Tsallis dynamics using the Nosé-Hoover approach

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On the basis of the Nosé-Hoover method, we developed a deterministic algorithm that produces an arbitrary probability density. An ordinary differential equation in the algorithm can realize the Tsallis distribution density. The Tsallis distribution has been considered a candidate of a distribution that represents a physical system in a heat bath. The Tsallis distribution density employed in this algorithm is defined using a full energy function form $E(x,p)$, along with the Tsallis index $q \geqslant 1$. Using the current equation, numerical simulations were performed for simple systems and the Tsallis distributions were observed.

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I. INTRODUCTION

Since Tsallis's proposal [1], Tsallis's statistics has been studied extensively. Research of its fundamental aspect and applications to various areas have been done [2]. Tsallis statistics is based on the Tsallis entropy, which is characterized by nonextensivity in contrast to the extensivity in the traditional Boltzmann-Shannon (BS) entropy. Tsallis distribution is obtained by extremization of the Tsallis entropy under some constraints (normalization condition and expectation values for some physical variables). Recently, it has been shown [3–6] that the canonical ensemble theory derived from microcanonical ensemble is not unique and that the Tsallis statistics can be derived. Namely, distribution representing a subsystem in a closed total system is not limited to the Boltzmann-Gibbs (BG) distribution (which is characterized by the maximum entropy principle for the BS entropy), but can be realized by the Tsallis distribution. This fact has been considered as one of the remarkable features of the Tsallis's nonextensive statistics. Furthermore, it has been reported [7] that the explanation in view of the Tsallis's statistics is possible for certain physical phenomena that are intractable by the traditional BG extensive statistics.

The Tsallis distribution approaches the BG distribution as the Tsallis index q tends to 1. Nosé and Hoover proposed a deterministic equation that represents a system constructed by adding (only) one degree of freedom to an objective physical system, and they showed that the equation can realize the BG distribution [8,9]. From this method, numerical simulations of the physical system in a heat bath can be done, in a deterministic way, without using numerous degrees of freedom to treat the heat bath, and knowledge of the canonical ensemble system has been intensively increased. Andricioaei and Straub [10] proposed a molecular dynamics (MD) and a Monte Carlo method for realizing the Tsallis distribution, and they showed the efficiency by its application to chemical systems. They dealt with Tsallis distribution represented by coordinate variables $x \equiv (x_1,\ldots,x_n)$ [i.e., potential energy $U(x)$ is used for energy for defining the distribution] along with the Tsallis index $q \geqslant 1$. Their MD method is based on the Newton equation and its ability of effective sampling of states in chemical systems has been shown [11]. The method proposed by Plastino and Antenodo [12] is a deterministic method based on the work of Kusnezov, Bulgac, and Bauer [13], and it can generate the Tsallis distribution represented by both coordinate variables x and momentum variables p [i.e., not only the potential energy $U(x)$, but also the kinetic energy $K(p)$ are used for defining the distribution]. Successful results using the method for the index range $0 < q \leqslant 1$ (their primary concern is in ''superextensive'' region), which is obtained by realizing the required ''Tsallis cut off condition,'' were reported, but a numerical overflow problem was pointed out for $q > 1$.

Our goal is (1) to obtain a deterministic equation that can realize the Tsallis distribution, which has been considered a candidate of a distribution that represents a physical system in a heat bath, and (2) to enable stable numerical simulations using the above equation for such a physical system. In contrast to the previous methods, we treat Tsallis distribution represented by variables (x, p) with the index $q \geqslant 1$. Physical phenomena were studied in relation to the Tsallis distribution with index $q > 1$ (''subextensive'' region) [2] for the Lévy flight [14], granular matter [15], and fully developed turbulence [16], and the efficiencies of the Tsallis statistics were reported.

For our purpose, we propose an ordinary differential equation (ODE) that produces the Tsallis distribution, on the basis of the Nosé-Hoover (NH) equation, which is an ODE that can realize the BG distribution. We first introduced a ''density dynamics'' to clarify the concept that distribution density is realized by a giving density function and a corresponding vector field. We then constructed an ODE to fulfill the density dynamics, so that an arbitrary density function was realized under ergodic assumption (Sec. II). Accordingly, arbitrary distribution density derived from canonical ensemble theory is produced, when the density is given as a smooth function. In Sec. III, we applied this dynamics to the Tsallis distribution density and constructed an ODE for the distribution. The validity of realization for the distribution was examined in numerical simulations using simple systems in Sec. IV. Section V summarizes the results of our study.

