# Canonical Theory of Dissipative Systems

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Contents

# Entropy production in Brownian motion

- Langevin eq. $m\dfrac{dv(t)}{dt} = -\zeta v(t) + \eta(t) + F$

$$\langle \eta(t)\eta(t')\rangle = 2\varepsilon\delta(t-t')$$

$$\zeta = \frac{1}{k_BT}\varepsilon = \frac{1}{k_BT}\int_0^\infty \langle \eta(0)\eta(t)\rangle dt \ ; \ \frac{1}{2}m\langle v^2(t)\rangle = \frac{1}{2}k_BT.$$

- odd part (antisymmetric part): **mass current**

$$\frac{d}{dt}J(t) = -\gamma J(t) + F \ ; \ \gamma \equiv \frac{\zeta}{m} \text{ and } J(t) \equiv m\langle v(t)\rangle$$

- even part (symmetric part):

Work $\langle v(t)\rangle F = \dfrac{dE(t)}{dt} + \dfrac{dU(t)}{dt}$ ; $E(t) = \dfrac{1}{2}m\langle v^2(t)\rangle$ and

$$\frac{dU(t)}{dt} = \zeta\langle v^2(t)\rangle - \langle v(t)\eta(t)\rangle = \zeta\langle v^2(t)\rangle - \frac{\varepsilon}{m} = \zeta\left(\langle v^2(t)\rangle - \underset{\substack{\uparrow \\ F=0}}{\langle v^2(t)\rangle_0}\right) = \zeta\langle v(t)\rangle^2.$$

entropy production $\sigma_S(t)$ is given by

$$\sigma_S(t) \equiv \left(\frac{dS}{dt}\right)_{irr} \equiv \frac{1}{T}\frac{dU}{dt} = \frac{\mu F^2}{T}\left(1-e^{-\gamma t}\right)^2 \ ; \ \mu \equiv \frac{1}{\zeta} \text{ and } \gamma = \frac{\zeta}{m}.$$

Langevin eq. of the electric current density $j(t)$:

$$\frac{dj(t)}{dt} = -\gamma j(t) + \frac{e}{m}\sum_{j=1}^{n} \eta_j(t) + \frac{ne^2}{m}E$$

entropy production $\sigma_s(t) \equiv \frac{1}{T}\frac{dU(t)}{dt}$ is given by

$$\sigma_s(t) = \frac{\zeta}{T}\langle j(t)\rangle^2 = \frac{\zeta\sigma^2E^2}{T}(1-e^{-\gamma t})^2 = \frac{\sigma E^2}{T}(1-e^{-\gamma t})^2 \to \frac{\sigma E^2}{T}$$

and $\sigma_s(t)$ satisfies differential eq.

$$T\frac{d\sigma_s(t)}{dt} + 2\gamma T\sigma_s(t) - 2\gamma(\sigma E^2)(1-e^{-\gamma t}) = 0$$

