Exact Invariants for a Class of Three-Dimensional Time-Dependent Classical Hamiltonians

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(Received 26 April 2000; revised manuscript received 8 June 2000)

An exact invariant is derived for three-dimensional Hamiltonian systems of N particles confined within a general velocity-independent potential. The invariant is found to contain a time-dependent function $f_2(t)$, embodying a solution of a third-order differential equation whose coefficients depend on the explicitly known trajectories of the particle ensemble. Our result is applied to a one-dimensional time-dependent nonlinear oscillator and to a system of Coulomb interacting particles in a time-dependent quadratic external potential.

PACS numbers: 41.85.–p, 45.50.Jf

We consider a system of a nonrelativistic ensemble of N particles of the same species moving in an explicitly time-dependent and velocity-independent potential, whose Hamiltonian H takes the form

$$H = \sum_{i=1}^{N} \tfrac{1}{2}[p_{x,i}^2 + p_{y,i}^2 + p_{z,i}^2] + V(\vec{x},\vec{y},\vec{z},t), \qquad (1)$$

with $\vec{x}$, $\vec{y}$, and $\vec{z}$ the N component vectors of the spatial coordinates of all particles. It is hereby assumed that the system may be completely described within $6N$-dimensional Cartesian phase space spanned by the $3N$ particle coordinates and their conjugate momenta. From the canonical equations, we derive for each particle i the equations of motion

$$\dot{x}_i = p_{x,i}, \qquad \dot{p}_{x,i} = -\frac{\partial V(\vec{x},\vec{y},\vec{z},t)}{\partial x_i}, \qquad (2)$$

and likewise for the y and z degrees of freedom. The solution functions $\vec{x}(t)$, $\vec{y}(t)$, $\vec{z}(t)$, and $\vec{p}_x(t)$, $\vec{p}_y(t)$, $\vec{p}_z(t)$ define a path within the $6N$-dimensional phase space that completely describes the system's time evolution. A quantity

$$I = I[\vec{x}(t),\vec{p}_x(t),\vec{y}(t),\vec{p}_y(t),\vec{z}(t),\vec{p}_z(t),t] \qquad (3)$$

constitutes an invariant of the particle motion if its total time derivative vanishes:

$$\frac{dI}{dt} = \frac{\partial I}{\partial t} + \sum_{i=1}^{N}\left[\frac{\partial I}{\partial x_i}\dot{x}_i + \frac{\partial I}{\partial y_i}\dot{y}_i + \frac{\partial I}{\partial z_i}\dot{z}_i + \frac{\partial I}{\partial p_{x,i}}\dot{p}_{x,i} + \frac{\partial I}{\partial p_{y,i}}\dot{p}_{y,i} + \frac{\partial I}{\partial p_{z,i}}\dot{p}_{z,i}\right] = 0.$$

We examine the existence of a conserved quantity (3) for a system described by (1) with a special ansatz for I being at most quadratic in the velocities [1]

$$I = \sum_i [f_2(t)(p_{x,i}^2 + p_{y,i}^2 + p_{z,i}^2) + f_1(x_i,t)p_{x,i} + g_1(y_i,t)p_{y,i} + h_1(z_i,t)p_{z,i}] + f_0(\vec{x},\vec{y},\vec{z},t). \qquad (4)$$

The set of functions $f_2(t)$, $f_1(x_i,t)$, $g_1(y_i,t)$, $h_1(z_i,t)$, and $f_0(\vec{x},\vec{y},\vec{z},t)$ that render I invariant are to be determined. With the single particle equations of motion (2), a vanishing total time derivative of Eq. (4) means explicitly

$$\sum_i\Bigg[(\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2)\frac{df_2}{dt} + \dot{x}_i\frac{\partial f_1}{\partial t} + \dot{y}_i\frac{\partial g_1}{\partial t} + \dot{z}_i\frac{\partial h_1}{\partial t} + \dot{x}_i^2\frac{\partial f_1}{\partial x_i} + \dot{y}_i^2\frac{\partial g_1}{\partial y_i} + \dot{z}_i^2\frac{\partial h_1}{\partial z_i} + \dot{x}_i\frac{\partial f_0}{\partial x_i} + \dot{y}_i\frac{\partial f_0}{\partial y_i} + \dot{z}_i\frac{\partial f_0}{\partial z_i} - (2f_2\dot{x}_i + f_1)\frac{\partial V}{\partial x_i} - (2f_2\dot{y}_i + g_1)\frac{\partial V}{\partial y_i} - (2f_2\dot{z}_i + h_1)\frac{\partial V}{\partial z_i}\Bigg] + \frac{\partial f_0}{\partial t} = 0. \qquad (5)$$