II. DENSITY DYNAMICS

On the basis of the Nosé-Hoover method, we construct a density dynamics that enables realization of an arbitrary density.

For a density, suppose that an arbitrary density function ρ (that is smooth, positive, and integrable) defined on a domain Ω in $\mathbf{R}^N$ is given. Regarding a dynamics, consider an ODE that has an invariant density ρ. That is, given ρ becomes the density (with respect to Lebesgue measure $d\omega$ on $\mathbf{R}^N$) of an invariant measure for the flow generated by an ODE

$$\dot{\omega} = X(\omega), \tag{1}$$

where $X:\mathbf{R}^N \supset \Omega \to \mathbf{R}^N$ is assumed to be smooth and complete. From a generalized Liouville's theorem, it is sufficient that the vector field X satisfies the Liouville equation [17]

$$\operatorname{div} \rho X = 0. \tag{2}$$

Then, by Birkhoff's individual ergodic theorem [18], the rate of sojourn time into an area $A \subset \Omega$ for a solution $t \mapsto \omega(t)$ of ODE (1) has a long-time limit value, for almost every initial point by the measure $\rho d\omega$. Further, if the flow is ergodic with respect to the measure $\rho d\omega$, then for almost every point, the value is constant and

$$\lim_{\tau\to\infty} \frac{1}{\tau} \int_0^\tau \chi_A(\omega(t))dt = \int_\Omega \chi_A(\omega)\rho(\omega)d\omega \Big/ \int_\Omega \rho(\omega)d\omega$$

$$= \text{const} \times \int_A \rho(\omega)d\omega, \tag{3}$$

where

$$\chi_A : \Omega \to \mathbf{R}, \omega \mapsto \begin{cases} 1, & \text{for } \omega \in A \\ 0, & \text{otherwise} \end{cases}$$

holds. Namely, probability density regarding realization for point $\omega \in \Omega$ is interpreted to be proportional to the given value $\rho(\omega)$. In the sense that an arbitrary density can be realized, we call (ρ, X), a doublet of objective density ρ and a corresponding field X, *density dynamics*.

A field X that satisfies Eq. (2) is not unique. The "Nosé-Hoover field"

$$X_{\mathrm{NH}} : \omega \equiv (x,p,\zeta) \mapsto (p, -\nabla U(x) - \zeta p, (\|p\|^2 - nT)/Q) \tag{4}$$

has been extensively studied including related ergodic property [19–21], and gives simple and powerful instruction to our trial of construction of a field X. In Eq. (4), $x \equiv (x_1,\ldots,x_n)$, $p \equiv (p_1,\ldots,p_n)$, and $U(x)$ represent coordinates, momenta, and potential energy of a physical system, respectively, $\zeta \in \mathbf{R}$ is a variable introduced to control a temperature of the physical system to $T>0$, and Q is a positive parameter [8,9,22] (we put all masses and Boltzmann's constant are unity). An approach inspired by the Nosé-Hoover field leads to the following ODE described by intended X (for simplicity, let $\Omega \equiv \mathbf{R}^N \equiv \mathbf{R}^{2n+1}$):

$$\begin{aligned} \dot{x}_i &= D_{p_i}\Theta(\omega), \quad i = 1,\ldots,n, \\ \dot{p}_i &= -D_{x_i}\Theta(\omega) - D_\zeta\Theta(\omega)p_i, \quad i = 1,\ldots,n, \\ \dot{\zeta} &= \sum_{j=1}^n D_{p_j}\Theta(\omega)p_j - n, \end{aligned} \tag{5}$$

