Microscopic theory for the time irreversibility and the entropy production

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Abstract. In stochastic thermodynamics, the entropy production of a thermodynamic system is defined by the irreversibility measured by the logarithm of the ratio of the path probabilities in the forward and reverse processes. We derive the relation between the irreversibility and the entropy production starting from the deterministic equations of motion of the whole system consisting of a physical system and a surrounding thermal environment. The derivation assumes the Markov approximation that the environmental degrees of freedom equilibrate instantaneously. Our approach provides a guideline for the choice of the proper reverse process to a given forward process, especially when there exists a velocity-dependent force. We demonstrate our idea with an example of a charged particle in the presence of a time-varying magnetic field.

Keywords: stochastic particle dynamics, fluctuation phenomena
1. Introduction

Over the past few decades, many efforts have been devoted to establishing thermodynamics for general nonequilibrium systems [1–10]. Among them, stochastic thermodynamics is one of the most widely used approaches [11, 12]. In stochastic thermodynamics, dynamics of a system surrounded by a thermal environment is described as a stochastic process governed by the Langevin equation or the master equation. Thermodynamic quantities such as heat, work, and entropy production are defined at the stochastic trajectory level in the way consistent with classical thermodynamics [5, 8, 9, 13].

Suppose that a system, whose configuration is denoted by \( s \), evolves along a stochastic path \( s[\tau] = \{s(t)|0 \leq t \leq \tau\} \) in contact with a thermal environment. The time evolution is accompanied by the entropy production, which is decomposed into the sum \( \Delta S_{\text{tot}}(s[\tau]) = \Delta S_{\text{sys}}(s[\tau]) + \Delta S_{\text{env}}(s[\tau]) \). In stochastic thermodynamics, the system entropy change \( \Delta S_{\text{sys}} \) is taken as the difference of the Shannon entropy of the system while the environment entropy change is taken as

\[
\Delta S_{\text{env}} = \ln \frac{\mathcal{P}(s[\tau]|s(0))}{\mathcal{P}(s[\tau]|s^{\dagger}(0))},
\]

where \( \mathcal{P}(s[\tau]|s(0)) \) denotes the conditional path probability of a system following the path \( s[\tau] \) to a given initial configuration \( s(0) \) and \( \mathcal{P}(s[\tau]|s^{\dagger}(0)) \) denotes the conditional path probability of a system following the time reversed path \( s^{\dagger}[\tau] \) to a given initial configuration \( s^{\dagger}(0) \) in the reverse process [6, 9, 14–16] (detailed notations will be explained later). The Boltzmann constant \( k_B \) is set to unity throughout the paper. From the definition of the entropy production, stochastic thermodynamics predicts several fluctuation theorems [6–10] for the statistical properties of the entropy production and related quantities, which have been examined experimentally [17–22].

Throughout this paper, we will use the term time irreversibility or irreversibility to denote the logarithm of the ratio of the conditional path probabilities in the forward and reverse processes. Equation (1) relates the environmental entropy production and
the time irreversibility. There have been several attempts to show the consistency of the entropy production of stochastic thermodynamics with that of classical thermodynamics. The consistency was first suggested for a stochastic system by invoking an analogy to a chemical reaction system [23]. For master equation systems, the entropy production in (1) is shown to be consistent with the second law of thermodynamics [6]. For Langevin equation systems driven by a velocity-independent force, the expression in (1) leads to the Clausius relation \( \Delta S_{\text{env}} = \frac{\Delta Q}{T} \) where \( \Delta Q \) is the heat dissipated into the thermal environment of temperature \( T \) [9].

Despite the consistency at the phenomenological level, the entropy production in terms of the time irreversibility still remains to be verified microscopically. Maes and Netočný tried to establish the relation (1) for a thermal equilibrium case by considering Hamiltonian dynamics for a coupled system consisting of a physical system and a surrounding environment [24]. Under the Markov approximation that the degrees of freedom of the environment should equilibrate instantaneously, they showed that the irreversibility of the physical system is equal to the change in the entropy of the environment. More recently, the similar approach is applied to discrete systems described by the master equation [25, 26].

