Double Density Dynamics: Dynamical Realization of Superstatistics

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Abstract

We create a deterministic method, double density dynamics, to realize an arbitrary distribution for both physical variables and associated parameters simultaneously. We specifically construct an ordinary differential equation that has an invariant density relating to a joint distribution of the physical system and parameter system. For a temperature parameter, a generalized temperature function leads to a physical system that develops under nonequilibrium temperature describing superstatistics. The joint distribution density of the physical system and temperature system appears as the Radon-Nikodym derivative of a distribution that is created by a scaled long-time average generated from the flow of the differential equation under an ergodic assumption. These ideas are based on the density dynamics molecular dynamics method and utilized for efficiently simulating physical systems in nonequilibrium. Along with general mathematical framework for aiming at further applications, specific settings of required functions together with associated numerical example for 1-D harmonic oscillator are given.

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I. INTRODUCTION

Numerical simulation for physical system is now an important tool for understanding the structures, phases, and mechanisms of the system in systematic manners. Molecular dynamics (MD) simulation is used for classical/quantum Hamiltonian/non-Hamiltonian system to understand characteristics of the systems in terms of microscopic descriptions [1].

Often, the physical system or rather equations of motion (EOM) in these methods includes some parameters, which may be keys for performing the simulations. For example, intensive-quantity parameters such as temperature and pressure are important for understanding equilibrium and nonequilibrium states. There would be a case that we are motivated to fluctuate these values to know the effect of these parameters. Typical situation is to change or fluctuate such intensive quantity parameters, which is relevant for nonequilibrium simulations [2, 3]. In other case, a parameter is included where its handling is not so clear. For example, optimal values of the parameters are unknown a priori, such as "mass" parameters for the thermostat or barostat in extended system methods [4, 5]. As well, the optimal parameter values in sampling method [6, 7] are often system-dependent and need efforts for their seeking.

In these situations, what should we do? Ad hoc manners for varying the parameter values do not give us the information such as the probability distribution that the physical system obeys, precluding an easy interpretation to compare the results with experiments. The current study is motivated to construct a route to solve this problem. A possible approach, which will be the issue of this paper, to is to control the dynamical variations of the parameter values by a certain protocol based on a probabilistic description.

We present deterministic equations of motion describing the physical system and a parameter system, realizing an arbitrary joint distribution in "physical-space × parameter-space." Specifically, we realize a joint distribution density of the physical system, described with coordinates $x \equiv (x_1, \ldots, x_n)$ and momenta $p \equiv (p_1, \ldots, p_n)$, and the parameter system, described with β, of a form:

$$\rho_{\mathrm{Phys}}(x, p, \beta) f(\beta). \tag{1}$$

Physically, $\rho_{\mathrm{Phys}}(x, p, \beta)$ stands for the distribution density value such that (x, p) emerges under the condition that the parameter takes a value of β, and f stands for the the distribution density of the parameter. In particular we emphasize on the temperature parameter.

Namely, the physical system interacts with a heat bath whose temperature is $1/\beta$ (Boltzmann's constant is unity) and obeys a distribution density $\rho_{\rm Phys}(x,p,\beta)$, and the temperature is also a dynamical variable and obeys a probability distribution density f. We derive an ordinary differential equation (ODE) that produces the density, equation (1), with dynamical variables including x, p, and β, via providing a invariant density (a density of an invariant measure) that is related to equation (1).

The distribution of the physical system regarding equation (1) is represented by the marginal distribution density,

$$\rho_{\rm R}(x,p) \equiv \int d\beta \rho_{\rm Phys}(x,p,\beta) f(\beta). \tag{2}$$

Here $\rho_{\rm R}(x,p)$ plays a main role in superstatistics [8–10], which describes nonequilibrium complex systems characterized by different time scales [11], and which offers a route [12] to non-extensive statistical mechanics [13–16] characterized by long-tail distributions. Superstatistics has been successfully applied to broad area of research, including hydrodynamic turbulence [17], complex networks [18], solar flares [19], high-energy physics [20], random matrix [21], and nanoscale electrochemical systems [22].

In this terminology, our method leads to a deterministic, time-reversible method generating a superstatistics distribution in a *dynamical* manner. Generating density (1), we observe that superstatistics distribution $\rho_{\rm R}(x,p)$ is realized by focusing only on the physical variables (x,p). With this realization, a physical system in a nonequilibrium environment, which is yet under control in light of equation (1), can be simulated. It must provide us a new gain due to the freedom of choosing $\rho_{\rm Phys}$ and f. In fact, approaches to realize the marginal distribution, $\rho_{\rm R}(x,p)$, have been taken into account [23]. Namely, they utilize the distribution in *static* manners, for which β is not a dynamical variable but just a variable of integration. One of the advantages of the *dynamical* realization of superstatistics distributions, viz., the realization of the density (1), is that we can directly observe the influence of temperature deviations to the physical system, leading to understanding dynamical features of the physical system in nonequilibrium. Another advantage is that we can generate the distribution and constitute reweighted distributions even if the integration, equation (2), which defines $\rho_{\rm R}(x,p)$, cannot be analytically (explicitly) done. The resulting ability to *freely* set f guides us to direct interpretations between simulations and experiments. Moreover, our target is a general density form of equation (1), in contrast to conventional approaches addressing a specific form, $\int d\beta \mathrm{e}^{-\beta U(x)} f(\beta)$, using potential energy $U(x)$. On the other hands, generation of $\rho_{\mathrm{R}}(x,p)$ based on a stochastic EOM, Langevin equation, was discussed by Beck [8], for which $f(\beta)$ is assumed to exist irrespective of descriptions of the detailed structure. Hahn *et al.* [24] characterized the EOM as stochastic differential equations driven by exchangeable processes. In our method, whereas, β is a realistic dynamical variable, and the specific mechanism to realize $f(\beta)$ is provided. In addition, the current deterministic method enables us to monitor numerical accuracies in integrating the ODE [25].

In this paper, we pursuit a method for generating distribution density, equation (1), in a deterministic manner by constructing an ODE. We constitute a general framework of the method and consider a mathematical structure of the resulting space of dynamical variables. In section II we present a vector filed defining the ODE and clarify the structure of the generated probability space. In section III we define density functions suitable for our purpose and state fundamental results regarding the realization of equation (1). In section IV we specifically set the required functions and discuss the related mathematical conditions. We present results of a brief numerical test to validate the current scheme in section V and conclude in section VI.

II. DOUBLE DENSITY DYNAMICS

Main idea.—Target probability density, ρ, of variables ω, including x, p and Q, where Q is a dynamical variable related to β, can be realized by a smooth vector field X having an invariant measure $P \equiv \rho d\omega$ on $\Omega \subset \mathbb{R}^N$. Namely, if we ensure a *normal* condition for ρ, then for any solution ϕ of an ODE, $\dot{\omega} = X(\omega)$, generated by complete field X, and for any P-integrable function g, we have $\lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau g\left(\phi\left(t\right)\right) dt = \int_\Omega g(\omega) dP(\omega)\, / P(\Omega)$ under an ergodic assumption [26]. Though it is not trivial to constitute such a suitable X for given ρ, the *density dynamics* approach [27, 28], modeled on the Nosé-Hoover (NH) method [29, 30], gives a solution of this, a kind of an *inverse*, problem. Generalizing this idea, we propose a vector field that reflects the two systems: physical system and parameter system. The density dynamics for a physical system and the density dynamics for a parameter system will be coupled in a consistent manner. To accurately demonstrate the realization of the density, we shall also manifest the resulting probability space that is described by a scaled long-time average for X. Note that the NH scheme has been actively utilized in revisiting thermostatting methods as detailed in reviews [31, 32].

A. Vector field

We begin with definitions of phase space Ω and a general form of vector field X.

Let the phase space Ω be a domain (open, connected set) of $\mathbb{R}^N$ with $N \equiv 2(n^{(1)}+n^{(2)}+1)$, specifically given by $\Omega \equiv D \times \mathbb{R}^{n^{(1)}} \times \mathbb{R} \times \mathbb{R}^{n^{(2)}} \times \mathbb{R}^{n^{(2)}} \times \mathbb{R}$, with D being a domain of $\mathbb{R}^{n^{(1)}}$. For state $\omega \equiv (x^{(1)}, p^{(1)}, \zeta^{(1)}, x^{(2)}, p^{(2)}, \zeta^{(2)}) \in \Omega$, the first three variables $(x^{(1)}, p^{(1)}, \zeta^{(1)}) \in D \times \mathbb{R}^{n^{(1)}} \times \mathbb{R}$ describe a physical system, and the last three variables $(x^{(2)}, p^{(2)}, \zeta^{(2)}) \in \mathbb{R}^{n^{(2)}} \times \mathbb{R}^{n^{(2)}} \times \mathbb{R}$ describe a parameter system. Here, only for $x^{(1)}$ the accessible area is defined to be not necessarily the whole but D, on which a potential function is defined in realistic applications.

Suppose an arbitrary given density $\rho : \Omega \to \mathbb{R}$, which is strictly positive and of class C^2 function. For this ρ, we define X as follows:

$$X : \Omega \to \mathbb{R}^N, \tag{3a}$$

$$\begin{aligned}\omega &\equiv (x^{(1)}, p^{(1)}, \zeta^{(1)}, x^{(2)}, p^{(2)}, \zeta^{(2)}) \\ &\mapsto (X_{x^{(1)}}(\omega), X_{p^{(1)}}(\omega), X_{\zeta^{(1)}}(\omega), X_{x^{(2)}}(\omega), X_{p^{(2)}}(\omega), X_{\zeta^{(2)}}(\omega)),\end{aligned} \tag{3b}$$

where

$$X_{x^{(a)}}(\omega) = h^{(a)}(\omega)\, \nabla_{p^{(a)}}\Theta(\omega) - \nabla_{p^{(a)}} h^{(a)}(\omega) \in \mathbb{R}^{n^{(a)}}, \tag{4a}$$

$$\begin{aligned}X_{p^{(a)}}(\omega) &= -h^{(a)}(\omega)\, \nabla_{x^{(a)}}\Theta(\omega) + \nabla_{x^{(a)}} h^{(a)}(\omega) \\ &\quad - \left[k^{(a)}(\omega)\nabla_{\zeta^{(a)}}\Theta(\omega) - \nabla_{\zeta^{(a)}} k^{(a)}(\omega)\right] p^{(a)} \in \mathbb{R}^{n^{(a)}},\end{aligned} \tag{4b}$$

$$\begin{aligned}X_{\zeta^{(a)}}(\omega) &= \left[(p^{(a)} | \nabla_{p^{(a)}}\Theta(\omega)) - n^{(a)}\right] k^{(a)}(\omega) \\ &\quad - (\nabla_{p^{(a)}} k^{(a)}(\omega) |\, p^{(a)}) \in \mathbb{R},\end{aligned} \tag{4c}$$

with $(\cdot\,|\,\cdot)$ being the inner product in $\mathbb{R}^{n^{(a)}}$, for $a = 1, 2$, and

$$\Theta \equiv -\ln \rho. \tag{5}$$

Here $h^{(a)}$ and $k^{(a)}$ $(a = 1, 2)$ are arbitrary C^2-functions, which will be suitably chosen according to the problem as seen below, on Ω. Namely, X is constructed from the given ρ and subordinate functions, $h^{(a)}$ and $k^{(a)}$. If we consider only $a = 1$ (viz., only consider the physical system) and put $h^{(1)} = k^{(1)} = 1$ (constant function), we have the original *density dynamics* [27].