We may arrange the terms of this equation with regard to their power in the velocities $\dot{x}_i$, $\dot{y}_i$, and $\dot{z}_i$. Equation (5) must hold independently of the specific phase-space location of each individual particle i. Therefore, the coefficients pertaining to the velocity powers must vanish separately for each index i. The condition for the terms proportional to $\dot{x}_i^2$ is

$$\frac{\partial f_1(x_i,t)}{\partial x_i} + \frac{df_2(t)}{dt} = 0,$$

and similarly for the functions g_1 and h_1. It follows that $f_1(x_i,t)$, $g_1(y_i,t)$, and $h_1(z_i,t)$ must be linear functions in x_i, y_i, and z_i, respectively,

$$f_1(x_i,t) = -\dot{f}_2(t)x_i + b_{x,i}(t), \qquad (6a)$$

$$g_1(y_i,t) = -\dot{f}_2(t)y_i + b_{y,i}(t), \qquad (6b)$$

$$h_1(z_i,t) = -\dot{f}_2(t)z_i + b_{z,i}(t), \qquad (6c)$$

with $b_{x,i}(t)$, $b_{y,i}(t)$, and $b_{z,i}(t)$ defined as arbitrary functions of time only.

The terms of Eq. (5) that are linear in $\dot{x}_i$ sum up to

$$\frac{\partial f_1}{\partial t} + \frac{\partial f_0}{\partial x_i} - 2f_2(t)\frac{\partial V}{\partial x_i} = 0. \qquad (7)$$

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In order to eliminate $\partial f_1/\partial t$ from (7), we calculate the partial time derivative of $f_1(x_i, t)$ from Eq. (6a):

$$\frac{\partial f_1}{\partial t} = -\ddot{f}_2(t)x_i + \dot{b}_{x,i}(t). \tag{8}$$

Again, similar expressions apply to $\partial g_1/\partial t$ and $\partial h_1/\partial t$. Inserting (8) into (7), and solving for the terms containing the partial derivatives of the yet unknown but arbitrary ancillary function $f_0(\vec{x}, \vec{y}, \vec{z}, t)$, one obtains the following three differential equations for f_0:

$$\frac{\partial f_0}{\partial x_i} = \ddot{f}_2(t)x_i - \dot{b}_{x,i}(t) + 2f_2(t)\frac{\partial V}{\partial x_i}, \tag{9a}$$

$$\frac{\partial f_0}{\partial y_i} = \ddot{f}_2(t)y_i - \dot{b}_{y,i}(t) + 2f_2(t)\frac{\partial V}{\partial y_i}, \tag{9b}$$

$$\frac{\partial f_0}{\partial z_i} = \ddot{f}_2(t)z_i - \dot{b}_{z,i}(t) + 2f_2(t)\frac{\partial V}{\partial z_i}. \tag{9c}$$

A function $f_0(\vec{x}, \vec{y}, \vec{z}, t)$ with partial derivatives (9) is obviously given by

$$f_0(\vec{x}, \vec{y}, \vec{z}, t) = 2f_2(t)V(\vec{x}, \vec{y}, \vec{z}, t) + \sum_i [\tfrac{1}{2}\ddot{f}_2(x_i^2 + y_i^2 + z_i^2) - \dot{b}_{x,i}x_i - \dot{b}_{y,i}y_i - \dot{b}_{z,i}z_i]. \tag{10}$$

The remaining terms of Eq. (5) do not depend on the velocities $\dot{x}_i$, $\dot{y}_i$, and $\dot{z}_i$. With (6), these terms impose the following condition for I to embody an invariant of the particle motion:

$$\sum_i \left[(\dot{f}_2 x_i - b_{x,i})\frac{\partial V}{\partial x_i} + (\dot{f}_2 y_i - b_{y,i})\frac{\partial V}{\partial y_i} + (\dot{f}_2 z_i - b_{z,i})\frac{\partial V}{\partial z_i} \right] + \frac{\partial f_0}{\partial t} = 0. \tag{11}$$