where the function is defined by

$$\Theta = -\ln\rho : \Omega \to \mathbf{R}, \tag{6}$$

and $D_{x_i}\Theta(\omega)$, $D_{p_i}\Theta(\omega)$, and $D_\zeta\Theta(\omega)$ denote the partial derivative of Θ at point $\omega \equiv (x,p,\zeta)$ with respect to x_i, p_i, and ζ, respectively. The field X becomes smooth and the Liouville equation (2) is proved to be satisfied. Thus, Eq. (3) holds under the ergodic assumption. Equation (3) has been formulated using an infinite time. A certain condition is required for the function Θ to ensure that all solutions of ODE (5) are defined for $-\infty < t < \infty$ (viz., completeness of X). We assume the fulfillment of that condition as well as the ergodicity. Note that Θ is considered to be dimensionless, but it can have a physical dimension. To show this, we use an arbitrariness that all properties required for X are invariant under scalar multiplication for X. Namely, if Eq. (6) is defined using scaled variable $\overline{\Theta} \equiv \Theta/\varepsilon \equiv -\ln\rho$, where ε is a constant having the same dimension as Θ, and if X [the right-hand side of Eq. (5)] formulated using $\overline{\Theta}$ in place of Θ is multiplied by ε, then an ODE represented by Θ having the dimension is obtained.

Equation (5), which realizes the density dynamics, is based on the Nosé-Hoover method. This can be understood from the fact that Eq. (5) with the function choice of $\Theta(x,p,\zeta) \equiv (1/T)[U(x) + \frac{1}{2}\|p\|^2 + (1/2Q)\zeta^2]$ becomes equivalent to the NH equation. It means "flow equivalent" [23], i.e., in this case, the transformations for variable $\zeta \mapsto Q^{-1}\zeta$ and for time $t \mapsto T^{-1}t$ yield the NH equation $\dot{\omega} = X_{\mathrm{NH}}(\omega)$.

Here, we give some remarks regarding ergodicity for (ρ, X) defined by Eqs. (5) and (6). First, $\operatorname{div} X \neq 0$ holds. Suppose that $\operatorname{div} X(\omega) = 0$ holds for all point $\omega \in \Omega$ when Eq. (2) applies. Then ρ becomes an invariant function. That is, for an arbitrary solution ω and arbitrary time t, $\rho(\omega(t)) = \rho(\omega(0))$. Now, ρ cannot be almost everywhere constant (otherwise $\int_{\mathbf{R}^N} |\rho| d\omega = +\infty$). Therefore, the system does not become ergodic. However, since $\operatorname{div} X = -nD_\zeta\Theta$ holds and $D_\zeta\Theta$ is proved to be not identically zero from the conditions for ρ, $\operatorname{div} X \neq 0$ is concluded. Second, fixed points for X, which can be obstructions to ergodicity, do not exist, since $n>0$. These favorable properties are inherited from the NH equation.

III. TSALLIS DYNAMICS

The method introduced in the preceding section is applied to a density for the Tsallis distribution, and an ODE is derived.

We deal with a density [24]

$$\rho_{\mathrm{Tsallis}}(x,p) = [1 - (1-q)\beta E(x,p)]^{q/(1-q)}. \tag{7}$$

Here, $E(x,p)$ is a total energy and set to be, for simplicity, the sum of potential energy $U(x) \geqslant 0$ and a kinetic energy $K(p) \equiv \frac{1}{2}\|p\|^2$. The parameter q is a real number called the "Tsallis index" and only the case for $q \geqslant 1$ is treated. The

