Construction of an extended invariant for an arbitrary ordinary differential equation with its development in a numerical integration algorithm

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For an arbitrary ordinary differential equation (ODE), a scheme for constructing an extended ODE endowed with a time-invariant function is here proposed. This scheme enables us to examine the accuracy of the numerical integration of an ODE that may itself have had no invariant. These quantities are constructed by referring to the Nosé-Hoover molecular dynamics equation and its related conserved quantity. By applying this procedure to several molecular dynamics equations, the conventional conserved quantity individually defined in each dynamics can be reproduced in a uniform, generalized way; our concept allows a transparent outlook underlying these quantities and ideas. Developing the technique, for a certain class of ODEs we construct a numerical integrator that is not only explicit and symmetric, but preserves a unit Jacobian for a suitably defined extended ODE, which also provides an invariant. Our concept is thus to simply build a divergence-free extended ODE whose solution is just a lift-up of the original ODE, and to constitute an efficient integrator that preserves the phase-space volume on the extended system. We present precise discussions about the general mathematical properties of the integrator and provide specific conditions that should be incorporated for practical applications.

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I. INTRODUCTION

Ordinary differential equations (ODEs) that are nonlinear and possess many degrees of freedom cannot be usually solved analytically, so that numerical solutions are of great value, e.g., for investigating physical phenomena or for a guide to understanding certain mathematical issues. To numerically solve an ODE, it is important to verify the accuracy of the numerical integration. If there exists a time-invariant function for the ODE, we can check the error generated by the numerical integration by monitoring this function value during the integrating process. For an ODE defined on a phase space Ω, we call a function $L:\Omega\rightarrow\mathbf{R}$ an *invariant* if for an arbitrary solution of the ODE, ϕ, the quantity $L(\phi(t))$ is constant with respect to time t. For instance, as is well known for a Hamiltonian system, the Hamiltonian function is an invariant; however, such an invariant does not always exist for an arbitrary ODE.

Also for the ODE used in molecular dynamics (MD) simulation [1], confirmation of the accuracy of the integration is critical because long-time integration is required to obtain expectation values of the physical quantities and because the employed vector field requires many operands derived from the complicated interactions among the particles. Newton dynamics has the total energy (Hamiltonian) as a common invariant. In contrast, "Boltzmann-Gibbs dynamics" (BGD), i.e., an ODE that can directly generate the Boltzmann-Gibbs (BG) distribution [2], can have a certain conserved quantity, but even in such a case the description of the quantity is proposed individually for each BGD equation, without a uniform outlook. As such a viewpoint, Terada and Kidera [3] defined a generalized form of the conserved quantity in constant-temperature MD simulation, and applied it to the Nosé-Hoover (NH) equation [4,5] and the Gaussian isokinetic (GI) equation [6–9]. Recently, in the development of an isothermal-isobaric MD algorithm, Stern [10] discussed a conserved quantity for equations satisfying the Liouville condition. However, the relation between these quantities is still unclear.

In this paper we first show that for an arbitrary ODE, the construction of quantities corresponding to an invariant is always possible. For this purpose we utilize techniques such as those used in MD: namely, the NH equation and its related invariant. In our proposed procedure, for a given ODE on Ω, we consider a space having an additional degree of freedom, $\Omega'\equiv\Omega\times\mathbf{R}$, and on Ω' constitute a new ODE, which turns out to have an invariant. Further, the projection of an arbitrary solution of this new ODE into Ω becomes a solution of the original ODE; namely, no solutions in the original ODE are affected by introducing the added variable. Thus, numerical integration can be done for this new ODE, and checking of the integration will be possible by monitoring the constructed invariant value. We also call such a conserved quantity an *extended invariant* with respect to the *original* ODE in order to distinguish the invariant, which is a phase-space function and represented for the new extended ODE (see Secs. II and III A). In addition to the general presentation of the quantities, we show that our extended invariant uniformly describes the conserved quantities provided for individual MD equations.

As well as serving as a tool for numerical integration, the proposed technique enables us to develop a numerical integration algorithm itself. Well-known conventional integrators such as the classical Runge-Kutta method or Gear method are made for general use and are easy to implement, so they are especially convenient to use as integrators for newly developed equations. However, such classical integrators do not generally preserve certain intrinsic properties of the ODE

that is of interest. This feature entails a disadvantage in accuracy, because the error caused from this nonpreservation can only be lessened by reducing the unit time step length.

By contrast, the recently developed "geometric integrator" captures the geometric features of the ODE and exactly preserves its corresponding geometric properties at *any* value of the unit time step. Such efficient integrator techniques [11–13] have been developed since the pioneering works including those for the so-called symplectic integrator for Hamiltonian system [14–16] and the systematic scheme of exponential operator decomposition [17,18]. They have been applied to a variety of systems, e.g., molecular [19], rigid body [20], spin liquid [21], quantum many-body [22], *ab initio* MD [23], separated time scale [24], and time-irreversible [25] systems. As well as the symplectic property of the Hamiltonian system, the following geometric issues have been addressed: momentum maps [26], Poisson brackets [26,27], (linear) reversibility [28], and phase-space volume [29–31]. In particular, volume preservation is broadly concerned with systems including the Hamiltonian system, and the preservation is considered to be intrinsically important in constructing an effective integrator. In fact, from studies of the nonsymplectic, volume-preserving integrator on several Hamiltonian systems [32] and divergence-free systems [33], it has been indicated that the volume-preserving integrator produces comparative results rather than the corresponding results of the symplectic integrator. In general, however, the theoretical assurance about the effectiveness of the geometric integrator is qualified for ODEs that have the corresponding geometric properties.

In this work, we construct a numerical integration method by using the present invariant construction technique with its suitable extension, together with the effective decomposition-composition technique recently developed for ODE flow. The characteristic feature is that in addition to the existence of the invariant in a newly constructed extended ODE, the ODE becomes divergence-free, and the resulting integrator has a constant unit Jacobian; namely, the integrator keeps the volume-preserving property for the extended ODE. This method provides a route to easily construct an efficient integrator for many kinds of ODEs, including non-Hamiltonian systems, via a theoretical concept based on a geometric view beyond the symmetric feature.

After a brief review in Sec. II of the NH equation and its related invariant, we construct in Sec. III the extended invariant and the extended equation for an arbitrary ODE. We present an extended invariant for each BGD equation and show that it is identical to the quantity conventionally proposed. In addition to BGD, we apply it to Tsallis dynamics [34], which can produce the Tsallis distribution [35], an extension of the BG distribution. Furthermore, we provide a general description to demonstrate the connections among our extended invariant and the quantities of Terada-Kidera and Stern. In Sec. IV, we further generalize the above technique and develop a protocol for constructing efficient numerical integrators. The efficiencies of the integrators are analyzed by theoretically capturing the characteristics with a consideration of suitable mathematical conditions for the validness. Finally, Sec. V summarizes our work.

II. THE NOSÉ-HOOVER EQUATION AND THE EXTENDED INVARIANT

The Nosé-Hoover equation can be represented by [1,4,5,36]

$$\dot{x}_i = p_i/m_i, \quad i = 1, \ldots, n, \tag{1a}$$

$$\dot{p}_i = -D_i U(x) - (\zeta/Q)p_i, \quad i = 1, \ldots, n, \tag{1b}$$

$$\dot{\zeta} = 2K(p) - nk_{\mathrm{B}}T, \tag{1c}$$

where $x \equiv (x_1, \ldots, x_n) \in D \subset \mathbf{R}^n$, $p \equiv (p_1, \ldots, p_n) \in \mathbf{R}^n$, $U(x)$, and $K(p) \equiv \Sigma_{i=1}^{n} p_i^2/2m_i$ represent the coordinates, momenta, potential energy, and kinetic energy, respectively, of a physical system, with m_i being a mass parameter, k_{B} Boltzmann's constant, $\zeta \in \mathbf{R}$ a variable to control the temperature of the physical system to $T > 0$, and Q a positive parameter. For an arbitrary solution of Eq. (1), $\phi \equiv (x, p, \zeta): \mathbf{R} \supset J \to \Omega \equiv D \times \mathbf{R}^n \times \mathbf{R}$, the quantity $\mathcal{I}: J \to \mathbf{R}$ defined by

$$\mathcal{I}(t) \equiv U(x(t)) + K(p(t)) + \frac{1}{2Q}\zeta(t)^2 + \frac{nk_{\mathrm{B}}T}{Q}\int_0^t \zeta(s)ds \tag{2}$$

is shown to be constant with respect to time t. Since $\mathcal{I}$ is not represented as a phase-space function on Ω due to the existence of the time functional in the last term (which is defined only when the time development of a solution is given), $\mathcal{I}$ does not become the invariant in the sense of the definition given in Sec. I; hence we call Eq. (2) an *extended invariant* with respect to Eq. (1). When we evaluate the last term in appropriate fashion, $\mathcal{I}$ can be used for a numerical integration check. However, we can get another simple insight when we employ the following form having an additional degree of freedom v:

$$\dot{x}_i = p_i/m_i, \quad i = 1, \ldots, n, \tag{3a}$$

$$\dot{p}_i = -D_i U(x) - (\zeta/Q)p_i, \quad i = 1, \ldots, n, \tag{3b}$$

$$\dot{\zeta} = 2K(p) - nk_{\mathrm{B}}T, \tag{3c}$$

$$\dot{v} = \zeta/Q. \tag{3d}$$

We then have an *invariant* $L: \Omega' \equiv \Omega \times \mathbf{R} \to \mathbf{R}$ defined by

$$L(\omega') \equiv U(x) + K(p) + \frac{1}{2Q}\zeta^2 + nk_{\mathrm{B}}Tv, \tag{4}$$

where $\omega' \equiv (x, p, \zeta, v)$ denotes the extended phase-space point, and we observe that this expression is surely independent of each solution's form, in contrast to Eq. (2). Obviously the solution ϕ in the original Eq. (1) is not affected by handling Eq. (3), because the variable v is decoupled from the other original variables. Accordingly, we can solve Eq. (3) numerically to seek ϕ and use the value of $L(\phi'(t))$ for the solution of Eq. (3), $\phi': J \to \Omega'$, to check the integration.