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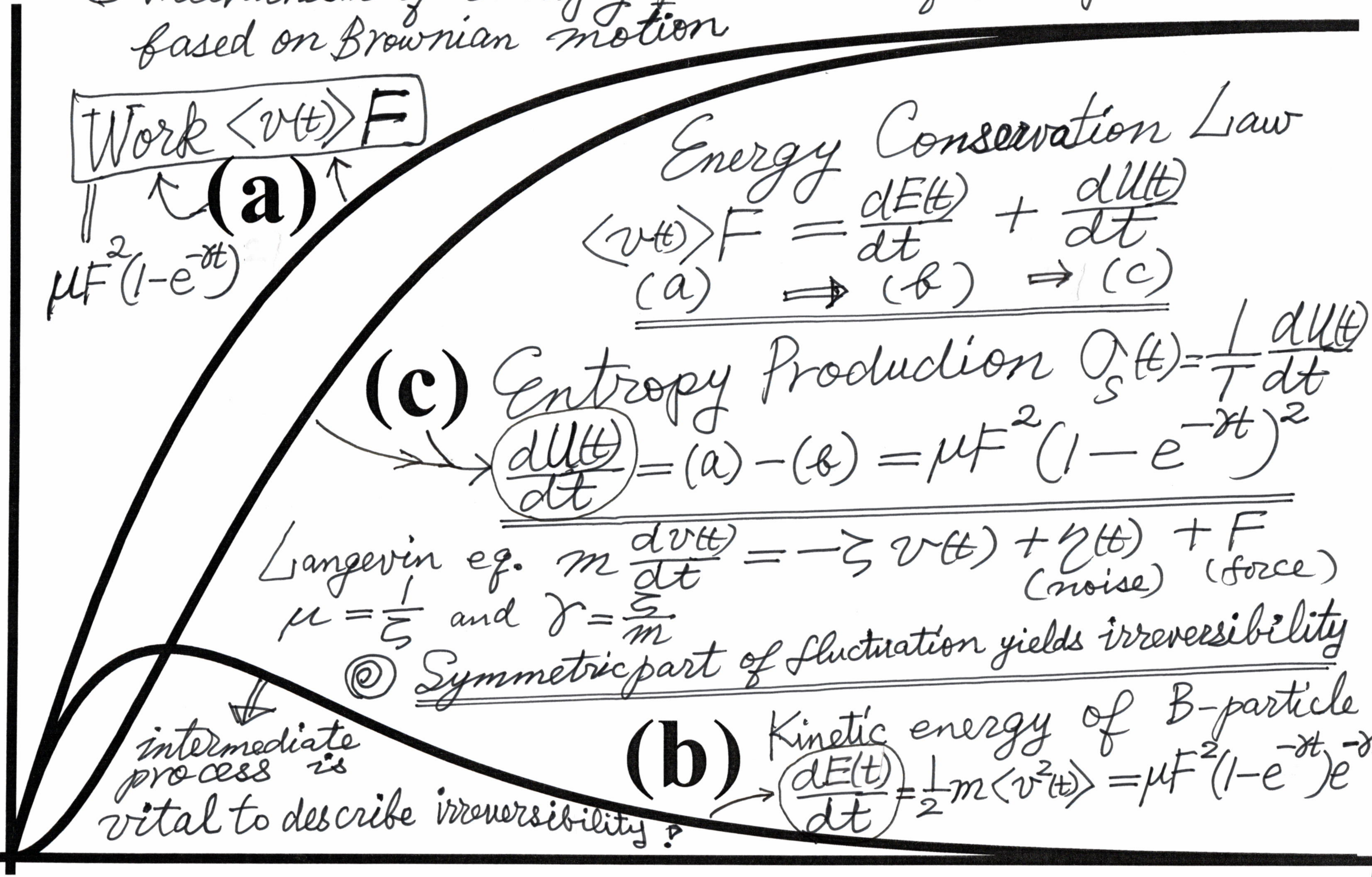
Solution:

$$\sigma_s(t) = \frac{\sigma E^2}{T}(1-e^{-\gamma t})^2$$

Entropy production in intermediate processes

# ◎ Mechanism of Entropy Production of Transport Phenomena based on Brownian motion



$\boxed{\text{Work } \langle v(t)\rangle F}$

**(a)**

$\parallel$

$\mu F^2(1-e^{-\gamma t})$

Energy Conservation Law

$$\langle v(t)\rangle F = \frac{dE(t)}{dt} + \frac{dU(t)}{dt}$$

(a) $\Rightarrow$ (b) $\Rightarrow$ (c)

**(c)** Entropy Production $\sigma_s(t) = \frac{1}{T}\frac{dU(t)}{dt}$

$$\frac{dU(t)}{dt} = (a) - (b) = \mu F^2 (1 - e^{-\gamma t})^2$$

Langevin eq. $m\frac{dv(t)}{dt} = -\zeta v(t) + \underset{(\text{noise})}{\eta(t)} + \underset{(\text{force})}{F}$

$\mu = \frac{1}{\zeta}$ and $\gamma = \frac{\zeta}{m}$

◎ Symmetric part of fluctuation yields irreversibility

intermediate process is vital to describe irreversibility?

**(b)** Kinetic energy of B-particle

$$\frac{dE(t)}{dt} = \frac{1}{2}m\langle v^2(t)\rangle = \mu F^2(1-e^{-\gamma t})e^{-\gamma t}$$

# Kubo's theory

linear response

# Zubarev's theory

exponential form

## Canonical Theory of Dissipative Dynamics

to describe both current and entropy production by discovering the effect of symmetric part of $\rho(t)$ or fluctuation : including thermal field $E_T = \frac{1}{\beta_0}\nabla\beta(x)$

$$\rho(t) = e^{\eta(t)} = \rho_{eq} + \underset{(\text{Kubo})}{\rho_1(t)} + \underset{\text{symmetric part}}{\rho_2(t)} + \cdots$$

$\because$) entropy production :

$$\sigma_S = \frac{dS}{dt} = \frac{1}{T}\frac{d}{dt}\mathrm{Tr}\,\mathcal{H}_0\,\rho_{sym}(t) = \frac{1}{T}\frac{d}{dt}\mathrm{Tr}\,\mathcal{H}_0\,\rho_2(t) + \cdots$$

# Variational Principles of Dissipative Dynamics

◎ Discovery of dissipative Lagrangians by introducing **integrated entropy production**

(or considering intermediate processes)

Consider the simplest dissipative system:

$$m\ddot{x}(t) + \zeta\dot{x}(t) + kx(t) = 0$$

a) a mathematical Lagrangian:

$$\mathcal{L}_{math}(t) = e^{\gamma t}\mathcal{L}_{dyn}(t);\ \mathcal{L}_{dyn}(t) = \frac{m}{2}\dot{x}^2(t) - \frac{k}{2}x^2(t)$$

where $\gamma = \zeta/m$. This is not physical.

