

Invariants for time-dependent Hamiltonian systems

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An exact invariant is derived for n -degree-of-freedom Hamiltonian systems with general time-dependent potentials. The invariant is worked out in two equivalent ways. In the first approach, we define a special *Ansatz* for the invariant and determine its time-dependent coefficients. In the second approach, we perform a two-step canonical transformation of the initially time-dependent Hamiltonian to a time-independent one. The invariant is found to contain a function of time $f_2(t)$, defined as a solution of a linear third-order differential equation whose coefficients depend in general on the explicitly known configuration space trajectory that follows from the system's time evolution. It is shown that the invariant can be interpreted as the time integral of an energy balance equation. Our result is applied to a one-dimensional, time-dependent, damped non-linear oscillator, and to a three-dimensional system of Coulomb-interacting particles that are confined in a time-dependent quadratic external potential. We finally show that our results can be used to assess the accuracy of numerical simulations of time-dependent Hamiltonian systems.

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I. INTRODUCTION

Analytical approaches to isolate conserved quantities for a given physical system is a key objective in the realm of Hamiltonian theory. In the special case of an autonomous system, where the Hamiltonian does not depend on time explicitly, one conserved quantity is immediately found: the Hamiltonian itself that then represents the system's total energy as a constant of motion. Unfortunately, the Hamiltonians of most real physical systems are explicitly time dependent, hence do not provide directly a conserved quantity.

One of the first approaches to identify conserved quantities for explicitly time-dependent systems has been worked out in the context of the Lagrangian formalism by Noether [1]. Lutzky [2] demonstrated that the well-known invariant for the one-dimensional time-dependent harmonic oscillator [3,4] follows straightforwardly from Noether's theorem. Subsequently, Chattopadhyay [5] extended this work to derive invariants from this theorem for certain one-dimensional non-linear systems.

Another approach to work out conserved quantities for explicitly time-dependent Hamiltonian systems has been pursued by Leach [6]. Performing a finite time-dependent canonical transformation, he mapped the Hamiltonian of the time-dependent damped harmonic oscillator onto a time-independent one. Expressing this new Hamiltonian in terms of the old coordinates, one immediately obtains an invariant in the original system.

A third way to find exact invariants for time-dependent classical Hamiltonians has been worked out systematically by Lewis and Leach [7] using direct *Ansätze* with different powers in the canonical momentum.

In this paper, we will show in Sec. II and III that both, the direct approach with an *Ansatz* quadratic in the canonical momenta, as well as the canonical transformation approach can straightforwardly be generalized to n -degree-of-freedom Hamiltonian systems with general time-dependent potentials. In either case, the same invariant is obtained. The invariant is found to contain an unknown function of time $f_2(t)$, which is

given as a solution of a linear third-order differential equation, referred to as the auxiliary equation. In general, this equation depends on the system's spatial degrees of freedom. As a consequence, the auxiliary equation can only be integrated in conjunction with the equations of motion.

From the energy balance equation for time-dependent Hamiltonian systems, it is shown that the invariant can be interpreted as the sum of the system's time-varying energy content and the energy fed into or detracted from it.

We will present two applications of our findings in Sec. IV. In the first example, the invariant and the associated auxiliary equation is worked out for the one-dimensional system of the damped asymmetric spring. It is shown that for the special case of a vanishing nonlinearity, the invariant agrees with the harmonic oscillator result. For the case of autonomous systems we will furthermore demonstrate that a solution of the auxiliary equation with $f_2(t) \neq \text{const}$ leads to a nontrivial invariant that exists in addition to the invariant given by the Hamiltonian.

In the second example, we will examine the more challenging case of a three-dimensional ensemble of N Coulomb-interacting particles of the same species that are confined within a time-dependent quadratic external potential. From the form of the related auxiliary equation, it will become obvious that the function $f_2(t)$ represents a kind of generalization of a beam envelope function. It is shown that the function $f_2(t)$ may become unstable, depending on the strength of the external focusing forces — similar to the behavior of envelope functions [8].

In Sec. V we will point out that the existence of an invariant for explicitly time-dependent Hamiltonian systems can be used to assess the accuracy of numerical simulations of such systems. In analogy to autonomous systems, where the actual conservation of the Hamiltonian can be used as an accuracy criterion, we may check in a simulation of an explicitly time-dependent system to what extent the numerically obtained invariant differs from the exact invariant of the ideal case.

II. ANSATZ APPROACH

We consider an n -degree-of-freedom system of particles of the same species moving in an explicitly time-dependent potential V that may be described by a Hamiltonian H of the form

$$H = \sum_{i=1}^n \frac{c(t)}{2} p_i^2 + V(\{x\}, t). \quad (1)$$

Herein, $c(t)$ is defined as an arbitrary twice differentiable function of time that combines the particles' kinetic energy and a velocity-dependent potential leading to isotropic friction forces with linear velocity dependence. For $c(t) \equiv 1$, the Hamiltonian (1) thus describes systems without friction [9]. The curly braces denote the set of n configuration space variables $\{x\} = x_1, \dots, x_n$.