We can confirm the smoothness (C^1) of X easily and the validity of the Liouville equation,

$$\mathrm{div}\,\rho X = 0, \tag{6}$$

via a straightforward calculation. Due to Liouville's theorem, these facts ensure that $\rho d\omega$ becomes an invariant measure of the flow $\{T_t : \Omega \to \Omega\}$ generated by field X which is assumed to be complete. We call this flow *double density dynamics (DDD).*

For our purpose, we formulate a probability space via this vector field, X, and set a specific form of density ρ in sections II B and III A, respectively.

B. Probability space

From now on we focus on a temperature as a parameter and consider a *temperature system* using relevant notations. This is done to smoothly introduce a notion of dynamical temperature, although the issues in this subsection are applicable to a general parameter system.

First, we rewrite $\omega \equiv (x^{(1)}, p^{(1)}, \zeta^{(1)}, x^{(2)}, p^{(2)}, \zeta^{(2)})$ as $(x, p, \zeta, Q, \mathcal{P}, \eta)$: $\mathbb{R}^{2n} \ni (x, p) \equiv (x^{(1)}, p^{(1)})$ is the physical variables with $n^{(1)} \equiv n$ degrees of freedom, $\mathbb{R}^1 \ni \zeta \equiv \zeta^{(1)}$ is a control variable for the physical-system temperature (here just imagine the NH mechanism for (x, p) via a friction variable ζ); $(Q, \mathcal{P}, \eta) \equiv (x^{(2)}, p^{(2)}, \zeta^{(2)})$ forms the temperature system yielding a *nonequilibrium* temperature against the physical system, via *coordinates* $Q \in \mathbb{R}^{n^{(2)}} \equiv \mathbb{R}^m$, their corresponding *momenta* $\mathcal{P} \in \mathbb{R}^m$, and a control variable $\eta \in \mathbb{R}^1$, which again forms an analog of the NH mechanism for $(Q, \mathcal{P})$ as seen below. Second, we specifically put

$$h^{(1)} \equiv k^{(1)} \equiv 1 \text{ (const. function)}, \tag{7a}$$

$$h^{(2)}(\omega) \equiv k^{(2)}(\omega) \equiv 1/T(x, p, Q) \tag{7b}$$

for a certain strictly positive, C^2-function T, and multiply X by this scalar field T. Then we have $X' : \Omega \to \mathbb{R}^N$, $\omega \overset{\mathrm{d}}{\mapsto} T(x,p,Q)X(\omega)$, represented by

$$X'_x(\omega) = T(x,p,Q)\,\nabla_p\Theta(\omega) \in \mathbb{R}^n, \tag{8a}$$

$$X'_p(\omega) = -T(x,p,Q)\nabla_x\Theta(\omega) - T(x,p,Q)\nabla_\zeta\Theta(\omega)p \in \mathbb{R}^n, \tag{8b}$$

$$X'_\zeta(\omega) = T(x,p,Q)\ [(p|\ \nabla_p\Theta(\omega)) - n] \in \mathbb{R}, \tag{8c}$$

$$X'_Q(\omega) = \ \nabla_{\mathcal{P}}\Theta(\omega) \in \mathbb{R}^m, \tag{8d}$$

$$X'_{\mathcal{P}}(\omega) = -\ \nabla_Q\tilde{\Theta}(\omega) - \nabla_\eta\Theta(\omega)\ \mathcal{P} \in \mathbb{R}^m, \tag{8e}$$

$$X'_\eta(\omega) = (\mathcal{P}|\ \nabla_{\mathcal{P}}\Theta(\omega)) - m \in \mathbb{R}, \tag{8f}$$

with

$$\tilde{\Theta}(\omega) \equiv \Theta(\omega) + \ln T(x,p,Q). \tag{9}$$

Although equation (7) is not the unique choice of the function forms, the fundamental variables we consider is (x,p,Q) so that this form may be a natural choice. The meaning of the multiplication of T is described in remark 3 below. To properly describe a probability-space structure we shall use the following definitions.

a. Definitions and notations We define projections: $\pi_1 : \Omega \to \Omega_1 := D \times \mathbb{R}^n \times \mathbb{R}^m$, $\omega \equiv (x,p,\zeta,Q,\mathcal{P},\eta) \mapsto (x,p,Q)$; $\pi_{\mathrm{R}} : \Omega \to D \times \mathbb{R}^n$, $\omega \mapsto (x,p)$; similarly, $\pi_{\mathrm{Q}}(\omega) := Q$ and $\pi_{\mathrm{x}}(\omega) := x$. To clarify a variable dependence, we denote $\tilde{T} \equiv T \circ \pi_1 : \Omega \to \mathbb{R}$, $\omega \mapsto T(x,p,Q)$. For any $n \in \mathbb{N}$, l_n and $\mathcal{L}_n$ represent the Lebesgue measure and the Lebesgue measurable sets on $\mathbb{R}^n$, respectively; $\mathcal{B}_n$ represents the Borel measurable sets on $\mathbb{R}^n$; $\mathcal{L}_n \cap \Omega$ is denoted by $\mathcal{L}_n^\Omega$ and so on. Basically, we consider a measure space $(\Omega, \mathcal{L}_N^\Omega, P)$, where $P := \rho dl_N$, or employ a measure $P' = \rho' dl_N$ using a modified density ρ' instead of the given density ρ, as described below. Put $L^1(P) \equiv \{g : \Omega \to \mathbb{R} \mid g \text{ is } \mathcal{B}_N^\Omega\text{-measurable and } P\text{-integrable}\}$. For any $n \in \mathbb{N}$ and $B \subset \mathbb{R}^n$, χ_B^n is the characteristic function of B [viz., $\chi_B^n(\omega) = 1$ if $\omega \in B$ and $\chi_B^n(\omega) = 0$ otherwise], but we may omit n if it is clear. $\mathbb{R}_+$ denotes the strictly positive real numbers.

Long-time behavior for the flow generated by vector field X' is described as follows:

Proposition 1 *Let $\int_\Omega \rho' dl_N < \infty$, where $\rho' \equiv \rho/\tilde{T}$. Assume $X' = \tilde{T}X$ is complete, so that its flow $\{T'_t : \Omega \to \Omega |\ t \in \mathbb{R}\}$ is generated. Then for $g \in L^1(P)$, the following hold:*

(i) *for a.e.* $\omega \in \Omega$ there exist a limit,

$$\lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau (g \cdot \tilde{T}))(T'_t(\omega))dt =: \overline{gT}(\omega) \in \mathbb{R}; \tag{10}$$

(ii) *if* $\{T'_t\}$ *is ergodic with respect to measure space* (Ω, L_N^Ω, P')*, then*

$$\overline{gT}(\omega) = \int_\Omega g\rho dl_N \Big/ \int_\Omega \rho' dl_N \in \mathbb{R} \;\; \textit{for a.e. } \omega \in \Omega; \tag{11}$$

(iii) *furthermore, if* ρ *is* l_N*-integrable, then*

$$\frac{\overline{gT}(\omega)}{\overline{T}(\omega)} = \int_\Omega g\rho dl_N \Big/ \int_\Omega \rho dl_N \in \mathbb{R} \;\; \textit{for a.e. } \omega. \tag{12}$$

Proof. Since $\rho' : \Omega \to \mathbb{R}$ becomes *normal*, i.e., smooth (C^2), strictly positive, and l_N-integrable, and since Ω is open, $P' = \rho' dl_N$ becomes a strictly positive, finite measure on $\mathcal{L}_N^\Omega$. For X', it becomes C^1, and the Liouville equations holds:

$$\operatorname{div} \rho' X' = \operatorname{div} \rho X = 0. \tag{13}$$

From these facts and the assumption of the completeness of X', P' becomes an invariant measure with respect to $\{T'_t\}$, i.e., $\forall t \in \mathbb{R}, \forall A \in \mathcal{L}_N^\Omega$, $P'(T_t'^{-1}A) = P'(A)$. Now for a function $g \in L^1(P)$, it holds that $g' \equiv g\tilde{T} \in L^1(P')$ due to

$$\mathbb{R} \ni \int_\Omega g dP = \int_\Omega g\rho dl_N = \int_\Omega g'\rho' dl_N = \int_\Omega g' dP', \tag{14}$$

and $g' \circ \Phi' : \mathbb{R}\times\Omega \to \mathbb{R}$ is $\mathcal{B}_1 \otimes \mathcal{L}_N^\Omega$-measurable, where $\Phi'(t,\omega) := T'_t(\omega)$ for $(t,\omega) \in \mathbb{R}\times\Omega$. (i) Thus, according to Birkhoff's ergodic theorem, for P'-a.e. $\omega \in \Omega$ there exists a time average of g', i.e., $\overline{g'}(\omega) \equiv \lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau g'(T'_t(\omega))dt \in \mathbb{R}$, which is equivalent to $\overline{gT}(\omega)$ defined in equation (10) [we abbreviate as $\overline{g'} = \overline{g\tilde{T}} \equiv \overline{gT}$]. Note "P'-a.e." can be replaced by P-a.e. or l_N-a.e., since P', P, and l_N become equivalent (i.e., absolutely continuous with each other) because $\rho, \rho' > 0$, so that we abbreviate them to just "a.e." (ii) It follows from the ergodicity that $\overline{g'}(\omega) = \int_\Omega g' dP' / P'(\Omega)$ for P'-a.e. ω, where the RHS equals $\int_\Omega g\rho dl_N / \int_\Omega \rho' dl_N$ due to equation (14). (iii) Since the l_N-integrability of ρ is nothing but the P-integrability of $g \equiv 1$ (constant function), above (i) and (ii) apply to $1 \in L^1(P)$, implying

$$\overline{T}(\omega) \equiv \exists \lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau \tilde{T}(T'_t(\omega))dt = \int_\Omega \rho dl_N \Big/ \int_\Omega \rho' dl_N \in \mathbb{R} \;\; \text{(a.e. } \omega). \tag{15}$$

Also note that $\overline{T}(\omega) \neq 0$ (a.e.) since $\int_\Omega \rho dl_N > 0$. Thus, the division of equation (11) by equation (15) leads to the validity of equation (12) for a.e. ω. ■

Here the LHS of equation (12) can be interpreted as a scaled long-time average of g, abbreviated as

$$\overline{\overline{g}}(\omega) \equiv \frac{\overline{gT}(\omega)}{\overline{T}(\omega)}, \tag{16}$$

and the RHS of equation (12) is the space average of g weighted by ρ and written as

$$\langle g \rangle \equiv \int_\Omega g(\omega)\rho(\omega)dl_N(\omega) \Big/ \int_\Omega \rho(\omega)dl_N(\omega) = \int_\Omega gdP \,/ P(\Omega) \,. \tag{17}$$

Therefore, in a simplified notation we have

$$\overline{\overline{g}}(\omega) = \langle g \rangle \quad \text{a.e. } \omega, \tag{18}$$

or more simply, $\overline{\overline{g}} = \langle g \rangle$.

