MS-1

非線形輸送現象におけるエントロピー生成速度最小の原理

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目次 (Refs. M.S., Physica A390 (2011) 1904, A391 (2012) 1074 and 準備中 [paper]

1. Onsager−Prigogineの原理 (エネルギー散逸最小：線形のみ成立

2. Feynmanの線形電気回路のジュール熱生成最小の説明
(1964年 Feynman lecture) 線形応答でのみ成立

3. M.S. (1994年岩波の「統計力学」) Feynmanとは
dualな一般の電気回路で議論 (線形応答のみ)

4. 新しい原理：非線形でも線形でも一般的に成立
新しい視点：瞬時のエネルギー散逸ではなく
"積分した"エネルギー散逸を最小

5. 何故，線形応答の場合には瞬時の値で正しい結
を与えるか

6. 熱伝導，化学反応などへの応用 (to be submitted to Physica A (Paper III))

Refs. Physica A390 (2011) 1904, A391 (2012) 1074.

MS-2

1. Onsager's reciprocity relation and
least energy dissipation theorem

1st law:

5. 何故、線形応答の場合には瞬時の値で正しい結果を与えるか

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MS-2

1. Onsager's reciprocity relation and least energy dissipation theorem

Def. Entropy production (due to 1st law thermodynamics)

$$\sigma = \sum_{i=1}^{n} J_i X_i = \sum_{i=1}^{n} \sum_{j=1}^{n} L_{ij} X_i X_j \geq 0$$

where the current J_i is given by

$$J_i = \sum_{j=1}^{n} L_{ij} X_j \quad \text{(linear response)}$$

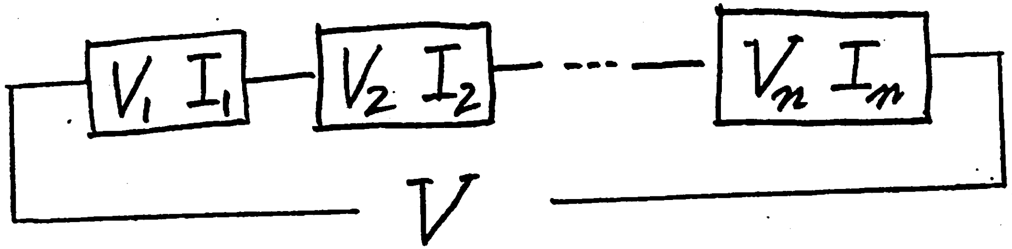
X_j : conjugate force

◎ Reciprocity relation

$L_{ij} = L_{ji}$ due to the time reversal sym. of fluctuation in equil.

→ least energy dissipation theorem $\frac{\partial \sigma}{\partial X_i} = 0$ $(i = k+1, \ldots, n)$ with $\frac{\partial \sigma}{\partial X_i} = 2J_i$ $(i = 1, 2, \ldots, k)$

2. Feynman's demonstration of least dissipation theorem in a linear electric circuit (The Feynman Lectures on Physics, Vol. II, 1964)



$\Rightarrow I_1 = I_2 = \cdots = I_n$,

entropy production for the fixed total voltage V

$$\sigma \equiv \frac{dS}{dt} = \frac{1}{T}\left(V_1 I_1 + V_2 I_2 + \cdots + V_n I_n\right)$$

$$= \frac{1}{T}\left(L_{11} V_1^2 + L_{22} V_2^2 + \cdots + L_{(n-1)(n-1)} V_{n-1}^2 + L_{nn}\left(V - \sum_{k=1}^{n-1} V_k\right)^2\right)$$

minimization of σ yields

$I_1 = I_2 = \cdots = I_n$, as it should be.

◎ Physics is very attractive, but this does not hold in nonlinear cases: $L_{jj} = L_{jj}(V_j)$ problem.
In particular, Prigogine emphasized the importance to solve this

MS-4

3. My demonstration of minimum entropy production in electric circuits dual to Feynman's example [illegible] for the fixed total current I

$I_1 = I_2 = \cdots = I_n$, as is shown above.

