Stochastic thermodynamics for systems described by a Fokker-Planck equation

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I. Langevin Equation

Now, let's considerer a system of particles in space that can be modeled as a continuos time Markovian system. We can make a model by the Langevin equation that is given in the following form:

$$m\frac{\mathrm{d}v_i}{\mathrm{d}t} = F_i - \alpha_i v_i + f_i(t) \tag{1}$$

in this equation with got some brief information as that m is the mass of each particle, $v_i = dx_i/dt$ and the term x_i is the position of the i-th particle. For a general case, we will consider that each particle is in contact with a different heat bath with temperature T_i.

Also in the equation (1), the forces that we consider are:

$$\begin{cases} F_i = f_i(x) + F_i^{\text{ext}}(t) & \text{force acting in the particle} \\ f_i^{\text{rand}}(t) & \text{Random force} \end{cases}$$

for the random force, we got the Gaussian Noise properties that are given by:

$$\left\langle f_i^{\text{rand}}(t) \right\rangle = 0 \tag{2}$$

$$\left\langle f_i^{\text{rand}}(t) f_i^{\text{rand}}(t') \right\rangle = 2\alpha k_B T_i \delta_{ij} \delta(t-t') \tag{3}$$

Above Langevin equation can be rewritten in the following form

$$m\frac{dv_i}{dt} = -\alpha_i v_i + F_i(t) + B_i(t), \tag{4}$$

where quantities v_i, α_i and $F_i(t)$ denote the particle velocity, the viscous constant and external force, respectively. From now on, we shall express them in terms of reduced quantities: $\gamma_i = \alpha_i/m$ and $f_i(t) = F_i(t)/m$. The stochastic force $\zeta_i(t) = B_i(t)/m$ accounts for the interaction between particle and the i-th environment and satisfies the properties

$$\langle \zeta_i(t) \rangle = 0, \tag{5}$$

and

$$\langle \zeta_i(t) \zeta_{i'}(t') \rangle = 2\gamma_i T_i \delta_{ii'} \delta(t-t'), \tag{6}$$

respectively, where T_i is the bath temperature. Let $P_i(v,t)$ be the velocity probability distribution at time t, its time evolution is described by the Fokker-Planck (FP) equation

$$\frac{\partial P_i}{\partial t} = -\frac{\partial J_i}{\partial v} - f_i(t)\frac{\partial P_i}{\partial v}, \tag{7}$$

where J_i is given by

$$J_i = -\gamma_i v P_i - \frac{\gamma_i T_i}{m}\frac{\partial P_i}{\partial v}. \tag{8}$$

It is worth mentioning that above equations are formally identical to description of the overdamped harmonic oscillator subject to the harmonic force $f_h = -\bar{k}x$ just by replacing $x \to v$, $\bar{k}/\alpha \to \gamma_i$, $1/\alpha \to \gamma_i/m$.

From the FP equation and by performing appropriate partial integrations together boundary conditions in which both $P_i(v,t)$ and $J_i(v,t)$ vanish at extremities, the time variation of the energy system $U_i = \langle E_i \rangle$ in contact with the i-th reservoir is given by

$$\frac{dU_i}{dt} = -\frac{m}{2}\int v^2\Big[\frac{\partial J_i}{\partial v} + f_i(t)\frac{\partial P_i}{\partial v}\Big]dv. \tag{9}$$

The right side of Eq. (19) can be rewritten as $dU_i/dt = -(\dot{W}_i + \dot{Q}_i)$, where $\dot{W}_i$ and $\dot{Q}_i$ denote the work per unity of time and heat flux from the system to the environment (thermal bath) given by

$$\dot{W}_i = -m\langle v_i \rangle f_i(t) \quad \text{and} \quad \dot{Q}_i = \gamma_i(m\langle v_i^2 \rangle - T_i), \tag{10}$$

respectively. In the absence of external forces $\dot{W}_i = 0$ and all heat flux comes from/goes to the thermal bath.

