Equation of motion

\[ H = \sum_i \frac{p_i^2}{2m} + U + \frac{p_s^2}{2\alpha} + gkT e^u s \]

\[
\begin{align*}
\dot{r}_i &= \frac{\partial H}{\partial p_i} = \frac{\bar{p}_i}{ms^2} \\
\dot{q}_i &= -\frac{\partial H}{\partial q_i} = -\frac{\partial U}{\partial r_i} = \bar{F}_i \\
\dot{s} &= \frac{\partial H}{\partial p_s} = \frac{p_s}{\alpha} \\
\dot{p}_s &= -\frac{\partial H}{\partial r} = 2 \sum_i \frac{p_i^2}{2ms^2} - \frac{gkT}{s}
\end{align*}
\]

Now we change variables

\[ \dot{t} \rightarrow \tau \quad \bar{p}_i \Rightarrow \bar{p}_i' = \frac{\bar{p}_i}{s} \]

\[ \frac{dt}{s^\alpha} = d\tau \]

We start from

\[ \dot{r}_i = \frac{dr_i}{dt} = \frac{\bar{p}_i}{ms^2} \Rightarrow \frac{dr_i}{dt} s^\alpha = \frac{\bar{p}_i}{m} s^\alpha \]

The relation between \( \frac{d\bar{r}_i}{dt} \) and \( \bar{p}_i' \) is CANONICAL if we fix \( \alpha = 1 \)

Thus, from now on we set \( \alpha = 1 \quad g = \omega \)
For $\alpha = 1 \; q = 3N$

(a) \[ \frac{d\vec{P}_i}{dt} = \frac{\vec{P}_i}{m} \]

(b) \[ \frac{d\vec{P}_i'}{dt} = S \frac{d}{dt} \left( \frac{\vec{P}_i}{S} \right) = S \left[ \frac{\dot{\vec{P}}_i}{S} - \frac{\vec{P}_i}{S^2} \right] \]

\[ = \frac{\dot{\vec{P}}_i}{S} - \frac{\vec{P}_i}{S} \cdot \dot{S} = \vec{F}_i - \frac{1}{\alpha} P_s \vec{P}_i' = \vec{F}_i - \frac{P_s}{\alpha} \vec{P}_i' \]

(c) \[ \frac{ds}{dt} = \dot{s} = \frac{S P_s}{\alpha} \]

(d) \[ \frac{dP_s}{dt} = S \dot{P}_s = 2S \sum \frac{P_i^2}{2mS} - 3NkT = 2 \left( \sum \frac{P_i^2}{2m} - \frac{3}{2} NkT \right) \]

**COMMENTS:** (a), (b), (d) are independent of $S$

We only need to solve them.

(a) + (b) give the "Newton" equation

\[ m \frac{d\vec{r}_i}{dt} = \vec{F}_i - \frac{1}{\alpha} P_s m \bar{v}_i \]

\[ \bar{v} = \frac{d\vec{r}}{dt} \]

There is a velocity-dependent term

- For $P_s > 0$ it acts as a friction, it decreases the energy of the system.

- For $P_s < 0$ it gives energy to the system

$P_s$ is the reservoir variable: the system exchanges energy with the reservoir by means of $P_s$
The dynamics of $p_s$ is controlled by

$$
\frac{dp_s}{dt} = 2 \left( \sum_i \frac{p_i^2}{2m} - \frac{3}{2} NkT \right)
$$

kinetic energy

average kinetic energy (equipartition)

If the kinetic energy is larger than $\frac{3}{2} NkT$, then

$$
\frac{dp_s}{dt} > 0 \quad \Rightarrow \quad p_s \text{ increases, eventually it becomes positive, therefore it acts as a friction on the system, reducing the kinetic energy}
$$

If instead the kinetic energy is smaller than $\frac{3}{2} NkT$

then

$$
\frac{dp_s}{dt} < 0 \quad \Rightarrow \quad p_s \text{ decreases, eventually it becomes negative, therefore it provides additional energy to the system and the kinetic energy increases}
$$

The role of $p_s$ is that of guaranteeing that the kinetic energy fluctuates around $\frac{3}{2} NkT$, the average value in the canonical ensemble.
The canonical energy is not conserved

\[
\frac{d}{dt} \left[ \sum_i \frac{p_i^2}{2m} + U \right] =
\]

\[
= \sum_i \frac{p_i}{m} \frac{dp_i}{dt} + \sum_i \frac{\partial U}{\partial F_i} \frac{dF_i}{dt} \quad \text{(using the eqs. of motion)}
\]

\[
= \sum_i \frac{p_i}{m} \left( \ddot{F}_i - \frac{p_i}{\alpha} \ddot{p}_i \right) - \sum_i F_i \dddot{p}_i
\]

\[
= -\frac{2p_s}{\alpha} \sum_i \frac{p_i^2}{2m} \quad \text{as expected}
\]

Correction: Reverse the inequalities at the right unceases for \( p_s < 0 \)

If we include the energy of the reservoir, the total energy is of course conserved

\[
\frac{d}{dt} \left( \frac{p_s^2}{2\alpha} + 3NkT \epsilon_s \right) = \frac{p_s}{\alpha} \frac{dp_s}{dt} + \frac{3NkT}{\epsilon_s} \frac{d\epsilon_s}{dt} =
\]

\[
= \frac{2p_s}{\alpha} \left( \sum_i \frac{p_i^2}{2m} - \frac{3}{2} NkT \right) + 3NkT \frac{1}{\epsilon} \frac{5p_s}{\alpha}
\]

\[
= \frac{2p_s}{\alpha} \sum_i \frac{p_i^2}{2m}
\]

The energy flows from system to reservoir but the total energy is constant.
Let $\overrightarrow{P} = \Sigma_i \overrightarrow{p}_i$ (total momentum)

$$\frac{d\overrightarrow{P}}{dt} = \frac{\Sigma}{i} \frac{d\overrightarrow{p}_i}{dt} = \Sigma_i \overrightarrow{F}_i - \frac{Ps}{Q} \Sigma_i \overrightarrow{p}_i$$

In the absence of external forces

$$\Sigma_i \overrightarrow{F}_i = 0 \ (\text{III principle of dynamics})$$

$$\frac{d\overrightarrow{P}}{dt} = -\frac{Ps}{Q} \overrightarrow{P} \quad \text{Now we use} \quad \frac{Ps}{Q} = \frac{1}{S} \frac{ds}{dt}$$

$$\downarrow$$

$$\frac{d\overrightarrow{P}}{dt} = -\frac{1}{S} \overrightarrow{P} \frac{ds}{dt} \Rightarrow s \frac{d\overrightarrow{P}}{dt} + \overrightarrow{P} \frac{ds}{dt} = 0 \Rightarrow \frac{d}{dt} (s \overrightarrow{P}) = 0$$

The quantity $(s \overrightarrow{P})$ is conserved

Same conjecture as in the standard case.

The relevant configuration correspond to $\overrightarrow{P} = 0$

(at least for $N$ not too small)