta(\vec{q}_i(t) - \vec{r})\, d^3\vec{r} \right\rangle$$

$$= \int d\Gamma\ \rho(\{\vec{q}_j, \vec{p}_j\}, t) \int_V d^3\vec{r} \sum_{i=1}^{N} \delta(\vec{q}_i - \vec{r})$$

$$= \int_V d^3\vec{r} \int d\Gamma\ \rho(\{\vec{q}_j, \vec{p}_j\}, t) \sum_{i=1}^{N} \delta(\vec{q}_i - \vec{r})$$

$$= \int_V d^3\vec{r} \left\langle \sum_{i=1}^{N} \delta(\vec{q}_i(t) - \vec{r}) \right\rangle$$

$$\Rightarrow \boxed{n(\vec{r}, t) = \left\langle \sum_{i=1}^{N} \delta(\vec{q}_i(t) - \vec{r}) \right\rangle}$$

One-body function:

$$n(\vec{r},t) = \sum_{i=1}^{N} \int \prod_{k} d^3\vec{q}_k\, d^3\vec{p}_k \;\; \rho(\{\vec{q}_j,\vec{p}_j\},t)\, \delta(\vec{q}_i - \vec{r})$$

$$= \sum_{i=1}^{N} \int \underbrace{d^3\vec{q}_i\, d^3\vec{p}_i}_{d\Gamma_i} \;\; \delta(\vec{q}_i - \vec{r}) \underbrace{\int \prod_{k\neq i} d^3\vec{q}_k\, d^3\vec{p}_k\, \rho(\{\vec{q}_j,\vec{p}_j\},t)}_{\equiv \rho_i(\vec{q}_i,\vec{p}_i,t)}$$

Particle indistinguishability All particles in the gas are indistinguishable so that ρ is invariant by permutations of $\vec{q}_i,\vec{p}_i$ & $\vec{q}_j,\vec{p}_j$.

Thus $\rho_i(\vec{q},\vec{p},t) = \rho_j(\vec{q},\vec{p},t) \equiv \rho_1(\vec{q},\vec{p},t)$

One-body density

One thus has

$$n(\vec{r},t) = \sum_{i=1}^{N} \int d^3\vec{p}_i \;\; \rho_1(\vec{r},\vec{p}_i) = N\int d^3\vec{p}\, \rho_1(\vec{r},\vec{p})$$

$$\boxed{n(\vec{r},t) = \int d^3\vec{p}\, f_1(\vec{r},\vec{p}) \quad ; \quad f_1(\vec{r},\vec{p}) = N\rho_1(\vec{r},\vec{p})}$$

f_1 has a simple interpretation: $f_1(\vec{q},\vec{p},t)\, d^3\vec{q}\, d^3\vec{p}$ is the average # of particle in the volume $d^3\vec{q}\, d^3\vec{p}$ near $\vec{q},\vec{p}$.

Equivalent definitions

$$\rho_1(\vec{q},\vec{p},t) = \langle \delta(\vec{q}-\vec{q}_1(t))\, \delta(p-\vec{p}_1(t))\rangle$$

$$= \frac{1}{N} \langle \sum_{i=1}^{N} \delta(\vec{q}-\vec{q}_i(t))\, \delta(p-\vec{p}_i(t))\rangle$$

$$= \int \prod_{i\geq 2} d\Gamma_i \;\; \rho(\; \vec{q},\vec{p}, \{\vec{q}_j,\vec{p}_j\}_{j\geq 2}, t)$$

It is normalized as $\int d^3\vec{q}\, d^3\vec{p}\; \rho_1(\vec{q},\vec{p},t) = 1$

The one-body density f_1 is then defined as

$$f_1(\vec{q},\vec{p},t) = \sum_{i=1}^{N} \langle \delta(\vec{q}-\vec{q}_i(t))\,\delta(\vec{p}-\vec{p}_i(t)) \rangle$$ & is normalized as

$$\int d^3\vec{p}\, d^3\vec{q}\; f_1(\vec{q},\vec{p},t) = N$$

They contain the same information and we will use them equivalently.

Comment:
$$\left.\begin{aligned} &\rho(\{\vec{q}_i,\vec{p}_i\},t) : \mathbb{R}^{6N}\times\mathbb{R} \to \mathbb{R} \\ &\rho_1(\vec{q},\vec{p},t) : \mathbb{R}^{6}\times\mathbb{R} \to \mathbb{R} \end{aligned}\right\}$$ Huge dimensional reduction

To sample ρ for $N=10$ particles & 10 points per dimension, you need 10^{60} pts $\sim 10^{42} \times (600 \cdot 10^{15}) \Rightarrow 10^{42}$ times more than the 600 petabytes of data generated by LHC run 3. For ρ_1, you need 10^6 pts $\simeq 8$ Mb...