By assuming the system entropy S is given by $S_i(t) = -\int P_i(v,t)\ln[P_i(v,t)]dv$ and from the expression for J_i, one finds that its time derivative is given by

$$\frac{dS_i}{dt} = -\int \Big(\frac{J_i}{P_i}\Big)\Big(\frac{\partial P_i}{\partial v}\Big)dv. \tag{11}$$

As for the mean energy, above expression can be rewritten in the following form

$$\frac{dS_i}{dt} = \frac{m}{\gamma_i T_i}\Big(\int \frac{J_i^2}{P_i}dv + \gamma_i \int v J_i dv\Big). \tag{12}$$

Above expression can be interpreted according to the following form $dS_i/dt = \Pi_i(t) - \Phi_i(t)$, where the former term corresponds to the entropy production rate $\Pi_i(t)$ and it is strictly positive (as expected). The second term is the the flux of entropy and can also be rewritten more conveniently as

$$\Phi_i(t) = \frac{\dot{Q}_i}{T_i} = \gamma_i\Big(\frac{m}{T_i}\langle v_i^2 \rangle - k_B\Big). \tag{13}$$

If external forces are null and the particle is placed in contact to a single reservoir, the probability distribution approaches for large times the Gibbs (equilibrium) distribution $P_i^{eq}(v) = e^{-E/T_i}/Z$, being $E = mv^2/2$ its kinetic energy and Z the partition function. In such case, $\langle v_i^2 \rangle = T_i/m$ and therefore $\Pi_{eq} = \Phi_{eq} = 0$ (as expected). Conversely, it will evolve to a nonequilibrium steady state (NESS) when placed in contact with sequential and distinct reservoirs, in which heat is dissipated and the entropy is produced and hence $\Pi_{NESS} = \Phi_{NESS} > 0$.

II. **Fokker-Planck equation-overdamped case-sequential approach**

The same setup We are dealing with a Brownian particle with mass m sequentially placed in contact with N different thermal reservoirs. Each contact has a duration of τ/N and occurs during the intervals $\tau_{i-1} \le t < \tau_i$, where $\tau_i = i\tau/N$ for $i = 1, .., N$, in which the particle evolves in time according to the following Langevin equation

$$m\frac{dv_i}{dt} = -\alpha_i v_i + F_i(t) + B_i(t), \tag{14}$$

where quantities v_i, α_i and $F_i(t)$ denote the particle velocity, the viscous constant and external force, respectively. From now on, we shall express them in terms of reduced quantities: $\gamma_i = \alpha_i/m$ and $f_i(t) = F_i(t)/m$. The stochastic force $\zeta_i(t) = B_i(t)/m$ accounts for the interaction between particle and the i-th environment and satisfies the properties

$$\langle \zeta_i(t) \rangle = 0, \tag{15}$$

and

$$\langle \zeta_i(t)\zeta_{i'}(t') \rangle = 2\gamma_i T_i \delta_{ii'}\delta(t-t'), \tag{16}$$

respectively, where T_i is the bath temperature. Let $P_i(v,t)$ be the velocity probability distribution at time t, its time evolution is described by the Fokker-Planck (FP) equation

$$\frac{\partial P_i}{\partial t} = -\frac{\partial J_i}{\partial v} - f_i(t)\frac{\partial P_i}{\partial v}, \tag{17}$$

where J_i is given by

$$J_i = -\gamma_i v P_i - \frac{\gamma_i T_i}{m}\frac{\partial P_i}{\partial v}. \tag{18}$$

It is worth mentioning that above equations are formally identical to description of the overdamped harmonic oscillator subject to the harmonic force $f_h = -\bar{k}x$ just by replacing $x \to v$, $\bar{k}/\alpha \to \gamma_i$, $1/\alpha \to \gamma_i/m$.

From the FP equation and by performing appropriate partial integrations together boundary conditions in which both $P_i(v,t)$ and $J_i(v,t)$ vanish at extremities, the time variation of the energy system $U_i = \langle E_i \rangle$ in contact with the i-th reservoir is given by

$$\frac{dU_i}{dt} = -\frac{m}{2}\int v^2\Big[\frac{\partial J_i}{\partial v} + f_i(t)\frac{\partial P_i}{\partial v}\Big]dv. \tag{19}$$

By integrating the right side of Eq. (19) by parts and using suited boundary conditions, in which the probability and J_i vanish at extremities, above expression can be rewritten as $dU_i/dt = -(\dot{W}_i + \dot{Q}_i)$, where $\dot{W}_i$ and $\dot{Q}_i$ denote the work per unity of time and heat flux from the system to the environment (thermal bath) given by

$$\dot{W}_i = -m\langle v_i\rangle f_i(t) \quad \text{and} \quad \dot{Q}_i = \gamma_i(m\langle v_i^2\rangle - T_i), \tag{20}$$

respectively. In the absence of external forces $\dot{W}_i = 0$ and all heat flux comes from/goes to the thermal bath.