From the canonical equations, we derive for each degree of freedom i the equations of motion

$$\dot{x}_i = c(t)p_i, \quad \dot{p}_i = -\frac{\partial V(\{x\}, t)}{\partial x_i}. \quad (2)$$

With $\{p\} = p_1, \dots, p_n$ the set of canonical momenta, a quantity

$$I = I(\{x\}, \{p\}, t) \quad (3)$$

constitutes an invariant of the particle motion if its total time derivative vanishes along the phase-space path representing the system's time evolution

$$\frac{dI}{dt} = \frac{\partial I}{\partial t} + \sum_{i=1}^n \left[\frac{\partial I}{\partial x_i} \dot{x}_i + \frac{\partial I}{\partial p_i} \dot{p}_i \right] = 0.$$

We examine the existence of a conserved quantity (3) for a system described by Eq. (1) with a special *Ansatz* for I being at most quadratic in the momenta

$$I = \sum_i \left[\frac{1}{2} f_2(t) p_i^2 + f_1(x_i, t) p_i \right] + f_0(\{x\}, t). \quad (4)$$

The set of functions $f_2(t)$, $f_1(x_i, t)$, and $f_0(\{x\}, t)$ that render I invariant are to be determined. With the equations of motion (2), $dI/dt = 0$ means explicitly

$$\sum_i \left[\frac{1}{2} p_i^2 \frac{df_2}{dt} + p_i \frac{\partial f_1}{\partial t} + p_i^2 c \frac{\partial f_1}{\partial x_i} + p_i c \frac{\partial f_0}{\partial x_i} - (p_i f_2 + f_1) \frac{\partial V}{\partial x_i} \right] + \frac{\partial f_0}{\partial t} = 0. \quad (5)$$

We now eliminate step by step the functions f_1 and f_0 contained in Eq. (4). To this end, one may arrange the terms of Eq. (5) with regard to their powers in the momenta p_i . Equation (5) is fulfilled if the coefficients pertaining to the powers of the momenta vanish separately for each index i . From the terms proportional to p_i^2 , we thus get the condition

$$\frac{1}{2} \dot{f}_2(t) + c(t) \frac{\partial f_1(x_i, t)}{\partial x_i} = 0.$$

It follows that $f_1(x_i, t)$ must be a linear function in x_i

$$f_1(x_i, t) = -\frac{\dot{f}_2}{2c} x_i, \quad (6)$$

omitting an integration constant that does not depend on the configuration space variables.

For the terms linear in p_i , the condition derived from Eq. (5) reads

$$\frac{\partial f_1}{\partial t} = f_2(t) \frac{\partial V}{\partial x_i} - c(t) \frac{\partial f_0}{\partial x_i}. \quad (7)$$

On the other hand, $\partial f_1 / \partial t$ is given as the partial time derivative of Eq. (6)

$$\frac{\partial f_1}{\partial t} = \left(\frac{\dot{f}_2 \dot{c}}{2c^2} - \frac{\ddot{f}_2}{2c} \right) x_i. \quad (8)$$

Inserting Eq. (8) into Eq. (7), and solving for the terms containing the partial derivatives of the yet unknown but arbitrary ancillary function $f_0(\{x\}, t)$, one obtains the following partial differential equation for f_0

$$\frac{\partial f_0}{\partial x_i} = \left(\frac{\ddot{f}_2}{2c^2} - \frac{\dot{f}_2 \dot{c}}{2c^3} \right) x_i + \frac{f_2}{c} \frac{\partial V}{\partial x_i}. \quad (9)$$

A function $f_0(\{x\}, t)$ with partial derivative (9) is obviously given by

$$f_0(\{x\}, t) = \left(\frac{\ddot{f}_2}{c^2} - \frac{\dot{f}_2 \dot{c}}{c^3} \right) \sum_i \frac{1}{4} x_i^2 + \frac{f_2}{c} V(\{x\}, t). \quad (10)$$

The remaining terms of Eq. (5) do not depend on the momenta p_i . The third condition for I to embody an invariant of the particle motion thus writes, making use of Eq. (6)

$$\frac{\partial f_0}{\partial t} + \frac{\dot{f}_2}{2c} \sum_i x_i \frac{\partial V}{\partial x_i} = 0. \quad (11)$$

In order to eliminate the *Ansatz* function f_0 contained in Eq. (11), we calculate the partial time derivative of Eq. (10), i.e., the time derivative at fixed x_i

$$\begin{aligned} \frac{\partial f_0}{\partial t} = & \left(\frac{\ddot{\ddot{f}}_2}{c^2} - \frac{3\dot{f}_2 \dot{c}}{c^3} - \frac{\ddot{f}_2 \ddot{c}}{c^3} + \frac{3\dot{f}_2 \dot{c}^2}{c^4} \right) \sum_i \frac{1}{4} x_i^2 + \left(\frac{\dot{f}_2}{c} - \frac{f_2 \dot{c}}{c^2} \right) V \\ & + \frac{f_2}{c} \frac{\partial V}{\partial t}. \end{aligned} \quad (12)$$

Inserting Eq. (12) into Eq. (11), we finally get a homogeneous linear third-order differential equation for $f_2(t)$ that only depends on the configuration space variables

$$\begin{aligned}
& (\dot{f}_2 c - f_2 \dot{c}) V + f_2 c \frac{\partial V}{\partial t} + \frac{1}{2} \dot{f}_2 c \sum_i x_i \frac{\partial V}{\partial x_i} \\
& + \left(\ddot{f}_2 - \frac{3\dot{f}_2 \dot{c} + \dot{f}_2 \ddot{c}}{c} + \frac{3\dot{f}_2 \dot{c}^2}{c^2} \right) \sum_i \frac{1}{4} x_i^2 = 0.
\end{aligned} \tag{13}$$

The invariant I is finally obtained if we insert Eqs. (6), (10), and the Hamiltonian (1) into the *Ansatz* (4)

$$I = \frac{f_2}{c} H - \frac{\dot{f}_2}{2c} \sum_i x_i p_i + \frac{\dot{f}_2 c - \dot{f}_2 \dot{c}}{4c^3} \sum_i x_i^2. \tag{14}$$

Reviewing our approach to work out the invariant (14), we recollect that equations of motion (2) have been plugged into the expression for $dI/dt=0$ in Eq. (5). This means that the subsequent Eq. (13) — in conjunction with the side condition $I=\text{const}$ from Eq. (14) — may be conceived as a conditional equation for a potential $V(\{x\},t)$ that is consistent with a solution of the equations of motion (2).

