Information geometrical characterization of the Onsager-Machlup process

Tanaka, Shigenori

(Citation)
Chemical Physics Letters,689:152-155

(Issue Date)
2017-12-01

(Resource Type)
journal article

(Version)
Accepted Manuscript

Information geometrical characterization of the Onsager-Machlup process

Shigenori Tanaka

Graduate School of System Informatics, Kobe University, 1-1 Rokkodai, Nada-ku, Kobe 657-8501, Japan

Abstract

The Onsager-Machlup (OM) relaxation process, which provides a prototypical example of linear nonequilibrium thermodynamics, is characterized in terms of information geometry over the two-dimensional temperature-time parameter space. After deriving the probability distribution function for the OM process under the harmonic potential within a theoretical framework based on a transformation into imaginary-time quantum mechanics, the Fisher information metric is explicitly obtained. Differential geometry in the temperature-time space then gives the scalar curvature $R = -1$, thus specifying the OM process in a topological manner.

Keywords: Nonequilibrium thermodynamics; Onsager-Machlup process; Information geometry; Fisher information metric; Differential geometry

Email address: `tanaka2@kobe-u.ac.jp; Fax:+81-78-803-6621` (Shigenori Tanaka)

1. Introduction

Relevant, coarse-grained description of nonequilibrium relaxation processes is a key to understanding a variety of time-dependent phenomena in many fields of chemical, biological and condensed-matter physics [1–4]. Among a plethora of theoretical approaches, one of the simplest and most comprehensive descriptions was based on the stochastic differential (Langevin) equation and the associated Fokker-Planck-Smoluchowski equation for the linear diffusion process [5], whose probability distribution function can be given analytically [6]. An extension to nonequilibrium steadt state is also feasible [7]. Moreover, beyond this linear (Onsager-Machlup) relaxation process, the Fokker-Planck equation with general (harmonic and other) potentials [8] can be analyzed with the aid of a classical-quantum correspondence [9–11], in which a path integral formalism is employed to describe the resultant quantum mechanics with imaginary-time Schrödinger equation; the classical nonequilibrium thermodynamics at given temperatures can then be formulated through, *e.g.*, diffusion Monte Carlo simulations [11]. First, in Sec. 2 of this Letter, we will illustrate how this classical-quantum correspondence scheme appropriately gives an exact description of the simple Onsager-Machlup process near equilibrium.

The main aim of this Letter is further to provide an information geometrical characterization for the Onsager-Machlup (OM) relaxation process. Given the probability distribution function for a stochastic process, the information geometry [12] develops a differential geometry in parameter space (μ, ν), in which the Fisher information metric $g_{\mu\nu}$ plays a pivotal role. In Sec. 3, the two-dimensional differential geometry on $g_{\mu\nu}$ in the temperature-time space is formulated for the nonequilibrium OM process. Consequently, it is found that the scalar curvarure of $R = -1$ specifically characterizes the OM process in the information geometry on the temperature-time space, whose implications are discussed.

2. Onsager-Machlup relaxation process

The present study considers a temporal relaxation process of dynamical variable x described by an overdamped Langevin equation at temperature T [2, 3, 9–11, 13],

$$\dot{x} = -\frac{D}{k_B T} U'(x) + \eta(t), \tag{1}$$

where k_B, D and $U'(x)$ refer to the Boltzmann constant, the diffusion coefficient and the derivative of potential energy, respectively. $\eta(t)$ is a Gaussian noise with zero average satisfying the fluctuation-dissipation relation,

$$\langle \eta(t)\eta(t') \rangle = 2D\delta(t - t'), \tag{2}$$

where $\langle \quad \rangle$ means the statistical average. The time-dependent probability distribution function $P(x,t)$ sampled by the stochastic differential equation (1) then obeys the Fokker-Planck-Smoluchowski equation [2, 3, 13],

$$\frac{\partial}{\partial t} P(x,t) = D \frac{\partial}{\partial x} \left[\frac{\partial}{\partial x} P(x,t) + \frac{1}{k_B T} U'(x) P(x,t) \right]. \tag{3}$$

In the long-time limit ($t \to \infty$), all the solutions of Eq. (3) converge to the equilibrium Boltzmann distribution, $P(x,t) \to C e^{-U(x)/k_B T}$, with a normalization constant C.