By assuming the system entropy S is given by $S_i(t) = -\int P_i(v,t)\ln[P_i(v,t)]dv$ and from the expression for J_i, one finds that its time derivative is given by

$$\frac{dS_i}{dt} = -\int\Big(\frac{J_i}{P_i}\Big)\Big(\frac{\partial P_i}{\partial v}\Big)dv. \tag{21}$$

As for the mean energy, above expression can be rewritten in the following form

$$\frac{dS_i}{dt} = \frac{m}{\gamma_i T_i}\Big(\int \frac{J_i^2}{P_i}dv + \gamma_i\int vJ_i dv\Big). \tag{22}$$

Above expression can be interpreted according to the following form $dS_i/dt = \Pi_i(t) - \Phi_i(t)$ (as verified in distinct previous cases) where the former term corresponds to the entropy production rate $\Pi_i(t)$ and it is strictly positive (as expected). The second term is the the flux of entropy and can also be rewritten more conveniently as

$$\Phi_i(t) = \frac{\dot{Q}_i}{T_i} = \gamma_i\Big(\frac{m}{T_i}\langle v_i^2\rangle - k_B\Big). \tag{23}$$

As before, if external forces are null and the particle is placed in contact to a single reservoir, the probability distribution approaches for large times the Gibbs (equilibrium) distribution $P_i^{eq}(v) = e^{-E/T_i}/Z$, being $E = mv^2/2$ its kinetic energy and Z the partition function. In such case, $\langle v_i^2\rangle = T_i/m$ and therefore $\Pi_{eq} = \Phi_{eq} = 0$ (as expected). Conversely, it will evolve to a nonequilibrium steady state (NESS) when placed in contact with sequential and distinct reservoirs, in which heat is dissipated and the entropy is produced and hence $\Pi_{\text{NESS}} = \Phi_{\text{NESS}} > 0$.

In order to obtain explicit and general results, the external forces will be expressed in the following form:

$$\tilde{f}_i(t) = \begin{cases} X_1 g_1(t), & t \in [0,\tau/2] \\ X_2 g_2(t), & t \in [\tau/2,\tau], \end{cases} \tag{24}$$

where $g_i(t)$ and X_i account for the kind of driving and its strength at stage i, respectively.It is worth mentioning that Eq. (24) describes generic drivings which do not depend on the velocity or position of the Brownian particle. Continuity of $P_i(v,t)$ at times $t = \tau/2$ and $t = \tau$ implies

$$\langle v_1\rangle(\tau/2) = \langle v_2\rangle(\tau/2) \quad ; \quad b_1(\tau/2) = b_2(\tau/2) \tag{25}$$

$$\langle v_1\rangle(0) = \langle v_2\rangle(\tau) \quad ; \quad b_1(0) = b_2(\tau) \tag{26}$$

From the above, we arrive at the following general expressions (evaluated for $= 1$ and $\gamma_1 = \gamma_2 \equiv \gamma$):

$$\langle v_1\rangle(t) = X_1\int_0^t e^{\gamma(t'-t)}g_1(t')dt' + \frac{1}{e^{\gamma\tau}-1}\Big\{X_1\int_0^{\tau/2} e^{\gamma(t'-t)}g_1(t')dt' + X_2\int_{\tau/2}^{\tau} e^{\gamma(t'-t)}g_2(t')dt'\Big\}, \tag{27}$$

$$\langle v_2\rangle(t) = X_2\int_{\tau/2}^t e^{\gamma(t'-t)}g_2(t')dt' + \frac{1}{e^{\gamma\tau}-1}\Big\{e^{\gamma\tau}X_1\int_0^{\tau/2} e^{\gamma(t'-t)}g_1(t')dt' + X_2\int_{\tau/2}^{\tau} e^{\gamma(t'-t)}g_2(t')dt'\Big\}, \tag{28}$$

$$b_1(t) = -\frac{1}{m}\frac{(T_1-T_2)}{(1+e^{-\gamma\tau})}e^{-2\gamma t} + \frac{T_1}{m} \quad ; \quad b_2(t) = -\frac{1}{m}\frac{(T_2-T_1)}{(1+e^{-\gamma\tau})}e^{-2\gamma(t-\tau/2)} + \frac{T_2}{m}. \tag{29}$$