In the current method, thus, we realize the probability measure $\hat{P} \equiv P\,/P(\Omega)$ and probability space $(\Omega, \mathcal{L}_N^\Omega, \hat{P})$, under the assumption of the ergodicity and the integrabilities of ρ and ρ'. This is done through the ability of calculating the expectation value, $\int_\Omega g d\hat{P}$, for any function $g \in L^1(P)$ via the scaled-time average $\overline{\overline{g}}$. Namely, as is explicitly stated, the probability for any set $B \in \mathcal{B}_N^\Omega$ can be defined and represented as

$$\nu(B) \overset{\mathrm{d}}{:=} \overline{\overline{\chi_B^N}} = \left\langle \chi_B^N \right\rangle = \hat{P}(B), \tag{19}$$

which implies that we get $(\Omega, \mathcal{B}_N^\Omega, \nu)$ and $\nu = \hat{P}|\mathcal{B}_N^\Omega$ [exactly speaking, the equality $\overline{\overline{\chi_B^N}} = \left\langle \chi_B^N \right\rangle$ in equation (19) is valid for l_N-a.e. initial point $\omega \in \Omega$, and the set of all such points should be written as Ω_B considering the dependence on uncountably many Bs. Thus it should be $\nu(B) := \overline{\overline{\chi_B^N}}(\omega_B)$ for any $\omega_B \in \Omega_B$. Similar notification applies hereafter]. Therefore, using the equivalence of $\hat{P}$ and l_N, the completion of $(\Omega, \mathcal{B}_N^\Omega, \nu)$ emerges as the whole probability space $(\Omega, \mathcal{L}_N^\Omega, \hat{P})$.

Example 2 *A marginal distribution for x-component is given by*

$$\mathcal{B}_n^D \to \mathbb{R}, \; B_1 \mapsto \overline{\overline{\chi_{B_1}^n \circ \pi_x}}, \tag{20}$$

as confirmed from $\chi_{B_1}^n \circ \pi_x = \chi^N_{B_1 \times \mathbb{R}^n \times \mathbb{R} \times \mathbb{R}^m \times \mathbb{R}^m \times \mathbb{R}}$ and equation (19), indicating

$$\overline{\overline{\chi_{B_1}^n \circ \pi_x}} = \hat{P}(B_1 \times \mathbb{R}^n \times \mathbb{R} \times \mathbb{R}^m \times \mathbb{R}^m \times \mathbb{R}) \;\; (\forall B_1 \in \mathcal{B}_n^D), \tag{21}$$

whose RHS implies the marginal distribution. Marginal distributions for other components are given similarly.

Remark 3 *Scalar-field multiplication, viz., $X \to \kappa X$ using a smooth, strictly positive scalar filed κ, is a general concept to re-parametrize the time for each orbit of the flow. Namely, it causes a time rescaling between a solution of ODE $\dot{\omega} = X(\omega)$ and the corresponding solution of $\dot{\omega} = (\kappa X)(\omega)$. In fact, we see that proposition 1 holds for any C^2, strictly-positive $\kappa : \Omega \to \mathbb{R}$, instead of $\tilde{T}$. This means that the probability-space description in a usual ergodic dynamical system generated by a vector field having a smooth invariant density ρ applies for a dynamical system described by a scalar-field-multiplied vector-field along with keeping the density ρ as long as we consider the scaled-time average. Of course $\kappa = 1$ reduces to the usual description. Thus we have considered a general situation to obtain a probability-space structure. The reason why we choose $\kappa \equiv \tilde{T}$ is to obtain a simple form of EOM as described below.*

III. DYNAMICAL REALIZATION OF SUPERSTATISTICS

A. Density form

In section II B, we have only assumed the smoothness, positivity, and integrability for ρ, and similarly the smoothness and positivity for T. To create the specific density, equation (1), we set as follows:

$$\rho : \Omega \to \mathbb{R},\ \omega \mapsto \rho_{\mathrm{Phys}}(x, p, \sigma(Q))\, \rho_f(Q)\, \rho_{\mathrm{Cntr}}(\mathcal{P}, \zeta, \eta), \tag{22}$$

$$\rho_f : \mathbb{R}^m \to \mathbb{R},\ Q \mapsto f(\sigma(Q))\, |\det D\sigma(Q)|. \tag{23}$$

Each function constituting ρ and function T have to satisfy the following six conditions:

(C1) $\sigma : \mathbb{R}^m \to \mathbb{R}^m$ is a C^3-diffeomorphism, and $\det D\sigma : \mathbb{R}^m \to \mathbb{R}$ has a definite signature.

Note that σ is introduced to control the admissible space of β via mapping $Q \mapsto \sigma(Q) \equiv \beta$ using variable Q that moves in a whole *free* space $\mathbb{R}^m$, which is convenient to constitute a flow.

(C2) $\rho_{\mathrm{Cntr}} : \mathbb{R}^m \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}_+$ is of class C^2 and l_{m+2}-integrable, viz., $Z_{\mathrm{Cntr}} \equiv \int_{\mathbb{R}^{m+2}} \rho_{\mathrm{Cntr}}(\mathcal{P}, \zeta, \eta) dl_{m+2}(\mathcal{P}, \zeta, \eta) \in \mathbb{R}$.

(C3) $\rho_{\mathrm{Phys}} : D \times \mathbb{R}^n \times \sigma(\mathbb{R}^m) \to \mathbb{R}_+,\ (x, p, \beta) \mapsto \rho_{\mathrm{Phys}}(x, p, \beta)$, is of class C^2.

(C4) $f : \sigma(\mathbb{R}^m) \to \mathbb{R}_+$ is (i) of class C^2 and (ii) l_m-integrable.

(C5) $D \times \mathbb{R}^n \times \sigma(\mathbb{R}^m) \to \mathbb{R}_+$, $(x, p, \beta) \mapsto \rho_{\text{Phys}}(x, p, \beta) f(\beta)$, is l_{2n+m}-integrable.

(C6) $T : D \times \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}_+$, $(x, p, Q) \mapsto T(x, p, Q)$, is (i) of class C^2; and (ii) $D \times \mathbb{R}^n \times \sigma(\mathbb{R}^m) \to \mathbb{R}_+$, $(x, p, \beta) \mapsto \rho_{\text{Phys}}(x, p, \beta) f(\beta)/T(x, p, \sigma^{-1}(\beta))$, is l_{2n+m}-integrable.

Note that (C4ii) seems to be a natural condition, but will be required only for ensuring equation (45) in the following contexts. Although (C6i) has already been assumed, we state here for the clarity.

We show that ρ defined above satisfies the required properties:

Proposition 4 *Under conditions (C1)–(C4i) and (C5), ρ becomes smooth (C^2), strictly positive, and l_N-integrable such that*

$$\int_\Omega \rho dl_N = \int_{D\times\mathbb{R}^n\times\sigma(\mathbb{R}^m)} \rho_{Phys}(x, p, \beta) f(\beta) dl_{2n+m}(x, p, \beta) \times Z_{Cntr} \in \mathbb{R}_+ \tag{24a}$$

$$= \int_{D\times\mathbb{R}^n} \rho_R(x, p) dl_{2n}(x, p) \times Z_{Cntr} \tag{24b}$$

$$= \int_{\sigma(\mathbb{R}^m)} f(\beta) Z(\beta) dl_m(\beta) \times Z_{Cntr}, \tag{24c}$$

where

$$\rho_R : D \times \mathbb{R}^n \to \bar{\mathbb{R}},\ (x, p) \overset{d}{\mapsto} \int_{\sigma(\mathbb{R}^m)} \rho_{Phys}(x, p, \beta)\, f(\beta)\, dl_m(\beta), \tag{25}$$

and

$$Z : \sigma(\mathbb{R}^m) \to \bar{\mathbb{R}},\ \beta \overset{d}{\mapsto} \int_{D\times\mathbb{R}^n} \rho_{Phys}(x, p, \beta) dl_{2n}(x, p), \tag{26}$$

are Borel measurable, strictly positive, and finite almost everywhere.

Proof. The smoothness and positivity of ρ are clear from the conditions (C1)–(C4i) [(C1) implies that $\mathbb{R}^m \ni Q \mapsto |\det D\sigma(Q)| = \pm \det D\sigma(Q)$ is C^2 and nonzero, where either sign is fixed]. $\int_\Omega \rho dl_N > 0$ is thus also clear. We begin with splitting the phase space Ω into $\Omega_1 = D \times \mathbb{R}^n \times \mathbb{R}^m$, to which the "main" variables (x, p, Q) belong, and $\Omega_2 := \mathbb{R}^m \times \mathbb{R} \times \mathbb{R}$, to which the "control" variables $(\mathcal{P}, \zeta, \eta)$ belong. Although $\Omega \neq \Omega_1 \times \Omega_2$ due to our definition, by using a variable-order exchange, we have

$$\int_\Omega \rho dl_N = \int_{\Omega_1} \rho_1 dl_{2n+m} \cdot \int_{\Omega_2} \rho_{\text{Cntr}} dl_{m+2}, \tag{27}$$

where

$$\rho_1 : \Omega_1 \to \mathbb{R},\ (x,p,Q) \overset{\mathrm{d}}{\mapsto} \rho_{\mathrm{Phys}}(x,p,\sigma(Q))\,\rho_f(Q) \tag{28}$$

and $\rho_{\mathrm{Cntr}} : \Omega_2 \to \mathbb{R}$ are strictly positive and C^2 functions. The integration of ρ_{Cntr} in equation (27) is Z_{Cntr} [see (C2)], and the integration of ρ_1 in equation (27) will be examined below. It follows from Fubini's theorem applying to positive, $\mathcal{B}^{\Omega_1}_{2n+m}(= \mathcal{B}^{D\times\mathbb{R}^n}_{2n} \otimes \mathcal{B}_m)$-measurable function ρ_1 that

$$\begin{aligned}
&\int_{\Omega_1} \rho_1 dl_{2n+m} \\
&= \int_{D\times\mathbb{R}^n} dl_{2n}(x,p) \int_{\mathbb{R}^m} \rho_1(x,p,Q) dl_m(Q) && \text{(29a)}\\
&= \int_{D\times\mathbb{R}^n} dl_{2n}(x,p) \int_{\mathbb{R}^m} g^{(x,p)}(\sigma(Q))\,|\det D\sigma(Q)| dl_m(Q), && \text{(29b)}
\end{aligned}$$

where $g^{(x,p)} : \sigma(\mathbb{R}^m) \to \mathbb{R}_+,\ \beta \overset{\mathrm{d}}{\mapsto} \rho_{\mathrm{Phys}}(x,p,\beta)f(\beta)$, viz., $\rho_1(x,p,Q) = g^{(x,p)}(\sigma(Q))\,|\det D\sigma(Q)|$. For all $(x,p) \in D\times\mathbb{R}^n$, $g^{(x,p)}$ is positive and $\mathcal{L}^{\sigma(\mathbb{R}^m)}_m$-measurable, so that a variable transformation formula applying to diffeomorphic σ leads to

$$\int_{\mathbb{R}^m} g^{(x,p)}(\sigma(Q))\,|\det D\sigma(Q)| dl_m(Q) = \int_{\sigma(\mathbb{R}^m)} g^{(x,p)}(\beta) dl_m(\beta) = \rho_{\mathrm{R}}(x,p). \tag{30}$$

Thus

$$\begin{aligned}
&\int_{\Omega_1} \rho_1 dl_{2n+m} \\
&= \int_{D\times\mathbb{R}^n} dl_{2n}(x,p) \rho_{\mathrm{R}}(x,p) && \text{(31a)}\\
&= \int_{D\times\mathbb{R}^n} dl_{2n}(x,p) \int_{\sigma(\mathbb{R}^m)} dl_m(\beta) \rho_{\mathrm{Phys}}(x,p,\beta)\, f(\beta) && \text{(31b)}\\
&= \int_{D\times\mathbb{R}^n\times\sigma(\mathbb{R}^m)} \rho_{\mathrm{Phys}}(x,p,\beta) f(\beta) dl_{2n+m}(x,p,\beta) \in \mathbb{R} && \text{(31c)}\\
&= \int_{\sigma(\mathbb{R}^m)} dl_m(\beta) \int_{D\times\mathbb{R}^n} dl_{2n}(x,p) \rho_{\mathrm{Phys}}(x,p,\beta) f(\beta) && \text{(31d)}
\end{aligned}$$

where we have applied Fubini's theorem to positive, $\mathcal{B}^{D\times\mathbb{R}^n\times\sigma(\mathbb{R}^m)}_{2n+m}(= \mathcal{B}^{D\times\mathbb{R}^n}_{2n} \otimes \mathcal{B}^{\sigma(\mathbb{R}^m)}_m)$-measurable function, $(D\times\mathbb{R}^n)\times\sigma(\mathbb{R}^m) \to \mathbb{R},\ (x,p,\beta) \mapsto \rho_{\mathrm{Phys}}(x,p,\beta)f(\beta)$, and used the integrability condition (C5) for the finiteness in equation (31c). Therefore we obtain the integrability of ρ and the integral formulae in equations (24a) and (24b).