To solve Eq. (3), we here introduce a "wave function" $\psi(x,t)$ by [9–11]

$$\psi(x,t) = P(x,t)\exp\left[\frac{U(x)}{2k_BT}\right], \tag{4}$$

and find an imaginary-time Schrödinger equation from Eq. (3),

$$-\frac{\partial}{\partial t}\psi(x,t) = \hat{H}_{\text{eff}}\psi(x,t). \tag{5}$$

The effective Hamiltonian is then expressed by

$$\hat{H}_{\text{eff}} = -D\frac{\partial^2}{\partial x^2} + V_{\text{eff}}(x) \tag{6}$$

with

$$V_{\text{eff}}(x) = \frac{D}{(2k_BT)^2}\left\{[U'(x)]^2 - 2k_BTU''(x)\right\}. \tag{7}$$

Let us consider a dynamics under the harmonic potential,

$$U(x) = \frac{1}{2}kx^2, \tag{8}$$

with the spring constant k in the following analysis. Then, assuming a localized initial distribution, $P(x,0) = \delta(x-x_0)$ ($x_0 \neq 0$), a relaxation process of the Onsager-Machlup (OM) type [5] is realized. Since the effective potential, Eq. (7), is given as

$$V_{\text{eff}}(x) = \frac{D}{4}(\beta^2k^2x^2 - 2\beta k) \tag{9}$$

with $\beta = 1/k_BT$, we find the solution (eigenfunctions) to the time-independent Schrödinger equation,

$$\hat{H}_{\text{eff}}\phi(x) = E\phi(x), \tag{10}$$

as [14]

$$\phi_n(x) = \sqrt{\frac{\alpha}{2^n n!\sqrt{\pi}}} H_n(\alpha x) \exp\left(-\frac{\alpha^2 x^2}{2}\right) \tag{11}$$

with the eigenvalues (energies) as

$$E_n = n\beta k D \tag{12}$$

and $\alpha = \sqrt{\beta k/2}$, where $H_n(x)$ refer to the Hermite polynomials [15] with $n = 0, 1, 2, ...$ representing the eigenstates.

The time-dependent wavefunction can then be expanded as

$$\psi(x,t) = \sum_{n=0}^{\infty} c_n e^{-E_n t}\phi_n(x) \tag{13}$$

with the initial condition,

$$\psi(x,0) = \sum_n c_n \phi_n(x) = \exp\left(\frac{\beta}{4}kx^2\right)\delta(x - x_0). \tag{14}$$

The expansion coefficients in Eq. (14) is given by

$$c_n = \int_{-\infty}^{\infty} dx \phi_n(x) \exp\left(\frac{\beta}{4}kx^2\right)\delta(x - x_0) = \phi_n(x_0)\exp\left(\frac{\beta}{4}kx_0^2\right). \tag{15}$$

Thus, the time-dependent wavefunction can be expressed by

$$\psi(x,t) = \sqrt{\frac{\beta k}{2\pi}} \exp\left(-\frac{\beta}{4}kx^2\right) \sum_{n=0}^{\infty} \frac{1}{2^n n!} e^{-n\beta k D t} H_n(\alpha x_0) H_n(\alpha x). \tag{16}$$

Recalling the integral representation for the Hermite polynomials [15],

$$H_n(x) = \frac{2^n}{\sqrt{\pi}} \int_{-\infty}^{\infty} (x + i\xi)^n e^{-\xi^2} d\xi, \tag{17}$$

the time-dependent wavefunction of Eq. (16) is written as

$$\psi(x,t) = \sqrt{\frac{\beta k}{2\pi(1-e^{-2\gamma t})}} \exp\left(\frac{\beta}{4}kx^2\right) \exp\left[-\frac{\beta k(x - x_0 e^{-\gamma t})^2}{2(1-e^{-2\gamma t})}\right] \tag{18}$$