Historically, before Eqs. (1) and (2) were developed, Eqs. (3) and (4) were derived in the form of $d \ln s/dt = \zeta/Q$, where s is Nosé's extended variable [4,5,36]. Equation (3) was derived through a nonsymplectic variable transformation μ and

a time transformation from the Nosé Hamiltonian equation with the Hamiltonian having the relation $H(x,s,p,p_s)=L(\mu(x,s,p,p_s))$, where p_s is the canonical momentum conjugate to s [36]. Although the equation $\dot{v}=\zeta/Q$ turns out to be separated from the other equations, to keep the form of Eq. (3) allows one to manage a good control on the accuracy of the numerical solution via Eq. (4). It is also noted that in recent developments in the field of non-Hamiltonian dynamics and noncanonical Hamiltonian descriptions [37], phase space with even dimensions is addressed: according to [38,39], this dimensionality is necessary to formulate an algebraic approach to non-Hamiltonian dynamics by means of generalized brackets, which can then be used to reformulate Dirac's approach to constrained dynamics [40].

We show that in Sec. III the above form of the equation for v is not a unique result if we consider only usefulness in the integration, and as described in Sec. IV it also leads to a device for the integration itself.

III. EXTENDED INVARIANT FOR AN ARBITRARY ODE: SIMPLE CASE

Referring to the equations introduced in Sec. II, for an arbitrary ODE we construct an extended ODE and its invariant. In general, the candidate constituting the invariant, such as "energy," as in the first three terms in the right-hand side of Eq. (2), is not given *a priori*. However, we show that the candidate can be generated from an arbitrary function. We consider first a simple case in this section; the more general case is discussed in Sec. IV.

A. Theory

Let Ω be a domain of $\mathbf{R}^N$ and $X:\Omega\to\mathbf{R}^N$ be a vector field, generating an ODE

$$\dot{\omega}=X(\omega). \tag{5}$$

Suppose a function $B:\Omega\to\mathbf{R}$ and assume that X and B are smooth (say, of class C^1). Then, for an arbitrary solution of the ODE, ϕ, defined on an interval $J\subset\mathbf{R}$,

$$I_\phi:J\to\mathbf{R},\ t\overset{\mathrm{d}}{\mapsto} B(\phi(t))+\int_{t_0}^{t}Y(\phi(s))ds \tag{6}$$

$$=\text{const}, \tag{7}$$

viz., $I_\phi(t)$ is constant with respect to time t (t_0 can be any value in J), where Y is defined by

$$Y:\Omega\to\mathbf{R},\ \omega\mapsto Y(\omega)\equiv-(X(\omega)|\operatorname{grad}B(\omega))$$

$$=-\sum_{i=1}^{N}X_i(\omega)D_iB(\omega), \tag{8}$$

$(\cdot|\cdot)$ denoting the standard inner product in $\mathbf{R}^N$ [viz., $-Y$ is the (Lie) derivative of B along X: $-Y=XB$]. The constant property, Eq. (7), is confirmed straightforwardly by differentiating Eq. (6) with respect to t; Eq. (6) is nothing but the time integration of the identity $0=\dot{B}-(\dot{\omega}|\operatorname{grad}B(\omega))$. We say that the quantity Eq. (6) is an *extended invariant* with respect to the original ODE (5). With the same notation and assumptions, we also obtain the following.

Proposition 1. Consider a vector field in $\mathbf{R}^{N+1}$ defined by

$$X':\Omega'\equiv\Omega\times\mathbf{R}\to\mathbf{R}^{N+1},\ \omega'\equiv(\omega,v)\mapsto(X(\omega),Y(\omega)), \tag{9}$$

and an ODE

$$\dot{\omega}'=X'(\omega'), \tag{10}$$

viz., the original Eq. (5) with

$$\dot{v}=Y(\omega). \tag{11}$$

Then the following holds.

(i) The solution of Eq. (10) with an initial value $(\omega_0,v_0)\in\Omega'$ is uniquely given by $\phi':J\to\Omega',t\overset{\mathrm{d}}{\mapsto}(\phi(t),\varphi(t))$, where ϕ is a solution on an open interval J ($0\in J\subset\mathbf{R}$) for Eq. (5) with an initial value $\omega_0\in\Omega$, and $\varphi(t)\equiv-B(\phi(t))+v_0+B(\omega_0)$.

(ii) For ODE (10), the function

$$L:\Omega'\to\mathbf{R},\ \omega'=(\omega,v)\overset{\mathrm{d}}{\mapsto}B(\omega)+v \tag{12}$$

is an invariant; i.e., for its arbitrary solution ϕ' in the form given in (i),

$$L(\phi'(t))=B(\phi(t))+\varphi(t) \tag{13}$$

$$=I_\phi(t)+\varphi(t_0) \tag{14}$$

is constant for all $t\in J$.

Again the proof is straightforward. (i) The existence of ϕ is clear. So, for $\forall t\in J$, $D\phi'(t)=(D\phi(t),-D(B\circ\phi)(t))=(X(\phi(t)),Y(\phi(t)))=X'(\phi'(t))$ holds, and $\phi'(0)=(\phi(0),-B(\phi(0))+v_0+B(\omega_0))=(\omega_0,v_0)$. Since the assumptions of X ensure the uniqueness of solutions for the initial value problem of Eq. (5) and since such a uniqueness property for

$$\dot{v}=Y(\phi(t)) \tag{15}$$

is valid, the uniqueness property for Eq. (10) also holds. Therefore the results follow. (ii) is clear, where the equality in Eq. (14), which is the relation between the extended invariant with respect to the original ODE and the invariant with respect to the extended ODE, comes from Eq. (15).

Instead of Eq. (6), using the quantity defined from

$$I:J\to\mathbf{R},\ t\overset{\mathrm{d}}{\mapsto}B(\phi(t))+\int_{0}^{t}Y(\phi(s))ds-B(\phi(0)) \tag{16}$$

may be useful, because $I(t)=0\ \forall t\in J$ holds for all $\phi(0)\in\Omega$, implying the invariance of $I(t)$ with respect to initial values of the solutions as well as the time invariance.

B. Application

For an application of the results in Sec. III A, this section deals with the case of

$$B\equiv-c\ln\rho, \tag{17}$$

where ρ is a function and c a constant. We consider a special case mainly encountered in MD equations. We show that when we suitably choose ρ and c according to the target field

X, several conventional conserved quantities individually proposed for MD equations can be uniformly represented by the current extended invariant. After we treat in an elemental manner the simple case in which ρ satisfies the Liouville equation (Sec. III B 1), we take into account a somewhat more intricate case in which the equation is satisfied locally (Sec. III B 2). In Sec. III B, we assume that X is a C^1 vector field on a domain Ω in $\mathbf{R}^N$, ρ is a smooth (being of class C^2 is natural in the below examples), positive function on Ω, and $c \neq 0$.

1. Liouvillian dynamics

Let us define a field X as being *Liouvillian* with respect to ρ, if

$$\mathrm{div}(\rho X)(\omega) = 0 \tag{18}$$

holds for *all* $\omega \in \Omega$. Adopting this condition means that the consideration is not intended for nonequilibrium dynamics, but restricted to equilibrium situations. Notice that Eq. (18) at ω implies

$$\mathrm{div}\, X(\omega) = -\frac{1}{\rho(\omega)}\sum_{i=1}^{N} D_i \rho(\omega) X_i(\omega) = \frac{1}{c}\sum_{i=1}^{N} D_i B(\omega) X_i(\omega)$$
$$= -Y(\omega)/c. \tag{19}$$

Thus, when X is Liouvillian with respect to ρ, Eq. (6) turns out to be

$$I_\phi(t) = -c\left(\ln \rho(\phi(t)) + \int_{t_0}^{t} \mathrm{div}\, X(\phi(s))ds\right). \tag{20}$$

It should be noted that when $c=-1$, Eq. (20) is the same quantity as that recently demonstrated in Ref. [10]. Below, we consider each specific case in which ρ provides the microcanonical, BG, or Tsallis distribution, and we observe the form of the (extended) invariant.

The first example is an illustration via recovering well-known results using a familiar system; i.e., $N(\equiv 2n)$-dimensional Hamiltonian equation with smooth Hamiltonian $\boldsymbol{H}: \Omega \equiv \mathbf{R}^N \to \mathbf{R}$, $\dot{\omega} = X(\omega) \equiv \mathbf{J} \cdot \boldsymbol{\nabla} H(\omega)$, where

$$\mathbf{J} \equiv \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix}$$

is the skew-symmetric matrix in $\mathbf{R}^{2n}$. For an arbitrary smooth function G on $\mathbf{R}$, $\rho \equiv \exp \circ -G \circ H$ satisfies

$$\mathrm{div}(\rho X)(\omega) = (\boldsymbol{\nabla}(\exp \circ -G \circ H)(\omega) | \mathbf{J} \cdot \boldsymbol{\nabla} H(\omega))$$
$$= D(\exp \circ -G)(H(\omega))(\nabla H(\omega) | \mathbf{J} \cdot \boldsymbol{\nabla} H(\omega)) = 0$$

for all $\omega \in \Omega$. Thus, from Eqs. (7) and (20), $\mathrm{const} = I_\phi(t) = cG(H(\phi(t)))$; and thus, on each energy surface $\{\omega | H(\omega) = e\}$, which becomes an invariant set, the $\rho(\omega)$ takes a constant value and so can provide the microcanonical distribution.

The vector field of BGD $\dot{\omega} = X(\omega)$ is Liouvillian with respect to the following:

$$\rho(\omega) \equiv \rho_{\mathrm{BG}}(x,p)\rho_z(\zeta), \tag{21}$$

where

$$\rho_{\mathrm{BG}}(x,p) \equiv \exp[-E(x,p)/k_{\mathrm{B}}T] \tag{22}$$

is the BG density with $E(x,p) \equiv U(x) + K(p)$, ρ_z is a certain function of "extended variables" $\zeta \equiv (\zeta_1, \ldots, \zeta_M) \in \mathbf{R}^M$, and $\omega \equiv (x,p,\zeta) \in \Omega \equiv D \times \mathbf{R}^n \times \mathbf{R}^M \subset \mathbf{R}^N$ $(N \equiv 2n+M)$. We consider here the Nosé-Hoover chain (NHC) equation [41] and the Kusnezov, Bulgac, and Bauer (KBB) [42] equation, as the BGD.