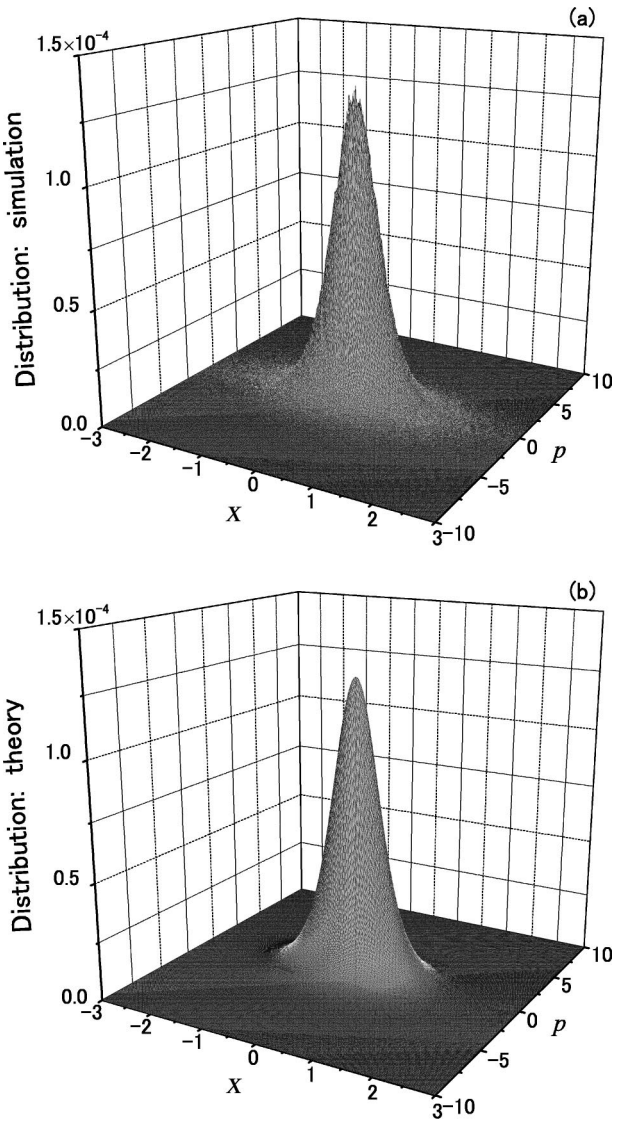

FIG. 1. Tsallis distribution for potential function $U(x)=2x^2$, Tsallis index $q=1.5$, and $\beta=1$. The values are evaluated on each mesh of the size $\Delta x\,\Delta p \equiv 0.01\times 0.04$. (a) Simulation results of histogram [left-hand side of Eq. (11)] obtained in integration of Eq. (9) with $\tau(\zeta)\equiv 400\zeta^3$; (b) theoretical values [right-hand side of Eq. (11)].

limit of the density as $q\to 1$ is $\rho_{\mathrm{BG}}(x,p)\equiv\exp[-\beta E(x,p)]$, which is proportional to the traditional BG distribution. The density of Eq. (7) becomes a continuous representation for the probability that is derived from extremizing the Tsallis entropy with considering the ''normalized q-expectation value'' of E (i.e., ''the third choice'' in Ref. [24]). Then, the form of Eq. (7) implies that β is defined using ''renormalized temperature'' T' by $\beta=1/T'>0$. In Eq. (7), normalization has not yet been done and the form raised to the qth power is used. This is because we have considered the ''escort probabilities'' [7,24] [see Eq. (10) below]. Note that our method is not restricted in the above density form nor the energy function form.

We apply the density of Eq. (7) to Eqs. (5) and (6). The density with respect to ζ component is not given *a priori*, so is put $\rho_z(\zeta)$, and a total density is defined as

$$\rho(x,p,\zeta)\equiv\rho_{\mathrm{Tsallis}}(x,p)\rho_z(\zeta). \tag{8}$$

Assume that the conditions for ρ are met. Then Eq. (5) turns to be

$$\begin{aligned}
&\dot{x}_i = g(x,p)p_i, \quad i=1,...,n,\\
&\dot{p}_i = -g(x,p)D_iU(x)-\tau(\zeta)p_i, \quad i,...,n,\\
&\dot{\zeta} = g(x,p)\|p\|^2-n,
\end{aligned} \tag{9}$$

where

$$g(x,p)\equiv\frac{q\beta}{1-(1-q)\beta E(x,p)},$$

$$\tau(\zeta)\equiv -D\ln\rho_z(\zeta).$$

As described in Sec. II, when we set a scaling factor as $\varepsilon\equiv 1/\beta$ and multiply the right-hand side of Eq. (9) by ε, we have variables x and p with the ordinary dimensions. In addition, we can see that the equation with a choice of $q\equiv 1$ and $\rho_z(\zeta)\equiv\exp[-(\beta/2Q)\zeta^2]$ yields the pure NH equation (with ζ scaled by the parameter Q).