In order to express Eq. (11) in a closed form for $f_2(t)$, one has to eliminate $\partial f_0/\partial t$. To this end, we calculate the partial time derivative of Eq. (10), i.e., the time derivative at fixed particle coordinates x_i, y_i, and z_i:

$$\frac{\partial f_0(\vec{x}, \vec{y}, \vec{z}, t)}{\partial t} = 2\dot{f}_2(t)V + 2f_2(t)\frac{\partial V}{\partial t} + \sum_i [\tfrac{1}{2}\dddot{f}_2(x_i^2 + y_i^2 + z_i^2) - \ddot{b}_{x,i}x_i - \ddot{b}_{y,i}y_i - \ddot{b}_{z,i}z_i]. \tag{12}$$

Inserting Eq. (12) into Eq. (13), we finally get a linear third-order differential equation for $f_2(t)$ and the $b_{x,y,z;i}(t)$ that depends only on the spatial variables of the particle ensemble

$$\begin{aligned} 2\dot{f}_2(t)V + 2f_2(t)\frac{\partial V}{\partial t} + \sum_i \Bigg[\tfrac{1}{2}\dddot{f}_2(t)(x_i^2 + y_i^2 + z_i^2) + \dot{f}_2(t)\left(x_i\frac{\partial V}{\partial x_i} + y_i\frac{\partial V}{\partial y_i} + z_i\frac{\partial V}{\partial z_i} \right) + \\ b_{x,i}\ddot{x}_i - \ddot{b}_{x,i}x_i + b_{y,i}\ddot{y}_i - \ddot{b}_{y,i}y_i + b_{z,i}\ddot{z}_i - \ddot{b}_{z,i}z_i \Bigg] = 0. \end{aligned} \tag{13}$$

At this point, it is helpful to review our derivation made so far. Speaking of an invariant I of the particle motion means explicitly to pinpoint a quantity (3) that is conserved along the phase-space path representing the system's time evolution. This path is defined as the subset of the $6N$-dimensional phase space on which the equations of motion (2) are fulfilled. In order to work out the invariant I of the particle motion, the equations of motion (2) have been inserted into the expression for $dI/dt = 0$ in Eq. (5). This means that the domain of (5), and hence the physical significance of the subsequent equation (13), is restricted to the actual phase-space path. Along the phase-space path, all terms of Eq. (13) that depend on the particle trajectories are in fact functions of the parameter t only. Accordingly, the potential $V[\vec{x}(t), \vec{y}(t), \vec{z}(t), t]$ and its derivatives are time-dependent coefficients of an ordinary differential equation for $f_2(t)$. In contrast to Ref. [1], Eq. (13) is not conceived as a partial differential equation for V in our context.

With $f_2(t)$ representing a solution of (13), the invariant I follows from (4), (6), and (10) together with the Hamiltonian (1) as

$$\begin{aligned} I = 2f_2(t)H + \sum_i [-\dot{f}_2(t)(x_i p_{x,i} + y_i p_{y,i} + z_i p_{z,i}) + \tfrac{1}{2}\ddot{f}_2(t)(x_i^2 + y_i^2 + z_i^2) \\ + b_{x,i}p_{x,i} - \dot{b}_{x,i}x_i + b_{y,i}p_{y,i} - \dot{b}_{y,i}y_i + b_{z,i}p_{z,i} - \dot{b}_{z,i}z_i]. \end{aligned} \tag{14}$$

The invariant (14) is easily shown to embody a time integral of Eq. (13) by calculating the total time derivative of (14) and by inserting the single particle equations of motion (2). Hence, Eq. (14) provides a time integral of Eq. (13) if and only if the system's evolution is governed by the equations of motion (2).

From their definition in Eqs. (6), $b_{x,i}(t)$, $b_{y,i}(t)$, and $b_{z,i}(t)$ are arbitrary functions of time that do not depend on $f_2(t)$. As a consequence, the sums over the terms containing the respective functions in Eq. (13) must vanish separately:

$$\dot{f}_2(t)\left(2V + \sum_{i=1}^{N}\left[x_i\frac{\partial V}{\partial x_i} + y_i\frac{\partial V}{\partial y_i} + z_i\frac{\partial V}{\partial z_i} \right] \right) + 2f_2(t)\frac{\partial V}{\partial t} + \dddot{f}_2(t)\sum_{i=1}^{N}\tfrac{1}{2}(x_i^2 + y_i^2 + z_i^2) = 0, \tag{15}$$

$$b_{x,i}\ddot{x}_i - \ddot{b}_{x,i}x_i = 0, \qquad b_{y,i}\ddot{y}_i - \ddot{b}_{y,i}y_i = 0, \qquad b_{z,i}\ddot{z}_i - \ddot{b}_{z,i}z_i = 0, \qquad i = 1, \ldots, N. \tag{15'}$$