The NHC equation [41] $\dot{\omega} = X_{\mathrm{NHC}}(\omega)$ is represented as

$$\dot{x}_i = p_i/m_i, \quad i = 1, \ldots, n, \tag{23a}$$

$$\dot{p}_i = -D_i U(x) - (\zeta_1/Q_1)p_i, \quad i = 1, \ldots, n, \tag{23b}$$

$$\dot{\zeta}_1 = 2K(p) - nk_{\mathrm{B}}T - (\zeta_2/Q_2)\zeta_1, \tag{23c}$$

$$\dot{\zeta}_j = \zeta_{j-1}^2/Q_{j-1} - k_{\mathrm{B}}T - (\zeta_{j+1}/Q_{j+1})\zeta_j, \quad j = 2, \ldots, M-1$$
$$\text{(if and only if } M \geqslant 3), \tag{23d}$$

$$\dot{\zeta}_M = \zeta_{M-1}^2/Q_{M-1} - k_{\mathrm{B}}T, \tag{23e}$$

where M is the "chain length" and Q_j is the positive parameter associated with the extended variable ζ_j $(j = 1, \ldots, M)$. The conserved quantity has been given [41] as

$$E(x(t),p(t)) + \sum_{j=1}^{M} \frac{1}{2Q_j}\zeta_j^2(t)$$
$$+k_{\mathrm{B}}T\int_0^t \left(n\zeta_1(s)/Q_1 + \sum_{j=2}^{M} \zeta_j(s)/Q_j\right)ds \tag{24}$$
$$= E(x(t),p(t)) + \sum_{j=1}^{M} \frac{1}{2Q_j}\zeta_j^2(t)$$
$$+k_{\mathrm{B}}T\left(n\eta_1(t) + \sum_{j=2}^{M} \eta_j(t)\right) \tag{25}$$
$$\equiv H'(p(t),x(t),\eta(t),\zeta(t)),$$

where $\eta(t) \equiv (\eta_1(t), \ldots, \eta_M(t))$ is defined through

$$\dot{\eta}_j = \zeta_j/Q_j, \quad \eta_j(0) = 0, \quad j = 1, \ldots, M. \tag{26}$$

Now, the field X_{NHC} becomes Liouvillian in the above sense when

$$\rho_z(\zeta) \equiv \exp\left[-\frac{1}{k_{\mathrm{B}}T}\left(\sum_{j=1}^{M} \frac{1}{2Q_j}\zeta_j^2\right)\right], \tag{27}$$

and yields $\mathrm{div}\, X_{\mathrm{NHC}}(\omega) = -(n\zeta_1/Q_1 + \Sigma_{j=2}^{M}\zeta_j/Q_j)$ for $\omega \in \Omega$. Thus, when we apply Eq. (7) using Eqs. (20)–(22) and (27) to any solution $\phi \equiv (x,p,\zeta): J \to \Omega$, we get the constancy of

$$I_\phi(t) = -c\left(\ln \rho(\phi(t)) + \int_0^t \mathrm{div}\, X_{\mathrm{NHC}}(\phi(s))ds\right)$$
$$= \frac{c}{k_\mathrm{B}T}\left(E(x(t),p(t)) + \sum_{j=1}^{M}\frac{1}{2Q_j}\zeta_j^2(t)\right)$$
$$+ c\int_0^t\left(n\zeta_1(s)/Q_1 + \sum_{j=2}^{M}\zeta_j(s)/Q_j\right)ds. \quad (28)$$

This quantity is equivalent to Eq. (24) when we choose $c=k_\mathrm{B}T$ [this constant indicates that Eq. (24) is surely an energy-originated quantity, as seen below in the conventional examples]; in other words, we can obtain the NHC conserved quantity in our fashion in the case of $B=-k_\mathrm{B}T\ln\rho$.

In a similar manner, we discuss the KBB equation with $E(x,p)$ as the Hamiltonian, represented [42] as

$$\dot{x}_i = p_i/m_i - h_2(\zeta_2)F_i(x,p), \quad i=1,\ldots,n, \quad (29a)$$

$$\dot{p}_i = -D_iU(x) - h_1(\zeta_1)G_i(x,p), \quad i=1,\ldots,n, \quad (29b)$$

$$\dot{\zeta}_1 = \alpha_1\sum_{i=1}^{n}[G_i(x,p)p_i/m_i - k_\mathrm{B}TD_{p_i}G_i(x,p)], \quad (29c)$$

$$\dot{\zeta}_2 = \alpha_2\sum_{i=1}^{n}[F_i(x,p)D_iU(x) - k_\mathrm{B}TD_{x_i}F_i(x,p)], \quad (29d)$$

where $h_j(\zeta_j)\equiv Dg_j(\zeta_j)$, $j=1,2$ $(M\equiv 2)$; g_j, F_i, and G_i are appropriate functions; and α_j represents a certain parameter. This vector field is also Liouvillian with respect to Eq. (21) with

$$\rho_z(\zeta) \equiv \exp\left[-\frac{1}{k_\mathrm{B}T}\left(\sum_{j=1}^{2}\frac{1}{\alpha_j}g_j(\zeta_j)\right)\right]. \quad (30)$$

The conserved quantity has been given [42] by

$$\mathcal{E}(x(t),p(t),\zeta(t)) \equiv E(x(t),p(t)) + \sum_{j=1}^{2}\frac{1}{\alpha_j}g_j(\zeta_j(t))$$
$$+ k_\mathrm{B}T\int_0^t ds\,\Lambda(x(s),p(s),\zeta(s)), \quad (31)$$

where

$$\Lambda(x,p,\zeta) \equiv \sum_{i=1}^{n}[h_1(\zeta_1)D_{p_i}G_i(x,p) + h_2(\zeta_2)D_{x_i}F_i(x,p)].$$

It has been pointed out in Ref. [42] that in the last term of Eq. (31) the relation $\mathrm{div}\, X_{\mathrm{KBB}}(\omega) = -\Lambda(\omega)$ holds. We can now address the reason for the appearance of this relation by applying Eq. (7) with Eqs. (20)–(22) and (30), and getting the extended invariant

$$I_\phi(t) = -c\left(\ln\rho(\phi(t)) + \int_0^t \mathrm{div}\, X_{\mathrm{KBB}}(\phi(s))ds\right)$$
$$= \frac{c}{k_\mathrm{B}T}\mathcal{E}(x(t),p(t),\zeta(t)). \quad (32)$$

Thus, we have again obtained the conventional conserved quantity Eq. (31), using our method.

The third example is the Tsallis dynamics (TD) equation [34] $\dot{\omega}=X_{\mathrm{TD}}(\omega)$, which can realize the Tsallis distribution [35], an extension of the BG distribution by the Tsallis index q. TD is derived from a non-Hamiltonian approach and the equation is given as

$$\dot{x}_i = g(x,p)p_i/m_i, \quad i=1,\ldots,n, \quad (33a)$$

$$\dot{p}_i = -g(x,p)D_iU(x) - \tau(\zeta)p_i, \quad i=1,\ldots,n, \quad (33b)$$

$$\dot{\zeta} = 2g(x,p)K(p) - nk_\mathrm{B}T, \quad (33c)$$

where $g(x,p)\equiv q/[1-(1-q)E(x,p)/k_\mathrm{B}T]$ and $\tau(\zeta)\equiv -k_\mathrm{B}TD\ln\rho_z(\zeta)$ for $\zeta\in\mathbf{R}$ $[\omega\equiv(x,p,\zeta);\ N\equiv 2n+1]$, with q and T being real parameters. The density

$$\rho(\omega) \equiv \rho_{\mathrm{Tsallis}}(x,p)\rho_z(\zeta) \quad (34)$$

with $\rho_{\mathrm{Tsallis}}(x,p)\equiv[1-(1-q)E(x,p)/k_\mathrm{B}T]^{q/(1-q)}$ [43] leads X_{TD} to be Liouvillian. Thus, the result of $\mathrm{div}\, X_{\mathrm{TD}}(x,p,\zeta) = -n\tau(\zeta)$ yields

$$I_\phi(t) = -c\left(\ln\rho(\phi(t)) + \int_0^t \mathrm{div}\, X_{\mathrm{TD}}(\phi(s))ds\right)$$
$$= -c\ln[\rho_{\mathrm{Tsallis}}(x(t),p(t))\rho_z(\zeta(t))] + cn\int_0^t\tau(\zeta(s))ds. \quad (35)$$

Note that as $q\to 1$, the density $\rho_{\mathrm{Tsallis}}(x,p)$ converges to $\rho_{\mathrm{BG}}(x,p)$ and so the extended invariant of TD [Eq. (35)] approaches that of NH [Eq. (2)] when $\rho_z(\zeta)\equiv\exp(-\zeta^2/2k_\mathrm{B}TQ)$ and $c=k_\mathrm{B}T$, as well as the fact that the TD equation (33) recovers the NH equation (1). From Proposition 1 in Sec. III A [and Eq. (19)], we can treat Eq. (33) coupled with

$$\dot{v} = cn\tau(\zeta)$$

and observe the value of the invariant

$$L(\omega') = -c[\ln\rho_{\mathrm{Tsallis}}(x,p) + \ln\rho_z(\zeta)] + v \quad (36)$$

for numerical integration check.

2. Locally Liouvillian dynamics

Thus far, we have considered the situation in which the condition of Eq. (18) holds at all phase-space points. We consider below a more general situation, i.e., one in which the condition holds locally, and we take account of the GI equation as an example.