2.1.4) The BBGKY hierarchy

Let us integrate the Liouville equation over $\{\vec{q}_j,\vec{p}_j\}_{j\geq 2}$ to construct the time evolution of ρ_1.

$$\partial_t \rho + \{\rho, H_1\} = \sum_{i=1}^{N} \frac{\partial \rho}{\partial \vec{p}_i} \cdot \sum_{k\neq i} \frac{\partial V}{\partial \vec{q}_i}(\vec{q}_i-\vec{q}_k) \qquad (*)$$

Left hand side

Since the LHS corresponds to free evolution, we expect that

$$\int \prod_{k>1} d\vec{q}_k\, d\vec{p}_k\; \partial_t \rho + \{\rho, H_1\} = \partial_t \rho_1 + \{\rho_1, H_1\} \qquad (**)$$

Derivation:

$$\int \partial_t \rho \prod_{k>1} d\vec{q}_k\, d\vec{p}_k = \partial_t \int \rho \prod_{k>1} d\vec{q}_k\, d\vec{p}_k = \partial_t \rho_1(\vec{q}_1, \vec{p}_1, t)$$

$$\{\rho, H_1\} = \underbrace{\int \prod_{k>1} d\vec{q}_k\, d\vec{p}_k \left\{ \frac{\partial}{\partial \vec{q}_1}\rho \cdot \frac{\partial H_1}{\partial \vec{p}_1} - \frac{\partial}{\partial \vec{p}_1}\rho \cdot \frac{\partial H_1}{\partial \vec{q}_1} \right\}}_{1}$$

$$+ \underbrace{\sum_{i>1} \int \prod_{k>1} d\vec{q}_k\, d\vec{p}_k\, \frac{\partial \rho}{\partial \vec{q}_i}\cdot\frac{\partial H}{\partial \vec{p}_i} - \frac{\partial \rho}{\partial \vec{p}_i}\cdot\frac{\partial H}{\partial \vec{q}_i}}_{2}$$

1: $\frac{\partial H}{\partial \vec{p}_1} = \vec{p}_1$ & $\frac{\partial H}{\partial \vec{q}_1} = \frac{\partial U}{\partial \vec{q}_1}$ do not depend on $\{\vec{q}_k, \vec{p}_k\}_{k\geq 2}$

$$\Rightarrow 1 = \frac{\partial}{\partial \vec{q}_1}\left(\int \prod_{k>1} d\Gamma_k\, \rho\right)\cdot\frac{\partial H_1}{\partial \vec{p}_1} - \frac{\partial}{\partial \vec{p}_1}\left(\int \prod_{k>1} d\Gamma_k\, \rho\right)\cdot\frac{\partial H}{\partial \vec{q}_1} = \{\rho_1(\vec{q}_1,\vec{p}_1), H_1\}$$

2: $i \in [\![2, N]\!] \Rightarrow$ integrated upon $\Rightarrow$ integration by parts

$$2 = \sum_{i>1} \int \prod_{k>1} d\vec{q}_k\, d\vec{p}_k \underbrace{-\rho \frac{\partial}{\partial \vec{q}_i}\cdot\frac{\partial}{\partial \vec{p}_i} H + \rho \frac{\partial}{\partial \vec{p}_i}\cdot\frac{\partial}{\partial \vec{q}_i} H}_{=0} + \text{boundary terms}$$

boundary terms: if periodic boundary conditions $\Rightarrow = 0$

else $\int \prod_k d\Gamma_k\, \rho \Rightarrow \rho \xrightarrow[|\vec{p}_i| \to \infty]{|\vec{q}_i| \to \infty} 0 \Rightarrow = 0$

$\Rightarrow 2 = 0$

$1 + 2 = \{\rho_1, H_1\}$ as announced.

Right-hand side

$$\int \prod_{l>1} d\Gamma_l \sum_{i=1}^{N} \frac{\partial \rho}{\partial \vec{p}_i} \cdot \sum_{k\neq i} \frac{\partial V(\vec{q}_i-\vec{q}_k)}{\partial \vec{q}_i} = \sum_{k\neq 1} \int d\Gamma_k \frac{\partial V}{\partial \vec{q}_1} \cdot \frac{\partial}{\partial \vec{p}_1} \overbrace{\int \prod_{l\neq 1,k} \rho}^{=\rho_2(\vec{q}_1,\vec{p}_1,\vec{q}_k,\vec{p}_k)}$$

$$+ \sum_{i=2}^{N} \underbrace{\int \prod_{l>1} d\Gamma_l \frac{\partial}{\partial \vec{p}_i} \cdot \left[\rho \sum_{k\neq i} \frac{\partial V(\vec{q}_i-\vec{q}_k)}{\partial \vec{q}_i} \right]}_{\text{total derivative integrated upon} \Rightarrow \text{boundary term} \Rightarrow =0}$$