In this paper, we extend the approach of [24] to a system which is driven by an arbitrary force and surrounded by a thermal environment. We obtain the expression for the irreversibility starting from the deterministic equations of motion and using the Markov approximation. The expression is shown to be the same as the one obtained from the Langevin equation formalism. We stress that the time irreversibility, the right hand side of (1), depends crucially on the choice of the reverse process especially when the driving force depends on the velocity. Our approach provides a systematic way for the proper choice of a reverse process. We apply our approach to a charged particle in the presence of the time-varying magnetic field.

This paper is organized as follows. In section 2, we introduce the setting of the problem. We consider deterministic Newtonian dynamics for the whole system that consists of a physical system of interest and a surrounding environment. The physical system is driven by a nonconservative force. We coarse-grain the environmental degrees of freedom to derive the effective dynamics of the physical system by adopting the Markov approximation. In section 3, we derive the expression for the irreversibility. We will show that the irreversibility is the same as that obtained from the Langevin equation approach. In order to calculate the irreversibility, one needs to define a reverse process. We suggest a rule for the choice of a proper reverse process. We explain the rule in a model system driven by a time-dependent magnetic Lorentz force in section 4. We summarize our results in section 5.

2. Coarse graining

We consider a classical system \( \mathcal{S} \) described by \( N \) Cartesian coordinates \( x_{1\leq i \leq N} \) for position and \( v_{1\leq i \leq N} \) for velocity. The system interacts with an environment \( \mathcal{E} \), which is described by \((M-N)\) Cartesian coordinates \( x_{N<i \leq M} \) and \( v_{N<i \leq M} \) for position and velocity, respectively. A configuration of the whole system \( \mathcal{U} \) corresponds to a point in.
the 2M-dimensional phase space $\Omega$. The phase space point is denoted by $c = (X, V)$ where $X \equiv (x_1, \ldots, x_N, x_{N+1}, \ldots, x_M)$ and $V \equiv (v_1, \ldots, v_N, v_{N+1}, \ldots, v_M)$. Similarly, a configuration of the system $\mathcal{S}$ corresponds to a point $s = (x, v)$ in the 2N-dimensional phase space with $x = (x_1, \ldots, x_N)$ and $v = (v_1, \ldots, v_N)$. The whole system evolves in time following the deterministic Newtonian equations of motion:

$$\dot{x}_i = v_i$$

$$\dot{v}_i = \left\{ \begin{array}{ll}
-\frac{\partial \Phi(X)}{\partial x_i} + f_i(s, \lambda) & (1 \leq i \leq N), \\
-\frac{\partial \Phi(X)}{\partial x_i} & (N < i \leq M),
\end{array} \right.$$  

(2)

where $\Phi(X)$ is a potential energy function of the whole system and $f(s, \lambda) = (f_1(s, \lambda), \ldots, f_N(s, \lambda))$ is an additional nonconservative driving force applied to the system $\mathcal{S}$ only. It may include $L$ control parameters denoted by $\lambda = \lambda(t) = (\lambda_1(t), \ldots, \lambda_L(t))$, each of which may depend on time. We set all masses to be unity without loss of generality. If the whole system starts with a configuration $c$ at time $t$, its subsequent state is determined uniquely. Let $T_{\Delta t}(c; t)$ be the configuration after the time interval $\Delta t$, which will be referred to as a trajectory function.

The total energy of $U$ is given by $H(c) \equiv \frac{1}{2} \sum_{i=1}^N v_i^2 + \Phi(X)$. All the states of same energy $E$ constitute a constant energy surface $\Omega_E \equiv \{c | H(c) = E \} \subset \Omega$. The total energy is not conserved in the presence of the driving force. If $c \in \Omega_E$, then the configuration $c' = T_{\Delta t}(c; t)$ belongs to another energy surface $\Omega_{E + \Delta E}$ where

$$dE = H(c') - H(c) = \sum_i f_i(s, \lambda(t)) v_i dt.$$  

(3)

Figure 1 illustrates the jump between energy surfaces.

The aim of this section is to derive the effective dynamics of the system $\mathcal{S}$ out of the deterministic dynamics of the whole system $U$. This can be done by coarse-graining the degrees of freedom of the environment. The most successful method is to introduce the Markovian approximation that the degrees of freedom of the environment equilibrate instantaneously to a given system configuration [24, 25]. The assumption is valid in the limiting case where the environment relaxes infinitely faster than the system [13, 25–31]. We adopt the Markov approximation to obtain the effective dynamics.