The GI equation [6–9] is frequently used in constant-temperature MD and also extensively used in multicanonical

MD [44] for the basis of the equation of motion. The GI equation $\dot{\omega}=X_{\mathrm{GI}}(\omega)$, with a phase-space point $\omega\equiv(x,p)\in\Omega\equiv D\times\{p\in\mathbf{R}^n|p\neq 0\}\subset\mathbf{R}^{2n}$, is of the form

$$\dot{x}_i = p_i/m_i, \quad i=1,\ldots,n, \tag{37a}$$

$$\dot{p}_i = -D_iU(x)-\xi(\omega)p_i, \quad i=1,\ldots,n, \tag{37b}$$

where $\xi(\omega)\equiv-\Sigma_{i=1}^n[D_iU(x)p_i/m_i]/(\Sigma_{i=1}^n p_i^2/m_i)$. Note that $\Gamma_c\equiv\{(x,p)\in\Omega|\Sigma_{i=1}^n p_i^2/m_i=c\}$ is an invariant set for every $c>0$ [i.e., an arbitrary solution of the ODE, ϕ: $J\to\Omega$, such that $\phi(0)\in\Gamma_c$ always lies in Γ_c], and so temperature, $\omega\mapsto(\Sigma_{i=1}^n p_i^2/m_i)/nk_{\mathrm{B}}$, is an invariant. (In an alternative choice [1,45] of a "friction" function such that $\xi:\Omega\equiv D\times\mathbf{R}^n\to\mathbf{R}$, $\omega\mapsto-\Sigma_{i=1}^n[D_iU(x)p_i/m_i]/\kappa$ with a constant $\kappa>0$, only for $c=\kappa$ does Γ_c become an invariant set and so the temperature is invariant locally on Γ_κ, except for the trivial case in which ∇U is identically zero.) Accordingly, monitoring the temperature value has been the usual simple check for the accuracy of the integration of this equation. The discussion in Sec. III A now presents an added equation $\dot{v}=Y(\omega)$ and defines the invariant of Eq. (12). When we choose B such that it contains the coordinate variable x, the invariant should contain the x (see also the example below), so that it will reinforce the conventional check, which uses only the p variable, reflecting an insufficiency of detection of the error derived from the x variable.

Now, in contrast to the cases in Sec. III B 1, X_{GI} is not recognized as Liouvillian in the global sense, but it can satisfy a local condition. Let us say that X is *locally Liouvillian* on Γ with respect to ρ, if $\mathrm{div}(\rho X)=0$ holds for a certain invariant subset Γ in Ω. We then admit that for each $c'>0$ the field X_{GI} is locally Liouvillian on $\Gamma_{c'}$ with respect to

$$\rho_{\mathrm{BG},1}(x,p)\equiv\exp[-\beta U(x)] \tag{38}$$

for $\beta=(n-1)/c'>0$; i.e., $\mathrm{div}(\rho_{\mathrm{BG},1}X_{\mathrm{GI}})(\omega)=0$ holds at all $\omega\in\Gamma_{c'}$ [although in the above alternative choice of ξ the field X_{GI} becomes Liouvillian in the global sense with respect to Eq. (38) when $\beta=(n+1)/\kappa$, the target to set constant temperature is only the explained local space Γ_κ]. When we construct the extended invariant according to Sec. III A in this local case, it is simpler to calculate Y directly from the definition, rather than through Eq. (20) as in the Liouvillian case, and we obtain the following: using Eq. (17) with $\rho\equiv\rho_{\mathrm{BG},1}$ (for any β), for a solution $\phi\equiv(x,p)$,

$$I_\phi(t) = B(\phi(t))+\int_0^t Y(\phi(s))ds \tag{39}$$

$$= c\beta\left(U(x(t))+K_0\int_0^t\xi(\phi(s))ds\right), \tag{40}$$

where $K_0\equiv\Sigma_{i=1}^n p_i^2(0)/m_i$ (or κ in the alternative choice of ξ). It should be noticed that this is the same *form* as (though not identical to) the conserved quantity discussed in Ref. [3] up to constants. In the following discussion, we clarify this statement in detail and explain the reason for this relation.

Terada and Kidera defined a conserved quantity for constant-temperature MD simulation by using a Jacobian [3]. We read that the quantity is defined by

$$\Delta H^*(t,\omega)\equiv k_{\mathrm{B}}T\ln\frac{\{\det[D\overline{T}_t(\omega)]\}^{-1}\rho(\omega)}{\rho(T_t(\omega))}, \tag{41}$$

where ρ is assumed to be given as the BG density at temperature T, which is of the form Eq. (22) or Eq. (38) of $\beta=1/k_{\mathrm{B}}T$; the target field X is assumed to be complete, and $\{T_t:\Omega\to\Omega|t\in\mathbf{R}\}$ is the corresponding flow, viz., $T_t(\omega)=\phi(t)$ for all t, with ϕ being a solution of the ODE $\dot{\omega}=X(\omega)$ such that $\phi(0)=\omega\in\Omega$. In addition, $\overline{T}_t:\Omega\to\Omega$ is a one-step map, representing an employed *integrator* with a unit time step of t [the 'integration' with initial value ω is to iterate the mapping: $\overline{T}_t\circ\cdots\circ\overline{T}_t(\omega)$], and having well-defined $\{\det[D\overline{T}_t(\omega)]\}^{-1}$, where $\det[D\overline{T}_t(\omega)]$ is the Jacobian of the map $\overline{T}_t$ at point ω. Now, for a function ρ (assuming positivity and smoothness, but not restricted to the BG density), we here present a quantity slightly deformed from Eq. (41); that is,

$$\Delta H^\bigstar(t,\omega)\equiv b\ln\frac{\{\det[DT_t(\omega)]\}^{-1}\rho(\omega)}{\rho(T_t(\omega))}, \tag{42}$$

where b is a constant. Replacing all T_t with $\overline{T}_t$ both in the Terada-Kidera conserved quantity of Eq. (41) and in the "Terada-Kidera extended invariant" of Eq. (42), and setting ρ as the BG density at temperature $T=b/k_{\mathrm{B}}$ in Eq. (42), we get the same quantity; namely, the two quantities can be the same when we evaluate them by an integrator $\overline{T}_t$, actually used in simulation.

However, it should be noticed that the Jacobian of a map permits several function forms and that such an arbitrary function form does not necessarily produce the same quantity in Eqs. (41) and (42) by the replacement of T_t with $\overline{T}_t$. Regarding such a function form, e.g., for the exact flow, Liouville's formula affirms that

$$\det DT_t(\omega)=\exp\left[\int_0^t(\mathrm{div}\,X)[T_s(\omega)]ds\right] \tag{43}$$

holds for all $t\in\mathbf{R}$ and all $\omega\in\Omega$ (see, e.g., Ref. [46] for Euclidean space or Ref. [47] for a smooth manifold). To clarify the discussion, let us denote the flow by the use of

$$\Phi:\mathbf{R}\times\Omega\to\Omega,\quad (t,\omega)\overset{\mathrm{d}}{\mapsto}T_t(\omega)$$

and the Jacobian by

$$J_0(\Phi)(t,\omega)\equiv\det[D_2\Phi(t,\omega)]=\det[DT_t(\omega)].$$

Likewise, we represent $\bar{\Phi}(t,\omega)=\overline{T}_t(\omega)$ for an integrator. Now, since X can be conversely correspondent to the flow, say $X=\nu(\Phi)$, we get another function form of the Jacobian, $J_1(\Phi)(t,\omega)\equiv\exp\{\int_0^t[\mathrm{div}\circ\nu(\Phi)][\Phi(s,\omega)]ds\}$. Furthermore, if the exact flow satisfies a certain condition [47], there exists a function g on Ω such that

$$J_2(\Phi)(t,\omega)\equiv\exp[g(\omega)-g(\Phi(t,\omega))] \tag{44}$$

$$= J_0(\Phi)(t,\omega) \tag{45}$$

holds for all (t,ω). In fact, the NH equation of the type Eq. (3) admits this J_2 form with $g=n\Pi_v$, Π_v being a projection $\omega\equiv(x,p,\zeta,v)\mapsto v$. Now, in these examples, we have a cer-

tain map I other than J_0 such that $I(\Phi)=J_0(\Phi)$ for exact flow Φ. However, we should take care that $I(\bar{\Phi})=J_0(\bar{\Phi})$ does not necessarily hold for an integrator and that a replacement of Φ with $\bar{\Phi}$ in Eq. (41) with use of J_0 and that in Eq. (42) with use of I thereby causes not generally identical results. Nevertheless, there is also a circumstance in which both $I(\Phi)=J_0(\Phi)$ and $I(\bar{\Phi})=J_0(\bar{\Phi})$ are valid. For instance, when we again use the exact flow of Eq. (3), Φ, and use $\bar{\Phi}$ constituted by the integrator as defined in Ref. [48], we can obtain $J_2(\bar{\Phi})=J_0(\bar{\Phi})$ using $g=n\Pi_v$ defined above [as such an integrator, actually, we can show that an arbitrary finite composition of the maps induced by the solvable decomposition of the field of Eq. (3) will suffice; cf. Sec. IV B]. Such an integrator thus becomes an integrator that preserves explicit volume-functional form, rather than a volume-preserving integrator (cf. Sec. IV).

Now, we show that our extended invariant Eq. (6) coincides (up to constants) with the current Terada-Kidera extended invariant Eq. (42), indicating that our invariant conceptually involves the Terada-Kidera quantity under a certain reconsideration. This can be done by assuming that X is locally Liouvillian with respect to a certain ρ on an invariant set $\Gamma \subset \Omega$. Then, for a solution ϕ with an arbitrary initial value of $\omega \in \Gamma$,

$$I_\phi(t) = B(\phi(t)) + \int_0^t Y(\phi(s))ds \tag{46}$$

$$= -c\left(\ln \rho(\phi(t)) + \int_0^t \operatorname{div} X(\phi(s))ds \right) \tag{47}$$

$$= c[-\ln\rho(T_t(\omega)) - \ln \det DT_t(\phi(0))] \tag{48}$$

$$= c \ln\left(\frac{[\det DT_t(\omega)]^{-1}}{\rho(T_t(\omega))} \right) \tag{49}$$

$$= (c/b)\Delta H^\star(t,\omega) + \text{const} \tag{50}$$

holds for any t. Here, Eq. (47) results from the fact that $\phi(s)$ is in the invariant set Γ for all s according to the initial condition, the property of being locally Liouvillian, and the use of Eq. (19). To get Eq. (48) from Eq. (47), we have used the Liouville formula Eq. (43). Note that if we exploit Eq. (16) with $c=b$, we have a perfect identity: $I(t)=\Delta H^\star(t,\omega)$.

