Physica A 392 (2013) 4279–4287

Contents lists available at SciVerse ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Irreversibility and entropy production in transport phenomena, IV: Symmetry, integrated intermediate processes and separated variational principles for multi-currents

Masuo Suzuki *

Computational Astrophysics Laboratory, RIKEN, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan

HIGHLIGHTS

- Mechanism of entropy production in transport phenomena is clarified using symmetry of states.
- Einstein's theory of Brownian motion is restudied to demonstrate how its entropy is produced.
- Variational principles of nonlinear steady states proposed by the author are extended to those of multi external fields.
- This new theory yields Gransdorff–Prigogine's evolution criterion inequality in a stronger form.
- Some explicit applications and validity conditions of our new theory are given in electric circuits.

ARTICLE INFO

Article history:
Received 13 February 2013
Received in revised form 8 April 2013
Available online 24 May 2013

Keywords:
Transport phenomena
Irreversibility
Entropy production
Brownian motion
Variational principle
Evolution criterion

ABSTRACT

The mechanism of entropy production in transport phenomena is discussed again by emphasizing the role of symmetry of non-equilibrium states and also by reformulating Einstein's theory of Brownian motion to derive entropy production from it. This yields conceptual reviews of the previous papers [M. Suzuki, Physica A 390 (2011) 1904; 391 (2012) 1074; 392 (2013) 314]. Separated variational principles of steady states for multi external fields $\{X_i\}$ and induced currents $\{J_i\}$ are proposed by extending the principle of minimum integrated entropy production found by the present author for a single external field. The basic strategy of our theory on steady states is to take in all the intermediate processes from the equilibrium state to the final possible steady states in order to study the irreversible physics even in the steady states. As an application of this principle, Gransdorff–Prigogine's evolution criterion inequality (or stability condition) $d_X P \equiv \int d\mathbf{r} \sum_i J_i dX_i \leq 0$ is derived in the stronger form $dQ_i \equiv \int d\mathbf{r} J_i dX_i \leq 0$ for individual force X_i and current J_i even in nonlinear responses which depend on all the external forces $\{X_k\}$ nonlinearly. This is called "separated evolution criterion".

Some explicit demonstrations of the present general theory to simple electric circuits with multi external fields are given in order to clarify the physical essence of our new theory and to realize the condition of its validity concerning the existence of the solutions of the simultaneous equations obtained by the separated variational principles. It is also instructive to compare the two results obtained by the new variational theory and by the old scheme based on the instantaneous entropy production. This seems to be suggestive even to the energy problem in the world.

* Tel.: +81 048 467 9074.
E-mail address: masuo.suzuki@riken.jp.

0378-4371/$ – see front matter
http://dx.doi.org/10.1016/j.physa.2013.05.019

1. Introduction concerning symmetry arguments on entropy production

The symmetry argument on the density matrix $\rho(t)$ is essential in understanding the irreversibility or entropy production of transport phenomena [1–3] even using the energy conservation of the input power and output heat dissipation as follows.

The density matrix $\rho(t)$ of the relevant system described by the Hamiltonian $\mathcal{H}(t)$ satisfies the von Neumann equation

$$i\hbar\frac{\partial}{\partial t}\rho(t) = [\mathcal{H}(t), \rho(t)] : \ \mathcal{H}(t) = \mathcal{H}_0 + \mathcal{H}_1 \quad \text{and} \quad \mathcal{H}_1 = -\boldsymbol{A}\cdot\boldsymbol{F}(t) \tag{1}$$

for a field $\boldsymbol{F}(t)$. For simplicity, we assume that $\boldsymbol{F}(t)$ is time-independent, as in static electric conduction and thermal conduction. The relevant system described by the static Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$ is still non-equilibrium with the current $\boldsymbol{J} = \langle\dot{\boldsymbol{A}}\rangle$. As was mentioned in the previous papers [1–3], the entropy production or energy dissipation in transport phenomena has been often argued [4] using the energy conservation law (i.e., the total energy $\langle\mathcal{H}\rangle$ is conserved). If we try to confirm explicitly this energy conservation, we have to note the following propositions. When the density matrix $\rho(t)$ is expanded as