with $\gamma = \beta k D$ after performing the summation over n and the Gaussian integrals. The time-dependent probability distribution function is then found to be

$$P(x,t) = \sqrt{\frac{\beta k}{2\pi(1-e^{-2\gamma t})}} \exp\left[-\frac{\beta k(x - x_0 e^{-\gamma t})^2}{2(1-e^{-2\gamma t})}\right], \tag{19}$$

which is a well-known expression [6]. This expression can also be derived by employing the path integral formalism [9–11] with the use of the kernel (propagator) for the harmonic oscillator [16] in imaginary time. It is also noted that, for $t \to \infty$, the time-dependent probability distribution function, Eq. (19), goes to the Boltzmann distribution, $P_{eq}(x) = \sqrt{\frac{\beta k}{2\pi}} \exp\left(-\frac{\beta}{2}kx^2\right)$.

We next discuss the nonequilibrium thermodynamics of this OM relaxation process. By using the time-dependent probability distribution function, Eq. (19), the time-dependent internal (potential) energy is expressed by

$$\begin{aligned} \bar{U}(t) &= \langle U(x) \rangle = \int dx U(x) P(x,t) \\ &= \frac{1}{2}kx_0^2 e^{-2\gamma t} + \frac{1-e^{-2\gamma t}}{2\beta}, \end{aligned} \tag{20}$$

where $\langle \quad \rangle$ means the average over the distribution function $P(x,t)$. The time-dependent entropy is given by [11]

$$\begin{aligned} S(t) &= -k_B \int dx P(x,t) \ln \frac{P(x,t)}{c} \\ &= \frac{k_B}{2} \ln \left[\frac{2\pi(1-e^{-2\gamma t})c^2}{\beta k} \right] + \frac{k_B}{2} \end{aligned} \tag{21}$$

with the normalization constant c which has the dimension of probability distribution function. We thus find an expression for the time-dependent free energy as

$$\begin{aligned} F(t) &= \bar{U}(t) - TS(t) \\ &= \frac{1}{2} k x_0^2 e^{-2\gamma t} - \frac{e^{-2\gamma t}}{2\beta} - \frac{1}{2\beta} \ln \left[\frac{2\pi(1-e^{-2\gamma t})c^2}{\beta k} \right]. \end{aligned} \tag{22}$$

The time derivative of the free energy is then given as

$$\dot{F}(t) = -\gamma e^{-2\gamma t} \left[k x_0^2 + \frac{e^{-2\gamma t}}{\beta(1-e^{-2\gamma t})} \right] \le 0, \tag{23}$$

thus showing that the free energy decreases temporally toward its minimum given by the Boltzmann distribution [11].

3. Information geometry with temperature-time metric

The Fisher information metric is a particular Riemannian metric in the space of probability distributions and plays a central role in information geometry [12]. It can be used to calculate the informational difference between measurements as the infinitesimal form of the relative entropy such as the Kullback-Leibler divergence. In the present study based on the time-dependent probability distribution function $P(x,t)$, the Fisher information metric is given by

$$g_{\mu\nu} = \langle(\partial_\mu \ln P)(\partial_\nu \ln P)\rangle = \int dx P(x,t)\,[\partial_\mu \ln P(x,t)]\,[\partial_\nu \ln P(x,t)] \tag{24}$$

in the parameter space represented by μ and ν.

In the following analysis we consider the two-dimensional parameter space formed by the inverse temperature $\beta = 1/k_B T$ and the time t to characterize the nonequilibrium process described by $P(x,t)$ of Eq. (19). The (covariant) metric tensor is then calculated to be

$$g_{\beta\beta} = \frac{1}{2\beta^2}\left(1 - 2\gamma t\frac{\varepsilon}{1-\varepsilon}\right)^2 + \frac{kx_0^2}{\beta}\gamma^2 t^2 \frac{\varepsilon}{1-\varepsilon}, \tag{25}$$

$$g_{tt} = 2\gamma^2\left(\frac{\varepsilon}{1-\varepsilon}\right)^2 + kx_0^2\beta\gamma^2\frac{\varepsilon}{1-\varepsilon}, \tag{26}$$