Vice versa, we may also assume the equations of motion (2) to be *previously* solved. Then, the trajectory $\{x(t)\}$, the potential $V(\{x(t)\},t)$, and its partial derivatives constitute known coefficients of Eq. (13) that depend on time only. In this understanding, Eq. (13) embodies an ordinary differential equation for $f_2(t)$. The invariant (14) then follows from the solution path $(\{x(t)\}, \{p(t)\})$ of Eqs. (2), and from $f_2(t)$ as a solution function of Eq. (13). According to the existence and uniqueness theorem for linear ordinary differential equations, a unique solution $f_2(t)$ of Eq. (13) exists — and consequently the invariant I — if V and its partial derivatives are continuous along $\{x(t)\}$.

With $f_2(t)$ a solution of Eq. (13), we may directly show that $dI/dt=0$ holds along solutions of the equations of motion (2). Substituting Eqs. (2) into the total time derivative of Eq. (14), we find that the resulting equation agrees with Eq. (13). Hence, Eq. (14) provides a conserved quantity as a time integral of Eq. (13) if and only if the system's evolution is governed by the equations of motion (2). We will use this relationship in Sec. V to estimate the numerical error of computer simulations of dynamical systems described by Eq. (2).

Conversely, the invariant $I=\text{const}$ from Eq. (14) in conjunction with the third-order equation (13) can easily be shown to imply the equations of motion (2) by inserting Eq. (13) into the total time derivative of Eq. (14). Since $dI/dt \equiv 0$ must hold for all solutions $f_2(t)$ of Eq. (13), the respective sums of terms proportional to $\ddot{f}_2(t)$, $\dot{f}_2(t)$, and $f_2(t)$ must vanish separately. For the terms proportional to $\ddot{f}_2(t)$, this means

$$\frac{\dot{f}_2}{2c^2} \sum_i x_i (\dot{x}_i - c(t)p_i) \equiv 0. \tag{15}$$

The identity (15) must be fulfilled for *all* initial conditions $(\{x(0)\}, \{p(0)\})$ and resulting phase-space trajectories $(\{x(t)\}, \{p(t)\})$ of the underlying dynamical system. Consequently, the expression in parentheses must vanish separately

for each index i , thereby establishing the first equation of motion (2). For the remaining terms of $dI/dt \equiv 0$, we find

$$\sum_i \left(f_2 p_i - \frac{1}{2c(t)} \dot{f}_2 x_i \right) \left(\dot{p}_i + \frac{\partial V}{\partial x_i} \right) \equiv 0.$$

Similar to the previous case, we may only fulfill this equation in general for any solution $f_2(t)$ of Eq. (13) and each index i if the second equation of motion (2) holds.

Summarizing, we may state that the triple made up by the equations of motion (2), the third-order equation (13), and the invariant $I=\text{const}$ of Eq. (14) forms a logical triangle: if two sides are given at a time, the third can be deduced.

The physical interpretation of the invariant (14) can be worked out considering the total time derivative of the Hamiltonian (1). Making use of the canonical equations (2), we find

$$\frac{d}{dt} \left[\sum_{i=1}^n \frac{1}{2} c(t) p_i^2 + V \right] - \sum_{i=1}^n \frac{1}{2} \dot{c}(t) p_i^2 - \frac{\partial V}{\partial t} = 0, \tag{16}$$

which represents just the explicit form of the general theorem $dH/dt = \partial H / \partial t$ for the Hamiltonian (1). Equation (16) can be interpreted as an energy balance relation, stating that the system's total energy change dH/dt is quantified by the dissipation and the explicit time dependence of the external potential. Multiplying Eq. (16) by the dimensionless quantity f_2/c , and inserting $\partial V / \partial t$ according to the auxiliary equation (13), the resulting terms sum up to the total time derivative

$$\frac{d}{dt} \left[\frac{f_2}{c} H - \frac{\dot{f}_2}{2c} \sum_i x_i p_i + \frac{\dot{f}_2 c - \dot{f}_2 \dot{c}}{4c^3} \sum_i x_i^2 \right] = 0.$$

The expression in brackets coincides with the invariant (14). With the initial conditions $f_2(0)/c(0)=1$, $\dot{f}_2(0)=\dot{f}_2(0)=0$ for the auxiliary equation (13), the invariant I can now be interpreted as the conserved *initial* energy H_0 for a non-autonomous system described by the Hamiltonian (1), comprising both the system's time-varying energy content H and the energy fed into or detracted from the system.

The meaning of $f_2(t)$ follows directly from the representation (14) of the invariant if the Hamiltonian H is treated formally as an independent variable: $I = I(\{x\}, \{p\}, t, H)$. A vanishing total time derivative of the invariant I then writes

$$\begin{aligned}
\frac{dI}{dt} &= \frac{\partial I}{\partial t} \Big|_{\{x\}, \{p\}, H} + \frac{\partial H}{\partial t} \frac{\partial I}{\partial H} \Big|_{\{x\}, \{p\}, t} \\
&+ \sum_i \left(\dot{x}_i \frac{\partial I}{\partial x_i} \Big|_{\{p\}, t, H} + \dot{p}_i \frac{\partial I}{\partial p_i} \Big|_{\{x\}, t, H} \right) = 0.
\end{aligned}$$

Inserting x_i and p_i from the canonical equations (2), and making again use of the auxiliary equation (13) to eliminate the third-order derivative $\ddot{f}_2(t)$, we find the expected result

$$\frac{\partial I}{\partial H} \Big|_{\{x\}, \{p\}, t} = \frac{f_2(t)}{c(t)}.$$

f_2/c thus provides the slope of the total energy I with respect to the actual system energy H .