The measurability of ρ_{R} follows from the fact that $D\times\mathbb{R}^n \to \mathbb{R}, (x,p) \mapsto \int_{\mathbb{R}^m} \rho_1(x,p,Q) dl_m(Q)$ becomes $\mathcal{B}^{D\times\mathbb{R}^n}_{2n}$-measurable [Fubini's theorem in equation (29)] and the fact that this map is ρ_{R} [equation (30)]. The positivity of ρ_{R} is evident. ρ_{R} is finite for l_{2n}-a.e., due to the integrability, equation (31c), through Fubini's theorem. Similarly, we see that $Z' : \sigma(\mathbb{R}^m) \to \bar{\mathbb{R}}$, $\beta \overset{\mathrm{d}}{\mapsto} \int_{D\times\mathbb{R}^n} \rho_{\mathrm{Phys}}(x,p,\beta) f(\beta) dl_{2n}(x,p)$ is well defined, $\mathcal{B}_m^{\sigma(\mathbb{R}^m)}$-measurable, finite for l_m-a.e. β, and strictly positive. So does Z'/f, which equals Z (note $0 < f < \infty$). Finally, observe that equation (31d) becomes $\int_{\sigma(\mathbb{R}^m)} dl_m(\beta) Z'(\beta) = \int_{\sigma(\mathbb{R}^m)} f(\beta) Z(\beta) dl_m(\beta)$, which leads to equation (24c). ■

As found from the above proof, without the integrability condition (C5), both ρ_{R} and Z are well defined and Borel measurable, and (C5) is equivalent to the finiteness of the integral in equation (24b) and that in equation (24c).

B. Fundamental results

The dynamics for flow $\{T_t'\}$, generated by vector field X and scalar function T, and the associated probability space $(\Omega, \mathcal{L}_N^{\Omega}, \hat{P})$ were formulated through proposition 1, where X was constructed from an abstract form of density function ρ which should satisfy just the normal three conditions. These conditions are satisfied for ρ defined by equations (22) and (23) under (a part of) conditions (C1)–(C5), as shown in proposition 4.

In what follows, ρ is the density defined by equations (22) and (23), and $\rho' = \rho/\tilde{T}$. In this section, first, we prove lemma 5 to show that the integrability of ρ' required in proposition 1 is ensured by (C6). Next, we explicitly show that by using ρ we can dynamically realize the superstatistics distributions, viz., realize the joint distribution density (1). This is stated in theorem 6, as a special case of equation (18) with $g(\omega) \equiv B(x,p,\sigma(Q))$, a function of fundamental variables (x,p,Q). Integral formulae for B are also shown in lemma 5.

Consider a condition:

(C7) (i) $B : \Omega_1' := D \times \mathbb{R}^n \times \sigma(\mathbb{R}^m) \to \mathbb{R}$, $(x,p,\beta) \mapsto B(x,p,\beta)$, is $\mathcal{B}_{2n+m}^{\Omega_1'}$-measurable, and
(ii) a function $\Omega_1' \to \mathbb{R}$, $(x,p,\beta) \mapsto B(x,p,\beta)\rho_{\mathrm{Phys}}(x,p,\beta)f(\beta)$, is l_{2n+m}-integrable.

Note, instead of B, we can treat $b : \Omega_1 = D \times \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$, $(x,p,Q) \mapsto b(x,p,Q)$, since B and b can be defined from one to another each other in a trivial manner such that $b(x,p,Q) = B(x,p,\sigma(Q))$ and $B(x,p,\beta) = b(x,p,\sigma^{-1}(\beta))$.

Lemma 5 *Under conditions (C1)–(C4i), (C5), and (C7i), condition (C7ii) is equivalent to* $\int_\Omega b(x,p,Q)\rho(\omega)dl_N(\omega) \in \mathbb{R}$. *Under (C1)–(C4i), (C5) and (C7), we have*

$$\mathbb{R}\ni \langle b\circ\pi_1\rangle \tag{32a}$$

$$= \frac{\int_{\Omega_1'} B(x,p,\beta)\rho_{\rm Phys}(x,p,\beta)f(\beta)dl_{2n+m}(x,p,\beta)}{\int_{\Omega_1'} \rho_{\rm Phys}(x,p,\beta)f(\beta)dl_{2n+m}} \tag{32b}$$

$$= \frac{\int_{D\times\mathbb{R}^n} dl_{2n}(x,p)\int_{\sigma(\mathbb{R}^m)} dl_m(\beta)B(x,p,\beta)\rho_{\rm Phys}(x,p,\beta)f(\beta)}{\int_{D\times\mathbb{R}^n}\rho_{\rm R}(x,p)dl_{2n}} \tag{32c}$$

$$= \frac{\int_{\sigma(\mathbb{R}^m)} dl_m(\beta)f(\beta)\int_{D\times\mathbb{R}^n} dl_{2n}(x,p)B(x,p,\beta)\rho_{\rm Phys}(x,p,\beta)}{\int_{\sigma(\mathbb{R}^m)} f(\beta)Z(\beta)dl_m(\beta)}. \tag{32d}$$

Proof. Assume (C1)–(C4i), (C5), and (C7i). Obviously $b\circ\pi_1$ is $\mathcal{B}_N^\Omega$-measurable. Below we shall calculate $\langle b\circ\pi_1\rangle$, for which similar procedures to the proof of proposition 4 will be used with a careful attention to the indefinite signature of B. We have

$$\int_\Omega |b\circ\pi_1|\rho dl_N = \int_{\Omega_1}|\rho_1'|dl_{2n+m}\cdot Z_{\rm Cntr}, \tag{33}$$

with $\rho_1' := b\rho_1 : \Omega_1 \to \mathbb{R}$ [see equation (28)], noting that this map is equal to $(x,p,Q)\mapsto \tilde{g}^{(x,p)}(\sigma(Q))\,|\det D\sigma(Q)|$, where $\mathcal{B}_m^{\sigma(\mathbb{R}^m)}$-measurable function $\tilde{g}^{(x,p)} : \sigma(\mathbb{R}^m)\to\mathbb{R}$, $\beta \overset{\rm d}{\mapsto} (B\rho_{\rm Phys})(x,p,\beta)f(\beta)$, is defined for every (x,p). Thus, a variable transformation formula and Fubini's theorem read

$$\int_{\Omega_1}|\rho_1'|dl_{2n+m}$$

$$= \int_{D\times\mathbb{R}^n} dl_{2n}(x,p)\int_{\sigma(\mathbb{R}^m)} dl_m(\beta)|(B\rho_{\rm Phys})(x,p,\beta)|\,f(\beta) \tag{34a}$$

$$= \int_{D\times\mathbb{R}^n\times\sigma(\mathbb{R}^m)} |B(x,p,\beta)|\rho_{\rm Phys}(x,p,\beta)f(\beta)dl_{2n+m}(x,p,\beta). \tag{34b}$$

Assume also (C7ii). Then we have $\int_{\Omega_1}|\rho_1'|dl_{2n+m}\in\mathbb{R}$, implying $b\circ\pi_1\in L^1(P)$. It follows from this integrability that $\int_\Omega b\circ\pi_1\rho dl_N = \int_{\Omega_1}\rho_1' dl_{2n+m}\cdot Z_{\rm Cntr}$ and

$$\mathbb{R}\ni\int_{\Omega_1}\rho_1' dl_{2n+m} = \int_{D\times\mathbb{R}^n} dl_{2n}(x,p)\int_{\mathbb{R}^m} dl_m(Q)\rho_1'(x,p,Q).$$

Here, for l_{2n}-a.e. (x,p), $\rho_{1,(x,p)}' : \mathbb{R}^m\to\mathbb{R}$, $Q\overset{\rm d}{\mapsto}\rho_1'(x,p,Q)$, becomes l_m-integrable, viz., $\mathbb{R}\ni\int_{\mathbb{R}^m}\rho_{1,(x,p)}'(Q)dl_m(Q) = \int_{\mathbb{R}^m}\tilde{g}^{(x,p)}(\sigma(Q))\,|\det D\sigma(Q)|dl_m(Q)$. So we can safely use a variable transformation formula to get

$$\mathbb{R}\ni\int_{\mathbb{R}^m}\rho_1'(x,p,Q)dl_m(Q) = \int_{\sigma(\mathbb{R}^m)}(B\rho_{\rm Phys})(x,p,\beta)f(\beta)dl_m(\beta)\ \text{ a.e. } (x,p).$$

Condition (C7ii) thus leads us to

$$\mathbb{R}\ni \int_{\Omega_1} \rho_1' dl_{2n+m} \tag{35a}$$
$$= \int_{D\times\mathbb{R}^n} dl_{2n}(x,p) \int_{\sigma(\mathbb{R}^m)} (B\rho_{\text{Phys}})(x,p,\beta) f(\beta) dl_m(\beta) \tag{35b}$$
$$= \int_{D\times\mathbb{R}^n\times\sigma(\mathbb{R}^m)} (B\rho_{\text{Phys}})(x,p,\beta) f(\beta) dl_{2n+m}(x,p,\beta) \tag{35c}$$
$$= \int_{\sigma(\mathbb{R}^m)} dl_m(\beta) f(\beta) \int_{D\times\mathbb{R}^n} dl_{2n}(x,p)(B\rho_{\text{Phys}})(x,p,\beta). \tag{35d}$$

Note $\int_\Omega \rho dl_N \in \mathbb{R}_+$ by proposition 4. From equation (35), the fact that $\langle b\circ\pi_1\rangle = \int_\Omega b\circ\pi_1\cdot \rho dl_N \,/ \int_\Omega \rho dl_N = \int_{\Omega_1} \rho_1' dl_{2n+m} \cdot Z_{\text{Cntr}} \,/ \int_\Omega \rho dl_N \in \mathbb{R}$, and equation (24), we see that $\langle b\circ\pi_1\rangle$ equals equations (32b)-(32d).

The above results have stated that "(C7ii) $\Longrightarrow \int_\Omega b\circ\pi_1 \rho dl_N \in \mathbb{R}$," under the conditions (C1)–(C4i), (C5), and (C7i). Conversely, if $\int_\Omega b\circ\pi_1\rho dl_N \in \mathbb{R}$ is assumed, then equations (33) and (34) manifest (C7ii) [note $Z_{\text{Cntr}} > 0$ due to (C2)]. ■

Theorem 6 *(i) Let ρ and T satisfy (C1)–(C6) [except (C4ii)]; and (ii) let $X' \equiv \tilde{T}X$ be complete and its flow $\{T_t' : \Omega\to\Omega |\ t\in R\}$ be ergodic with respect to measure space (Ω, L_N^Ω, P'). Then for B satisfying (C7) we have, for a.e. ω,*

$$\mathbb{R} \ni \overline{\overline{b\circ\pi_1}}(\omega) = \langle b\circ\pi_1\rangle\,, \tag{36}$$

which is also represented by equations (32b)–(32d).