◎ Physics is very attractive, but this does not hold in nonlinear cases : $L_{jj} = L_{jj}(V_j)$ ↗problem.
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MS-4

3. My demonstration of minimum entropy production in electric circuits dual to Feynman's example
↳ for the fixed total current I
(1994, 『Statistical mechanics』 (M.S., Iwanami, in Japanese)

p. 254 → これは定常状態では σ が最小になることを意味する．これをエントロピー生成速度最小の原理という．ただし，以上の議論は，線形応答の範囲で，Onsager の相反定理が成り立つ場合に正当化される．

簡単な応用例としては，Kirchhoff の法則をエントロピー生成速度最小の原理，すなわち，Joule 熱発生最小の条件より導くことができる．図 4-6 のような電気回路を例にとると，Joule 熱 W は，

$$W = I_1^2R_1 + (I - I_1)^2R_2 + (I_1 - I_5)^2R_3 + (I - I_1 + I_5)^2R_4 + I_5^2R_5 \tag{4.318}$$

と与えられ，変分条件

$$\frac{\partial W}{\partial I_1} = 0, \quad \frac{\partial W}{\partial I_5} = 0 \tag{4.319}$$

から，容易に Kirchhoff の法則，すなわち，$I_1R_1 + I_3R_3 = I_2R_2 + I_4R_4$ などが導かれる*．電荷保存は最初から仮定した．

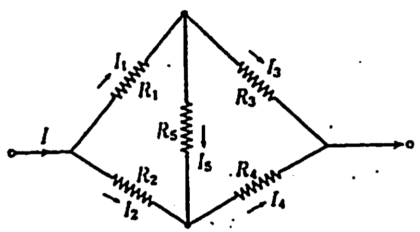


図 4-6　Kirchhoff の法則とエントロピー生成速度（すなわち Joule 熱発生）最小の原理．

* エントロピー生成速度を一定，すなわち Joule 熱発生速度を一定にする条件の下では，電流が最大原理によって Kirchhoff の法則が導かれる．すなわち，(4.318) で W = 一定 とおいて，I を I_1 の関数とみなし，偏微分すると，$\partial I/\partial I_1 = (I_2R_2 + I_4R_4 - I_1R_1 - I_3R_3)/(I_2R_2 + I_4R_4)$ となり，

◎ Unfortunately, this does not work when $\{R_j\}$ depend on current $\{I_j\}$: $R_j = R_j(I_j)$

nonlinear responses.

This has been a long-term basic difficult problem!

. New theory: General theorem of minimum entropy production including nonlinear responses (to be in Physica A (2012) Paper III)

Before giving my general theory, it will be interesting to explain my many trials to extend this theorem to nonlinear responses. (From a half century experience.)

— Stay hungry. Stay foolish. (S. Jobs) (愚直であれ)

4-a) A simple example of nonlinear resistance: $R_j = R_j(I_j) = a_j I_j^m$ $(m>0)$

Minim. of $\tilde{Q} = \sum I_j^2 R_j(I_j)$ gives a correct result!

However, if we add another term (ex. $R_j = \underset{(\text{constant})}{a_{0j}} + a_j I_j^m$), then we fail!

4-b) Answer!

These many trials suggest to consider a new type of the integral form

$$\tilde{Q}^I = \sum_j \int_0^{I_j} R_j(I) I dI \Leftarrow \sum_j \int_0^t I_j(t) R_j(I_j(t)) \dot{I}_j(t) dt \quad \text{with } I_j(t) = I_j$$

This integrated energy dissipation does give finally a desired correct law!

a new type of the integral form

$$\circledcirc \quad \tilde{Q}^{I} = \sum_{j} \int_{0}^{I_j} R_j(I) I \, dI \leftarrow \sum_{j} \int_{0}^{t} I_j(t) R_j(I_j(t)) \dot{I}_j(t) dt \quad \text{with } I_j(t) = I_j$$

This integrated energy dissipation does give finally a desired correct law!

In Feynman's case, we consider

$$Q^{I} = \sum_{j} \int_{0}^{V_j} I_j(V) dV = \sum_{j} \int_{0}^{t} I_j(V_j(t)) \dot{V}(t) dt \quad \text{with } V_j(t) = V_j$$

4-c) General formulation

$$O^{I} = \int d\mathbf{r} \int_{0}^{X(\mathbf{r})} J(X(\mathbf{r})) dX(\mathbf{r}) = \int d\mathbf{r} \int_{0}^{t} J(X(\mathbf{r},t)) \dot{X}(\mathbf{r},t) dt \quad \text{with } X(\mathbf{r},t) = X(\mathbf{r})$$