Inserting the above expressions into expressions for work and heat and averaging over a complete cycle, we finally arrive at

$$\begin{aligned}
\overline{\dot{W}}_1 &= -\frac{m}{\tau\,(e^{\gamma\tau}-1)}\left[X_1^2\left((e^{\gamma\tau}-1)\int_0^{\tau/2} g_1(t)e^{-\gamma t}\int_0^t g_1(t')e^{\gamma t'}\,dt'dt+\int_0^{\tau/2} g_1(t)e^{-\gamma t}\,dt\int_0^{\tau/2} g_1(t')e^{\gamma t'}\,dt'\right)\right.\\
&+\left. X_1X_2\int_0^{\tau/2} g_1(t)e^{-\gamma t}\,dt\int_{\tau/2}^{\tau} g_2(t')e^{\gamma t'}\,dt'\right], \qquad (30)\\
\overline{\dot{Q}}_1 &= \frac{\gamma m}{\tau}\left[\int_0^{\tau/2}\langle v_1\rangle^2 dt-\frac{1}{2\gamma m}\tanh(\gamma\tau/2)(T_1-T_2)\right], \qquad (31)
\end{aligned}$$

and

$$\begin{aligned}
\overline{\dot{W}}_2 &= -\frac{m}{\tau(e^{\gamma\tau}-1)}\left[X_2^2\left(\int_{\tau/2}^{\tau} g_2(t)e^{-\gamma t}dt\int_{\tau/2}^{\tau} g_2(t')e^{\gamma t'}dt'+(e^{\gamma\tau}-1)\int_{\tau/2}^{\tau} g_2(t)e^{-\gamma t}\int_{\tau/2}^{t} g_2(t')e^{\gamma t'}dt'dt\right).\right.\\
&\left.+X_1X_2e^{\gamma\tau}\left(\int_{\tau/2}^{\tau} g_2(t)e^{-\gamma t}\,dt\int_0^{\tau/2} g_1(t')e^{\gamma t'}\,dt'\right)\right], \qquad (32)\\
\overline{\dot{Q}}_2 &= \frac{m\gamma}{\tau}\left[\int_{\tau/2}^{\tau}\langle v_2\rangle^2 dt+\frac{1}{2\gamma m}\tanh(\gamma\tau/2)(T_1-T_2)\right], \qquad (33)
\end{aligned}$$

for first and second stages, respectively and $\overline{\sigma}$ is promptly obtained by inserting above expressions in Eq. (23). It is worth emphasizing that Eqs. (30)-(33) are general and valid for any kind of drivings and temperatures. Close to equilibrium the entropy production, given by Eq. (23), assumes the familiar *flux times force* form $\overline{\sigma}\approx J_1f_1+J_2f_2+J_Tf_T$ where

$$f_1=X_1/T\ \ ;\ \ f_2=X_2/T\ \ ;\ \ f_T=\Delta T/T^2 \qquad (34)$$

($\Delta T=T_2-T_1$) and fluxes defined by

$$\overline{\dot{W}}_1=-TJ_1f_1\ \ ;\ \ \overline{\dot{W}}_2=-TJ_2f_2\ \ ;\ \ \overline{\dot{Q}}_1-\overline{\dot{Q}}_2=2J_T. \qquad (35)$$

Up to first order in the forces these fluxes can be expressed in terms of Onsager coefficients $J_1=L_{11}f_1+L_{12}f_2$, $J_2=L_{21}f_1+L_{22}f_2$ and $J_T=L_{TT}f_T$ which results in