The coarse-graining is done by the mapping

$$\pi(c) = s,$$  

(4)

which decimates the degrees of the freedom of the environment. For a given $c \in \Omega_E$, the corresponding system configuration $s = \pi(c)$ is unique. On the other hand, there are many states in $\Omega_E$ that are coarse-grained to the same state $s$. The set of all such states are denoted by

$$V(s; E) \equiv \{c | \pi(c) = s \text{ and } H(c) = E \}.$$  

(5)

These subsets are represented as the rectangular regions in figure 1.

We are interested in the transition probability that the system configuration jumps from $s$ to $s'$ in the infinitesimal time interval $dt$ given that the whole system is distributed according to the probability distribution $P(c)$ in the energy surface $\Omega_E$ initially. Such a transition is accompanied with the energy change $dE = \sum_i f_i v_i dt$. It can be written as

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\[ W_{dt}(s \to s'; E, t) = \frac{\int_{V(s; E)} \text{d}c \int_{V(s'; E+dE)} \text{d}c' P(c) \delta(c' - T_{dt}(c; t))}{\int_{V(s; E)} \text{d}c P(c)} \]  

where \( \delta(\cdot) \) is the Dirac delta function, and \( \int_{V(s; E)} \text{d}c \) represents the integration over the space \( V(s; E) \). The denominator is the probability that the system \( S \) is in the configuration \( s \), while the numerator is the joint probability that the system is at \( s \) initially and at \( s' \) after time \( dt \).

The Markov approximation simplifies the transition probability. Since the environment is assumed to be in the equilibrium state, \( P(c) \) is uniform within each \( V(s; E) \) sector [24]. Thus the factors \( P(c) \) in the denominator and the numerator cancel each other. The remaining factor in the numerator is equal to the volume of \( V_{dt}(s \to s'; E, t) \) that is defined as

\[ V_{dt}(s \to s'; E, t) = \{ c | c \in V(s; E) \text{ and } \pi(T_{dt}(c; t)) = s' \}. \]

It is the subset of \( V(s; E) \) consisting of configurations \( c \in V(s; E) \) that are coarse-grained to \( s' \) after time \( dt \). Therefore, the transition probability is given by

\[ W_{dt}(s \to s'; E, t) = \frac{\text{Volume of } V_{dt}(s \to s'; E, t)}{\text{Volume of } V(s; E)}. \]
where $|(-)|$ denotes the volume of the set $(-)$ in the phase space. The time evolution under the Markov approximation is illustrated in figure 1. The transition probability depends on $t$ explicitly because of the $t$ dependence of the trajectory function $T_{dt}(c; t)$.

3. Irreversibility

In this section, we quantify the time irreversibility by comparing the transition probability of a trajectory $s[\tau]$ in a given dynamical process, called the forward process, with that of a time-reversed trajectory denoted by $s^\dagger[\tau] = \{\epsilon s(\tau - t) | 0 \leq t \leq \tau\}$ in the corresponding reverse process. Here, $\epsilon$ is the time-reversal operator that changes the sign of all the velocity coordinates. That is, $\epsilon s = (x, -v)$ for $s = (x, v)$.

We first remark on the way how one should define the reverse process to a given forward process. Consider, for example, a charged particle in the presence of the uniform magnetic field $B$. The magnetic Lorentz force acts on the particle as a driving force. Many literatures take it for granted that the magnetic field should be flipped ($B \rightarrow -B$) in the reverse process so that the system traces back the original trajectory [32–35]. On the other hand, some studies claim that one should use the same driving force for the reason that a forward trajectory and its time-reversed trajectory should be compared on the equal footing [16, 36–39]. According to this claim, one should use the same magnetic field $B$ in the reverse process. Such an ambiguity always arises when the driving force $f$ depends explicitly on the velocity so that it breaks the time-reversal symmetry. We will provide an argument that guides us to choose the appropriate driving force in the reverse process.