We finally note that for the special case $\dot{c} \equiv \partial V / \partial t \equiv 0$, i.e., for autonomous systems, $f_2(t) \equiv c \equiv 1$ is always solution of Eq. (13). For this case, the invariant (14) reduces to $I = H$, hence provides the system's total energy, which is a known invariant for Hamiltonian systems with no explicit time dependence. Nevertheless, Eq. (13) also admits solutions $f_2(t) \neq \text{const}$ for these systems. We thereby obtain another nontrivial invariant that exists in addition to the invariant representing the energy conservation law. This will be demonstrated in an example at the end of Sec. IV A.

III. CANONICAL TRANSFORMATION APPROACH

This approach aims to transform the Hamiltonian (1) to a new Hamiltonian \bar{H} that no longer depends on time explicitly, hence embodies the total energy of the transformed system as a constant of motion. It happens that this procedure is most clearly performed in two steps. In the first step, we canonically transform the Hamiltonian (1) to a new set of coordinates $\{x\} \rightarrow \{\bar{x}\}$, $\{p\} \rightarrow \{\bar{p}\}$ to obtain an intermediate Hamiltonian \bar{H} . The explicitly time-dependent generating function of this transformation may be expressed in terms of the new locations and the old momenta as

$$F_3(\{\bar{x}\}, \{p\}, t) = \sum_{i=1}^n \left[\frac{\dot{f}_2(t)}{4c(t)} \bar{x}_i^2 - \sqrt{f_2(t)} \bar{x}_i p_i \right]. \quad (17)$$

The coordinate transformation rules derived from (17) are

$$x_i = - \frac{\partial F_3}{\partial p_i} = \sqrt{f_2} \bar{x}_i$$

$$\bar{p}_i = - \frac{\partial F_3}{\partial \bar{x}_i} = \sqrt{f_2} p_i - \frac{\dot{f}_2}{2c} \bar{x}_i.$$

In matrix notation, this phase-space preserving linear transformation writes

$$\begin{pmatrix} x_i \\ p_i \end{pmatrix} = \begin{pmatrix} \sqrt{f_2} & 0 \\ \dot{f}_2 / (2c \sqrt{f_2}) & 1 / \sqrt{f_2} \end{pmatrix} \begin{pmatrix} \bar{x}_i \\ \bar{p}_i \end{pmatrix}. \quad (18)$$

Expressed in the new (barred) coordinates, the partial time derivative of the generating function (17) follows as

$$\frac{\partial F_3}{\partial t} = \sum_i \left[\left(\frac{\dot{f}_2}{c} - \frac{\dot{f}_2^2}{cf_2} - \frac{\dot{f}_2 \ddot{c}}{c^2} \right) \frac{1}{4} \bar{x}_i^2 - \frac{\dot{f}_2}{2f_2} \bar{x}_i \bar{p}_i \right]. \quad (19)$$

Writing finally the old Hamiltonian H in terms of the new coordinates, the transformed Hamiltonian $\bar{H} = H + \partial F_3 / \partial t$ is obtained as

$$\bar{H} = \frac{c(t)}{f_2(t)} \left[\sum_{i=1}^n \frac{1}{2} \bar{p}_i^2 + \bar{V}(\{\bar{x}\}, t) \right] \quad (20)$$

with the potential \bar{V} in the transformed system given by

$$\bar{V}(\{\bar{x}\}, t) = \left(\frac{f_2 \ddot{f}_2}{c^2} - \frac{\dot{f}_2^2}{2c^2} - \frac{f_2 \dot{f}_2 \dot{c}}{c^3} \right) \sum_{i=1}^n \frac{1}{4} \bar{x}_i^2 + \frac{f_2}{c} V(\{\sqrt{f_2} \bar{x}\}, t). \quad (21)$$

The new potential \bar{V} consists of two components, namely a term related to the original potential V , and an additional quadratic potential that describes the linear forces of inertia occurring due to the time-dependent linear transformation (18) to a new frame of reference.

Up to now, the function $f_2 = f_2(t)$ contained in the generating function (17) has been defined as an arbitrary regular function of time. We now require the potential $\bar{V}(\{\bar{x}\}, t)$ — as defined by Eq. (21) — to be independent of time explicitly:

$$\frac{\partial \bar{V}(\{\bar{x}\}, t)}{\partial t} = 0. \quad (22)$$

This means that $f_2(t)$ is now tailored to eliminate the explicit time dependence of Eq. (21) exactly at $\{\bar{x}\}$. The explicit time dependence that is introduced if the original potential $V(\{x\}, t)$ is expressed in the new spatial coordinates yields

$$\frac{\partial V}{\partial(\sqrt{f_2} \bar{x}_i)} \frac{\partial(\sqrt{f_2} \bar{x}_i)}{\partial t} = \frac{\dot{f}_2}{2f_2} x_i \frac{\partial V}{\partial x_i}. \quad (23)$$

In detail, Eq. (22) with (23) means in terms of the old spatial coordinates

$$\frac{\partial \bar{V}}{\partial t} = \left(\frac{\ddot{f}_2}{c^2} - \frac{3\dot{f}_2 \dot{c}}{c^3} + \frac{3f_2 \ddot{c}}{c^4} \right) \sum_i \frac{1}{4} x_i^2 + \left(\frac{\dot{f}_2}{c} - \frac{f_2 \dot{c}}{c^2} \right) V$$

$$+ \frac{f_2}{c} \frac{\partial V}{\partial t} + \frac{\dot{f}_2}{2c} \sum_i x_i \frac{\partial V}{\partial x_i} = 0. \quad (24)$$