Proof. From (C1)–(C4i), and (C5), we can apply proposition 4, so that ρ satisfies the three conditions. Due to this fact and (C6i), $P = \rho dl_N$ and $P' = \rho' dl_N$ are well-defined measures on $(\Omega, \mathcal{L}_N^\Omega)$ in the course of applying proposition 1. Lemma 5 states $b\circ\pi_1 \in L^1(P)$. In addition, by temporarily putting $b \equiv 1/T$, the corresponding B satisfies (C7) due to the condition of T, viz., (C6), so that lemma 5 also states $\mathbb{R} \ni \int_\Omega b(x,p,Q)\rho(\omega) dl_N(\omega) = \int_\Omega \rho' dl_N$. From these results and assumption (ii), proposition 1 with $g \equiv b\circ\pi_1$ [this b is the one in equation (36)] demonstrates $\exists\overline{\overline{b\circ\pi_1}}(\omega) = \langle b\circ\pi_1\rangle \in \mathbb{R}$ for a.e. ω. Lemma 5 shows the equality among $\langle b\circ\pi_1\rangle$ and equations (32b)–(32d). ■

In this subsection we shall assume that the conditions (i) and (ii) in theorem 6 hold, so that propositions 1 and 4 are also applicable ($\int_\Omega \rho' dl_N < \infty$ is concluded) as shown in the proof of theorem 6.

Theorem 6 shows that the joint distribution density, equation (1), can be created by the scaled long-time average generated by the flow $\{T'_t\}$. This is explicitly stated as follows. For any $M \in \mathcal{B}_{2n+m}^{\Omega'_1}$, $B \equiv B_M \equiv \chi_M^{2n+m}$ satisfies (C7), so that theorem 6 demonstrates

$$\mathbb{R} \ni \overline{\overline{b_M \circ \pi_1}}(\omega) \tag{37a}$$

$$= \frac{\int_{\Omega'_1} \chi_M^{2n+m}(x,p,\beta)\rho_{\text{Phys}}(x,p,\beta)f(\beta)dl_{2n+m}(x,p,\beta)}{\int_{\Omega'_1} \rho_{\text{Phys}}(x,p,\beta)f(\beta)dl_{2n+m}} \quad \text{(a.e. } \omega) \tag{37b}$$

$$= \int_M \rho_0(x,p,\beta)dl_{2n+m}(x,p,\beta), \tag{37c}$$

where

$$\rho_0(x,p,\beta) := \rho_{\text{Phys}}(x,p,\beta)f(\beta) \Bigg/ \int_{\Omega'_1} \rho_{\text{Phys}}(x,p,\beta)f(\beta)dl_{2n+m}\ , \tag{38}$$

and $b_M(x,p,Q)$ takes 1 if $(x,p,\sigma(Q)) \in M$ and otherwise 0. Thus we obtain, via the scaled long-time average, a specific probability measure (distribution),

$$\nu_0 : \mathcal{B}_{2n+m}^{\Omega'_1} \to \mathbb{R},\ M \overset{\text{d}}{\mapsto} \overline{\overline{b_M \circ \pi_1}} = \int_M \rho_0 dl_{2n+m}, \tag{39}$$

whose Radon-Nikodym derivative with respect to l_{2n+m} is ρ_0 for l_{2n+m}-a.e. (note ρ_0 is positive and integrable), viz., $\frac{d\nu_0}{dl_{2n+m}}(x,p,\beta) = \rho_0(x,p,\beta)$ (a.e.), which is proportional to $\rho_{\text{Phys}}(x,p,\beta)f(\beta)$. This fact indicates the realization of density (1).

The following indicates the realization of the superstatistics distribution.

Corollary 7 *For $A(x,p)$, a function of pure physical variables such that*

(C8) $\quad A : D \times \mathbb{R}^n \to \mathbb{R}$ *is $\mathcal{B}_{2n}^{D\times\mathbb{R}^n}$-measurable and $\rho_R dl_{2n}$-integrable,*

we have

$$\overline{\overline{A \circ \pi_R}}(\omega) = \langle A \rangle_R := \frac{\int_{D\times\mathbb{R}^n} A(x,p)\rho_R(x,p)dl_{2n}(x,p)}{\int_{D\times\mathbb{R}^n} \rho_R dl_{2n}} \in \mathbb{R} \quad \textit{a.e. } \omega. \tag{40}$$

Here the integrability condition in (C8) can be replaced by a condition such that $\Omega'_1 \to \mathbb{R}$, $(x,p,\beta) \mapsto A(x,p)\rho_{Phys}(x,p,\beta)f(\beta)$, is l_{2n+m}-integrable.

Proof. Note the two integrability conditions are equivalent:

$$\int_{\Omega'_1} |A(x,p)|\rho_{\text{Phys}}(x,p,\beta)f(\beta)dl_{2n+m}(x,p,\beta) \tag{41a}$$

$$= \int_{D\times\mathbb{R}^n} dl_{2n}(x,p) \int_{\sigma(\mathbb{R}^m)} |A(x,p)|\rho_{\text{Phys}}(x,p,\beta)f(\beta)dl_m(\beta) \tag{41b}$$

$$= \int_{D\times\mathbb{R}^n} dl_{2n}(x,p)|A(x,p)|\rho_{\text{R}}(x,p). \tag{41c}$$

Thus, if we define $B_A : \Omega_1' \to \mathbb{R}$, $(x,p,\beta) \overset{\mathrm{d}}{\mapsto} A(x,p)$, then B_A meets (C7). Applying theorem 6 with $B \equiv B_A$, where $b_A \circ \pi_1 = A \circ \pi_{\mathrm{R}}$, we get

$$
\begin{aligned}
&\overline{\overline{A \circ \pi_{\mathrm{R}}}}(\omega) = \langle b_A \circ \pi_1 \rangle \quad \text{(a.e.)} \\
&= \frac{\int_{D\times\mathbb{R}^n} dl_{2n}(x,p) \int_{\sigma(\mathbb{R}^m)} dl_m(\beta) B_A(x,p,\beta) \rho_{\mathrm{Phys}}(x,p,\beta) f(\beta)}{\int_{D\times\mathbb{R}^n} \rho_{\mathrm{R}} dl_{2n}} \\
&= \frac{\int_{D\times\mathbb{R}^n} dl_{2n}(x,p) A(x,p) \rho_{\mathrm{R}}(x,p)}{\int_{D\times\mathbb{R}^n} \rho_{\mathrm{R}} dl_{2n}}.
\end{aligned}
$$

■

Equation (40) states that superstatistics distribution ρ_{R} is realized in calculating the scaled long-time average of physical quantities. It should be noted that for realizing ρ_{R} the current scheme needs no explicit form of ρ_{R}, which is defined by the integration formula (25). It is an advantage of the *dynamical* realization of superstatistics that ρ_{R} is realized regardless of whether the integration can be explicitly done or not.

b. Note on ergodicity So far, we have assumed the ergodicity with respect to $\{T_t'\}$ and $(\Omega, \mathcal{L}_N^{\Omega}, P')$. The proof of the ergodicity is hard in general, and we here just note that the following two obstacles [27] of the ergodicity vanish in the current system: fixed points [i.e., $\omega_0 \in \Omega$ such that $X'(\omega_0) = 0$] and zero divergence [i.e., $\operatorname{div} X'(\omega) = 0$ for $\forall \omega \in \Omega$]. For the first issue, we can easily observe from equations (8d) and (8f) and $m > 0$ that the fixed points do not exist. For the second issue, we have

$$
\begin{aligned}
\operatorname{div} X'(\omega) = &(\nabla_x T(x,p,Q) \mid \nabla_p \Theta(\omega)) - (\nabla_p T(x,p,Q) \mid \nabla_x \Theta(\omega)) \\
&- D_\zeta \Theta(\omega) \left[(p | \nabla_p T(x,p,Q)) + nT(x,p,Q) \right] \\
&- m D_\eta \Theta(\omega)
\end{aligned}
\tag{43}
$$

for any $\omega = (x,p,\zeta,Q,\mathcal{P},\eta) \in \Omega$. As long as we consider a case that $\rho_{\mathrm{Cntr}}(\mathcal{P},\zeta,\eta)$ takes a form of $\rho_2(\mathcal{P},\zeta)\rho_{\mathrm{Y}}(\eta)$, where ρ_2 and ρ_{Y} are strictly positive, C^2 functions, such as those will appear in (S2) (section IV A), we conclude that $\operatorname{div} X' \neq 0$. Otherwise, in the case, the result $0 = \operatorname{div} X'(\omega) = G(x,p,\zeta,Q,\mathcal{P}) + H(\eta)$ for $\forall \omega \in \Omega$, where $H(\eta) \equiv mD \ln \rho_{\mathrm{Y}}(\eta)$ becomes the last term of equation (43) and where $G(x,p,\zeta,Q,\mathcal{P})$ is the remaining contributions, implies $\rho_{\mathrm{Y}}(\eta) \propto \mathrm{e}^{\mathrm{const.}\times\eta}$, which leads to a contradiction to the integrability condition in (C2).

1. Special types of distributions

A formula for a special type of distribution can be obtained as an examples of corollary 7 or theorem 6.

Example 8 (marginal distribution) *As for equation (20), since* $A \equiv \chi_{B_1 \times \mathbb{R}^n}$ *for* $B_1 \in \mathcal{B}_n^D$ *satisfies (C8), corollary 7 states*

$$\overline{\overline{\chi^n_{B_1} \circ \pi_x}} = \overline{\overline{\chi^{2n}_{B_1 \times \mathbb{R}^n} \circ \pi_R}} = \left\langle \chi^{2n}_{B_1 \times \mathbb{R}^n} \right\rangle_R$$
$$= \int_{B_1 \times \mathbb{R}^n} \rho_R(x,p) dl_{2n}(x,p) \Big/ \int_{D \times \mathbb{R}^n} \rho_R dl_{2n} \, . \tag{44}$$

The following two examples are direct consequences of theorem 6.