It immediately follows from Eq. (49) with the results of $I_\phi(t)=I_\phi(0)$ that

$$\rho(T_t(\omega)) = [\det DT_t(\omega)]^{-1}\rho(\omega) \quad \forall\, \omega \in \Gamma, \quad \forall\, t \in \mathbf{R}. \tag{51}$$

Conversely, as stated in Ref. [3], we exactly assert that Eq. (51) leads to the locally Liouvillian property of X. This can be done by a differentiation of Eq. (51) with respect to t at 0, using Eq. (43): for $\forall \omega \in \Gamma$,

$$\begin{aligned}
&\operatorname{div} \rho X(\omega) - \rho(\omega)\operatorname{div} X(\omega) \\
&= \sum_{i=1}^N D_i\rho(\omega)X_i(\omega) \\
&= D(\rho \circ \phi)(0) \\
&= \frac{d}{dt}\rho(\omega)\exp\left[-\int_0^t (\operatorname{div} X \circ \phi)(s)ds \right]\Bigg|_{t=0} \\
&= -\rho(\omega)\operatorname{div} X(\omega).
\end{aligned}$$

Thus, the locally Liouvillian property on Γ and the relation of Eq. (51) are equivalent. In this sense, for a locally Liouvillian field, our extended invariant function is considered to measure disruptions of the locally Liouvillian property in the numerical integration process.

The "application" in Sec. III B is to discuss the theoretical general-purpose character of our approach such that our extended invariant coincides with the conserved quantity (or intimate conserved quantity) of an MD equation that adapts to Eq. (18) (globally or locally) for a *known* density ρ, using the choice of B via Eq. (17). The Newton equation and the BGD described so far are examples. However, the important point to note is that in a specific application in which an equation of motion is given but such a density is not known, we can set an arbitrary smooth function as B in order to constitute the invariant. Actually, in the TD equation (33) we selected B and ρ that satisfy Eqs. (17) and (18), but this is only to take into account the correspondence of TD with BGD in the $q \to 1$ extensive limit about densities, equations of motion, and the extended invariants.

IV. EXTENDED INVARIANT: GENERALIZED CASE

In the previous section we developed a technique for constructing the invariant; here, in Sec. IV A, the foundation of a generalization of the technique is evolved and in Sec. IV B it is applied to construct a numerical integrator.

A. Theory

We generalize Eq. (9) by renewing the equation for v. Suppose that $X:\Omega \to \mathbf{R}^N$ and $B:\Omega \to \mathbf{R}$ satisfy the same conditions given in Sec. III A, and that Y is defined by Eq. (8). Consider a continuous function

$$\lambda:\mathbf{R} \supset U \to \mathbf{R}\setminus\{0\}, \tag{52}$$

where U is an arbitrary disjoint union of open intervals U_α, $U=\Sigma_{\alpha\in A}U_\alpha$.

Proposition 2. Consider a vector field in $\mathbf{R}^{N+1}$ defined by

$$X'':\Omega'' \equiv \Omega \times U \to \mathbf{R}^{N+1},$$

$$\omega' \equiv (\omega, v) \mapsto (X(\omega), Y(\omega)\lambda(v)), \tag{53}$$

and the ODE

$$\dot{\omega}' = X''(\omega'), \tag{54}$$

viz., $\dot{\omega}=X(\omega)$ with

$$\dot{v} = Y(\omega)\lambda(v). \tag{55}$$

Then the following holds.

(i) The solution of Eq. (54) with an initial value $(\omega_0, v_0) \in \Omega''$ is uniquely given as

$$\phi'':\mathbf{R}\supset J_\phi\to\Omega'',\ t\overset{\mathrm{d}}{\mapsto}(\phi(t),\varphi_\phi(t)),$$

where $\phi:J$ (an open interval containing 0) $\to\Omega$ is a solution of $\dot{\omega}=X(\omega)$ with an initial value $\omega_0\in\Omega$, and $\varphi_\phi:J_\phi\to U$ is a solution of

$$\dot{v}=Y(\phi(t))\lambda(v) \tag{56}$$

with an initial value $v_0\in U_\alpha\subset U$, defined by

$$\varphi_\phi(t)\equiv\Lambda_\alpha^{-1}(F_\phi(t)+\Lambda(v_0)). \tag{57}$$

Here, Λ_α is a restriction of the following function to U_α:

$$\Lambda:U\to\mathbf{R},\ v\overset{\mathrm{d}}{\mapsto}\int_{v_{\alpha'}}^{v}\frac{1}{\lambda(u)}du\quad\text{for } v\in U_{\alpha'}, \tag{58}$$

where $v_{\alpha'}\in U_{\alpha'}$ is a fixed arbitrary point for each $\alpha'\in A$;

$$F_\phi:J\to\mathbf{R},\ t\overset{\mathrm{d}}{\mapsto}\int_0^t Y(\phi(s))ds=B(\phi(0))-B(\phi(t)); \tag{59}$$

and J_ϕ is an open interval such that

$$0\in J_\phi\subset J^\phi\equiv\{t\in J|F_\phi(t)+\Lambda(v_0)\in\Lambda_\alpha(U_\alpha)\}. \tag{60}$$

(ii) For ODE (54), the function

$$L:\Omega''\to\mathbf{R},\ \omega'=(\omega,v)\overset{\mathrm{d}}{\mapsto}B(\omega)+\Lambda(v) \tag{61}$$

is an invariant; i.e., for its arbitrary solution ϕ'' in the form given in (i), $L(\phi''(t))=B(\phi(t))+\Lambda(\varphi_\phi(t))$ is constant for all $t\in J_\phi$.

To prove the above, first, notice that for every α the map $\Lambda_\alpha:U_\alpha\to\Lambda_\alpha(U_\alpha)$ has the inverse (since the assumptions for λ and U_α with the intermediate value theorem ensure that λ is either positive on the whole U_α or negative on the whole U_α, the map Λ_α becomes strictly monotone) and that J^ϕ and φ_ϕ are independent of the choice of v_α, as can be easily checked. The existence of J_ϕ is derived from the property of J and the fact that $\Lambda_\alpha(U_\alpha)-\Lambda(v_0)$ becomes an open set containing $F_\phi(0)$ and that F_ϕ is continuous. Since Eq. (56) forms an ODE of the separation of variables, its unique solution with an initial condition of $(t,v)=(0,v_0)$ is shown to take the form of Eq. (57). The remaining proof of (i) can be performed along the same lines as given in Proposition 1 (Sec. III A). (ii) is due to the fact that $D(L\circ\phi'')(t)=-Y(\phi(t))+D\Lambda(\varphi_\phi(t))Y(\phi(t))\lambda(\varphi_\phi(t))=0$ for $\forall t\in J_\phi$.

The case of $\lambda(v)=1$ is the simplest example, being the situation argued in Sec. III A. Another important example is obtained in the case when B satisfies Eq. (17) with $c=1$ and Eq. (18) and when

$$\lambda(v)=v \tag{62}$$

with $U=\mathbf{R}\backslash\{0\}$. Then Eq. (54) defines

$$\dot{\omega}=X(\omega), \tag{63}$$

$$\dot{v}=Y(\omega)\lambda(v)=-\operatorname{div}X(\omega)v, \tag{64}$$

and Eq. (61) defines the invariant (up to a constant)

$$L(\omega,v)=B(\omega)+\ln v. \tag{65}$$

The key characteristic in Eqs. (63) and (64) is the invariance of the domain of definition, $J=J^\phi=J_\phi$ [derived from $\Lambda_\alpha(U_\alpha)=\mathbf{R}$; also obvious because Eq. (64) turns out to be a nonautonomous linear ODE], and is the divergence-free feature

$$\operatorname{div}X''=0. \tag{66}$$

Equation (66) gives the important result that the map T_t'', where $\{T_t''|t\in\mathbf{R}\}$ is the (exact) flow generated by X'' (assumed to be complete and C^1), has a unit Jacobian for all t: we define this term by stating that a differentiable map f from an open set O of $\mathbf{R}^N$ into $\mathbf{R}^N$ *has a unit Jacobian* if $\det[Df(\omega)]=1$ holds for *all* $\omega\in O$. This result is clear, e.g., from Eq. (43) such that for all t and all $\omega\in\Omega''$,

$$\det[DT_t''(\omega)]=\exp\left(\int_0^t(\operatorname{div}X'')[T_s''(\omega)]ds\right)=1. \tag{67}$$

Actually, from the Liouville theorem, the following three properties are all equivalent for exact flow $\{T_t\}$ of C^1, complete field X: X is divergence-free, T_t has a unit Jacobian for all t, and T_t is volume preserving for all t; here, volume preserving for $f:\mathbf{R}^N\supset O\to\mathbf{R}^N$ means that $m(f(E))=m(E)$ for any set $E\subset O$, where m is the volume [i.e., m: Lebesgue measure on $\mathbf{R}^N$; O, E, $f(E)$: measurable set]; notice that if f is a C^1-diffeomorphism on an open set O,

$$m(f(E))=\int_E|\det Df(\omega)|dm(\omega). \tag{68}$$

B. Application

As an application of Sec. IV A, for a certain class of ODEs, we construct on the extended space an efficient numerical integration method, which has the following advantages: (1) the symmetric property holds; (2) the invariant can be used; (3) the Jacobian is exactly preserved; (4) any order with respect to local error for time step h can be implemented; (5) explicitness holds. These properties have been achieved by (i) adopting the extended-invariant production technique described in Sec. IV A, (ii) using a symmetric composition method in conjunction with the order condition theory [49,50], and (iii) constructing a divergence-free solvable decomposition of the vector field. Demonstrating (ii) and (iii) above, Sec. IV B 1 introduces the integrator and investigates the properties (1)–(5). Section IV B 2 illustrates our scheme by applying it to the NH equation.

1. A development in numerical integration

The following two techniques for integration are combined to achieve (ii) above: solvable decomposition (or splitting) of the vector field, and effective composition of the corresponding maps. We begin with a brief review of these techniques [51], before going to the point (iii) in Sec. IV B 1 b.

a. Symmetric composition. Solvable decomposition of a

smooth vector field X on an open set $\Omega \subset \mathbf{R}^N$ means a decomposition of X for which each exact flow generated by the decomposed field can be represented by an explicitly given complete flow; namely, a vector field $X:\Omega \to \mathbf{R}^N$ can be decomposed as

$$X = X^{[1]} + X^{[2]} + \cdots + X^{[L]}, \tag{69}$$

with the condition that every $X^{[i]}$ is smooth and complete and that

$$\dot{\omega} = X^{[i]}(\omega) \tag{70}$$

is solved explicitly, meaning that the one-parameter transformation for $X^{[i]}$, $\Phi_t^{[i]}:\Omega \to \Omega$, can be obtained exactly in an explicit form [$\mathbf{R} \ni t \mapsto \Phi_t^{[i]}(\omega)$ is a solution of Eq. (70) for an initial value ω; recall the group property, which will be used below in, e.g., Eq. (75), such that $\Phi_t^{[i]} \circ \Phi_s^{[i]} = \Phi_{t+s}^{[i]}$ for all t, s, and $\Phi_0^{[i]} = \mathrm{id}_\Omega$].