We observe that Eq. (24) agrees with the linear differential equation (13) for $f_2(t)$, as obtained in Sec. II. Provided that f_2 is a solution of Eq. (24), the explicit time dependence of transformed Hamiltonian \bar{H} is imposed by the preceding factor c/f_2 only

$$\bar{H} = \frac{c(t)}{f_2(t)} \left[\sum_{i=1}^n \frac{1}{2} \bar{p}_i^2 + \bar{V}(\{\bar{x}\}) \right]. \quad (25)$$

This explicit time dependence of the Hamiltonian (25) can be eliminated in the second step with the help of a time-scale transformation $t \rightarrow \tau$ defined by

$$\tau(t) = \int_{t_0}^t \frac{c(t')}{f_2(t')} dt'. \quad (26)$$

With τ the independent variable, the canonical equations

$$\frac{d\bar{x}_i}{d\tau} = \frac{\partial \bar{H}}{\partial \bar{p}_i}, \quad \frac{d\bar{p}_i}{d\tau} = - \frac{\partial \bar{H}}{\partial \bar{x}_i}$$

follow from Eq. (25). The new Hamiltonian $\tilde{H} = \bar{H}f_2/c$ contained herein no longer depends on time explicitly

$$\tilde{H} = \sum_{i=1}^n \frac{1}{2} \bar{p}_i^2 + \bar{V}(\{\bar{x}\}). \quad (27)$$

Expressing (27) in terms of the original coordinates according to Eq. (18), we get an invariant I of the original system H

$$\begin{aligned} \tilde{H} = \frac{f_2}{c} \left[\sum_i \frac{c}{2} p_i^2 + V(\{x\}, t) \right] - \frac{\dot{f}_2}{2c} \sum_i x_i p_i \\ + \frac{\ddot{f}_2 c - \dot{f}_2 \dot{c}}{4c^3} \sum_i x_i^2 = I, \end{aligned} \quad (28)$$

which has been derived previously in Eq. (14) on the basis of the *Ansatz* (4).

IV. NUMERICAL EXAMPLES

A. Time-dependent damped asymmetric spring

As a simple example, we investigate the one-dimensional nonlinear system of a time-dependent ‘‘damped asymmetric spring.’’ With $c(t) = \exp[-F(t)]$, its Hamiltonian is defined by

$$H = \frac{1}{2} e^{-F(t)} p^2 + \left(\frac{1}{2} \omega^2(t) x^2 + a(t) x^3 \right) e^{F(t)}. \quad (29)$$

Writing $f(t) \equiv \dot{F}(t)$, the equation of motion follows as

$$\dot{x} = p e^{-F(t)}, \quad \ddot{x} + f(t) \dot{x} + \omega^2(t) x + 3a(t) x^2 = 0. \quad (30)$$

The invariant I is immediately found writing the general invariant (14) for one degree of freedom with the Hamiltonian H given by Eq. (29)

$$\begin{aligned} I = \frac{1}{2} e^{2F(t)} \left[f_2 \dot{x}^2 - \dot{f}_2 x \dot{x} + x^2 \left\{ \frac{1}{2} \ddot{f}_2 + \frac{1}{2} \dot{f}_2 f(t) \right. \right. \\ \left. \left. + f_2 \omega^2(t) + 2x f_2 a(t) \right\} \right]. \end{aligned} \quad (31)$$

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

$$\begin{aligned} \ddot{f}_2 + 3\dot{f}_2 f(t) + \dot{f}_2 \dot{f}(t) + 2\dot{f}_2 f^2(t) + 4\dot{f}_2 \omega^2(t) + 4f_2 f(t) \omega^2(t) \\ + 4f_2 \omega \dot{\omega}(t) + 2x(t) [2f_2 \dot{a}(t) + 4f_2 a(t) f(t) + 5\dot{f}_2 a(t)] \\ = 0, \end{aligned} \quad (32)$$

which follows from Eq. (13) or, equivalently, from Eq. (24). Since the particle trajectory $x = x(t)$ is explicitly contained in Eq. (32), the solution $f_2(t)$ can only be obtained integrating Eq. (32) simultaneously with the equation of motion (30).

We may easily convince ourselves that I is indeed a conserved quantity. Calculating the total time derivative of Eq. (31), and inserting the equation of motion (30), we end up with Eq. (32), which is fulfilled by definition of $f_2(t)$ for the given trajectory $x = x(t)$.

The third-order equation (32) may be converted into a coupled set of first- and second-order equations. The second-order equation

$$\ddot{f}_2 - \frac{\dot{f}_2^2}{2f_2} + \dot{f}_2 f(t) + 2f_2 \omega^2(t) = \frac{g_x(t)}{f_2} e^{-2F(t)} \quad (33)$$

is equivalent to Eq. (32) if the time derivative of $g_x(t)$, introduced in Eq. (33), is given by

$$\dot{g}_x(t) = -2x(t) f_2 e^{2F(t)} (2f_2 \dot{a} + 4f_2 a f + 5\dot{f}_2 a). \quad (34)$$

With the help of the auxiliary equation (33), the invariant (31) may be expressed in the alternative form

$$I = \frac{e^{2F(t)}}{2f_2} \left[\left(f_2 \dot{x} - \frac{1}{2} \dot{f}_2 x \right)^2 + 2x^3 f_2^2(t) a(t) \right] + \frac{g_x(t)}{4f_2} x^2. \quad (35)$$

In contrast to Eq. (32), the equivalent coupled set of equations (33) and (34) does not contain the time derivatives of the external functions $f(t)$ and $\omega(t)$. The invariant (35) reduces to the well-known invariant [6] for the time-dependent damped harmonic oscillator if $a(t) \equiv 0$, which means that $g_x(t) = g_0 = \text{const}$. For this particular linear system, Eq. (33) no longer depends on the specific particle trajectory $x = x(t)$. The solution functions $f_2(t)$ and $\dot{f}_2(t)$ then apply to all trajectories emerging as integrals of the equation of motion (30) with $a(t) \equiv 0$. With regard to the general form of the differential equation for $f_2(t)$, as given by Eq. (13), we conclude that a decoupling from the equations of motion (2) may occur for isotropic linear systems only.