Consider a forward process with a driving force $f(s, \lambda)$ for a time interval $0 \leq t \leq \tau$. Suppose that the system evolves along a trajectory $s[\tau]: s(t_0 = 0) \rightarrow \cdots \rightarrow s(t_l) \rightarrow \cdots \rightarrow s(t_n = \tau)$ with $t_l = l dt$. The forward trajectory is to be compared with the time-reversed one $s^\dagger[\tau]: s^\dagger(t_0) \rightarrow \cdots \rightarrow s^\dagger(t_l) \rightarrow \cdots \rightarrow s^\dagger(t_n)$ with $s^\dagger(t_l) = \epsilon s(t_{n-l} = \tau - t_l)$ in the reverse process. Since the driving force $f$ does work on the system, the whole system $\mathcal{U}$ jumps from one energy surface $\Omega_E$ to another $\Omega_{E+dE}$ with d$E$ in (3) at each step (see also figure 1). Let $f^\dagger(s, \lambda^\dagger)$ be the driving force in the reverse process. We require that the system $\mathcal{S}$ should return back from $\epsilon s(t_{l+1})$ to $\epsilon s(t_l)$ and the whole system $\mathcal{U}$ from $\Omega_{E+dE}$ to $\Omega_E$ at each time step in the reverse process. The energy surface requirement constraints the possible form of $f^\dagger(s, \lambda^\dagger)$. The work d$E^\dagger$ done by $f^\dagger$ in the reverse process should cancel d$E$, which yields

$$
\sum_i f^\dagger_i(\epsilon s, \lambda^\dagger(t))(-dx_i) = -\sum_i f_i(s, \lambda(\tau - t))dx_i
$$

(8)

up to the leading order in dt. It suggests that the driving force in the reverse process should be chosen as

$$
f^\dagger(s, \lambda^\dagger(t)) = f(\epsilon s, \lambda(\tau - t)).
$$

(9)
Note that $f^\dagger$ may have a different function form from $f$ when the force depends on the velocity $v$. An explicit example involving a charged particle in the presence of the magnetic field will be discussed in section 4.

The meaning of this choice is clear. The forces acting on the system at each time step constitute a sequence $\{F_0, \ldots, F_l, \ldots, F_n\}$ with $F_l = f(s(t_l), \lambda(t_l))$. The choice in (9) implies that the forces in the reverse process constitute the sequence $\{F_0^\dagger, \ldots, F_l^\dagger, \ldots, F_n^\dagger\}$ with $F_l^\dagger = f^\dagger(s^\dagger(t_l), \lambda^\dagger(t_l)) = f(s(t_{n-l}), \lambda(t_{n-l})) = F_{n-l}$. The system is acted on by the *same force values* in the time-reversed order. Another important property of the choice (9) is that every trajectory $c[\tau] = \{c(t) | 0 \leq t \leq \tau\}$ of the whole system $\mathcal{U}$ in the forward process is traced back in the reverse process. Formally we have

$$\mathcal{T}^\dagger_l(\epsilon \mathcal{T}_l(c; 0); \tau - t) = \epsilon c$$

with the trajectory function $\mathcal{T}^\dagger$ of the reverse process.

Once the reverse process is defined, the transition probability during the infinitesimal time interval is given by

$$W_{dt}^\dagger(s \to s'; E, t) = \frac{|V_{dt}^\dagger(s \to s'; E, t)|}{|V(s; E)|},$$

where

$$V_{dt}^\dagger(s \to s'; E, t) = \{c | c \in V(s; E) \text{ and } \pi(\mathcal{T}_{dt}^\dagger(c, t)) = s' \}.$$ 

Thus, the irreversibility, given by the log ratio of the path probabilities as appeared in the right hand side of (1), is given by the sum of

$$\mathrm{d}I = \ln \frac{W_{dt}^\dagger(s \to s'; E, t)}{W_{dt}^\dagger(\epsilon s' \to \epsilon s; E + \mathrm{d}E, \tau - t)} = \mathrm{d}I_1 + \mathrm{d}I_2,$$

where

$$\mathrm{d}I_1 = \ln \frac{|V(\epsilon s'; E + \mathrm{d}E)|}{|V(s; E)|},$$

$$\mathrm{d}I_2 = \ln \frac{|V_{dt}^\dagger(s \to s'; E, t)|}{|V_{dt}^\dagger(\epsilon s' \to \epsilon s; E + \mathrm{d}E, \tau - t)|}.$$ 

Using the property in (10), one finds that $V_{dt}^\dagger(\epsilon s' \to \epsilon s; E + \mathrm{d}E, \tau - t) = \epsilon \mathcal{T}_{dt}(V(s \to s'; E, t))$. One also finds that $V(s; E) = \epsilon V(s; E)$ and that the phase space volume is invariant under the operation of $\epsilon$. Therefore, the irreversibility is given by

$$\mathrm{d}I_1 = \ln \frac{|V(s'; E + \mathrm{d}E)|}{|V(s; E)|},$$

$$\mathrm{d}I_2 = \ln \frac{|V(s \to s'; E, t)|}{|\mathcal{T}_{dt}(V(s \to s'; E, t))|}.$$ 

We stress that we take into account the time reversed trajectory of the whole system including the physical system and the environment in the expression of $\mathrm{d}I$. The choice
in (9) guarantees that the environment returns to the original energy surface in the reverse process.