$$\begin{aligned}
L_{11} &= \frac{mT}{\tau\,(e^{\gamma\tau}-1)}\left[(e^{\gamma\tau}-1)\int_0^{\tau/2} g_1(t)e^{-\gamma t}\int_0^t g_1(t')e^{\gamma t'}\,dt'dt+\int_0^{\tau/2} g_1(t)e^{-\gamma t}dt\int_0^{\tau/2} g_1(t')e^{\gamma t'}\,dt'\right], \qquad (36)\\
L_{22} &= \frac{mT}{\tau\,(e^{\gamma\tau}-1)}\left[\int_{\tau/2}^{\tau} g_2(t)e^{-\gamma t}\,dt\int_{\tau/2}^{\tau} g_2(t')e^{\gamma t'}\,dt'+(e^{\gamma\tau}-1)\int_{\tau/2}^{\tau} g_2(t)e^{-\gamma t}\int_{\tau/2}^{t} g_2(t')e^{\gamma t'}\,dt'dt\right], \qquad (37)\\
L_{12} &= \frac{mT}{\tau\,(e^{\gamma\tau}-1)}\int_0^{\tau/2} g_1(t)e^{-\gamma t}\,dt\int_{\tau/2}^{\tau} g_2(t')e^{\gamma t'}\,dt' \quad ; \quad L_{21}=\frac{mTe^{\gamma\tau}}{\tau\,(e^{\gamma\tau}-1)}\int_0^{\tau/2} g_1(t')e^{\gamma t'}\,dt'\int_{\tau/2}^{\tau} g_2(t)e^{-\gamma t}\,dt, \qquad (38)\\
L_{TT} &= \frac{T^2}{2\tau}\tanh\left(\frac{\gamma\tau}{2}\right). \qquad (39)
\end{aligned}$$

Four remarks are in order. First, Eqs. (30) and (32) state that average powers are independent on the velocities. Second, Onsager coefficients L_{ij}'s ($i,j=1,2$) are exact and valid for arbitrary values of f_i's. Third, to verify Onsager-Casimir symmetry for the cross coefficients L_{12} and L_{21} it is necessary not only to reverse the drivings but also to exchange the indices $1\leftrightarrow 2$. Fourth and last, there is no coupling between work fluxes and heat flux. That is, the cross coefficients L_{T1}, L_{1T}, L_{T2} and L_{2T} are absent. Hence this class of engines does not convert heat into work (nor work is converted into heat) and always loses its efficiency when the difference of temperatures ΔT between thermal baths is large, because heat can not be converted into output work. In the regime of low temperatures, efficiency properties can be solely expressed in terms of Onsager coefficients and their derivatives.

III. **Fokker-Planck equation-underdamped case**

For this Brownian motion system, we can associate a probability distribution function $P(x,v,t)$ in what we got the set that $x=(x_1,x_2,\ldots,x_n)$ and $v=(v_1,v_2,\ldots,v_n)$.

The Fokker-Planck equation associated to this system with N particles, in that each one has a thermal reservoir with temperature T_i, is given by:

$$\frac{\partial P}{\partial t}=-\sum_i\frac{\partial}{\partial v_i}\left[\frac{1}{m}F_iP-\gamma_iv_iP\right]-\sum_i\frac{\partial}{\partial x_i}(v_iP)+\frac{k_B}{m}\sum_i\gamma_iT_i\frac{\partial^2P}{\partial v_i^2}$$

in the case that all particles are submited by the same $\gamma_i=\alpha_i/m$, we make that $\gamma_i=\gamma$, $\forall i$, so we reach in:

$$\frac{\partial P}{\partial t} = -\sum_i \frac{\partial}{\partial v_i}\left[\frac{1}{m}F_i P - \gamma v_i P\right] - \sum_i \frac{\partial}{\partial x_i}(v_i P) + \frac{k_B \gamma}{m}\sum_i T_i \frac{\partial^2 P}{\partial v_i^2} \tag{40}$$

As we said before, we're gonna consider a case with multiples Brownian particles in that each one is submited to a different thermal reservoir. For start some general analysis, let's make the equation (40) in a different form:

$$\frac{\partial P}{\partial t} = -\sum_i \frac{\partial J_{x_i}}{\partial x_i} - \sum_i \frac{\partial J_{v_i}}{\partial v_i} - \sum_i \frac{\partial}{\partial v_i}\left(\frac{1}{m}F_i P\right) \tag{41}$$

in this form, we write some terms as probabilities currents and can be analysed as a diffusion function. Each current is given by:

$$\begin{cases} J_{x_i} &= v_i P \\ J_{v_i} &= -\gamma v_i P - \dfrac{\gamma T_i k_B}{m}\dfrac{\partial P}{\partial v_i} \end{cases}$$