A long-time average value of any physical variable O represented by a function of x and p exists for almost everywhere, and under the ergodic assumption similarly to Eq. (3), it equals to a space average with weight ρ_{Tsallis} (expectation of O in the Tsallis distribution). That is,

$$\begin{aligned}
&\lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau O(x(t),p(t))dt\\
&\quad=\int_\Omega O(x,p)\rho(\omega)d\omega \Big/ \int_\Omega \rho(\omega)d\omega\\
&\quad=\int_{\mathbf{R}^{2n}} O(x,p)\rho_{\mathrm{Tsallis}}(x,p)\\
&\qquad\times dx\,dp \Big/ \int_{\mathbf{R}^{2n}}\rho_{\mathrm{Tsallis}}(x,p)dx\,dp.
\end{aligned} \tag{10}$$

Here, we have assumed $\int_\Omega|O\rho|d\omega<+\infty$. Similarly, for each point $(\overline{x},\overline{p})$ with a suitable area $\Delta(\overline{x},\overline{p})\subset\mathbf{R}^{2n}$ that includes $(\overline{x},\overline{p})$, is sufficiently small, and has a constant volume, the following equation holds:

$$\begin{aligned}
&\lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau \chi_{\Delta(\overline{x},\overline{p})}(x(t),p(t))dt\\
&\quad=\int_{\Delta(\overline{x},\overline{p})}\rho_{\mathrm{Tsallis}}(x,p)dx\,dp \Big/ \int_{\mathbf{R}^{2n}}\rho_{\mathrm{Tsallis}}(x,p)dx\,dp\\
&\quad\approx\rho_{\mathrm{Tsallis}}(\overline{x},\overline{p})\times\mathrm{const},
\end{aligned} \tag{11}$$

where

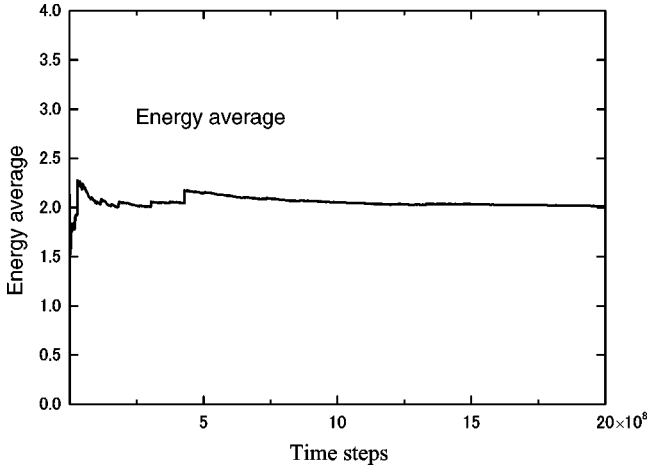

FIG. 2. Simulation results of the energy average in the Tsallis distribution for the potential function $U(x)=2x^2$. Time average of the energy $(1/t)\int_0^t E(x(s),p(s))ds$ is shown as a function of time steps. See Fig. 1 for simulation conditions. Theoretical value of the energy average is 2.0.

$$\chi_{\Delta(\overline{x},\overline{p})}:\mathbf{R}^{2n}\to\mathbf{R},(x,p)\mapsto\begin{cases}1, & \text{for } (x,p)\in\Delta(\overline{x},\overline{p})\\ 0, & \text{otherwise.}\end{cases}$$

The left-hand side of Eq. (11) represents the rate of sojourn time into $\Delta(\overline{x},\overline{p})$ of $t\mapsto(x(t),p(t))$ obtained from the ODE (9). Thus, a probability density regarding realization for point $(\overline{x},\overline{p})$ is proportional to $\rho_{\text{Tsallis}}(\overline{x},\overline{p})$.

IV. NUMERICAL SIMULATION

Realization of the Tsallis distribution via Eq. (9) is examined in numerical simulations using simple systems.