The subspace $V(s; E)$ comprises the accessible states of the environment to a given system state $s$ in the energy surface $\Omega_E$. The environment is assumed to equilibrate instantaneously in the Markovian approximation. Thus, $\ln |V(s; E)|$ is the Boltzmann entropy of the environment and $dI_1$ in (14) is equal to the change in the Boltzmann entropy of the environment. The contribution $dI_1$ represents the irreversibility produced by the equilibration process of the environment. It can also be written in the Clausius form in the weak coupling limit. The energy $E$ of the whole system $\mathcal{U}$ is decomposed into the sum $E = E_{\text{sys}} + E_{\text{env}} + E_{\text{int}}$, where $E_{\text{sys}}$ ($E_{\text{env}}$) is the energy of the system (environment) and $E_{\text{int}}$ is the interaction energy between them. In the weak coupling limit, $E_{\text{int}}$ is negligible so that $E \simeq E_{\text{sys}} + E_{\text{env}}$. Hence, we have $\ln |V(s; E)| = S_{\text{env}}(E_{\text{env}} = E - E_{\text{sys}}(s))$ and $\ln |V(s'; E + dE)| = S_{\text{env}}(E_{\text{env}} = E + dE - E_{\text{sys}}(s'))$, where $S_{\text{env}}(E_{\text{env}})$ denotes the entropy of the environment as a function of the energy. We note that $dE$ is the work done by the driving force on the system. The first law of thermodynamics implies that $E_{\text{sys}}(s') - E_{\text{sys}}(s) = dE - dQ$ where $dQ$ denotes the heat dissipated to the environment. Consequently, we obtain that

$$dI_1 = \frac{dQ}{T},$$

(15)

where $T = (\partial S_{\text{env}}/\partial E_{\text{env}})^{-1}$ is the temperature of the environment. Extension to systems at strong coupling with the environment would be interesting [40], which we do not pursue in this work.

The quantity $dI_2$ involves the expansion rate of the phase space volume during the time evolution. It is determined by the determinant of the Jacobian matrix $J = \partial \mathbf{c}'/\partial \mathbf{c}$ with $\mathbf{c}' = \mathcal{T}_\mathbf{dt}(\mathbf{c}; t)$ for $\mathbf{c} \in V(s; E)$. The Jacobian matrix $J$ is a block matrix of size $2M \times 2M$ in the form of

$$J = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

(16)

where $A_{mn} = (\partial x'_m/\partial x_n) = \delta_{mn}$, $B_{mn} = (\partial x'_m/\partial v_n) = \delta_{mn}dt$,

$$C_{mn} = \frac{\partial v'_m}{\partial x_n} = \left(-\frac{\partial^2 \Phi}{\partial x_m \partial x_n} + \sum_{i,j=1}^N \delta_{im} \delta_{jn} \frac{\partial f_i}{\partial x_j}\right)dt,$$

(17)

and

$$D_{mn} = \frac{\partial v'_m}{\partial v_n} = \delta_{mn} + \sum_{i,j=1}^N \delta_{im} \delta_{jn} \frac{\partial f_i}{\partial v_j} dt$$

(18)

are the submatrices of size $M \times M$ ($m, n = 1, \cdots, M$) up to the first order in $dt$, where $\delta_{mn}$ is the Kronecker delta symbol. The determinant of the block matrix is given by $\det(J) = \det(D) \det(A - BD^{-1}C)$ [41]. Note that $A = I$, $B = (dt)I$, $C = \mathcal{O}(dt)$, and $D = I + \mathcal{O}(dt)$. Thus, we obtain that $\det(J) = \det(D) = \prod_{m=1}^M D_{mm} = 1 + dt \sum_{i=1}^N \partial f_i/\partial v_i$ up to $\mathcal{O}(dt)$, which yields that

$$dI_2 = \ln \det J^{-1} = -dt \left(\nabla_v \cdot f\right)$$

(19)
with the shorthand notation \((\nabla_v \cdot f) \equiv \sum_{i=1}^{N} \partial f_i/\partial v_i\). Combining (15) and (19), we finally obtain
\[
dI = \frac{dQ}{T} - dt [\nabla_v \cdot f(s, \lambda)] . \tag{20}
\]