IV. Entropy and entropy production

Following the Boltzmann entropy definition, that we represented for the discrete case in equation(**??**), we can get the continuous form by replacing the sum by the integral:

$$S(t) = -k_B \int P(x,v,t)\log P(x,v,t)d\tau \tag{42}$$

taking the time derivative of the equation above:

$$\begin{aligned} \frac{\mathrm{d}S(t)}{\mathrm{d}t} &= -k_B \int \left[\frac{\partial P}{\partial t}\log P + P\frac{1}{P}\frac{\partial P}{\partial t}\right] d\tau \\ &= -k_B \int \left[\frac{\partial P}{\partial t}(\log P + 1)\right] d\tau \end{aligned}$$

Now, plugging the equation (41) in the equation above, we reach in the following expression:

$$\frac{\partial S}{\partial t} = -k_B \sum_i \int \left\{\left[-\frac{\partial J_{x_i}}{\partial x_i} - \frac{\partial J_{v_i}}{\partial v_i} - \frac{\partial}{\partial v_i}\left(\frac{1}{m}F_i P\right)\right](\log P + 1)\right\} d\tau \tag{43}$$

$$= k_B \sum_i \int \left\{\left[\frac{\partial J_{x_i}}{\partial x_i} + \frac{\partial J_{v_i}}{\partial v_i} + \frac{\partial}{\partial v_i}\left(\frac{1}{m}F_i P\right)\right](\log P + 1)\right\} d\tau \tag{44}$$

$$= k_B \left[\underbrace{\sum_i \int \frac{\partial J_{x_i}}{\partial x_i}(\log P + 1)\,d\tau}_{\mathcal{I}_1} + \underbrace{\sum_i \int \frac{\partial J_{v_i}}{\partial v_i}(\log P + 1)\,d\tau}_{\mathcal{I}_2} + \underbrace{\sum_i \int \frac{\partial}{\partial v_i}\left(\frac{1}{m}F_i P\right)(\log P + 1)\,d\tau}_{\mathcal{I}_3}\right] \tag{45}$$

For calculate each of the integrals, we need first to assure some conditions:

- $\lim_{x \text{ or } v \to \pm\infty} P(x,v,t) = 0$
- $\lim_{x \text{ or } v \to \pm\infty} J_{v_i} = 0$

Now, let's calculate each one of the integrals:

■(Integral $\mathcal{I}_1$)

$$
\begin{aligned}
\mathcal{I}_1 &= \sum_i \int \frac{\partial J_{x_i}}{\partial x_i} (\log P + 1)\, d\tau \\
&= \sum_i \int \frac{\partial}{\partial x_i} (v_i P)\, (\log P + 1)\, d\tau \\
&= \sum_i \int \left[\underbrace{\frac{\partial v_i}{\partial x_i}}_{=0} P + v_i \frac{\partial P}{\partial x_i} \right] (\log P + 1)\, d\tau \\
&= \sum_i \int v_i \frac{\partial P}{\partial x_i} (\log P + 1)\, d\tau \\
&= \sum_i \left\{ \underbrace{v_i P\, (\log P + 1)\Big|_{-\infty}^{\infty}}_{=0} - \int P \frac{\partial}{\partial x_i} [v_i (\log P + 1)] d\tau \right\} \\
&= -\sum_i \left\{ \int v_i P \frac{1}{P} \frac{\partial P}{\partial x_i} d\tau \right\} \\
&= -\sum_i \left\{ \int v_i \frac{\partial P}{\partial x_i} d\tau \right\} \\
&= -\sum_i \left\{ \underbrace{v_i P\Big|_{-\infty}^{\infty}}_{=0} - \int P \underbrace{\frac{\partial v_i}{\partial x_i}}_{=0} d\tau \right\} \\
&= 0
\end{aligned}
$$

■(Integral $\mathcal{I}_2$)

$$
\begin{aligned}
\mathcal{I}_2 &= \sum_i \int \frac{\partial J_{v_i}}{\partial x_i} (\log P + 1)\, d\tau \\
&= \sum_i \left\{ \underbrace{J_{v_i} (\log P + 1)\Big|_{-\infty}^{\infty}}_{=0} - \int \frac{J_{v_i}}{P} \frac{\partial P}{\partial v_i} d\tau \right\}
\end{aligned}
$$

knowing that $\dfrac{\partial P}{\partial v_i} = \dfrac{m}{\gamma k_B T_i} [-\gamma v_i P - J_{v_i}]$. we reach in:

$$
\begin{aligned}
\mathcal{I}_2 &= -\sum_i \left\{ \int \frac{J_{v_i}}{P} \left[\frac{m}{\gamma k_B T_i} (-\gamma v_i P - J_{v_i}) \right] d\tau \right\} \\
&= \sum_i \left\{ \frac{m}{\gamma k_B T_i} \int \frac{J_{v_i}^2}{P} d\tau + \frac{m}{\gamma k_B T_i} \int \gamma v_i J_{v_i} d\tau \right\}
\end{aligned}
$$