We thus obtain the following distinct invariants:

$$I_{f_2} = 2f_2(t)H - \dot{f}_2(t)\sum_{i=1}^{N}(x_i p_{x,i} + y_i p_{y,i} + z_i p_{z,i}) + \ddot{f}_2(t)\sum_{i=1}^{N}\tfrac{1}{2}(x_i^2 + y_i^2 + z_i^2), \tag{16}$$

$$I_{b_{x,i}} = b_{x,i}p_{x,i} - \dot{b}_{x,i}x_i, \qquad I_{b_{y,i}} = b_{y,i}p_{y,i} - \dot{b}_{y,i}y_i, \qquad I_{b_{z,i}} = b_{z,i}p_{z,i} - \dot{b}_{z,i}z_i, \qquad i = 1,\dots,N. \tag{16'}$$

Regarding Eq. (15), one finds that for the special case $\partial V/\partial t \equiv 0$; hence for autonomous systems, $f_2(t) = \text{const}$ is always a solution of Eq. (15). For this case, the invariant (16) reduces to $I_{f_2} \propto H$, thus providing the system's total energy, which is a known invariant for Hamiltonian systems with no explicit time dependence. Nevertheless, Eq. (15) also allows for solutions $f_2(t) \neq \text{const}$ for these systems. We thereby obtain other nontrivial invariants for autonomous systems that exist in addition to the invariant representing the energy conservation law.

Equation (15) can be significantly simplified for potentials V that may be expressed as a sum of homogeneous functions $V = \sum_m V_m$. By definition, V_m is referred to as homogeneous if for every real $\lambda > 0$ and all $\vec{x}$, $\vec{y}$, and $\vec{z}$ the condition

$$V_m(\lambda\vec{x}, \lambda\vec{z}, \lambda\vec{z}, t) = \lambda^{k_m} V_m(\vec{x}, \vec{z}, \vec{z}, t)$$

is satisfied, k_m specifying the degree of homogeneity of V_m. With V a sum of homogeneous functions, Euler's relation may be written as

$$\sum_{i=1}^{N}\left[x_i\frac{\partial V}{\partial x_i} + y_i\frac{\partial V}{\partial y_i} + z_i\frac{\partial V}{\partial z_i}\right] = \sum_m k_m V_m. \tag{17}$$

Using (17), the differential equation (15) for $f_2(t)$ finally reads for homogeneous potential functions V_m

$$2f_2\frac{\partial V}{\partial t} + \dot{f}_2\sum_m (k_m + 2)V_m + \dddot{f}_2\sum_{i=1}^{N}\tfrac{1}{2}(x_i^2 + y_i^2 + z_i^2) = 0. \tag{18}$$

As a simple example, we investigate the one-dimensional nonlinear Hamiltonian system of a time-dependent "asymmetric spring," defined by

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}\omega^2(t)x^2 + a(t)x^3. \tag{19}$$

The related equation of motion follows as

$$\ddot{x} + \omega^2(t)x + 3a(t)x^2 = 0. \tag{20}$$

The invariant I_{f_2} is immediately found writing down the general invariant (16) for one dimension and one particle with the Hamiltonian H given by (19)

$$I_{f_2} = f_2(p^2 + \omega^2x^2 + 2ax^3) - \dot{f}_2xp + \tfrac{1}{2}\ddot{f}_2x^2. \tag{21}$$

The function $f_2(t)$ for this particular case is given as a solution of the third-order differential equation

$$\dddot{f}_2 + 4\dot{f}_2\omega^2 + 4f_2\omega\dot{\omega} + x(t)(4f_2\dot{a} + 10\dot{f}_2a) = 0, \tag{22}$$

which follows from (15) or, equivalently, from (18). Since the particle trajectory $x = x(t)$ is explicitly contained in Eq. (22), it must be known prior to integrating Eq. (22). The trajectory is obtained integrating the equation of motion (20).