$$= \sum_{k\neq 1} \int d\Gamma_k \frac{\partial V(\vec{q}_1-\vec{q}_k)}{\partial \vec{q}_1} \cdot \frac{\partial}{\partial \vec{p}_1} \rho_2(\vec{q}_1,\vec{p}_1,\vec{q}_k,\vec{p}_k)$$

$$= (N-1) \int d\Gamma_2 \frac{\partial V}{\partial \vec{q}_1}(\vec{q}_1-\vec{q}_2) \cdot \frac{\partial}{\partial \vec{p}_1} \rho_2(\vec{q}_1,\vec{p}_1,\vec{q}_2,\vec{p}_2)$$

Since the particles $2, 3, \ldots, N$ are statistically indistinguishable.

Two-body functions $\rho_2(\vec{q},\vec{p},\vec{q}',\vec{p}')$ is the probability density to find particle 1 at $\vec{q},\vec{p}$ & particle 2 at $\vec{q}',\vec{p}'$. It is defined as

$$\rho_2(\vec{q},\vec{p},\vec{q}',\vec{p}') = \langle \delta(\vec{q}-\vec{q}_1(t))\,\delta(\vec{p}-\vec{p}_1(t))\,\delta(\vec{q}'-q_2(t))\,\delta(\vec{p}'-p_2(t)) \rangle$$

& is normalized as $\int d\vec{q}\,d\vec{p}\,d\vec{q}'\,d\vec{p}'\, \rho_2(\vec{q},\vec{p},\vec{q}',\vec{p}',t) = 1$.

We then define $f_2(\vec{q},\vec{p},\vec{q}',\vec{p}') = N(N-1)\,\rho_2(\vec{q},\vec{p},\vec{q}',\vec{p}',t)$ such that

$$\boxed{\underbrace{\partial_t f_1(\vec{q}_1,\vec{p}_1,t)+\{f_1,H_1\}}_{\text{free evolution}} = \underbrace{\int d\vec{q}_2\, d\vec{p}_2\, \frac{\partial V(\vec{q}_1-\vec{q}_2)}{\partial \vec{q}_1}\cdot \frac{\partial f_2(\vec{q}_1,\vec{p}_1,\vec{q}_2,\vec{p}_2)}{\partial \vec{p}_1}}_{\text{interaction term}}} \qquad \text{(F1)}$$

Comments:

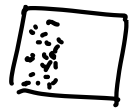
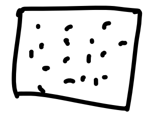
(I) We find the same structure as in Liouville's equation, because it comes from the same physics, but for lower dimensional object $\Rightarrow$ Good!

(II) In terms of computational cost, we could put equation (F1) in a computer, but we do not know f_2... (F1) is not a closed equation for f_1.

(III) We can integrate Liouville's equation over $d\Gamma_{k,\,k\geq 3}$ to get the time evolution of f_2. The right-hand side would involve $f_3(\vec{q}_1,\vec{p}_1,\vec{q}_2,\vec{p}_2,\vec{q}_3,\vec{p}_3)$. Each n-point function depends on the $(n+1)$-point function, for $n<N \Rightarrow$ BBGKY hierarchy of equations. As complex as Liouville's equation!

We need some approximation to close this hierarchy.

(IV) Time reversibility

Can (F1) predict the irreversible dynamics from  to  ?

Hamilton's equations are time reversible

If $\vec{q}(t), \vec{p}(t)$ solutions of $\dot{\vec{q}} = \frac{\partial H}{\partial \vec{p}}$; $\dot{\vec{p}} = -\frac{\partial H}{\partial \vec{q}}$.

Then $\vec{q}^{R}(t) = \vec{q}(t_f - t)$ & $\vec{p}^{R}(t) = -\vec{p}(t_f - t)$ are also solutions

$$\frac{d}{dt}\vec{q}^{R}(t) = \frac{d}{dt}\vec{q}(t_f - t) = -\dot{\vec{q}}(t_f - t) = -\left.\frac{\partial H}{\partial \vec{p}}\right|_{t_f - t} = \left.\frac{\partial H}{\partial -\vec{p}}\right|_{t_f - t} = \left.\frac{\partial H}{\partial \vec{p}^{R}}\right|_{t}$$

$$\frac{d}{dt}\vec{p}^{R}(t) = -\frac{d}{dt}\vec{p}(t_f - t) = \dot{\vec{p}}(t_f - t) = -\left.\frac{\partial H}{\partial \vec{q}}\right|_{t_f - t} = -\left.\frac{\partial H}{\partial \vec{q}^{R}}\right|_{t}$$