$$g_{\beta t} = g_{t\beta} = -\frac{\gamma}{\beta}\frac{\varepsilon}{1-\varepsilon}\left(1 - 2\gamma t\frac{\varepsilon}{1-\varepsilon}\right) + kx_0^2\gamma^2 t\frac{\varepsilon}{1-\varepsilon}, \tag{27}$$

with the determinant,

$$g = \det(g_{\mu\nu}) = |g_{\mu\nu}| = \frac{kx_0^2\gamma^2\varepsilon}{2\beta(1-\varepsilon)}, \tag{28}$$

where $\varepsilon = e^{-2\gamma t} = e^{-2\beta k D t}$ has been introduced. The contravariant metric tensor, *i.e.*, the inverse matrix of the Fisher information metric, is accordingly obtained as

$$g^{\beta\beta} = g_{tt}/g, \tag{29}$$

$$g^{tt} = g_{\beta\beta}/g, \tag{30}$$

$$g^{\beta t} = g^{t\beta} = -g_{\beta t}/g = -g_{t\beta}/g. \tag{31}$$

We further calculate basic quantities in differential geometry [17]. The derivatives of the metric tensor with respect to the two-dimensional parameters, β and t, are

$$\begin{aligned}\partial_\beta g_{\beta\beta} &= -\frac{1}{\beta^3}\left(1-2\gamma t\frac{\varepsilon}{1-\varepsilon}\right)^2 - \frac{2\gamma t}{\beta^3}\frac{\varepsilon}{1-\varepsilon}\left(1-2\gamma t\frac{\varepsilon}{1-\varepsilon}\right)\left(1-\frac{2\gamma t}{1-\varepsilon}\right)\\ &+ \frac{kx_0^2}{\beta^2}\gamma^2 t^2\frac{\varepsilon}{1-\varepsilon}\left(1-\frac{2\gamma t}{1-\varepsilon}\right),\end{aligned} \tag{32}$$

$$\begin{aligned}\partial_t g_{\beta\beta} &= -\frac{2\gamma}{\beta^2}\frac{\varepsilon}{1-\varepsilon}\left(1-2\gamma t\frac{\varepsilon}{1-\varepsilon}\right)\left(1-\frac{2\gamma t}{1-\varepsilon}\right)\\ &+ \frac{2kx_0^2}{\beta}\gamma^2 t\frac{\varepsilon}{1-\varepsilon}\left(1-\frac{\gamma t}{1-\varepsilon}\right),\end{aligned} \tag{33}$$

$$\partial_\beta g_{tt} = \frac{4\gamma^2}{\beta}\left(\frac{\varepsilon}{1-\varepsilon}\right)^2\left(1-\frac{2\gamma t}{1-\varepsilon}\right) + kx_0^2\gamma^2\frac{\varepsilon}{1-\varepsilon}\left(3-\frac{2\gamma t}{1-\varepsilon}\right), \tag{34}$$

$$\partial_t g_{tt} = -8\gamma^3\frac{\varepsilon^2}{(1-\varepsilon)^3} - 2kx_0^2\beta\gamma^3\frac{\varepsilon}{(1-\varepsilon)^2}, \tag{35}$$

$$
\begin{aligned}
\partial_\beta g_{\beta t} &= \partial_\beta g_{t\beta} \\
&= \frac{2\gamma^2 t}{\beta^2}\frac{\varepsilon}{(1-\varepsilon)^2}\left(1+\varepsilon-4\gamma t\frac{\varepsilon}{1-\varepsilon}\right) \\
&+ 2kx_0^2\frac{\gamma^2 t}{\beta}\frac{\varepsilon}{1-\varepsilon}\left(1-\frac{\gamma t}{1-\varepsilon}\right),
\end{aligned} \tag{36}
$$

$$
\begin{aligned}
\partial_t g_{\beta t} &= \partial_t g_{t\beta} \\
&= \frac{2\gamma^2}{\beta}\frac{\varepsilon}{(1-\varepsilon)^2}\left(1+\varepsilon-4\gamma t\frac{\varepsilon}{1-\varepsilon}\right) \\
&+ kx_0^2\gamma^2\frac{\varepsilon}{1-\varepsilon}\left(1-\frac{2\gamma t}{1-\varepsilon}\right).
\end{aligned} \tag{37}
$$