■**(Integral $\mathcal{I}_3$)**

$$
\begin{aligned}
\mathcal{I}_3 &= \sum_i \int \frac{\partial}{\partial v_i}\left(\frac{1}{m}F_i P\right)(\log P + 1)\, d\tau \\
&= \frac{1}{m}\sum_i \left\{ \int \left[P \underbrace{\frac{\partial F_i}{\partial v_i}}_{=0} + F_i \frac{\partial P}{\partial v_i} \right] (\log P + 1)\, d\tau \right\} \\
&= \frac{1}{m}\sum_i \left\{ \int F_i \frac{\partial P}{\partial v_i}(\log P + 1)\, d\tau \right\} \\
&= \frac{1}{m}\sum_i \left\{ \underbrace{F_i P (\log P + 1)\Big|_{-\infty}^{\infty}}_{=0} - \int P \frac{\partial}{\partial v_i}[F_i(\log P + 1)] d\tau \right\} \\
&= -\frac{1}{m}\sum_i \left\{ \int F_i P \frac{1}{P}\frac{\partial P}{\partial v_i} d\tau \right\} \\
&= -\frac{1}{m}\sum_i \left\{ \int F_i \frac{\partial P}{\partial v_i} d\tau \right\} \\
&= -\frac{1}{m}\sum_i \left\{ F_i P \Big|_{-\infty}^{\infty} \right\} \\
&= 0
\end{aligned}
$$

With all the integrals evaluated for a general case, we can input the above results in equation (45) and get the following form for the entropy production for a system like that:

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \sum_i \frac{m}{\gamma T_i}\left\{ \int \frac{J_{v_i}^2}{P} d\tau + \int \gamma v_i J_{v_i} d\tau \right\} \tag{46}$$

Analysing the equation (46) we know that the term of J_{v_i} is such that:

$$\sum_i \frac{m}{\gamma T_i} \int \frac{J_{v_i}^2}{P} d\tau \geq 0$$

beyond that, we know that we can represent dS/dt as the form of (**??**):

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \Pi(t) - \phi(t)$$

in what the entropy production is always greater or equal to 0. Due to that, we are gonna define the entropy production and the entropy flux of this kind of system by the following form:

$$\boxed{\Pi(t) = \sum_i \frac{m}{\gamma T_i} \int \frac{J_{v_i}^2}{P} d\tau (47)}$$

$$\boxed{\phi(t) = -\sum_i \frac{m}{T_i} \int v_i J_{v_i} d\tau (48)}$$

V. Mean energy, work and dissipated power

In this following section, we're gonna derive some other relations starting from some ensembles definitions.

For the mean energy $U = \langle E \rangle$, we start from the definition:

$$U = \langle E \rangle = \int EP(x, v, t) d\tau$$

For the case we're considering, we got the fact that the energy function is composed by only a kinetic energy(T) and a potential energy(V) that does not have an explicit time dependence. In other words:

$$\frac{\partial E}{\partial t} = 0$$

Now, plugging the energy definition for the case in the above expression, we got:

$$U = \int (T + V) P d\tau \tag{49}$$

deriving in respect to time:

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \int (T + V) \frac{\partial P}{\partial t} d\tau \tag{50}$$

in this equation above, we insert the equation (41):

$$\frac{\mathrm{d}U}{\mathrm{d}t} = -\int \left\{ (T + V) \left[\sum_i \frac{\partial J_{x_i}}{\partial x_i} + \sum_i \frac{\partial J_{v_i}}{\partial v_i} + \sum_i \frac{\partial}{\partial v_i} \left(\frac{1}{m} F_i P \right) \right] \right\} d\tau \tag{51}$$

$$= -\sum_i \left\{ \underbrace{\int \left[(T + V) \frac{\partial J_{x_i}}{\partial x_i} \right] d\tau}_{\mathcal{I}_1} + \underbrace{\int \left[(T + V) \frac{\partial J_{v_i}}{\partial v_i} \right] d\tau}_{\mathcal{I}_2} + \underbrace{\int \left[(T + V) \frac{\partial}{\partial v_i} \left(\frac{1}{m} F_i P \right) \right] d\tau}_{\mathcal{I}_3} \right\} \tag{52}$$

