Equations of motion

$$H = \sum_i \frac{p_i^2}{2ms^2} + U + \frac{p_s^2}{2Q} + gkT\ln s$$

$$\begin{cases} \dot{r}_i = \dfrac{\partial H}{\partial \vec{p}_i} = \dfrac{\vec{p}_i}{ms^2} \\ \dot{p}_i = -\dfrac{\partial H}{\partial \vec{q}_i} = -\dfrac{\partial U}{\partial \vec{r}_i} = \vec{F}_i \\ \dot{s} = \dfrac{\partial H}{\partial p_s} = \dfrac{p_s}{Q} \\ \dot{p}_s = -\dfrac{\partial H}{\partial s} = 2\sum_i \dfrac{p_i^2}{2ms^3} - \dfrac{gkT}{s} \end{cases}$$

Now we change variables

$$t \to \tau \qquad \vec{p}_i \Rightarrow \vec{p}_i' = \frac{\vec{p}_i}{s}$$

$$\frac{dt}{s^\alpha} = d\tau$$

We start from

$$\dot{r}_i = \frac{dr_i}{dt} = \frac{\vec{p}_i}{ms^2} \implies \frac{d\bar{r}_i}{d\tau} = \frac{d\bar{r}_i}{dt} s^\alpha = \frac{\bar{p}_i}{ms^2} s^\alpha = \frac{\bar{p}_i'}{m} s^{\alpha-1}$$

The relation between $\dfrac{d\bar{r}_i}{d\tau}$ and $\bar{p}_i'$ is CANONICAL if we fix $\boxed{\alpha = 1}$

Thus, from now on we set $\boxed{\alpha = 1 \quad g = 3N}$

For $\alpha = 1$ $\quad g = 3N$

(a) $\dfrac{d\bar{r}_i}{d\tau} = \dfrac{\bar{p}'_i}{m}$

(b) $\dfrac{d\bar{p}'_i}{d\tau} = s\dfrac{d}{dt}\left(\dfrac{\bar{p}_i}{s}\right) = s\left[\dfrac{\dot{\bar{p}}_i}{s} - \dfrac{p_i\,\dot{s}}{s^2}\right]$

$= \dot{\bar{p}}_i - \bar{p}'_i\,\dot{s} = \bar{F}_i - \dfrac{1}{Q}p_s\,\bar{p}'_i = \bar{F}_i - \dfrac{p_s}{Q}\,\bar{p}'_i$

(c) $\dfrac{ds}{d\tau} = s\dot{s} = \dfrac{s\,p_s}{Q}$

(d) $\dfrac{dp_s}{d\tau} = s\,\dot{p}_s = 2s\sum_i \dfrac{p_i'^2}{2ms^3} - 3NkT = 2\left(\sum_i \dfrac{p'^2}{2m} - \dfrac{3}{2}NkT\right)$

<u>COMMENTS</u>: (a), (b), (d) are independent of s
We only need to solve them.

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

$$m\frac{d^2\bar{r}_i}{d\tau^2} = \bar{F}_i - \frac{1}{Q}p_s\,m\bar{v}_i \qquad \bar{v} = \frac{d\bar{r}}{d\tau}$$

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

$$\frac{dp_s}{d\tau} = 2\left(\underbrace{\sum_i \frac{p_i'^2}{2m}}_{\text{kinetic energy}} - \underbrace{\frac{3}{2}NkT}_{\text{average kinetic energy (equipartition)}} \right)$$

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

$\frac{dp_s}{d\tau} > 0 \Rightarrow$ p_s 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

$\frac{dp_s}{d\tau} < 0 \Rightarrow$ p_s 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

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

$$= \sum_i \frac{p_i'}{m} \cdot \frac{dp_i'}{d\tau} + \sum_i \frac{\partial U}{\partial \bar{r}_i} \cdot \frac{d\bar{r}_i}{d\tau} \qquad \text{(using the eqs. of motion)}$$

$$= \sum_i \frac{\bar{p}_i'}{m} \cdot \left(\bar{F}_i - \frac{p_s}{Q}\bar{p}_i'\right) - \sum_i \bar{F}_i \cdot \frac{\bar{p}_i'}{m}$$

$$= -\frac{2p_s}{Q}\sum_i \frac{p_i'^2}{2m} \quad \leftarrow$$

AS EXPECTED
the energy decreases for $p_s < 0$

Correction: Reverse the inequalities at the right increases for $p_s > 0$

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

$$\frac{d}{d\tau}\left(\frac{p_s^2}{2Q} + 3NkT \ln s\right) = \frac{p_s}{Q}\frac{dp_s}{d\tau} + \frac{3NkT}{s}\frac{ds}{d\tau} =$$

$$= \frac{2p_s}{Q}\left(\sum_i \frac{p_i'^2}{2m} - \frac{3}{2}NkT\right) + 3NkT\frac{1}{s}\frac{sp_s}{Q}$$

$$= \frac{2p_s}{Q}\sum_i \frac{p_i'^2}{2m}$$

The energy flows from system to reservoir but the total energy is constant.

Momentum conservation

Let $\vec{P} = \sum_i \vec{p}_i'$ (total momentum)

$$\frac{d\bar{P}}{d\tau} = \sum_i \frac{d\vec{p}_i'}{d\tau} = \sum_i \bar{F}_i - \frac{p_s}{Q} \sum_i \vec{p}_i'$$

In the absence of external forces

$$\sum_i \vec{F}_i = 0 \quad (\text{III principle of dynamics})$$

$$\frac{d\bar{P}}{d\tau} = -\frac{p_s}{Q}\vec{P} \qquad \text{Now we use} \quad \frac{p_s}{Q} = \frac{1}{s}\frac{ds}{d\tau}$$

$$\Downarrow$$

$$\frac{d\bar{P}}{d\tau} = -\frac{1}{s}\bar{P}\frac{ds}{d\tau} \implies s\frac{d\bar{P}}{d\tau} + \bar{P}\frac{ds}{d\tau} = 0 \implies \frac{d}{d\tau}(s\bar{P}) = 0$$

$\boxed{\text{The quantity } (s\bar{P}) \text{ is conserved}}$

Same conjecture as in the standard case.

The relevant configurations correspond to $\bar{P} = 0$
(at least for N not too small)