Another property of the linear system [$a(t) \equiv 0$] follows directly from Eq. (35). For a positive integration constant $g_x(t) = g_0 > 0$, one finds that $f_2(t) I \geq 0$. Consequently, $f_2(t)$ can never change sign, thus remains non-negative for the initial condition $f_2(0) > 0$, which means that $I > 0$. The generating function (17) then remains real at all times t , and accordingly the Hamiltonian \tilde{H} of the transformed system.

On the other hand, $f_2(t)$ may change sign for the general nonlinear system (30), depending on the strength of the nonlinear forces. Then, the time-dependent canonical transformation (18) becomes imaginary, which means that the autonomous system ceases to exist as a physical system. Under these circumstances, the particle motion within the time-dependent nonlinear system can no longer be expressed as the linearly transformed motion within a *real* autonomous system.

Figure 1 shows a special case of a numerical integration of the equation of motion (30). Included in this figure, we see the result of a simultaneous numerical integration of Eqs. (33) and (34). The coefficients of Eq. (30) are defined as $\omega(t) = \cos(t/2)$, $a(t) = 5 \times 10^{-3} \sin(t/3)$, and $f(t) = 1.76 \times 10^{-3} \cos^2(t/\pi)$. The initial conditions were set to $x(0) = 1$, $\dot{x}(0) = 0$, $f_2(0) = 1$, $\dot{f}_2(0) = 0$, and $\ddot{f}_2(0) = 0$. According to Eq. (35), we hereby define an invariant of $I = 0.5$ for

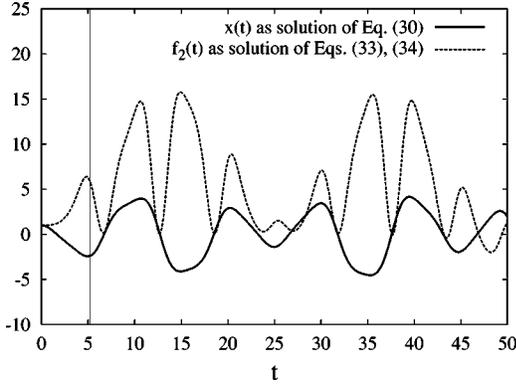


FIG. 1. Example of a numerical integration of Eq. (30) and the simultaneous numerical integration of Eqs. (33) and (34). The vertical line marks the instant of time $t=5.2$, referred to in Fig. 2.

the sample particle. With both results, we are able to calculate the phase-space curve of constant invariant $I(x, \dot{x}, t) = 0.5$, as defined by Eq. (35).

Figure 2 displays both a snapshot of this curve at $t=5.2$, and the instantaneous location of the sample particle. As expected, the particle lies exactly on the line of constant I , thereby providing a numerical verification of Eq. (35).

For the special case of an autonomous system, we define $c(t) = \exp(-F) = 1$, $\omega(t) = \omega_0 = \text{const}$, and $a(t) = a_0 = \text{const}$. It follows that $\dot{F} = \dot{f} = \dot{\omega} = \dot{a} = 0$, which means that Eq. (32) reduces to

$$\ddot{f}_2 + \dot{f}_2(4\omega_0^2 + 10x(t)a_0) = 0. \quad (36)$$

Obviously, this equation has the special solution $f_2(t) \equiv 1$. In that case, the invariant (31) is given by

$$I = \frac{1}{2}\dot{x}^2 + \frac{1}{2}\omega_0^2 x^2 + a_0 x^3 = H,$$

thus coincides with the system's Hamiltonian that represents the conserved total energy. A further nontrivial invariant is obtained for solutions of Eq. (36) with $f_2(t) \neq \text{const}$ as

$$I = \frac{1}{2}[f_2 \dot{x}^2 - \dot{f}_2 x \dot{x} + x^2 \{ \frac{1}{2} \ddot{f}_2 + f_2 \omega_0^2 + 2x f_2 a_0 \}]. \quad (37)$$

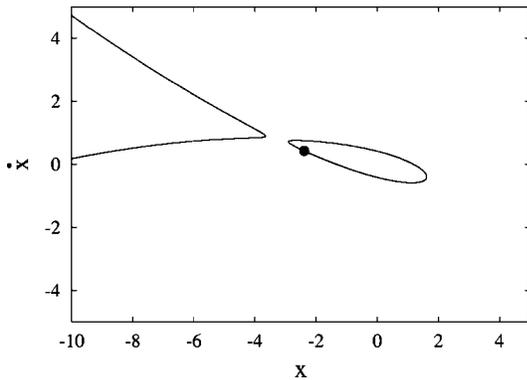


FIG. 2. Lines of constant invariant $I=0.5$ in the (x, \dot{x}) phase-space plane and location of the sample particle at $t=5.2$, $f_2=6.1$.

For the harmonic oscillator, i.e., for $a_0=0$, we may substitute the integral of Eq. (36)

$$\ddot{f}_2(t) + 4\omega_0^2 f_2(t) = 0 \quad (38)$$

into Eq. (37) to derive the invariant in the form

$$I = \frac{1}{2}[f_2(\dot{x}^2 - \omega_0^2 x^2) - \dot{f}_2 x \dot{x}].$$

With $f_2(t)$ a solution of Eq. (38), this expression agrees with the invariant presented earlier by Lutzky [10].