When the driving force does not depend on the velocity, the irreversibility in (20) is equal to the change in the entropy of the environment \(dS_{\text{env}} = dQ/T\). The same is true even in the presence of the velocity-dependent force as long as it has the vanishing divergence with respect to the velocity \((\nabla_v \cdot f = 0)\). The additional contribution \(dI_2\) becomes nonzero when \(\nabla_v \cdot f \neq 0\).

As is evident from (14), \(dI_2\) represents the contraction rate of the phase space volume during the infinitesimal time step. The phase space volume contraction rate has been identified with the entropy production rate in deterministic thermostatted dynamical systems [2, 24, 42–49]. In deterministic dynamics, one needs to introduce a phenomenological thermostat force to maintain a nonequilibrium steady state. The thermostat force plays a role of an effective damping force and depends on velocity. The explicit form of \(dI_2\) suggests that the velocity dependent force \(f\) generates an additional entropy production as if there were a thermostat associated with the velocity-dependent force. The physical meaning of the additional thermostat remains unknown yet.

We now show that the irreversibility in (20) based on the deterministic dynamics incorporated with the Markovian approximation and the weak coupling limit is reproduced in the phenomenological Langevin equation approach. Consider the Langevin equations
\[
\begin{align*}
\dot{x}_i &= v_i \\
\dot{v}_i &= f_{c,i}(x) + f_i(s, \lambda) - \gamma v_i + \xi_i(t) .
\end{align*} \tag{21}
\]
In comparison with (2), interactions with the environment are treated with the damping force and the thermal white noise satisfying \(\langle \xi_i(t) \rangle = 0\) and \(\langle \xi_i(t)\xi_j(t') \rangle = 2\gamma T \delta_{ij} \delta(t - t')\). The system is driven by the conservative force denoted by \(f_c(x)\) and the nonconservative driving force \(f\). The Langevin equations for the reverse process are given by
\[
\begin{align*}
\dot{x}_i &= v_i \\
\dot{v}_i &= f_{c,i} + f_i^\dagger(s, \lambda^\dagger) - \gamma v_i + \xi_i(t) .
\end{align*} \tag{22}
\]

The Onsager–Machlup formalism allows one to write down the path probability for the Langevin equation system [50]. Using the formalism, we obtain the logarithm of the path probability ratio of the forward and reverse processes during the infinitesimal time interval \(dt\). It is given by
\[
dI = \frac{dQ}{T} - dt [\nabla_v \cdot [f(s, \lambda) - \delta f]] + \frac{\delta f}{\gamma T} \circ dv + \frac{dt}{\gamma T} \delta f \cdot [-f_c(x) - f(s, \lambda) + \delta f - \gamma v] , \tag{23}
\]
where \(\delta f \equiv [f(s, \lambda) - f^\dagger(\epsilon s, \lambda^\dagger)]/2\) and the notation \((\cdot) \circ dv\) stands for the stochastic integral in the Stratonovich sense [51] (see appendix for derivation).
When we choose the driving force $f^\dagger$ in the reverse process according to (9), $\delta f$ is identically zero and the two irreversibilities in (20) and (23) become the same. Our theory substantiates the Langevin equation approach under the choice of (9).

4. Charged particle under the Lorentz force

The irreversibility in (12) depends crucially on the definition of the reverse process to a given forward process. We have proposed that the force $f^\dagger$ should be chosen as in (9) on the ground that the whole system should move back to the original energy surface in the reverse process. This choice is characterized by the fact that the sequence of the force values in the reversed process is the same as that in the forward process in the time-reversed order. In order to stress that the force values are the same, we refer to this choice as the V rule. There is an alternative choice where the function form of the force is taken to be the same [16, 36–39]. It is formulated as

$$f^\dagger(s, \lambda^\dagger(t)) = f(s, \lambda(\tau - t)).$$

(24)

In order to distinguish it from $f^\dagger$ according to the V rule, we use the superscript $\dagger$. This choice will be referred to as the F rule. The merit of the F rule is that the forward and the reverse processes are compared in the same physical system characterized by the driving force of same form. When the force depends on the velocity, the forces in the reverse processes $f^\dagger$ and $f^\ddagger$ are different, so are the irreversibility. In this section, we compare the two choices for a charged particle under the Lorentz force.