We may easily convince ourselves that I_{f_2} is indeed a conserved quantity. Calculating the total time derivative of Eq. (21), and inserting the equation of motion (20), we end up with Eq. (22), which is fulfilled by a definition of $f_2(t)$ for the given trajectory $x = x(t)$.

The third-order equation (22) may be converted into a coupled set of first- and second-order equations. With the substitution $\rho_x^2(t) \equiv f_2(t)$, the second-order equation writes

$$\ddot{\rho}_x + \omega^2(t)\rho_x - \frac{g_x(t)}{\rho_x^3} = 0. \tag{23}$$

Equation (23) is equivalent to (22), provided that the time derivative of the function $g_x(t)$, introduced in (23), is given by

$$\dot{g}_x(t) = -x(t)(2\dot{a}\rho_x^4 + 10a\rho_x^3\dot{\rho}_x). \tag{24}$$

Expressing the invariant (21) in terms of $\rho_x(t)$, we get inserting the auxiliary equation (23)

$$I_{\rho_x} = (\rho_x p - \dot{\rho}_x x)^2 + \frac{x^2}{\rho_x^2}g_x(t) + 2a(t)\rho_x^2x^3. \tag{25}$$

The invariant (25) reduces to the well-known Lewis invariant [2,3] for the time-dependent harmonic oscillator if $a(t) \equiv 0$, which means that $g_x(t) = \text{const}$. For this particular case, Eq. (24), and hence Eq. (23), no longer depends on the specific particle trajectory $x = x(t)$. Consequently, the solution functions $\rho_x(t)$ and $\dot{\rho}_x(t)$ apply to all trajectories that follow from $\ddot{x} + \omega^2(t)x = 0$. With regard to Eq. (15), we conclude that a decoupling from the equations of motion (2) may occur for linear systems only.

A more challenging example is constituted by an ensemble of Coulomb interacting particles of the same species moving in a time-dependent quadratic external potential, as typically given in the comoving frame for charged particle beams that propagate through linear external focusing devices

$$V(\vec{x}, \vec{y}, \vec{z}, t) = \sum_i\left[\tfrac{1}{2}\omega_x^2(t)x_i^2 + \tfrac{1}{2}\omega_y^2(t)y_i^2 + \tfrac{1}{2}\omega_z^2(t)z_i^2 + \tfrac{1}{2}\sum_{j\neq i}\frac{c_1}{r_{ij}}\right], \tag{26}$$

with $r_{ij}^2 = (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2$ and $c_1 = q^2/4\pi\epsilon_0 m$, q and m denoting the particles' charge and mass, respectively. The equations of motion that follow from (2) with (26) are

$$\ddot{x}_i + \omega_x^2(t)x_i - c_1\sum_{j\neq i}\frac{x_i - x_j}{r_{ij}^3} = 0, \tag{27}$$

and likewise for the y and z degrees of freedom. We note that the factor $1/2$ in front of the Coulomb interaction term in (26) disappears since each term occurs twice in the symmetric form of the double sum.

Equation (26) may be split into a sum of two homogeneous functions, namely, the focusing potential part with the degree of homogeneity $k_1 = 2$, and the Coulomb interaction part, the latter with the degree $k_2 = -1$. Consequently, the third-order differential equation (18) for $f_2(t)$ reads (after rearranging)

$$\sum_i \bigg[\dot{f}_2 \sum_{j \neq i} \frac{c_1}{r_{ij}} + x_i^2(\dddot{f}_2 + 4\dot{f}_2\omega_x^2 + 4f_2\omega_x\dot{\omega}_x) + y_i^2(\dddot{f}_2 + 4\dot{f}_2\omega_y^2 + 4f_2\omega_y\dot{\omega}_y) + z_i^2(\dddot{f}_2 + 4\dot{f}_2\omega_z^2 + 4f_2\omega_z\dot{\omega}_z)\bigg] = 0. \quad (28)$$

Of course, the same result is obtained if the potential function (26) is directly inserted into Eq. (15).

The invariant I_{f_2} for a system determined by the Hamiltonian (1) containing the potential (26) is given by (16), provided that $f_2(t)$ is a solution of (28).