$$\rho(t) = \rho_0 + \rho_1(t) + \rho_2(t) + \cdots + \rho_n(t) + \cdots, \tag{2}$$

with respect to the external force $\boldsymbol{F}$, the following results on the average $\langle\mathcal{H}\rangle$ taken over each order of the density matrix $\hat{\rho}_n(t) \equiv \rho_0 + \rho_1(t) + \cdots + \rho_n(t)$ can be proven easily:

$$\begin{aligned}
&\mathrm{Tr}\mathcal{H}(\rho_0 + \rho_1(t)) = \text{not conserved},\\
&\mathrm{Tr}\mathcal{H}(\rho_0 + \rho_1(t) + \rho_2(t)) = \text{conserved},\\
&\cdots\\
&\mathrm{Tr}\mathcal{H}(\rho_0 + \rho_1(t) + \cdots + \rho_{2n-1}(t)) = \text{not conserved},\\
&\mathrm{Tr}\mathcal{H}(\rho_0 + \rho_1(t) + \cdots + \rho_{2n}(t)) = \text{conserved}.
\end{aligned}$$

Note that $\mathrm{Tr}\hat{\rho}_n = \mathrm{Tr}\rho_0 = 1$ for all n. The above results support the previous statement that the entropy production comes from the symmetric part $\rho_{\mathrm{sym}}(t)$ of the density matrix [1–3]:

$$\sigma_S(t) = \left(\frac{\mathrm{d}S}{\mathrm{d}t}\right)_{\mathrm{irr}} = \frac{1}{T}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}\mathcal{H}_0\rho_{\mathrm{sym}}(t) = \frac{1}{T}\langle\boldsymbol{J}\rangle_F\cdot\boldsymbol{F} = \frac{\sigma_F F^2}{T} > 0 \tag{3}$$

at the temperature T, where

$$\rho_{\mathrm{sym}}(t) = \rho_0 + \rho_2(t) + \cdots + \rho_{2n}(t) + \cdots, \tag{4}$$

and

$$\langle\boldsymbol{J}\rangle_F = \mathrm{Tr}\boldsymbol{J}\rho_{\mathrm{antisym}}(t) = \mathrm{Tr}\dot{\boldsymbol{A}}\rho_{\mathrm{antisym}}(t) \tag{5}$$

with

$$\rho_{\mathrm{antisym}}(t) = \rho(t) - \rho_{\mathrm{sym}}(t) = \rho_1(t) + \cdots + \rho_{2n-1}(t) + \cdots. \tag{6}$$

This symmetry argument will be more directly realized by deriving the entropy production in Einstein theory of Brownian motion described by the following Langevin equation

$$m\frac{\mathrm{d}v(t)}{\mathrm{d}t} = -\zeta v(t) + \eta(t) + F. \tag{7}$$

Here, m denotes the mass of the relevant Brownian particle, ζ its friction constant and $\eta(t)$ the random force acting to the particle. For simplicity, $\eta(t)$ is assumed to be a Gaussian white noise satisfying the relation

$$\langle\eta(t)\eta(t')\rangle = 2\epsilon\delta(t-t'). \tag{8}$$

The strength ϵ of the noise $\eta(t)$ satisfies Einstein's relation [6], namely the fluctuation–dissipation theorem [4–8]

$$\zeta = \frac{1}{k_B T}\epsilon = \frac{1}{k_B T}\int_0^\infty \langle\eta(0)\eta(t)\rangle \mathrm{d}t. \tag{9}$$

This is equivalent to the equi-partition law

$$\frac{1}{2}m\langle v^2(t)\rangle_0 = \frac{\epsilon}{2\zeta} = \frac{1}{2}k_B T, \tag{10}$$

as is well known. Here, $\langle v^2(t)\rangle_0$ denotes the average of $v^2(t)$ for $F = 0$. Thus, the mass current $J(t) = m\langle v(t)\rangle$ in the presence of the external force F is given by the following equation with odd symmetry

$$\frac{\mathrm{d}}{\mathrm{d}t}J(t) = -\gamma J(t) + F; \quad \gamma = \frac{\zeta}{m}. \tag{11}$$