Consider a charged particle of mass $m$ and of charge $q$ in the three-dimensional space with cylindrical symmetry around the $\hat{z}$ direction. The time-dependent magnetic field $B(t) = bt\hat{z}$ is applied to the $z$ direction with a constant $b > 0$. According to the Maxwell equation $\nabla \times E = -\frac{\partial}{\partial t} B$, the time-varying magnetic field induces the electric field $E(x) = \frac{1}{2} b(y\hat{x} - x\hat{y}) = -\frac{1}{2} br\hat{\theta}$ with $r = \sqrt{x^2 + y^2}$ and the unit vector $\hat{\theta}$ in the azimuthal direction. The electric field line circulates around the origin in the clockwise direction. The particle is then applied to the Lorentz force

$$f(x, v, \lambda(t)) = qv \times B(t) + qE(x).$$

(25)

The field strengths are regarded as the parameters $\lambda$.

According to the V rule the force $f^\dagger$ in the reverse process is given by

$$f^\dagger(x, v, \lambda^\dagger(t)) = f(x, -v, \lambda(\tau - t)) = -qv \times B(\tau - t) + qE(x).$$

(26)

It amounts to the situation that the particle is subject to the Lorentz force under the fields

$$B^\dagger(t) = -B(\tau - t), \quad E^\dagger(x) = E(x).$$

(27)

Note that the magnetic field is flipped to the opposite direction. We compare the field configurations in the forward and the reverse processes in figure 2. The electro-magnetic fields in the reverse process also satisfy the Maxwell’s equation, $\nabla \times E^\dagger = -\frac{\partial}{\partial t} B^\dagger$.  

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On the other hand, the reverse process force according to the F rule, denoted by $f^\dagger$, is given by

$$f^\dagger(x, v, \lambda^\dagger(t)) = f(x, v, \lambda(\tau - t)) = qv \times B(\tau - t) + qE(x). \quad (28)$$

It corresponds to a Lorentz-like force under the fields

$$B^\dagger(t) = B(\tau - t), \quad E^\dagger(x) = E(x). \quad (29)$$

These fields do not satisfy the Maxwell's equation, $\nabla_x \times E^\dagger \neq -\frac{\partial}{\partial t} B^\dagger$. Namely, the reverse process in the F rule is an artificial process with non-physical electro-magnetic fields.

The consistency with electromagnetism suggests that the V rule be the proper way to define the reverse process for systems driven by a velocity-dependent force. Under the V rule, the irreversibility consists of the Clausius entropy change of the environment and the additional term $-dt[\nabla_v \cdot f]$. We do not know whether the additional term can be related to any thermodynamic quantity. In nature, the magnetic Lorentz force is the unique example of a velocity-dependent force among the fundamental forces. If we restrict ourselves to the fundamental Lorentz force, the additional term vanishes because the magnetic Lorentz force is divergence-free. Then, the irreversibility reduces to the conventional entropy production of the environment. One may consider velocity-dependent forces. However, they are not the fundamental forces but the phenomenological forces [52].

5. Summary

In stochastic thermodynamics, the entropy production is given by the logarithm of the ratio of the path probabilities of the system. In this work, we derived the connection between the irreversibility and the entropy production starting from the microscopic deterministic equations of motion of the whole system $\mathcal{U}$ consisting of a physical system $\mathcal{S}$ and an environment $\mathcal{E}$. The key assumption behind the connection is the Markovian approximation that the environmental degrees of freedom equilibrates so fast that they are always in the equilibrium state to a given configuration of $\mathcal{S}$. Our approach is an
extension of those in [24–26] to systems having the continuous degrees of freedom and being driven by an external force. We have shown that the irreversibility derived from the microscopic point of view has the same expression as the entropy production of the corresponding Langevin equation system.