This is not (directly) related to the energy dissipation

$$Q(t) = \zeta\int_0^t \dot{x}^2(s)\,ds$$

b) physical dissipative Lagrangian:

$$◎\ \mathcal{L}_{diss}(t) = \underset{\overset{\|}{\frac{m}{2}\dot{x}^2(t) - e^{-\gamma(\tau-t)}\times\frac{k}{2}x^2(t)}}{\mathcal{L}_{dyn}(t;\tau)} - \frac{\zeta}{2}\int_0^t e^{-(t-s)}\dot{x}^2(s)\,ds \quad ⊛$$

for $0 \leq t \leq \tau$

## Action

$$I = \int_0^\tau \mathcal{L}_{diss}(t)\,dt$$ (double integral)

∵) $\mathcal{L}_{diss}(t)$ depends on the intermediate processes.

→ Variational principles

$$\delta I = 0$$

yields the original dissipative equation, using the identity: For any $f(t)$ and $\tau$,

$$\int_0^\tau e^{\gamma(t-\tau)} f(t)\,dt = \int_0^\tau \left( f(t) - \gamma \int_0^t e^{\gamma(s-t)} f(s)\,ds \right) dt$$

⊛ $\mathcal{L}_{diss}(t)$ is expressed by the integrated heat generation.

# ◎ Entropy Change in Relaxation

We study first a simple phenomenological model of relaxation:

$\rho(t)$ : density matrix

$$◎ \quad \frac{\partial \rho(t)}{\partial t} = \frac{1}{i\hbar}[\mathcal{H}, \rho(t)] - \lambda(\rho(t) - \rho_f)$$

Solution:

$$\rho(t) = e^{-\lambda t} e^{\frac{t\mathcal{H}}{i\hbar}} \rho_i e^{-\frac{t\mathcal{H}}{i\hbar}} + (1 - e^{-\lambda t})\rho_f$$

where $\rho_f = \rho_f(\mathcal{H})$

Entropy change of the system ($\mathcal{H}$):

$$\frac{dS(t)}{dt} = \frac{1}{T(t)} \frac{d}{dt}\langle \mathcal{H} \rangle_t = \frac{\lambda}{T(t)}\left(\langle \mathcal{H} \rangle_f - \langle \mathcal{H} \rangle_t\right)$$

a) $T_f > T_{ini} \Longrightarrow \frac{dS(t)}{dt} > 0$

b) $T_f < T_{ini} \Longrightarrow \frac{dS(t)}{dt} < 0$,

as is expected. This suggests the next problem.

# Entropy Decrease in Order Formation

We study nonlinear Fokker–Planck eq.:

$$\frac{\partial}{\partial t}P(x,t) = -\frac{\partial}{\partial x}\alpha(x)P(x,t) + \varepsilon\frac{\partial^2}{\partial x^2}P(x,t),$$

where $\alpha(x) = \gamma x - g x^3$. This is equivalent to the nonlinear Langevin eq.:

$$\frac{dx}{dt} = \gamma x - g x^3 + \eta(t); \quad \underline{\gamma > 0,\ g > 0.}$$

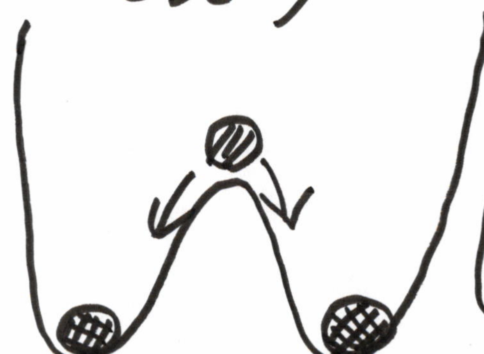
My <u>scaling solution in the time region of order formation</u> : M.S. 1976~1980.

$$P_{sc}(t) = \exp\left(-t\frac{\partial}{\partial x}\alpha(x)\right)\exp\left(t\tilde{\varepsilon}(t)\frac{\partial^2}{\partial x^2}\right)P(x,0)$$

**New result**

where

$$\tilde{\varepsilon}(t) = \frac{1-e^{-2\gamma t}}{2\gamma t}\cdot\varepsilon.$$



$$\boxed{\frac{dS(t)}{dt} < 0}$$

decrease

# Summary

1. Demonstration of mechanism of entropy production in transport phenom. using Einstein's Brownian motion.
2. Unified treatment of current J and entropy production $\sigma_S$, by formulating "canonical theory of t.p."
   — unification of Kubo & Zubarev's theories.
   (symmetry is important)
4. Discovery of dissipative physical Lagrangian including heat generation.
5. Demonstration of entropy decrease even in some "relaxation".
6. Entropy decrease in order formation based on my scaling solution.