B. System of Coulomb-interacting particles

We now analyze a three-dimensional example, namely an ensemble of N Coulomb-interacting particles of the same species moving in a time-dependent quadratic external potential, as typically given in the co-moving frame for charged particle beams that propagate through linear focusing lattices. The particle coordinates in the three spatial directions are distinguished by x_i , y_i , and z_i , the canonical momenta correspondingly by $p_{x,i}$, $p_{y,i}$, and $p_{z,i}$. Setting $c(t) \equiv 1$ in Eq. (1), the Hamiltonian H of this system may now be written as

$$H = \sum_{i=1}^N \frac{1}{2}(p_{x,i}^2 + p_{y,i}^2 + p_{z,i}^2) + V(\{x\}, \{y\}, \{z\}, t). \quad (39)$$

The effective potential contained herein is given by

$$V(\{x\}, \{y\}, \{z\}, t) = \sum_{i=1}^N \left[\frac{1}{2} \omega_x^2(t) x_i^2 + \frac{1}{2} \omega_y^2(t) y_i^2 + \frac{1}{2} \omega_z^2(t) z_i^2 + \frac{1}{2} \sum_{j \neq i} \frac{c_1}{r_{ij}} \right], \quad (40)$$

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 Eq. (2) with Eq. (40) are

$$\dot{x}_i = p_{x,i}, \quad \ddot{x}_i + \omega_x^2(t) x_i - c_1 \sum_{j \neq i} \frac{x_i - x_j}{r_{ij}^3} = 0, \quad (41)$$

and likewise for the y and z directions. We note that the factor $1/2$ in front of the Coulomb interaction term in Eq. (40) disappears in Eq. (41) since each term occurs twice in the symmetric form of the double sum.

For the effective potential (40) and $c(t) \equiv 1$, the third-order differential equation (13) for f_2 specializes to

$$\sum_i \left[\dot{f}_2 \sum_{j \neq i} \frac{c_1}{r_{ij}} + x_i^2 (\ddot{f}_2 + 4\dot{f}_2 \omega_x^2 + 4f_2 \omega_x \dot{\omega}_x) + y_i^2 (\ddot{f}_2 + 4\dot{f}_2 \omega_y^2 + 4f_2 \omega_y \dot{\omega}_y) + z_i^2 (\ddot{f}_2 + 4\dot{f}_2 \omega_z^2 + 4f_2 \omega_z \dot{\omega}_z) \right] = 0. \quad (42)$$

With $f_2(t)$ a solution of Eq. (42) and H the Hamiltonian (39), the invariant follows directly from Eq. (14) as

$$\begin{aligned}
 I = & f_2(t)H - \frac{1}{2}\dot{f}_2 \sum_i (x_i p_{x,i} + y_i p_{y,i} + z_i p_{z,i}) \\
 & + \frac{1}{4}\dot{f}_2 \sum_i (x_i^2 + y_i^2 + z_i^2). \quad (43)
 \end{aligned}$$

Equation (42) 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 coordinates. Likewise, the double sum over the Coulomb interaction terms may be expressed as electric field energy $W(t)$ of all particles

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

A similar notation will be used for all quadratic terms of the particle coordinates. Corresponding to the previous example, the third-order equation (42) may be split into a coupled set of first- and second-order differential equations. Similar to Eq. (33), we define the function $g = g(t)$ by

$$f_2 \ddot{f}_2 - \frac{1}{2} \dot{f}_2^2 + 2f_2^2 \omega^2(t) = g(t). \quad (44)$$

The function $\omega^2(t)$ contained herein is defined as the “average focusing function” according to

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

Comparing the time derivative of Eq. (44) with Eq. (42), one finds that the time derivative of $g(t)$ must satisfy

$$\begin{aligned}
 \dot{g}(t) = & \frac{1}{\langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle} \left[-2f_2 \dot{f}_2 \frac{W}{mN} + 4f_2^2 \{ \langle x p_x \rangle \right. \\
 & \left. \times (\omega_x^2 - \omega^2) + \langle y p_y \rangle (\omega_y^2 - \omega^2) + \langle z p_z \rangle (\omega_z^2 - \omega^2) \right]. \quad (45)
 \end{aligned}$$

Unlike the third-order equation (42), the equivalent coupled set of equations (44) and (45) no longer contains the time derivatives of the external focusing functions $\omega_x(t)$, $\omega_y(t)$, and $\omega_z(t)$. We observe that $\dot{g}(t)$ is determined by two quantities of different physical nature: the field energy constituted by all particles as a measure for the strength of the Coulomb interaction, and the system’s anisotropy. In contrast to $g_x(t)$ of the one-dimensional example of Sec. IV A, the function $g(t)$ is generally *not* constant in the linear case, which is given here for a vanishing Coulomb interaction ($W \rightarrow 0$).