We tried two potential functions; a harmonic oscillator and a double well oscillator both in one-dimension,

$$U(x)=2x^2, \tag{12}$$

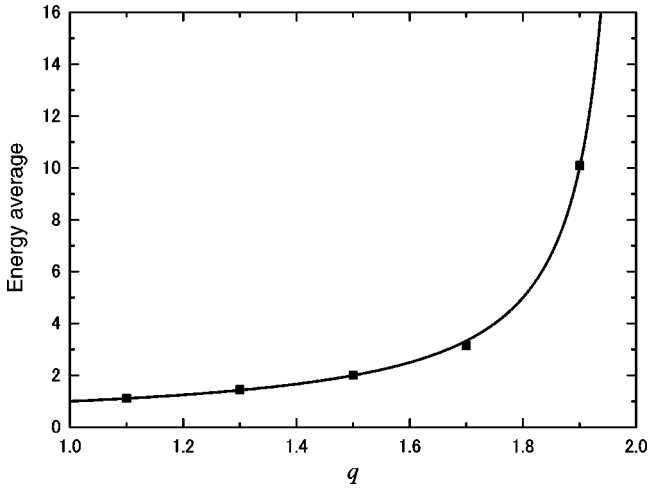

FIG. 3. Energy average in the Tsallis distribution for the potential function $U(x)=2x^2$. Square symbols indicate the values of simulation results at final time step for each Tsallis index q. The curve shows theoretical values [Eq. (14)].

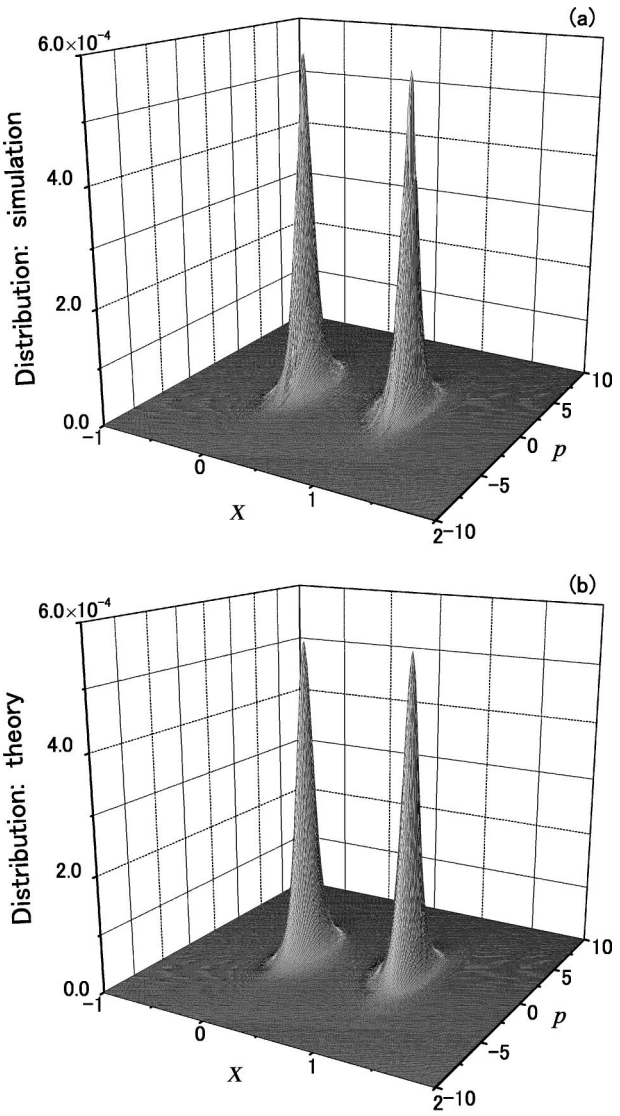

FIG. 4. Tsallis distribution for the potential function $U(x)=160x^2(x-1)^2$, Tsallis index $q=1.8$, and $\beta=1$. The values are evaluated on each mesh of the size $\Delta x\,\Delta p\equiv 0.01\times 0.04$. (a) Simulation results of histogram obtained in integration of Eq. (9) with $\tau(\zeta)\equiv 2000\zeta$; (b) theoretical values.