Using the solvable decomposition, the ODE

$$\dot{\omega} = X(\omega) \tag{71}$$

has one integrator, i.e., a map $\Phi_t:\Omega \to \Omega$, defined by

$$\Phi_t = \Phi_t^{[1]} \circ \Phi_t^{[2]} \circ \cdots \circ \Phi_t^{[L]}. \tag{72}$$

It is shown that this integrator Φ_t and its adjoint

$$\Phi_t^* \equiv (\Phi_{-t})^{-1} \tag{73}$$

$$= (\Phi_{-t}^{[L]})^{-1} \circ \cdots \circ (\Phi_{-t}^{[2]})^{-1} \circ (\Phi_{-t}^{[1]})^{-1} \tag{74}$$

$$= \Phi_t^{[L]} \circ \cdots \circ \Phi_t^{[2]} \circ \Phi_t^{[1]} \tag{75}$$

are first-order integrators of Eq. (71).

Several constructions of higher-order integrators exist. On the basis of the first-order map Φ_t, we now consider the following symmetric composition with the adjoint:

$$\Psi_h = \Phi_{\alpha_s h} \circ \Phi^*_{\beta_s h} \circ \cdots \circ \Phi_{\alpha_2 h} \circ \Phi^*_{\beta_2 h} \circ \Phi_{\alpha_1 h} \circ \Phi^*_{\beta_1 h}, \tag{76}$$

where the coefficients $\{\alpha_i, \beta_i\} \subset \mathbf{R}$ satisfy the symmetric condition:

$$\alpha_i = \beta_{s+1-i}, \quad i = 1, \ldots, s. \tag{77}$$

Owing to Eq. (77), the obtained integrator Ψ_h is symmetric, i.e., $\Psi_h^* = \Psi_h$ [or time-reversible: $(\Psi_h)^{-1} = \Psi_{-h}$]. According to the values of the order, several effective algorithms, i.e., the values of the stage s and the coefficients, are known. We here exhibit them regarding the lowest order.

Order 2. For $s=1$, the simplest integrator is obtained as

$$\Psi_h = \Phi_{h/2} \circ \Phi^*_{h/2}. \tag{78}$$

This form is frequently used; e.g., for the Newton equation $(\dot{x}, \dot{p}) = X_{\mathrm{N}}(x,p) \equiv (p, F(x)) \in \mathbf{R}^{2n}$, Eq. (78) gives the Störmer/Verlet method when we decompose X_{N} as $X^{[1]}(\omega) \equiv (0, F(x))$ and $X^{[2]}(\omega) \equiv (p, 0)$. For $s=2$,

$$\Psi_h = \Phi_{\alpha h} \circ \Phi^*_{(1/2-\alpha)h} \circ \Phi_{(1/2-\alpha)h} \circ \Phi^*_{\alpha h} \tag{79}$$

can be derived, where the several values of the parameter α are known as effective ones: $\alpha = 0.25$ or 0.1932 was set such that a norm of a certain error function takes the minimum [52]; $\alpha = 0.22$ is an intermediate value of these [51].

An alternative choice of the symmetric composition is

$$\Psi_h = \Phi_{\gamma_s h} \circ \Phi_{\gamma_{s-1} h} \circ \cdots \circ \Phi_{\gamma_2 h} \circ \Phi_{\gamma_1 h}, \tag{80}$$

where Φ_t is a symmetric second-order map with symmetric coefficients of

$$\gamma_i = \gamma_{s+1-i}. \tag{81}$$

Several effective algorithms have been developed; see, e.g., Ref. [53].

b. Divergence-free solvable decomposition. Let us consider the solvable decomposition in Eq. (69). It can be shown that also the field of Eqs. (63) and (64), $X'':\Omega'' \equiv \Omega \times U \to \mathbf{R}^{N+1}$, $\omega' \equiv (\omega, v) \mapsto (X(\omega), -\mathrm{div}\, X(\omega) v)$, has the following solvable decomposition:

$$X'' = X''^{[1]} + X''^{[2]} + \cdots + X''^{[L]}, \tag{82}$$

defined by

$$X''^{[j]}:\Omega'' \to \mathbf{R}^{N+1}, \ (\omega, v) \mapsto (X^{[j]}(\omega), -\mathrm{div}\, X^{[j]}(\omega) v), \tag{83}$$

$j = 1, \ldots, L$. It must be noted that each new field is divergence-free; viz.,

$$\mathrm{div}\, X''^{[j]} = 0 \tag{84}$$

for $j = 1, \ldots, L$. This enables us to construct an integrator with a constant unit Jacobian for Eqs. (63) and (64), as explained below. Notice that this Jacobian for the integrator is *exact*, because the map of the exact flow also has a unit Jacobian due to $\mathrm{div}\, X'' = 0$, according to Eq. (67).

Now, the solvability of Eq. (83) is based on the observation that for $j = 1, \ldots, L$ the solution of $\dot{\omega}' = X''^{[j]}(\omega')$ with an arbitrary initial value $\omega_0' \equiv (\omega_0, v_0) \in \Omega''$ is given by

$$\Phi^{[j]\omega_0'}:\mathbf{R} \to \Omega'', \ t \overset{\mathrm{d}}{\mapsto} (\phi^{[j]}(t), \varphi^{[j]}(t)),$$

where $\phi^{[j]}:\mathbf{R} \to \Omega$ is a solution of

$$\dot{\omega} = X^{[j]}(\omega) \tag{85}$$

with an initial value $\omega_0 \in \Omega$, the form of $\phi^{[j]}$ being explicitly given from the assumption regarding Eq. (69), and

$$\varphi^{[j]}(t) \equiv v_0 \exp\left(\int_0^t -(\mathrm{div}\, X^{[j]})[\phi^{[j]}(s)] ds \right). \tag{86}$$

Therefore, we can get the integrator via the definition of $\Phi_t^{[j]}(\omega') \equiv \Phi^{[j]\omega'}(t)$ and use of Eqs. (72) and (76).

Regarding the Jacobian for the current integrator, we should note that the integrator with any s and any coefficients is constructed purely from the composition of the map of the exact flow of $X''^{[j]}$, $\Phi_t^{[j]}:\Omega'' \to \Omega''$, for $j = 1, \ldots, L$. Notice that the composition of any two differentiable maps f_1, $f_2:\mathbf{R}^N \supset O$ (open) $\to O$, each of which has a unit Jacobian [see the statement above Eq. (67)], also has a unit Jacobian: for *all* ω, $\det[D(f_2 \circ f_1)(\omega)] = \det[Df_2(f_1(\omega))] \det[Df_1(\omega)] = 1$. Now, for all j and for all t, $\Phi_t^{[j]}$ has a unit Jacobian, since Eqs. (43) and (84) establish $\det[D\Phi_t^{[j]}(\omega')]$

$=\exp\{\int_0^t(\mathrm{div}\, X''^{[j]})[\Phi_s^{[j]}(\omega')]ds\}=1$ $(\forall\omega'\in\Omega'')$. Therefore, an arbitrary finite composition for $\Phi_{t_1}^{[1]},\Phi_{t_2}^{[2]},\ldots,\Phi_{t_L}^{[L]}$ with any values of $t_1,t_2,\ldots,t_L$, especially the type of Eqs. (72), (75), and (76), has a unit Jacobian, certifying the volume-preserving property [see, e.g., Eq. (68)] of the integrator Ψ_h (for any h) and the integration $\Psi_h\circ\cdots\circ\Psi_h$.

Let us summarize the discussion about the application of Eq. (62) to the integrator. If X has a solvable decomposition, we can construct a symmetric integrator with a unit Jacobian for an extended ODE defined by Eqs. (63) and (64). The extended ODE does not affect the solution of the original ODE (63) and has flow characterized by a constant unit Jacobian, with the result that the integrator's Jacobian is exact. Moreover, if B satisfies Eq. (17) with $c=1$ and Eq. (18), the extended ODE has the invariant defined by Eq. (65). It is worth noting that even if we lose this condition Eq. (18), the current integrator properties (1)–(5), stated at the beginning of Sec. IV B, hold except (2) ("the invariant can be used"), by considering that Eq. (64) is defined directly by $\dot{v}=-\mathrm{div}\, X(\omega)v$, rather than through $Y(\omega)$. Such a reconsideration concerning this issue will be discussed later.

There are many volume-preserving integrators for divergence-free system; they involve several elaborate devices, e.g., decomposing the vector field into pieces of two-dimensional Hamiltonian fields [30] or constructing an implicitly represented map from the old variables to new variables such that it yields a unit Jacobian [31]. In our method, however, the volume-preserving property arises naturally from the composition of the unit Jacobian map, and each procedure is generally explicit, which are technical aspects distinct from those of the above methods. In addition, our method converts the original ODE into a divergence-free system. One integrator that involves conceptually similar points as ours is the method devised by Legoll and Monneau [54]. There, by devising a suitable change of variables, the original ODE is switched into a system of normal form, which is a stronger condition than the divergence-free property. As explained below, our method accepts also a generalized normal form, which reduces the effort to make up the constitution of geometric integrator.