Equation (28) may be cast into a compact form if the sums over the particle coordinates are written in terms of "second beam moments," denoted as $\langle x^2 \rangle$ for the x direction. The double sum over the Coulomb interaction terms constitutes the electric field energy $W(t)$ of all particles

$$\langle x^2 \rangle (t) = \frac{1}{N} \sum_i x_i^2(t), \qquad W(t) = \frac{m}{2} \sum_i \sum_{j \neq i} \frac{c_1}{r_{ij}}.$$

Substituting $\rho^2(t) \equiv f_2(t)$ and defining the function $g = g(t)$ according to

$$g(t) = \langle x^2 \rangle \rho^3[\ddot{\rho} + \omega_x^2(t)\rho] + \langle y^2 \rangle \rho^3[\ddot{\rho} + \omega_y^2(t)\rho] + \langle z^2 \rangle \rho^3[\ddot{\rho} + \omega_z^2(t)\rho], \quad (29)$$

the third-order equation (28) can be transformed into an equivalent coupled system of a second-order equation for $\rho(t)$, and a first-order equation for $g(t)$, thereby eliminating the derivatives $\dot{\omega}_{x,y,z}(t)$ of the lattice functions. Solving (29) for $\ddot{\rho}(t)$ means to express it in the form of an "envelope equation"

$$\ddot{\rho} + \omega^2(t)\rho - \frac{g(t)}{\rho^3(\langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle)} = 0, \quad (30)$$

with the "average focusing function" $\omega^2(t)$ defined as

$$\omega^2(t) = \frac{\omega_x^2\langle x^2 \rangle + \omega_y^2\langle y^2 \rangle + \omega_z^2\langle z^2 \rangle}{\langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle}.$$

Equation (30) is equivalent to (28) if the derivative of $g(t)$ satisfies

$$\dot{g}(t) = 2\rho^3\bigg(\langle xp_x \rangle(\ddot{\rho} + \omega_x^2\rho) + \langle yp_y \rangle(\ddot{\rho} + \omega_y^2\rho) + \langle zp_z \rangle(\ddot{\rho} + \omega_z^2\rho) - \frac{W}{mN}\dot{\rho}\bigg). \quad (31)$$

Expressed in terms of $\rho(t)$ and $g(t)$, the invariant (16) writes

$$I_\rho/N = \langle(\rho p_x - \dot{\rho}x)^2\rangle + \langle(\rho p_y - \dot{\rho}y)^2\rangle + \langle(\rho p_z - \dot{\rho}z)^2\rangle + \rho^2\frac{2W}{mN} + \frac{g(t)}{\rho^2}.$$

We used the function $\rho(t)$ resulting from a numerical integration of the coupled set of differential equations (30) and (31) for given focusing functions $\omega_x^2(t)$, $\omega_y^2(t)$, $\omega_z^2(t)$ and initial conditions $g(0)$, $\rho(0)$, $\dot{\rho}(0)$. The time-dependent coefficients contained herein, namely the second-order beam moments as well as the field energy $W(t)$, were obtained from a three-dimensional simulation of a charged particle beam propagating through a periodic focusing lattice with non-negligible Coulomb interaction, as described by the potential function (26). We observe that for appropriate initial conditions the obtained evolution of $\rho(t)$ is approximately periodic, as imposed by the cell length of the periodic focusing lattice.

With regard to Eq. (30), we may interpret the function $\rho(t)$ as a "generalized beam envelope." Since the individual interparticle forces are included in (26), non-Liouvillean effects [4] emerging from the granular nature of charge distributions are also covered.

As an outlook, we point out that a major benefit of our result may be derived in the realm of numerical simulations of systems described by (1). Equation (16) embodies a time integral of Eq. (15), provided that the phase-space flow of the particle ensemble is *strictly* consistent with the equations of motion (2). This strict consistency can never be accomplished if the time evolution of the particle ensemble is obtained from a computer simulation because of the generally limited accuracy of numerical methods. Under these circumstances, the quantity I_{f_2} as given by Eq. (16)—with $f_2(t)$, $\dot{f}_2(t)$, and $\ddot{f}_2(t)$ following from (15)—can no longer be expected to be strictly constant. The deviation of a numerically obtained I_{f_2} from a constant of motion may thus be used as *a posteriori* error estimation for the respective simulation.

We finally note that the procedure to derive a quantity I that is conserved along a system's phase-space path can straightforwardly be generalized on the basis of (4) to potentials with quadratic velocity dependence.

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