The Christoffel symbols defined by (with the use of Einstein's convention)

$$
\Gamma^\lambda_{\mu\nu} = \frac{1}{2}g^{\lambda\tau}\left(\partial_\mu g_{\nu\tau}+\partial_\nu g_{\mu\tau}-\partial_\tau g_{\mu\nu}\right) \tag{38}
$$

are then calculated to be

$$
\Gamma^\beta_{\beta\beta} = -\frac{1}{\beta}\left(1-2\gamma t\frac{\varepsilon}{1-\varepsilon}-2\gamma^2t^2\frac{\varepsilon}{1-\varepsilon}\right)-kx_0^2\gamma^2t^2\frac{\varepsilon}{1-\varepsilon}, \tag{39}
$$

$$
\Gamma^t_{\beta\beta} = \frac{t}{\beta^2}\left(2-\gamma t-4\gamma t\frac{\varepsilon}{1-\varepsilon}-2\gamma^2t^2\frac{\varepsilon}{1-\varepsilon}\right)+kx_0^2\frac{\gamma^2t^3}{\beta}\frac{\varepsilon}{1-\varepsilon}, \tag{40}
$$

$$
\Gamma^\beta_{tt} = 2\beta\gamma^2\frac{\varepsilon}{1-\varepsilon}-kx_0^2\beta^2\gamma^2\frac{\varepsilon}{1-\varepsilon}, \tag{41}
$$

$$
\Gamma^t_{tt} = -\frac{\gamma}{1-\varepsilon}(1+\varepsilon+2\gamma t\varepsilon)+kx_0^2\beta\gamma^2t\frac{\varepsilon}{1-\varepsilon}, \tag{42}
$$

$$\Gamma^{\beta}_{\beta t} = \Gamma^{\beta}_{t\beta} = \gamma(1+2\gamma t)\frac{\varepsilon}{1-\varepsilon} - kx_0^2\beta\gamma^2 t\frac{\varepsilon}{1-\varepsilon}, \tag{43}$$

$$\Gamma^{t}_{\beta t} = \Gamma^{t}_{t\beta} = \frac{1}{2\beta}\left(3 - 2\gamma t - 6\gamma t\frac{\varepsilon}{1-\varepsilon} - 4\gamma^2 t^2\frac{\varepsilon}{1-\varepsilon}\right) + kx_0^2\gamma^2 t^2\frac{\varepsilon}{1-\varepsilon}. \tag{44}$$

It is thus straightforward to verify that the covariant derivatives of the metric tensor actually vanish,

$$g_{\mu\nu;\lambda} = \partial_\lambda g_{\mu\nu} - \Gamma^{\tau}_{\lambda\mu} g_{\tau\nu} - \Gamma^{\tau}_{\lambda\nu} g_{\mu\tau} = 0. \tag{45}$$

Then, after some algebra, the Ricci tensor given by

$$R_{\mu\nu} = \partial_\sigma \Gamma^{\sigma}_{\mu\nu} - \partial_\nu \Gamma^{\sigma}_{\mu\sigma} + \Gamma^{\sigma}_{\rho\sigma}\Gamma^{\rho}_{\mu\nu} - \Gamma^{\sigma}_{\rho\nu}\Gamma^{\rho}_{\mu\sigma} \tag{46}$$

is found to satisfy a relation,

$$R_{\mu\nu} = -\frac{1}{2} g_{\mu\nu}, \tag{47}$$

in the present case. This leads to the scalar curvature given by

$$R = g^{\mu\nu} R_{\mu\nu} = -\frac{1}{2} g^{\mu\nu} g_{\mu\nu} = -1 \tag{48}$$

in two dimension. The Einstein tensor is then

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} = 0, \tag{49}$$

which should be the case due to the symmetries in two dimension [18].