$$U(x)=160x^2(x-1)^2. \tag{13}$$

To confirm the validity of Eq. (11) concerning the density, we calculated the left-hand side of Eq. (11) by the histogram obtained from simulations for each mesh $\Delta(\overline{x},\overline{p})$ and compared with the theoretical value of the right-hand side. Regarding Eq. (10), we chose the total energy E as a physical variable, evaluated the left-hand side of Eq. (10) by time average $(1/t)\int_0^t E(x(s),p(s))ds$ in simulations, and compared with the theoretical value $\langle E\rangle$ defined by the right-hand side. For simplicity, all variables were treated as dimensionless. Parameter β was set as 1.0. We set parameter q within the range that the value of $\langle E\rangle$ remains finite. In numerical integrations of the ODE, the fourth-order Runge-Kutta method with a unit time step of $\Delta t=5\times 10^{-4}$ was used. An initial value was $x(0)=0.1$, $p(0)=1.0$, and $\zeta(0)=0.0$.

In harmonic oscillator case, simulation results regarding Eq. (11) (histogram calculated from $N=2\times10^9$ time steps) and the theoretical values are shown in Figs. 1(a) and 1(b), respectively. Here, we set $q=1.5$. Agreement between them can be seen. Integration with respect to x and p in Eq. (10) yields exactly

$$\langle E\rangle=\frac{1}{\beta}\frac{1}{2-q}. \tag{14}$$

Thus the theoretical value $\langle E\rangle$ in this case is 2.0. Figure 2 shows simulation results for the time average of energy as a function of time steps. It converged to the theoretical value. In addition, simulations were performed for several initial values chosen randomly within $|x|<2.0$, $|p|<10.0$, and $|\zeta|<1.0$. In these cases, results similar to the above were obtained. We carried out simulations for different q. Figure 3 shows the result of energy averages for several q's. These simulation results coincide well with the theoretical values.

In the NH equation, generating the BG distribution (viz., $q\rightarrow1$ case) for one-dimensional harmonic oscillator was difficult owing to the existence of comparatively wide ''regular motion'' regions [19] in Ω and many extensions of the method have thereby been proposed to overcome that problem [25]. In our study, we observed this difficulty of nonergodiclike behavior when we chose $\tau(\zeta)\equiv c\zeta$ ($c>0$ is some constant). However, the choice of $\tau(\zeta)\equiv c\zeta^3$ seems to work well in comparison to the linear case.

Regarding the double well oscillator [Eq. (13)], Fig. 4 shows simulation results (a) and the theoretical values (b) for the distribution. We set $q=1.8$. Simulation results for time average of energy was 3.388 (final time step) and the theoretical value $\langle E\rangle$ is evaluated as about 3.285. Agreement between these simulation results and theoretical values can be seen.

We now remark on computational costs for calculating energy average. The value $\langle E\rangle$ is obtained from the integral of $E\rho_{\mathrm{Tsallis}}$ and the contribution of each point (x,p) to $\langle E\rangle$ is $E(x,p)\rho_{\mathrm{Tsallis}}(x,p)/\int_{\mathbf{R}^{2n}}E\rho_{\mathrm{Tsallis}}dx\,dp$. The high energy region in which each point significantly contributes to $\langle E\rangle$ is, in general, larger than that for the BG density ρ_{BG}, since ρ_{Tsallis} decreases only in power with increasing E, while ρ_{BG} follows the exponential decreasing for E. Such a high energy region for the Tsallis density contains points for which $\rho_{\mathrm{Tsallis}}(x,p)$ is relatively small. These points constitute a rare event. If the volume of this rare event is considerably small, we may ignore the contribution of this event at a small expense of the accuracy for $\langle E\rangle$. Suppose the contrary case. Accurate evaluation for the energy average requires that such a rare event must be realized with an accurate frequency. That is, a statistical fully long time series is generally required. Consequently, such evaluation for the energy average in numerical simulation needs a lot of computational time. In our simulations for the above potential functions, this tendency was found for relatively large q, for which the corresponding distribution is apart from the BG distribution.

V. CONCLUSION

We have demonstrated a density dynamics and on the basis of the Nosé-Hoover method we have constructed an ODE that enables realization of an arbitrary smooth density. We have applied this equation to the Tsallis density and obtained an ODE that can realize the Tsallis distribution with the Tsallis index $q\geqslant1$. The Tsallis density has been defined by an energy that is defined using both the potential energy and kinetic energy for a physical system. Realization of the Tsallis distribution was verified in numerical simulations for simple systems.

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