Example 9 (reweighted distribution) *Under condition (C4ii), the current method enables to produce an arbitrarily target density* $\rho_{TRG}(x,p)$*, instead of* $\rho_R(x,p)$*, for the physical system, by a reweighting which needs no explicit form of* ρ_R*. That is,*

$$\overline{\overline{A\rho_{TRG}/\rho_{Phys}}} \Big/ \overline{\overline{\rho_{TRG}/\rho_{Phys}}} = \frac{\int_{D\times\mathbb{R}^n} A\rho_{TRG} dl_{2n}}{\int_{D\times\mathbb{R}^n} \rho_{TRG} dl_{2n}} =: \langle A \rangle_{TRG} \, , \tag{45}$$

where the functions satisfy

(C9) $\rho_{TRG} : D \times \mathbb{R}^n \to \mathbb{R}_+$ *is* $\mathcal{B}_{2n}^{D\times\mathbb{R}^n}$*-measurable and* l_{2n}*-integrable,*

(C10) $A : D \times \mathbb{R}^n \to \mathbb{R}$ *is* $\mathcal{B}_{2n}^{D\times\mathbb{R}^n}$*-measurable and* $\rho_{TRG} dl_{2n}$*-integrable.*

Defining a map $B_{R_A} : \Omega_1' \to \mathbb{R}$*,* $(x,p,\beta) \overset{d}{\mapsto} (A\rho_{TRG})(x,p)/\rho_{Phys}(x,p,\beta)$*, we have used an abbreviated form,* $\overline{\overline{A\rho_{TRG}/\rho_{Phys}}}$ *in equation (45), regarding the scaled long-time average of* $b_{R_A} \circ \pi_1 : \Omega \to \mathbb{R}$*,* $\omega \mapsto (A\rho_{TRG})(x,p)/\rho_{Phys}(x,p,\sigma(Q))$*. To show (45), we first look at*

$$\int_{\Omega_1'} |B_{R_A}(x,p,\beta)| \rho_{Phys}(x,p,\beta) f(\beta) dl_{2n+m}(x,p,\beta)$$
$$= \int_{\Omega_1'} (|A|\rho_{TRG})(x,p) f(\beta) dl_{2n+m}(x,p,\beta)$$
$$= \int_{D\times\mathbb{R}^n} |A(x,p)| \rho_{TRG}(x,p) dl_{2n}(x,p) \int_{\sigma(\mathbb{R}^m)} dl_m(\beta)\, f(\beta) \in \mathbb{R},$$

where we have used (C10) and (C4ii) in the last line to ensure the finiteness. Thus we can *apply theorem 6 with* $B \equiv B_{R_A}$ *to obtain*

$$\overline{\overline{A\rho_{TRG}/\rho_{Phys}}} \equiv \overline{\overline{b_{R_A} \circ \pi_1}}(\omega) = \langle b_{R_A} \circ \pi_1 \rangle \in \mathbb{R} \quad (a.e.) \tag{47a}$$

$$= \frac{\int_{D\times\mathbb{R}^n} dl_{2n}(x,p) \int_{\sigma(\mathbb{R}^m)} dl_m(\beta) B_{R_A}(x,p,\beta)\rho_{Phys}(x,p,\beta) f(\beta)}{\int_{D\times\mathbb{R}^n} \rho_R dl_{2n}} \tag{47b}$$

$$= \frac{\int_{D\times\mathbb{R}^n} dl_{2n}(x,p)(A\rho_{TRG})(x,p) \int_{\sigma(\mathbb{R}^m)} dl_m(\beta)\, f(\beta)}{\int_{D\times\mathbb{R}^n} \rho_R dl_{2n}}. \tag{47c}$$

We can also put $A = 1$ *due to (C9), having*

$$\overline{\overline{\rho_{TRG}/\rho_{Phys}}} \equiv \overline{\overline{b_{R_1} \circ \pi_1}}(\omega) \in \mathbb{R} \quad (a.e.) \tag{48a}$$

$$= \frac{\int_{D\times\mathbb{R}^n} dl_{2n}(x,p)\rho_{TRG}(x,p) \int_{\sigma(\mathbb{R}^m)} dl_m(\beta)\, f(\beta)}{\int_{D\times\mathbb{R}^n} \rho_R dl_{2n}}. \tag{48b}$$

Dividing equation (47) by equation (48) (note the latter is strictly positive) yields equation (45).

Example 10 (distribution regarding β***)*** *For a Borel measurable function* $h : \sigma(\mathbb{R}^m) \to \mathbb{R}$, $\beta \mapsto h(\beta)$, *such that* $\Omega_1' \to \mathbb{R}$, $(x,p,\beta) \mapsto h(\beta)\rho_{Phys}(x,p,\beta)f(\beta)$, *is* l_{2n+m}*-integrable, or equivalently,* hfZ *is integrable, we can apply theorem 6 with putting* $B \equiv B_h : \Omega_1' \to \mathbb{R}$, $(x,p,\beta) \overset{d}{\mapsto} h(\beta)$. *Noting* $b_h \circ \pi_1(\omega) = B_h(x,p,\sigma(Q)) = h \circ \sigma \circ \pi_Q(\omega)$, *we thus have*

$$\mathbb{R} \ni \overline{\overline{h(\beta)}} := \overline{\overline{h \circ \sigma \circ \pi_Q}} = \langle b_h \circ \pi_1 \rangle \quad (a.e.) \tag{49a}$$

$$= \frac{\int_{\sigma(\mathbb{R}^m)} dl_m(\beta) f(\beta) \int_{D\times\mathbb{R}^n} dl_{2n}(x,p) B_h(x,p,\beta)\rho_{Phys}(x,p,\beta)}{\int_{\sigma(\mathbb{R}^m)} fZ dl_m} \tag{49b}$$

$$= \frac{\int_{\sigma(\mathbb{R}^m)} h(\beta) f(\beta) Z(\beta) dl_m(\beta)}{\int_{\sigma(\mathbb{R}^m)} f(\beta) Z(\beta) dl_m(\beta)}. \tag{49c}$$

For instance, the distribution of $\beta \equiv \sigma(Q)$ *is given by*

$$\mu : \mathcal{B}_m^{\sigma(\mathbb{R}^m)} \to \mathbb{R},\ B \overset{d}{\mapsto} \overline{\overline{\chi_B^m \circ \sigma \circ \pi_Q}} = \frac{\int_B f(\beta) Z(\beta) dl_m(\beta)}{\int_{\sigma(\mathbb{R}^m)} fZ dl_m}, \tag{50}$$

which is not just the marginal distribution with respect to Q *represented by* $\mu' : \mathcal{B}_m \to \mathbb{R}$, $B' \mapsto \overline{\overline{\chi_{B'}^m \circ \pi_Q}} = \hat{P}(D \times \mathbb{R}^n \times \mathbb{R} \times B' \times \mathbb{R}^m \times \mathbb{R})$, *but is an induced measure for* μ' *by a map* σ, *viz.,* $\mu = \mu' \sigma^{-1}$.

IV. EXAMPLE OF FUNCTION SETTING

A. Fundamental functions

For dynamically realizing superstatistics in a target physical system, we should set specific forms of functions: $\rho_{\rm Phys}$ and $\rho_{\rm Cntr}$ in equation (22), σ and f in equations (22) and (23), and T in equation (8). These functions should be compatible with (C1)-(C6). First, we shall consider $\rho_{\rm Phys}$, $\rho_{\rm Cntr}$, and T, while just assume (C1) and (C4i) for σ and f, respectively. We here concentrate on an important case such that $\rho_{\rm Phys}(x,p,\beta) = \rho_{\rm E}(E(x,p),\beta)$, where $E(x,p)$ is the energy of the physical system. The details are as follows:

(S1) $\rho_{\rm Phys} : D \times \mathbb{R}^n \times \sigma(\mathbb{R}^m) \to \mathbb{R}$, $(x,p,\beta) \mapsto \rho_{\rm E}(E(x,p),\beta)$,

where

$E : D \times \mathbb{R}^n \to \mathbb{R}$, $(x,p) \mapsto U(x) + K(p)$ with

$U : D \to \mathbb{R}$ is of class C^2,

$K : \mathbb{R}^n \to \mathbb{R}$, $p \mapsto (p|\mathbf{M}^{-1}p)/2$, with $\mathbf{M}$ being a symmetric, positive-definite square matrix of size n (over $\mathbb{R}$);

$\rho_{\rm E} : \mathbb{R} \times \mathbb{R}^m \supset O \times \sigma(\mathbb{R}^m) \to \mathbb{R}$, $(\epsilon,\beta) \mapsto \rho_{\rm E}(\epsilon,\beta)$, is of class C^3, satisfying

$$\rho_{\rm E} > 0 \text{ and } D_1\rho_{\rm E} < 0, \quad -(\blacklozenge 1)$$

with O being an open set containing $E(D \times \mathbb{R}^n)$.

(S2) $\rho_{\rm Cntr} : \mathbb{R}^m \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$, $(Q,\mathcal{P},\eta) \mapsto \exp\left[-K_{\rm T}(\mathcal{P})\right] \rho_{\rm Z}(\zeta)\, \rho_{\rm Y}(\eta)$,

where

$K_{\rm T} : \mathbb{R}^m \to \mathbb{R}$, $\mathcal{P} \mapsto (\mathcal{P}\,|\,\mathbf{M}_{\rm T}^{-1}\mathcal{P})/2$, with $\mathbf{M}_{\rm T}$ being a symmetric, positive-definite square matrix of size m (over $\mathbb{R}$),

$\rho_{\rm Z}$, $\rho_{\rm Y} : \mathbb{R}^1 \to \mathbb{R}_+$, which are of class C^2 and l_1-integrable. $-(\blacklozenge 2)$

(S3) $T : D \times \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$, $(x,p,Q) \overset{\rm put}{\mapsto} -\frac{1}{D_1 \ln \rho_{\rm E}(E(x,p),\sigma(Q))}$.

Then we see that (C2), (C3), and (C6i) hold. In molecular simulation, potential energy function U is given as a force field and K is the kinetic energy with $\mathbf{M}$ such as $\mathrm{diag}(m_1, \cdots, m_n)$. It follows from (S1) and (S3) that (C6ii) is equivalent to l_{2n+m}-integrability of a function

$\Omega_1' \to \mathbb{R}$, $(x,p,\beta) \mapsto f(\beta)D_1\rho_{\rm E}(E(x,p),\beta)$, which is now a similar condition to (C5), viz., $(x,p,\beta) \mapsto f(\beta)\rho_{\rm E}(E(x,p),\beta)$ is l_{2n+m}-integrable.

Applying (S1) and (S2) into equation (22) and substituting the resultant density and temperature-function (S3) into equation (8), we have the following EOM:

$$\left.\begin{aligned}
&\dot{x} = \mathbf{M}^{-1}p \in \mathbb{R}^n,\\
&\dot{p} = -\nabla U(x) - T(x,p,Q)\,\tau_{\rm Z}(\zeta)\; p \in \mathbb{R}^n,\\
&\dot{\zeta} = 2K(p) - nT(x,p,Q) \in \mathbb{R}^1,\\
&\dot{Q} = \mathbf{M}_{\rm T}^{-1}\mathcal{P} \in \mathbb{R}^m,\\
&\dot{\mathcal{P}} = -\nabla \tilde{U}_{E(x,p)}(Q) - \tau_{\rm Y}(\eta)\;\mathcal{P} \in \mathbb{R}^m,\\
&\dot{\eta} = 2K_{\rm T}(\mathcal{P}) - m \in \mathbb{R}^1,
\end{aligned}\right\} \tag{51}$$

where $\tau_{\rm Z}(\zeta) \equiv -D\ln\rho_{\rm Z}(\zeta)$, $\tau_{\rm Y}(\eta) \equiv -D\ln\rho_{\rm Y}(\eta)$, and

$$\tilde{U}_\epsilon(Q) \equiv -\ln[\rho_f(Q)|D_1\rho_{\rm E}(\epsilon,\sigma(Q))|]. \tag{52}$$

Here, (x,p,ζ) forms the NH equations with *dynamical temperature* $T(x,p,Q)$, instead of a constant external temperature, along with the temperature-dependent friction $T(x,p,Q)\,\tau_{\rm Z}(\zeta)$. In addition, $(Q,\mathcal{P},\eta)$ takes again the NH form with *temperature-system potential energy,* $\tilde{U}_{E(x,p)}(Q)$, which is a function of temperature coordinates Q and depends also on the physical-system energy $\epsilon \equiv E(x,p)$, along with a friction $\tau_{\rm Y}(\eta)$ and a unit *temperature.* In this respect, we call this *coupled NH* EOM.