Thus, we have found that the Fisher information metric given by Eqs. (25)-(27), derived from the $P(x,t)$ for the OM process, gives $R = -1$ in the two-dimensional differential geometry for the parameter space of β and t, irrespective of the values of D, k and x_0.

4. Concluding remarks

As seen above, the Fisher information metric $g_{\mu\nu}$ for the time-dependent probability distribution function to describe the OM process satisfies a simple equation, $R = -1$, in the two-dimensional parameter space formed by β and t. Since the scalar curvature R may be regarded as only one independent variable in the two-dimensional differential geometry [18], the present relaxation process can thus be understood to be characterized by the equation of $R = -1$ in the context of information geometry in the β-t space. Then, while the present $g_{\mu\nu}$ gives a solution to the equation of $R = -1$ (that is, a two-dimensional counterpart of the Einstein equation in the four-dimensional space-time continuum), a question is raised as to whether there are other solutions to the identical equation. This question is related to a problem that what wide class of relaxation processes are contained as solutions to $R = -1$, because the present OM type process may be regarded as one of the simplest relaxation processes conceivable. In this regard, it is noted that an extension of OM theory to nonequilibrium steady state [7] gives the identical form of $g_{\mu\nu}$ to Eqs. (25)-(27) with a redefinition of x_0. Further, a more general question could be raised as to how the types (classes) of nonequilibrium processes can be characterized according to the values of the scalar curvature R. These questions and problems remain to be answered in the future, probably in the context of topological classification of various relaxation processes.

Acknowledgement

The author would like to acknowledge the Grants-in-Aid for Scientific Research (Nos. 26460035 and 17H06353) from the Ministry of Education, Cultute, Sports, Science and Technology (MEXT).

References

[1] H.C. Öttinger, Beyond Equilibrium Thermodynamics, John Wiley & Sons, Inc., Hoboken, New Jersey, 2005.

[2] A. Nitzan, Chemical Dynamics in Condensed Phases, Oxford University Press, New York, 2006.

[3] K. Sekimoto, Stochastic Energetics (Lecture Notes in Physics 799), Springer, Berlin Heidelberg, 2010.

[4] D.J. Evans, D.J. Searles, S.R. Williams, Fundamentals of Classical Statistical Thermodynamics, Wiley-VCH, Weinheim, 2016.

[5] L. Onsager, S. Machlup, Phys. Rev. 91 (1953) 1505.

[6] S. Chandrasekhar, Rev. Mod. Phys. 15 (1943) 1.

[7] T. Taniguchi, E.G.D. Cohen, J. Stat. Phys. 126 (2007) 1.

[8] K. Yasue, J. Math. Phys. 19 (1978) 1671.

[9] P. Faccioli, M. Sega, F. Pederiva, H. Orland, Phys. Rev. Lett. 97 (2006) 108101.

[10] M. Sega, P. Faccioli, F. Pederiva, G. Garberoglio, H. Orland, Phys. Rev. Lett. 99 (2007) 118102.

[11] S. Tanaka, J. Chem. Phys. 144 (2016) 094103.

[12] S. Amari, Information Geometry and Its Applications, Springer Japan, Tokyo, 2016.

[13] A.B. Adib, J. Phys. Chem. B 112 (2008) 5910.

[14] L.I. Schiff, Quantum Mechanics, 3rd ed., McGraw-Hill, Singapore, 1968.

[15] I.S. Gradshteyn, I.M. Ryzhik, A. Jeffrey, Table of Integrals, Series, and Products, 5th ed., Academic Press, San Diego, 1994.

[16] R.P. Feynman, A.R. Hibbs, Quantum Mechanics and Path Integrals, McGraw-Hill, New York, 2005.

[17] L.D. Landau, E.M. Lifshitz, The Classical Theory of Fields, 4th ed., Butterworth-Heinemann, Oxford (UK), 1980.

[18] J.D. Brown, Lower Dimensional Gravity, World Scientific, Singapore, 1988.

*Graphical Abstract (pictogram) (for review)