It is crucial to consider a proper reverse process to a given forward process in characterizing the time irreversibility. In this work, we suggest the V rule that the sequence of the force values in the reverse process should be the same as that in the forward process in the time-reversed order. It is formulated in (9). This rule is favored because it guarantees that the whole system returns to the original energy surface in the reverse process. This choice is contrasted to the F rule in (24), where the force in the reverse process has the same function form as the force in the forward process. The two choices are compared for a charged particle in the presence of time-varying magnetic field and the induced electric field.

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Appendix. Irreversibility in the Langevin system

In this appendix, we derive the relation (23) for the entropy production in the Langevin system. The forward dynamics and the reverse dynamics of the system are governed by (21) and (22) respectively. Suppose that the system evolves from a configuration $\mathbf{s} = (\mathbf{x}, \mathbf{v})$ to $\mathbf{s}' = (\mathbf{x}', \mathbf{v}')$ during the infinitesimal time interval $[t : t + dt]$ in the forward dynamics. Such a transition occurs with the transition probability denoted by $W_{dt}(\mathbf{s} \to \mathbf{s}' ; t)$. Similarly, $W_{dt}^\dagger(\epsilon \mathbf{s}' \to \epsilon \mathbf{s} ; \bar{t})$ denotes the transition probability in the reverse process. During the time interval, the control parameters change from $\lambda(t)$ to $\lambda(t + dt)$ in the forward dynamics and from $\lambda(\bar{t} - dt)$ to $\lambda(\bar{t})$ in the reverse dynamics with $\bar{t} = \tau - t$.

With the help of the Onsager–Machlup formalism [50], the transition probabilities can be written as

$$W_{dt}(\mathbf{s} \to \mathbf{s}' ; t) = \frac{\delta(d\mathbf{x} - \mathbf{v}dt)}{(4\pi \gamma T dt)^N/2} e^{-\frac{1}{4\gamma T dt} \{d\mathbf{v} - d\mathbf{v}' df_c(x) + df(s, \lambda(t)) - \gamma \mathbf{v}\}^2}$$ \hspace{1cm} (A.1)

and

$$W_{dt}^\dagger(\epsilon \mathbf{s}' \to \epsilon \mathbf{s} ; \bar{t}) = \frac{\delta(d\mathbf{x} - \mathbf{v}'d\bar{t})}{(4\pi \gamma T d\bar{t})^N/2} e^{-\frac{1}{4\gamma T d\bar{t}} \{d\mathbf{v}' - d\mathbf{v} df_c(x') + df(\epsilon \mathbf{s}', \lambda(\bar{t})) + \gamma \mathbf{v}'\}^2}$$ \hspace{1cm} (A.2)

with $d\mathbf{x} = \mathbf{x}' - \mathbf{x}$ and $d\mathbf{v} = \mathbf{v}' - \mathbf{v}$. Here, we used the Itô discretization scheme. Keeping the terms up to $O(dt)$, we obtain that the irreversibility $dI = \ln W_{dt}(\mathbf{s} \to \mathbf{s}' ; t)/W_{dt}^\dagger(\epsilon \mathbf{s}' \to \epsilon \mathbf{s} ; \bar{t})$ is given by
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\[ dI = -\frac{\mathbf{v}}{T} \circ \{d\mathbf{v} - dt [f_e(x) + f(s, \lambda(t)) - \delta f]\} \]
\[ + \frac{\delta f}{\gamma T} \circ \{d\mathbf{v} - dt [f_e(x) + f(s, \lambda(t)) - \delta f]\} \]
\[ - dt \nabla_v \cdot [f(s, \lambda(t)) - \delta f] \tag{A.3} \]

where \( \delta f = [f(s, \lambda(t)) - f^e(\epsilon s, \lambda(t))] / 2 \) and the notation \( d\mathbf{v} \circ \mathbf{v} = d\mathbf{v} \cdot [\mathbf{v} + (\mathbf{v} + d\mathbf{v})] / 2 \) stands for the stochastic integral in the Stratonovich sense [51].

According to stochastic thermodynamics, the heat dissipated to the environment is given by [5]

\[ dQ = [-d\mathbf{v} + dt f_e(x) + dt f(s, \lambda(t))] \circ \mathbf{v}. \tag{A.4} \]

Substituting the part in the first line in (A.3) and rearranging all the terms, we obtain (23).

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