Remark 11 *Since (S1) contains potential function $U(x)$, it may be natural to investigate the dependence of the key quantities upon a shift of the origin of U, viz., $U \to U + u_0$ for constant $u_0 \in \mathbb{R}$. Such key quantities are ρ [equation (22)], space average $\langle g\rangle$ of any g [equation (17)], and the EOM [equation (51)]. We can find a simple dependence upon u_0 of the behaviors of the quantities, if we restrict our attention to the case that there exists a function $\lambda : \mathbb{R}\times\sigma(\mathbb{R}^m) \to \mathbb{R}_+$ such that*

$$\rho_E(\epsilon + u_0,\beta) = \lambda(u_0,\beta)\rho_E(\epsilon,\beta) \tag{53}$$

for all possible $\epsilon, u_0,$ and β [viz., the ratio, $\rho_E(\epsilon+u_0,\beta)/\rho_E(\epsilon,\beta)$, is independent of ϵ]. Such an example of ρ_E will be seen in (S1-1) below [set $\lambda(u_0,\beta) = \exp(-\beta u_0)$]. In this case, $\rho|_{U\to U+u_0}(\omega) = \rho(\omega)\lambda(u_0,\sigma(Q)) \equiv \rho(\omega)\lambda_{u_0}(\sigma(Q))$ for all $\omega \in \Omega$, or simply,

$$\rho|_{U\to U+u_0} = \rho|_{f\to f\lambda_{u_0}}, \tag{54}$$

viz., the shift for U in ρ is equivalent to a factorization of f [see equations (22) and (23)]. Despite the fact that T in (S3) depends on E, we see the invariance:

$$T|_{U\to U+u_0} = T. \tag{55}$$

Thus, vector field X' [defining equation (51)], which is made from ρ and T, obeys

$$X'|_{U\to U+u_0} = X'|_{f\to f\lambda_{u_0}}. \tag{56}$$

Hence, if we have the converse factorization $f \to f/\lambda_{u_0}$ as well as the shift $U \to U+u_0$, then we recover an invariance for density, $\rho|_{U\to U+u_0,\ f\to f/\lambda_{u_0}} = \rho$, together with the invariances for $\langle g\rangle$ and X'. Note that these invariances are a matter for a theoretical interest. In applications, the relationships, (54)–(56), are really concerned, since ρ defines a realized density, T specifies the long-time averages [equations (10) and (16)], and X' defines the EOM [equation (51)].

Remark 12 *$T(x, p, Q)$ has a dimension of energy (Boltzmann's constant is unity). This is because we consider the physical system to be described such that the derivative of each coordinate with respect to time is given by $\frac{dx_i}{dt} = X'_{x_i}(\omega)$, which equals to $T(x, p, Q)\, D_{p_i}\Theta(\omega)$ in equation (8), and because $\Theta(\omega)$ is dimensionless as seen from equation (4). This result is consistent with the result derived from (S3). Note that insightful ideas regarding temperature function are seen in [33, 34].*

B. Remaining functions

We here consider subordinate functions defined in (S1) and (S2), the transform function σ, and the density function of the inverse temperature, f. As a natural choice we can set these functions as follows:

(S1-1) $\rho_{\mathrm{E}} : \mathbb{R}\times\mathbb{R}_+ \to \mathbb{R}_+,\ (\epsilon, \beta) \overset{\text{put}}{\mapsto} \exp[-\beta\epsilon]$, with $m = 1$,

(S2-1) $\rho_{\mathrm{Z}} : \mathbb{R}^1 \to \mathbb{R}_+,\ \zeta \overset{\text{put}}{\mapsto} \exp\left[-c_{\mathrm{Z}}\zeta^2\right]$, with $c_{\mathrm{Z}} > 0$,

(S2-2) $\rho_{\mathrm{Y}} : \mathbb{R}^1 \to \mathbb{R}_+,\ \eta \overset{\text{put}}{\mapsto} \exp[-c_{\mathrm{Y}}\eta^2]$, with $c_{\mathrm{Y}} > 0$,

(S4) $m = 1$, and $\sigma : \mathbb{R}^1 \to \mathbb{R}_+,\ Q \overset{\text{put}}{\mapsto} c\exp[Q/l]$, with $c,\ l > 0$.

Here $c_{\rm Z}$, $c_{\rm Y}$, c, and l are real parameters. $\rho_{\rm E}$ is a usual Boltzmann-Gibbs (BG) density, and $\rho_{\rm Z}$ and $\rho_{\rm Z}$ are Gaussians, which are familiar forms having nice properties. In fact, they are C^∞, and both (♦1) [in (S1)] and (♦2) [in (S2)] are satisfied. σ in (S4) ensures $\beta \equiv \sigma(Q) > 0$ for any $Q \in \mathbb{R}$. We also see the validity of (C1) [where $\det D\sigma > 0$], and thus (C6i) holds. In fact, (S3) obeying (S1-1) signifies

$$T(x, p, Q) = 1/\sigma(Q). \tag{57}$$

The remaining setting is for f, and we set $f \equiv f_{\rm G}$ defined by

(S5) $f_{\rm G} : \mathbb{R}_+ \longrightarrow \mathbb{R}^1$, $\beta \overset{\rm put}{\mapsto} \frac{d^\alpha}{\Gamma(\alpha)} \beta^{\alpha-1} \exp[-d\beta]$ with α, $d > 0$, where Γ is the gamma function.

Then we see that (C4) is satisfied [(ii) holds as $\int_{\mathbb{R}_+} f_{\rm G}(\beta) d\beta = 1$]. The remaining conditions, (C5) and (C6ii), are not trivial to confirm their validities in general. Note that, as is shown by lemma 5 with putting $b \equiv 1/T$, (C6ii) can be replaced with the condition that $\left\langle 1/\tilde{T} \right\rangle < \infty$, viz., the inverse (dynamical) temperature has a finite average. Considering this fact, (C6ii) seems to be a physically natural requirement, even if it may be omitted under a certain alternative consideration (e.g. considering a transformation of the simple long-time average instead of considering the transformed measure P'). For a toy model system, the validities of (C5) and (C6ii) are confirmed, and in fact they are valid for a 1-D harmonic oscillator model used in the current numerical study (see section V B 1) as long as we set

$$\alpha > 1. \tag{58}$$

The choice of (S5) for f here is due to these reasons and physically highly interesting features coming from the intimate relationship to nonextensive statistical mechanics [8, 12, 13]. For general systems, we assume the validities of (C5) and (C6ii).

V. NUMERICS

A. Numerical integrator

We introduce a numerical integration scheme for the ODE, (51). To do this, we define an extended ODE, according to the scheme in [25, 35], on an extended space $\Omega' \equiv \Omega \times \mathbb{R}$:

$$\dot{\omega} = X'(\omega), \tag{59a}$$

$$\dot{v} = \mathcal{Y}(\omega) \tag{59b}$$

for $\omega \in \Omega$, where equation (59a) represents equation (51), v is introduced as an extended variable on $\mathbb{R}$, and

$$\mathcal{Y}(\omega) \equiv -T(x, p, Q) \operatorname{div} X(\omega), \tag{60}$$

with $X(\omega) = X'(\omega)/T(x, p, Q)$ ($\forall \omega \in \Omega$) in equation (60). Then, ODE (59) has an invariant function [25] defined by

$$L : \Omega' \to \mathbb{R},\ \omega' \equiv (\omega, v) \mapsto -\ln \rho(\omega) + v. \tag{61}$$

Thus the numerical error of the integration can be checked by monitoring the value of equation (61) in the integration process.

For ODE (59) we can use a natural decomposition of its field, $\Omega' \to \mathbb{R}^{N+1} : \omega' \mapsto (X'(\omega), \mathcal{Y}(\omega))$, by assuming that $T(x, p, Q)$ is independent of p, which is satisfied e.g., in (S1-1) case [see equation (57)]. Namely we take account of the forms,

$$S_1(x, Q, \zeta) \equiv T(x, p, Q)\, \tau_{\mathrm{Z}}(\zeta), \tag{62}$$

$$S_2(x, Q) \equiv nT(x, p, Q), \tag{63}$$

for the 2nd and 3rd equations for equation (51). Then the fundamental maps corresponding to individual fields are easily obtained [25], and thus symmetric, desired order numerical integrator can be constructed. The fundamental maps are

$$\Phi_t^{[1]}(\omega') = (t\mathbf{M}^{-1}p + x, p, \zeta, Q, \mathcal{P}, \eta, v), \tag{64a}$$

$$\Phi_t^{[2]}(\omega') = (x, tF(x) + p, \zeta, Q, \mathcal{P}, \eta, v), \tag{64b}$$

$$\Phi_t^{[3]}(\omega') = (x, v, [2K(p) - S_2(x, Q)]\, t + \zeta, Q, \mathcal{P}, \eta, v), \tag{64c}$$

$$\Phi_t^{[4]}(\omega') = (x, \exp[-tS_1(x, Q, \zeta)]p, \zeta, Q, \mathcal{P}, \eta, v), \tag{64d}$$

$$\Phi_t^{[T1]}(\omega') = (x, p, \zeta, t\mathbf{M}_{\mathrm{T}}^{-1}\mathcal{P} + Q, \mathcal{P}, \eta, v), \tag{64e}$$

$$\Phi_t^{[T2]}(\omega') = (x, p, \zeta, Q, tF_{\mathrm{T}}(x, p, Q) + \mathcal{P}, \eta, v), \tag{64f}$$

$$\Phi_t^{[T3]}(\omega') = (x, p, \zeta, Q, \mathcal{P}, t[2K_{\mathrm{T}}(\mathcal{P}) - m] + \eta, v), \tag{64g}$$

$$\Phi_t^{[T4]}(\omega') = (x, p, \zeta, Q, \exp[-t\tau_{\mathrm{Y}}(\eta)]\mathcal{P}, \eta, v), \tag{64h}$$

$$\Phi_t^{[5]}(\omega') = (x, p, \zeta, Q, \mathcal{P}, \eta, t\mathcal{Y}(\omega) + v), \tag{64i}$$

where $F(x) \equiv -\nabla U(x)$ and $F_{\mathrm{T}}(x, p, Q) \equiv -\nabla \tilde{U}_{E(x,p)}(Q)$ are the forces for the physical system and the temperature system, respectively. The simplest symmetric, second-order integrator with time step h is given, e.g., by

$$\begin{aligned}&\Phi^{[5]}_{h/2}\circ\Phi^{[T4]}_{h/2}\circ\Phi^{[T3]}_{h/2}\circ\Phi^{[T2]}_{h/2}\circ\Phi^{[T1]}_{h/2}\circ\Phi^{[4]}_{h/2}\circ\Phi^{[3]}_{h/2}\circ\Phi^{[2]}_{h/2}\circ\Phi^{[1]}_{h}\\&\circ\Phi^{[2]}_{h/2}\circ\Phi^{[3]}_{h/2}\circ\Phi^{[4]}_{h/2}\circ\Phi^{[T1]}_{h/2}\circ\Phi^{[T2]}_{h/2}\circ\Phi^{[T3]}_{h/2}\circ\Phi^{[T4]}_{h/2}\circ\Phi^{[5]}_{h/2}.\end{aligned}\tag{65}$$

Here, although $\Phi^{[T2]}_t$ requires the value of $U(x)$ in general through the evaluation of $F_{\mathrm{T}}(x,p,Q)$ [and $\Phi^{[3]}_t$ and $\Phi^{[4]}_t$ may also require it through the evaluation of $T(x,p,Q)$ in a general case], the above map ordering ensures that the evaluations of the potential energy $U(x)$ and the force $F(x)$ is once at the one stage. Maps, $\Phi^{[5]}_t$, at the both ends do not need this kind of evaluations but just refer the values. Note that S_1 and S_2 can be used for an EOM that has a more generalized form than equation (51), and equation (64) can be extended to apply into such a generalized form.