Now, actually, one must evaluate Eq. (86) by a suitable manner in the process. Let us consider a practical condition that enables us to easily evaluate Eq. (86) for $j\in\{1,\ldots,L\}$. The most general condition is that the mapping $t\mapsto\varphi^{[j]}(t)$ in Eq. (86) can be specifically provided for any solution $\phi^{[j]}$ of Eq. (85). A more definite sufficient condition is

$$(\mathrm{grad}\,\mathrm{div}\, X^{[j]}|X^{[j]})=0. \tag{87}$$

If so, using the relation of

$$\frac{d}{dt}\mathrm{div}\, X^{[j]}(\phi^{[j]}(t)) = \left(\mathrm{grad}\,\mathrm{div}\, X^{[j]}(\phi^{[j]}(t))|X^{[j]}(\phi^{[j]}(t))\right)\ (\forall t\in\mathbf{R}),$$

we can conclude that $\mathrm{div}\, X^{[j]}(\phi^{[j]}(t))$ is constant with respect to t. Hence, the total solution is given explicitly as a simple form

$$\Phi^{[j]\omega_0'}(t)=(\phi^{[j]}(t),v_0\exp[-t\,\mathrm{div}\, X^{[j]}(\omega_0)]). \tag{88}$$

So, it is natural to inquire how general the situation is such that X has a solvable decomposition along with fulfillment of the condition of Eq. (87). We will answer this by presenting once more a sufficient condition and by observing its applicability. The first example of the sufficient condition is that a smooth vector field $X=(X_1,\ldots,X_N)$ on $\Omega\subset\mathbf{R}^N$ has the following "pseudonormal form:"

$$X_i(\omega_1,\ldots,\omega_N)=V_i(\omega_1,\ldots,\omega_{i-1},\omega_{i+1},\ldots,\omega_N) + W_i(\omega_1,\ldots,\omega_{i-1},\omega_{i+1},\ldots,\omega_N)\omega_i, \tag{89}$$

$i=1,\ldots,N$ (note that the normal form is the case of $W_i=0$; viz., X_i is independent of ω_i). We demonstrate the above issue from a second example that takes a more general form: grouping (and permuting if necessary) the variables as $\omega=(\omega_{(1)},\ldots,\omega_{(M)})$ with

$$\omega_{(k)}\in\mathbf{R}^{n_k}\ (k=1,\ldots,M;\textstyle\sum_{k=1}^M n_k=N),$$

we address

$$X=(X_{(1)},\ldots,X_{(M)}):\Omega\to\mathbf{R}^N,\ \omega\mapsto(X_{(1)}(\omega),\ldots,X_{(M)}(\omega))$$

defined by

$$X_{(k)}(\omega_{(1)},\ldots,\omega_{(M)})=V_{(k)}(\overset{k}{\omega^\vee})+\omega_{(k)}\cdot W_{(k)}(\overset{k}{\omega^\vee}), \tag{90}$$

with the abbreviation

$$\overset{k}{\omega^\vee}\equiv(\omega_{(1)},\ldots,\omega_{(k-1)},\omega_{(k+1)},\ldots,\omega_{(M)}), \tag{91}$$

where $V_{(k)}$ and $W_{(k)}$ are smooth maps such that $V_{(k)}(\overset{k}{\omega^\vee})\in\mathbf{R}^{n_k}$ and $W_{(k)}(\overset{k}{\omega^\vee})$ is a real $n_k\times n_k$ matrix, for $k=1,\ldots,M$. Now, when we decompose the X possessing this grouped form of Eq. (90) as

$$X=\sum_{j=1}^{L}X^{[j]} \tag{92}$$

in the following manner, we can straightforwardly see both the validity of Eq. (87) and the solvability of $X^{[j]}$ for each j [even when we cannot have eigenvalues of $W_{(k)}(\overset{k}{\omega^\vee})$ we can reach them by decomposing ω in a suitable way]:

$$X^{[j]}(\omega)\equiv\left(\overset{n_1}{\breve{0}},\ldots,\overset{n_{j-1}}{\breve{0}},V_{(j)}(\overset{j}{\omega^\vee}),\overset{n_{j+1}}{\breve{0}},\ldots,\overset{n_M}{\breve{0}}\right), \tag{93}$$

$$X^{[M+j]}(\omega)\equiv\left(\overset{n_1}{\breve{0}},\ldots,\overset{n_{j-1}}{\breve{0}},\omega_{(j)}\cdot W_{(j)}(\overset{j}{\omega^\vee}),\overset{n_{j+1}}{\breve{0}},\ldots,\overset{n_M}{\breve{0}}\right), \tag{94}$$

for $j=1,\ldots,M$ with $L\leqslant 2M$ [identically vanishing fields are omitted from Eq. (92)]. Now, the condition of Eq. (90) still admits the following application to MD equations. The fundamental form can already be observed through the NH field in Eq. (1); viz., the friction term corresponds to $\omega_{(k)}W_{(k)}(\overset{k}{\omega^\vee})$ and the other term corresponds to $V_{(k)}(\overset{k}{\omega^\vee})$ (see Sec. IV B 2). The NHC field X_{NHC} in Eq. (23) is also in the

form of Eq. (90), and some *NTV* equations, such as those in Refs. [38,55], take this form. The *NTP* equation demonstrated in, e.g., Refs. [19,56] (both the isotropic-cell and full-cell forms) falls into this category. Note that, of course, our formalism also accepts an intermediate case such that $X=Y+Z$, where Y has this form and Z may not have the form but is solvable and is endowed with specifically given $\int_0^t(\mathrm{div}\, Z)[\phi^Z(s)]ds$ for any solution ϕ^Z of $\dot{\omega}=Z(\omega)$.

Although the current method explained so far is acceptable to any number of dimensions of the original phase space, the parity of the space dimension is changed by adding one extended variable v. However, there is a case in which one would start from an original phase space of even dimensions and get the extended space also of even dimensions [38,39]. Adding two extended variables v_1 and v_2 and considering an extended ODE

$$\dot{\omega}'' = X''(\omega'') \tag{95}$$

with $\omega'' \equiv (\omega, v_1, v_2)$ can satisfy such a requirement for an original smooth field X on Ω. In what follows, we introduce two specific formulations. Likewise in Eqs. (63) and (64), we assume that B satisfies Eq. (17) (by smooth ρ with $c=1$) and Eq. (18). The first one is to assume $\lambda(v) \equiv v/2$ and consider on $\Omega'' \equiv \Omega \times \mathbf{R}_\times \times \mathbf{R}_\times$ ($\mathbf{R}_\times \equiv \mathbf{R}\backslash\{0\}$) an extended ODE (95) defined by

$$\dot{\omega} = X(\omega), \tag{96a}$$

$$\dot{v}_a = Y(\omega)\lambda(v_a) = -\frac{1}{2}\,\mathrm{div}\, X(\omega) v_a, \quad a = 1,2, \tag{96b}$$

in which Eqs. (8) and (19) are operated. As seen from a similar consideration given in Proposition 2, we can assert that the two functions defined by

$$L_a(\omega, v_1, v_2) \equiv B(\omega) + 2 \ln v_a \quad (a = 1,2) \tag{97}$$

are invariants of the extended ODE. Under the assumption of the solvable decomposition of X in Eq. (69), $X''=\Sigma_{j=1}^L X''^{[j]}$, designated by

$$X''^{[j]}(\omega'') \equiv \left(X^{[j]}(\omega), -\frac{1}{2}\,\mathrm{div}\, X^{[j]}(\omega) v_1, -\frac{1}{2}\,\mathrm{div}\, X^{[j]}(\omega) v_2 \right), \tag{98}$$

$j=1,\ldots,L$, brings a divergence-free solvable decomposition. For $j=1,\ldots,L$, as well as the validity of $\mathrm{div}\, X''^{[j]}=0$, the solvability can be easily checked: the solution of $\dot{\omega}''=X''^{[j]}(\omega'')$ with an initial value

$$\omega_0'' \equiv (\omega_0, v_{1,0}, v_{2,0}) \tag{99}$$

in Ω'' is given by the same manner with that for the single extended-variable case except that

$$\varphi^{[j]}: t \mapsto \exp\left(-\frac{1}{2}\Upsilon^{[j]}(t) \right)(v_{1,0}, v_{2,0}) \in \mathbf{R}^2 \tag{100}$$

[cf. Eq. (86)], where

$$\Upsilon^{[j]}(t) \equiv \int_0^t (\mathrm{div}\, X^{[j]})[\phi^{[j]}(s)]ds. \tag{101}$$

The second one is to consider $\lambda(v) \equiv v$ and an extended ODE:

$$\dot{\omega} = X(\omega), \tag{102a}$$

$$\dot{v}_1 = Y(\omega)\lambda(v_1) = -\,\mathrm{div}\, X(\omega) v_1, \tag{102b}$$

$$\dot{v}_2 = Y(\omega) = -\,\mathrm{div}\, X(\omega). \tag{102c}$$

Again using the procedure similar above, we get invariants of the extended ODE, $\omega'' \mapsto B(\omega) + \ln v_1$ and $\omega'' \mapsto B(\omega) + v_2$, and get a divergence-free solvable decomposition $X''=\Sigma_{j=1}^L X''^{[j]}$ as

$$X''^{[j]}(\omega'') \equiv (X^{[j]}(\omega), -\,\mathrm{div}\, X^{[j]}(\omega) v_1, -\,\mathrm{div}\, X^{[j]}(\omega)), \tag{103}$$

from the assumption of the solvable decomposition of X. The extended components of the solution of $\dot{\omega}''=X''^{[j]}(\omega'')$ are now described by

$$\varphi^{[j]}(t) \equiv (\exp[-\Upsilon^{[j]}(t)] v_{1,0}, -\Upsilon^{[j]}(t) + v_{2,0}) \in \mathbf{R}^2, \tag{104}$$

for $j=1,\ldots,L$. Note that the analysis given in the previous two paragraphs also applies to the current two formulations, wherein the issues addressed are the solvable decomposition of an original field X and the evaluation of the time integral in Eq. (86), viz., Eq. (101).