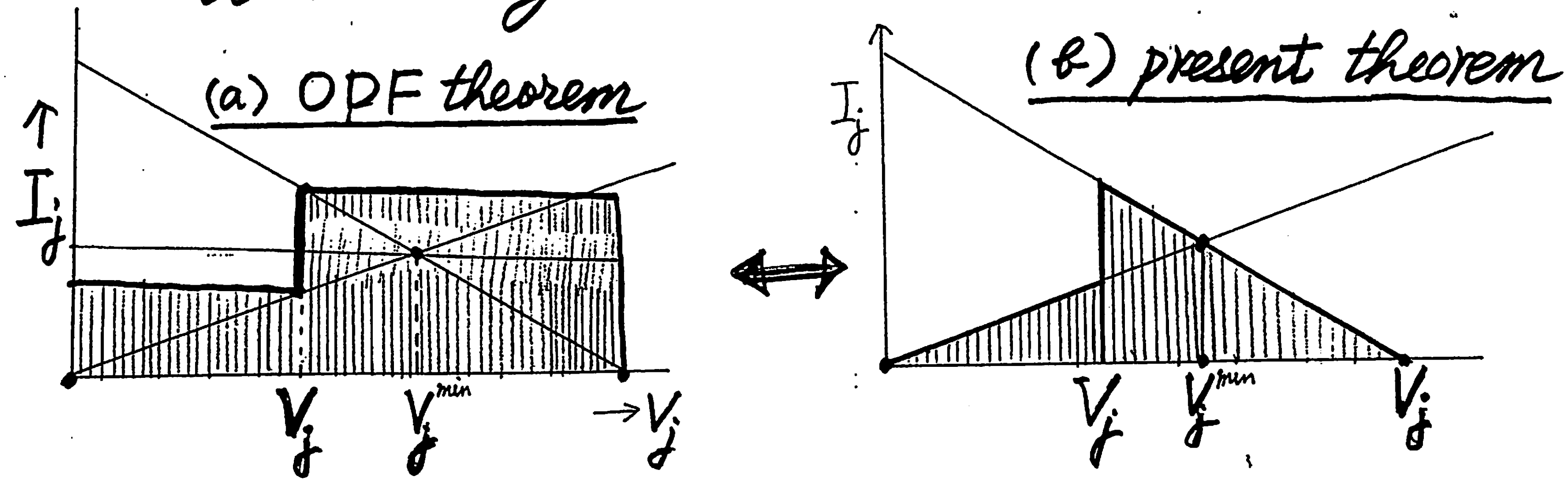
where $\int d\mathbf{r}$ denotes the volume integral in continuous systems such as thermal conduction and chemical reaction.

We have also

$$\tilde{O}^{I} = \int d\mathbf{r} \int^{J(\mathbf{r})} J(\mathbf{r},t) R(J(\mathbf{r},t)) dJ(\mathbf{r},t) = \int d\mathbf{r} \int^{t} J(\mathbf{r},t) R(J(\mathbf{r},t)) \dot{J}(\mathbf{r},t) dt$$

5. Why valid is OPF theorem in the linear regime?

We explain the reason in an electric circuit.
to minimize both areas.



They differ only by the factor 2.
This does not affect the rational treatment.
Thus, the instantaneous min. dissipation happens to be valid.

6. Applications to electric conduction, MS-8

heat conduction, chemical reaction, etc.

This does not affect the variational treatment.

Thus, the instantaneous min. dissipation happens to be valid.

6. Applications to electric conduction, heat conduction, chemical reaction, etc. MS-8

a) heat conduction : heat current J

x-coordinate x

$$J = -\lambda(T)\frac{dT}{dx}, \quad X = \frac{\partial}{\partial x}\left(\frac{1}{T}\right); \; T = T(x)$$

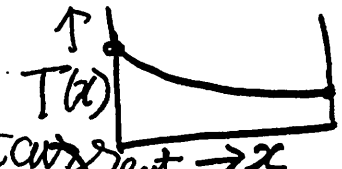
entropy production $\sigma_S = \dfrac{dS}{dt} = \displaystyle\int \frac{\lambda(T)}{T^2}\left(\frac{\partial T}{\partial x}\right)^2 dx$

(a) linear case (λ = constant) → minimiz. of σ_S yields $\lambda \nabla^2 T = 0 \quad \therefore \; \underline{T(x) = ax + b}$

(b) nonlinear case : present theory

minimization of the integrated entropy production yields

$$\frac{d}{dx}\left(\lambda(T(x))\frac{\partial T(x)}{\partial x}\right) = 0$$



~~Euler の式より~~ $\cancel{\dfrac{d}{dx}\left(\dfrac{\partial f}{\partial y'}\right) - \dfrac{\partial f}{\partial y} = 0}$ →

$$\lambda(T(x))\frac{\partial T(x)}{\partial x} = c \quad (= \text{constant}) \rightarrow J \text{ heat current}$$

c) chemical reaction : similar