B. Numerical test

1. *Protocol*

As an example of numerical verification of the present method we chose 1-dimensional harmonic oscillator (1HO), defined by energy

$$E(x,p)=\frac{1}{2}x^2+\frac{1}{2}p^2$$

for $(x,p)\in\mathbb{R}^2$ (viz., $n=1$). It is suitable to validate the method because it gives a typical and important model that describes physical system behavior around the equilibrium state and because it is simple enough such that the exact distributions are analytically obtained. There also includes a complexity in that the BG distribution is not trivially achieved via the sampling by use of the single NH equations due to the lack of the ergodicity [36].

For numerical simulation, we used the functions defined in (S1)–(S5). The following parameter values were used: $\mathbf{M}_{\mathrm{T}}=1$ [see (S2)], $c_{\mathrm{Z}}=c_{\mathrm{Y}}=1$ [see (S2-1) and (S2-2)], and $c=1$ [see (S4)]. For (S5), we put $\alpha=d=4$, so that equation (58) is satisfied. We used $l=2.24$ to set $1\sim(\alpha+1)/l^2$ [see (S4)]. We integrated 10^8 time steps using equation (65) with a unit time of 1×10^{-3}.

Distribution of each variable was obtained by the corresponding marginal distribution. For example, the distribution of x is represented by equation (21) with B_1 being each bin,

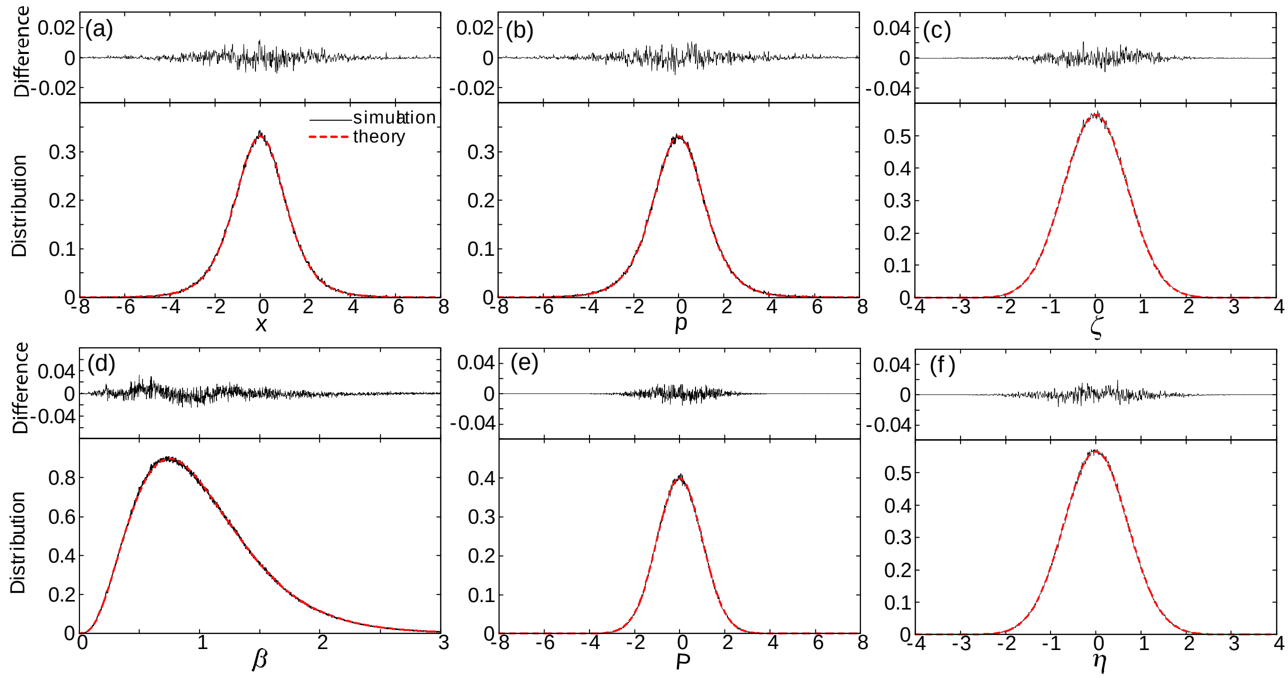

FIG. 1: Distribution densities of dynamical variables for the 1HO system. Those from simulation and theory are shown on the bottom, while their differences are shown on the top. (a)-(c) physical-system related variables: coordinate x, momentum p, and control variable ζ. (d)-(f) temperature-system variables: inverse temperature $\beta = \sigma(Q)$, momentum $\mathcal{P}$, and control variable η.

where the theoretical distribution is represented by the RHS of the equation, which turns out to be the RHS of equation (44), and the simulated distribution was estimated by the LHS, $\overline{\overline{\chi_{B_1} \circ \pi_{\mathrm{x}}}}$, with a finite-time approximation. Similar procedures were taken for $p, \zeta, \mathcal{P}$, and η. The distribution of $\beta \equiv \sigma(Q)$ was obtained from equation (50) for each bin B. The reweighting to the BG distribution density, $\rho_{\mathrm{BG}} : \mathbb{R}^2 \to \mathbb{R}, (x,p) \mapsto \mathrm{e}^{-\beta_{\mathrm{BG}} E(x,p)}$, at $\beta_{\mathrm{BG}} = 1$ was done by equation (45), where (C9) is obviously satisfied with $\rho_{\mathrm{TRG}} \equiv \rho_{\mathrm{BG}}$ for any $\beta_{\mathrm{BG}} > 0$ and $A \equiv \chi_B^2$ satisfies (C10) for any bin $B \in \mathcal{B}_2$.

2. Results

We show numerical results to confirm the realization of the distribution, equation (22) with (S1)-(S5), via equation (51). Figure 1 shows the distribution densities of coordinate x, momentum p, and control variable ζ for the physical system, and the inverse dynamical temperature $\beta = \sigma(Q)$, momentum $\mathcal{P}$, and control variable η for the temperature system.

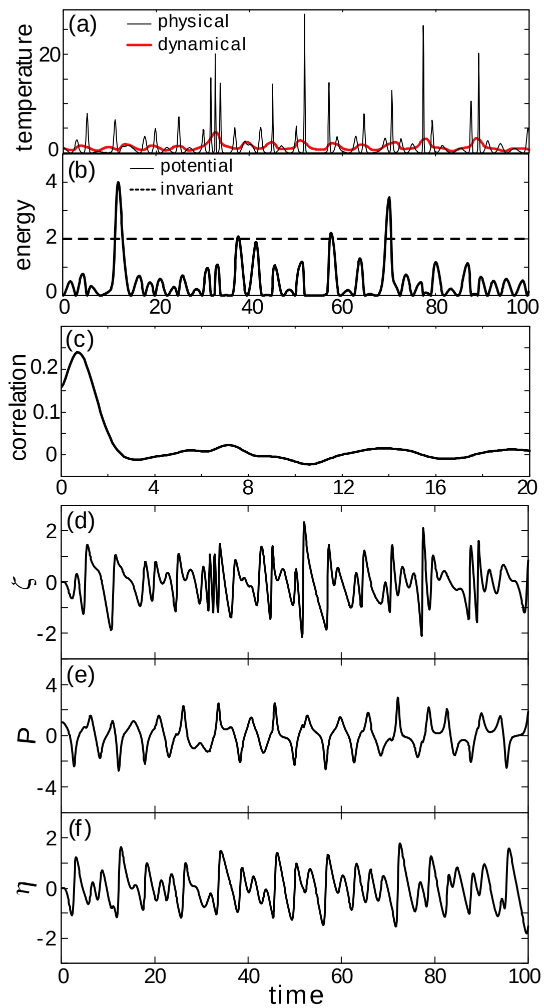

FIG. 2: Time development of quantities: (a) physical temperature $T_{\rm P}= p^2$ and dynamical temperature $T_{\rm D}= \sigma(Q)^{-1}$; (b) potential energy U and invariant L; (c) time-correlation between U and $T_{\rm P}$; (d) control variable ζ for the physical system; (e) momentum $\mathcal{P}$ and (f) control variable η for the temperature system.

Simulated and exact results agree well as were seen in small standard deviations of the discrepancies from the exact distributions for x, p, ζ, β, $\mathcal{P}$, and η, being 2.3×10^{-3}, 2.2×10^{-3}, 3.6×10^{-3}, 4.5×10^{-3}, 2.4×10^{-3}, and 3.2×10^{-3}, respectively. These results indicate that the present method produced a sufficiently accurate distribution. Reweighted result to the BG distributions was also satisfactory, where the standard deviations of the discrepancies from the exact distributions for x and p were 3.1×10^{-3} and 3.0×10^{-3}, respectively.

The behavior of the physical system in the nonequilibrium environment provided by the temperature system is shown in figure 2 (a)–(b). The time developments of physical temperature, $T_{\mathrm{P}} \equiv 2K(p)/n = p^2$, is perturbed from the pure 1HO Hamiltonian system, which should have period π for p^2. Compared with T_{P}, the dynamical temperature, $T_{\mathrm{D}} \equiv T(x,p,Q) = \sigma(Q)^{-1}$, changes more slowly [figure 2 (a)]. Around the time when T_{D} is large in oscillating-like motions, the amplitudes of T_{P} also become larger in an interesting manner. As shown in figure 2 (d)–(f), ζ, $\mathcal{P}$, and η show oscillation-like behaviors in nonlinear regime. As expected from the EOM, $\dot{\zeta} = T_{\mathrm{P}} - T_{\mathrm{D}}$ [the 3rd equation in (51)], ζ mainly obeys T_{P}, which shows faster oscillating motion than that of T_{D} [figure 2 (d)]. On the other hand, $\mathcal{P}$ mainly changes according to T_{D} [figure 2 (e)], as suggested by the relations, $\mathcal{P} = \dot{Q}$ and $T_{\mathrm{D}} \propto \exp\left[-Q/l\right]$. Similar correspondence appears in η [figure 2 (f)] and $\mathcal{P}$, via $\dot{\eta} = \mathcal{P}^2 - 1$. Figure 2(b) shows a time development of physical potential energy $U(x)$, suggesting a correlated motion with T_{P}. In fact, the correlation with a retarded time is seen by a correlation function [figure 2 (c)], defined by $G(t) \equiv \sum_{t_0} K(p(t_0))U(x(t+t_0))$. These correlations must be due to the nonlinear feature of ODE (51) and help to surmount nonergodic behaviors seen in conventional methods [37]. Keeping constant in the trajectory of invariant-function [equation (61)] in figure 2 (b) shows the success in the numerical integration.

VI. CONCLUSION

We have developed a new formalism, DDD, to realize densities of both physical system and parameters through the scaled long-time average generated by an ODE. The joint distribution density of the physical system and the parameter system is realized under the ergodic assumption of the flow, and the physical system density ρ_{R} is realized without its explicit form. Temperature-parameter application realizes superstatistics in a dynamical manner. The functions employed here to constitute the vector field is an example among the many choices. Beyond these applications, DDD demonstrates its potential for being (i) fruitfully utilized for various problems via creation of arbitrarily designed nonequilibrium temperatures [(S3)], (ii) exerted for well-planned parameters instead of temperature [equation (8)], and (iii) generalized for addressing multiple densities hierarchically for e.g., multiscale problems [equation (4)]. These new, general ideas are utilized for efficiently simulating a physical system in nonequilibrium, and it aims at the advance in molecular simulation, which is now a standard tool for atomic, molecular, soft-matter, and biological physics. We have focused on a theoretical study, and extensive applications are now under study.

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