Now, in the approach examined thus far, compatibility of the four properties of the integrator [(1), (3)–(5) indicated at the top of Sec. IV B] and having the invariant is attained under the assumption of Eqs. (17) and (18). We remark that one solution to get rid of this assumption for this compatibility can be presented by "twisting" Eqs. (102a)–(102c) with the simplest technique prepared in Sec. III A. That is to consider an extended ODE on $\Omega'' \equiv \Omega \times \mathbf{R}_\times \times \mathbf{R}$:

$$\dot{\omega} = X(\omega), \tag{105a}$$

$$\dot{v}_1 = -\,\mathrm{div}\, X(\omega) v_1, \tag{105b}$$

$$\dot{v}_2 = Y(\omega). \tag{105c}$$

It should be noted that the completely distinguishable point in Eqs. (105b) and (105c) from that in Eqs. (102b) and (102c) is that (i) Y in Eq. (105c) is defined only through an arbitrary smooth function B by Eq. (8), so that $Y(\omega)$ is no longer necessarily equal to $-\mathrm{div}\, X(\omega)$ [like Eq. (102c)] since we now lose the assumption stated above; (ii) the equation form of v_1 is fixed and independent of Y (viz., irrelevant to the choice of B and ρ). The quantity $B(\omega)+v_2$ defines an invariant, and a divergence-free solvable decomposition $X''=\Sigma_{j=1}^L X''^{[j]}$ is constituted by

$$X''^{[j]}(\omega'') \equiv (X^{[j]}(\omega), -\,\mathrm{div}\, X^{[j]}(\omega) v_1, Y^{[j]}(\omega)), \tag{106}$$

with $Y^{[j]}(\omega) \equiv -(X^{[j]}(\omega) \,|\, \mathrm{grad}\, B(\omega))$ ($\omega \in \Omega$, $j=1,\ldots,L$) by means of the solvable decomposition of X [Eq. (69)]. For the solution of $\dot{\omega}''=X''^{[j]}(\omega'')$ with an initial value ω_0'' [Eq. (99)]

in Ω'', the components for ω and v_1 are the same with those given previously, and the component for v_2 is presented explicitly as $v_{2,0}+\int_0^t Y^{[j]}(\phi^{[j]}(s))ds=v_{2,0}+B(\phi^{[j]}(0))-B(\phi^{[j]}(t))$. Thus, in fact, this decomposition provides the solvability, and also the previous discussion about the solvable decomposition of X and the evaluation of Eq. (101) exactly applies.

2. Integrator for the Nosé-Hoover equation

To illustrate the proposed integrator demonstrated in Sec. IV B 1, we here apply the single-extended-variable formulation to the NH equation. Although the applicability is clear from the previous demonstration, we present the concrete procedure to make the discussion explicit. The NH field in Eq. (1) takes the form of Eq. (90) as

$$X_{\mathrm{NH}}:\Omega \equiv D \times \mathbf{R}^n \times \mathbf{R}^1 \to \mathbf{R}^{2n+1},$$

$$\begin{aligned}\omega \equiv (x,p,\zeta) &\equiv (\omega_{(1)},\omega_{(2)},\omega_{(3)}) \\ &\mapsto (p\cdot\mathbf{M}^{-1},-\nabla U(x)-p\cdot(\zeta/Q)\mathbf{1},2K(p)-nk_{\mathrm{B}}T) \\ &\equiv (X_{(1)}(\omega),X_{(2)}(\omega),X_{(3)}(\omega)),\end{aligned} \tag{107}$$

where $\mathbf{M}\equiv\mathrm{diag}(m_1,\ldots,m_n)$ is the matrix for the mass parameter and U is a smooth function on domain $D\subset\mathbf{R}^n$, so that $X_{\mathrm{NH}}=\Sigma_{j=1}^{L}X^{[j]}$ with $L\equiv 4$ described by

$$X^{[1]}(\omega) \equiv (p\cdot\mathbf{M}^{-1},0,0), \tag{108}$$

$$X^{[2]}(\omega) \equiv (0,-\nabla U(x),0), \tag{109}$$

$$X^{[3]}(\omega) \equiv (0,0,2K(p)-nk_{\mathrm{B}}T), \tag{110}$$

$$X^{[4]}(\omega) \equiv (0,-p\cdot(\zeta/Q)\mathbf{1},0) \tag{111}$$

comprises a solvable decomposition and satisfies Eq. (87). Consequently, we have the extended vector field represented, for $\omega'\equiv(\omega,v)=(x,p,\zeta,v)$, by

$$X''^{[1]}(\omega') \equiv (p\cdot\mathbf{M}^{-1},0,0,0), \tag{112}$$

$$X''^{[2]}(\omega') \equiv (0,-\nabla U(x),0,0), \tag{113}$$

$$X''^{[3]}(\omega') \equiv (0,0,2K(p)-nk_{\mathrm{B}}T,0), \tag{114}$$

$$X''^{[4]}(\omega') \equiv (0,-(\zeta/Q)p,0,(n\zeta/Q)v) \tag{115}$$

and the corresponding complete exact flows $\Phi_t^{[j]}$:

$$\Phi_t^{[1]}:\omega' \mapsto (tp\cdot\mathbf{M}^{-1}+x,p,\zeta,v), \tag{116}$$

$$\Phi_t^{[2]}:\omega' \mapsto (x,-t\nabla U(x)+p,\zeta,v), \tag{117}$$

$$\Phi_t^{[3]}:\omega' \mapsto (x,p,(2K(p)-nk_{\mathrm{B}}T)t+\zeta,v), \tag{118}$$

$$\Phi_t^{[4]}:\omega' \mapsto (x,e^{-(\zeta/Q)t}p,\zeta,e^{(n\zeta/Q)t}v). \tag{119}$$

If we define B by Eq. (17) with $c=1$ using Eq. (21) and $\rho_z(\zeta)\equiv\exp(-\zeta^2/2k_{\mathrm{B}}TQ)$, then Eq. (18) is fulfilled (globally), so that the extended ODE has the invariant of Eq. (65).

Now, as observed in Eq. (76), our integrator is constructed from the basic form of

$$\Phi_t\circ\Phi_{t'}^{*} \tag{120}$$

$$=\Phi_t^{[1]}\circ\Phi_t^{[2]}\circ\Phi_t^{[3]}\circ\Phi_{t+t'}^{[4]}\circ\Phi_{t'}^{[3]}\circ\Phi_{t'}^{[2]}\circ\Phi_{t'}^{[1]}, \tag{121}$$

ensuring that the force evaluation among the particles is performed once; this is the most time-consuming operand in Eqs. (116)–(119): such evaluation is done only in the $\Phi_t^{[2]}$ map and appears twice in Eq. (121); actually, the left $\Phi_t^{[2]}$ needs just the reference of the $\nabla U(x)$ value evaluated in the right $\Phi_{t'}^{[2]}$ because the coordinate change is done only in the $\Phi_h^{[1]}$ map and because no such a map exists between the $\Phi_t^{[2]}$ and $\Phi_{t'}^{[2]}$. So the evaluation is performed once for Eq. (78) and twice for Eq. (79). Also note that although indefiniteness exists in the arrangements among $\{\Phi_t^{[1]},\Phi_t^{[2]},\Phi_t^{[3]},\Phi_t^{[4]}\}$ for Φ_t in the construction of Eq. (120) (they are not equivalent in general; however, they have the same order of accuracy as integrator), the force evaluation is always done once against any permutation. This is because the sequence appears only in the form of either $(\cdots1\cdots2\cdots2\cdots1\cdots)$ or $(\cdots2\cdots1\cdots1\cdots2\cdots)$ due to the symmetry in Eq. (120); the former is the case of Eq. (121) while in the latter, the force value for the right $\Phi_{t'}^{[2]}$ can be referenced to that obtained in the preceding stage. Accordingly, the number of force evaluations corresponds to the value of s and depends only on it.

We remark that Klein has investigated the isothermal-isobaric MD equation in detail with a consideration of integrators and boundary conditions [57]. For the NH equation, in fact, an integrator has already been derived, which is essentially the same as that in our simplest example, Eq. (78). However, Klein's work is based on the partial error cancellation technique while ours is based on the effective symmetric composition, resulting in different integrators, e.g., Eq. (79). Furthermore, for general ODEs we have constructed a theoretical framework and provided several specific conditions for acquiring a practical divergence-free solvable decomposition, resulting in the construction of an integrator with an exact unit Jacobian. Also, our integrator is distinguishable from that obtained by Refs. [19,48], because the latter integrators are based on hierarchical use of the composition along the lines of the Yoshida/Suzuki method [15,58,59] (note that commutative maps among $\{\Phi_{h_1}^{[1]},\Phi_{h_2}^{[2]},\Phi_{h_3}^{[3]},\Phi_{h_4}^{[4]}\}$ with respect to arbitrary values of h_j are only $\Phi_{h_1}^{[1]}$ and $\Phi_{h_3}^{[3]}$ when $\nabla U\neq 0$, so that differences in their arrangement as well as the coefficient values yield no equivalence) together with, in principle, a nonunity Jacobian.

In view of the computational overhead and accuracy, a numerical comparison among the current integrators and the conventional one for applications to various systems and conditions is being studied and will be given elsewhere.

V. CONCLUSION

For an arbitrary ODE, we provided a method for constructing an extended ODE and the extended invariant,

which is not necessarily based on the concept of energy. The extended ODE retains every solution of the original ODE and accompanies the invariant function. To investigate the connection between the current invariant and the conventional relevant quantities in MD, we considered a situation such that the phase-space function applied in our formulation is $B \equiv -c \ln \rho$. In the case that the ODE globally satisfies the Liouville condition for a density ρ, our extended invariant has been shown to agree with Stern's quantity. Specifically, for NHC and KBB equations, which are BGD carrying the BG distribution density, our extended invariant recovers each conserved quantity conventionally provided. The next case demonstrates the system described by the local Liouville condition with a characterization of the GI equation as a specific example; we showed that the current extended invariant coincides with the Terada-Kidera extended invariant, which is intimately related to the originally proposed Terada-Kidera conserved quantity. In addition, we derived an (extended) invariant for the TD equation carrying the Tsallis distribution density instead of the BG density. The current method thereby allows a unified description of conserved quantities in MD equations and enables us to easily constitute an invariant for an arbitrary ODE, including that newly developed for a variety of purposes.

As well as the simple construction of an invariant that helps to check the accuracy of a numerical integration, for a certain class of ODEs this constitution idea was shown to facilitate the development of the numerical integrator itself. For an arbitrary ODE having a solvable decomposition of the vector field, we derived a framework for the construction of an efficient numerical integrator regarding a renewed extended ODE. This was done by generalizing the above protocol and developing a technique of divergence-free solvable decomposition of the extended vector field, and by combining them with the symmetric composition method. The resulting integrator is symmetric and carries an exact unit Jacobian together with the invariant function on the extended ODE. We theoretically investigated their characteristics in detail with comparison to other methods and provided several specific conditions for practical constitution of an explicit integrator. We expect that the current simple technique for constructing an explicit symmetric volume-preserving integrator on an extended system will be efficiently used in many applications.

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