As we've done before, let's solve these integrals separately:

■(Integral $\mathcal{I}_1$)

$$\begin{aligned}
\mathcal{I}_1 &= \int \left[(T + V) \frac{\partial J_{x_i}}{\partial x_i} \right] d\tau \\
&= \underbrace{(T + V) J_{x_i} \Big|_{-\infty}^{\infty}}_{=0} - \int J_{x_i} \frac{\partial (T + V)}{\partial x_i} d\tau \\
&= -\int J_{x_i} \frac{\partial V}{\partial x_i} d\tau \\
&= \int J_{x_i} f_i d\tau \\
&= \int v_i F_i P d\tau \\
&= \langle v_i f_i \rangle
\end{aligned}$$

■(Integral $\mathcal{I}_2$)

$$\begin{aligned}
\mathcal{I}_2 &= \int \left[(T + V) \frac{\partial J_{v_i}}{\partial v_i} \right] d\tau \\
&= \underbrace{(T + V) J_{v_i} \Big|_{-\infty}^{\infty}}_{=0} - \int J_{v_i} \underbrace{\frac{\partial T}{\partial v_i}}_{=mv_i} d\tau \\
&= -m \int v_i J_{v_i} d\tau
\end{aligned}$$

■**(Integral $\mathcal{I}_3$)**

$$\begin{aligned}
\mathcal{I}_3 &= \int \left[(T+V)\frac{\partial}{\partial v_i}\left(\frac{1}{m}F_i P\right)\right] d\tau \\
&= \underbrace{\frac{1}{m}(T+V)F_i P\Big|_{-\infty}^{\infty}}_{=0} - \frac{1}{m}\int F_i P \underbrace{\frac{\partial T}{\partial v_i}}_{=mv_i} d\tau \\
&= -\int F_i v_i P d\tau \\
&= -\langle F_i v_i \rangle \\
&= -\langle v_i f_i \rangle - \langle v_i \rangle F_i^{\text{ext}}(t)
\end{aligned}$$

Now, plugging the integrals above in the equation (52):

$$\frac{\mathrm{d}U}{\mathrm{d}t} = -\sum_i \left[\langle v_i f_i \rangle - m\int v_i J_{v_i} d\tau - \langle v_i f_i \rangle - \langle v_i \rangle F_i^{\text{ext}}(t)\right]$$

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \underbrace{\sum_i m\int v_i J_{v_i} d\tau}_{\text{Heat per time}} + \underbrace{\sum_i \langle v_i \rangle F_i^{\text{ext}}(t)}_{\text{Work per time}} \tag{53}$$

As we know, the term J_{v_i} is given by:

$$J_{v_i} = -\gamma v_i P - \frac{\gamma T_i k_B}{m}\frac{\partial P}{\partial v_i}$$

now, replacing this in the integral term of (53):

$$\begin{aligned}
\int v_i J_{v_i} d\tau &= -\int \left[v_i \left(\gamma v_i P + \frac{\gamma T_i k_B}{m}\frac{\partial P}{\partial v_i}\right)\right] d\tau \\
&= -\gamma \int v_i^2 P d\tau - \frac{\gamma T_i k_B}{m}\int v_i \frac{\partial P}{\partial v_i} d\tau \\
&= -\gamma \left\langle v_i^2 \right\rangle - \frac{\gamma T_i k_B}{m}\left(\underbrace{v_i P\Big|_{-\infty}^{\infty}}_{=0} - \underbrace{\int P d\tau}_{=1}\right) \\
&= -\gamma \left\langle v_i^2 \right\rangle + \frac{\gamma k_B T_i}{m}
\end{aligned}$$

Plugging this relation above in (52):

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \underbrace{\sum_i \langle v_i \rangle F_i^{\text{ext}}(t)}_{\text{Work}} - \underbrace{\sum \left[m\gamma \left\langle v_i^2 \right\rangle + \gamma k_B T_i \right]}_{\text{Heat}} \tag{54}$$

References