With the help of Eq. (44), we may substitute $\ddot{f}_2(t)$ and the external focusing functions in Eq. (43) to express the invariant in the alternative form

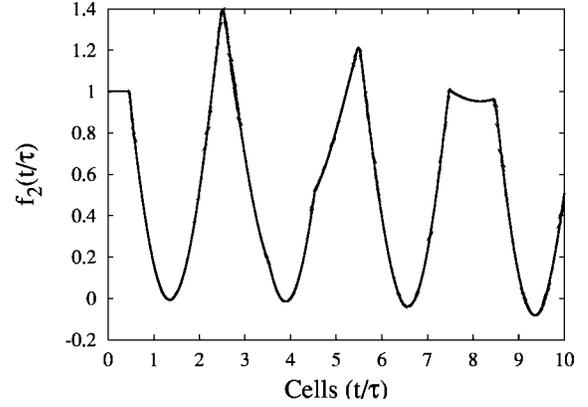


FIG. 3. $f_2(t)$ as stable solution of Eq. (42) for $\sigma_0 = 45^\circ$, $\sigma = 9^\circ$. τ denotes the focusing period common to all three directions.

$$\begin{aligned}
 2f_2 I/N = & \left\langle \left(f_2 p_x - \frac{1}{2} \dot{f}_2 x \right)^2 \right\rangle + \left\langle \left(f_2 p_y - \frac{1}{2} \dot{f}_2 y \right)^2 \right\rangle \\
 & + \left\langle \left(f_2 p_z - \frac{1}{2} \dot{f}_2 z \right)^2 \right\rangle + f_2^2(t) \frac{2W}{mN} + \frac{1}{2} g(t) (\langle x^2 \rangle \\
 & + \langle y^2 \rangle + \langle z^2 \rangle). \quad (46)
 \end{aligned}$$

Similar to the previous example, the function $g(t)$ accounts for an eventual change of sign of $f_2(t)$, owing to the fact that all other terms on the right-hand side of Eq. (46) may not turn negative.

The canonical transformation (18) becomes undefined for instants of time t with $f_2(t) = 0$. Furthermore, for time intervals with a negative value of $f_2(t)$, the elements of the transformation matrix (18) turn imaginary. For these cases, the equivalent autonomous system of Eqs. (39) and (40) that is defined by the canonical transformation rules (18) and (26) ceases to exist in a physical sense. This indicates that the beam evolves within the nonautonomous system in a way that can no longer be correlated to the beam evolution within an autonomous system by the linear canonical transformation (18). In contrast, the invariant (43) itself exists for *all* $f_2(t)$ that are solutions of the auxiliary equation (42).

Figures 3 and 4 show the function $f_2(t)$ as the result of numerical integrations of the coupled set (44) and (45). The second-order moments—denoted by the angle brackets—and the field energy function $W(t)$ were taken from simulations of a fictitious three-dimensional anisotropic focusing lattice that is described by the Hamiltonian (39) with the potential (40). The simulation leading to Fig. 3 was performed at the zero-current tune of $\sigma_0 = 45^\circ$, and a space charge depressed tune of $\sigma = 9^\circ$ in each direction.

As a result of various simulations, we found that $f_2(t)$ becomes unstable for $\sigma_0 \geq 60^\circ$. Furthermore, it turned out that this limit value for an unstable evolution of $f_2(t)$ decreases as the field energy $W(t)$ increases. A case with a growing amplitude of $f_2(t)$ is displayed in Fig. 4 for a beam propagating under the conditions of a zero-current tune of $\sigma_0 = 60^\circ$ and the depressed tune of $\sigma = 15^\circ$. In agreement with earlier studies on high current beam transport [11], the simulation results show that the beam moments remain

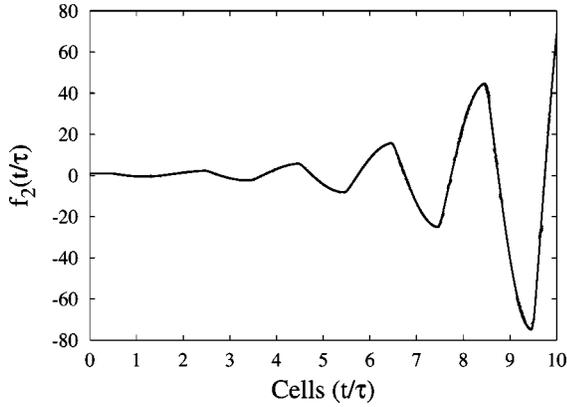


FIG. 4. $f_2(t)$ as unstable solution of Eq. (42) for $\sigma_0=60^\circ$, $\sigma=15^\circ$. τ denotes the focusing period common to all three directions.

bounded under these conditions. This means that an instability of $f_2(t)$ is *not* necessarily associated with an instability of the beam moments. Nevertheless, the phase-space planes of constant I become more and more distorted as $f_2(t)$ and its derivatives diverge. This may indicate a transition from a regular to a chaotic motion of the beam particles.

V. CHECKING THE ACCURACY OF NUMERICAL SIMULATIONS OF HAMILTONIAN SYSTEMS

The conserved quantity I that has been shown to exist for explicitly time-dependent Hamiltonian systems can be used to test the results of numerical simulations of such systems. As already stated in Sec. II, Eq. (14) embodies a time integral of eq. (13) if the system’s time evolution is *strictly* consistent with the equations of motion (2). In the ideal case, i.e., if no numerical inaccuracies were included in a computer simulation of a system governed by Eq. (1), and no numerical errors were added performing the subsequent integration of Eq. (13), we would not see any deviation $\Delta I/I_0$ calculating the invariant (14) as a function of time.

Of course, we can never avoid numerical errors in computer simulations of dynamical systems because of the generally limited accuracy of numerical methods. For the same reason, the numerical integration of Eq. (13) is also associated with a specific finite error tolerance. Under these circumstances, the quantity I as given by Eq. (14) — with $f_2(t)$, $\dot{f}_2(t)$, and $\ddot{f}_2(t)$ following from Eq. (13) — can no longer be expected to be *exactly* constant. Both numerical tasks — the numerical integration of the equations of motion (2), and the subsequent numerical integration of Eq. (13) contribute to a nonvanishing $\Delta I/I_0$ along the integration time span. Nevertheless, since both tasks do not depend on each other with respect to their specific error tolerances, we can regard the obtained $\Delta I/I_0$ curve as a cross check of both numerical methods. Since the error tolerance for the numerical integration of Eq. (13) is a known property of the underlying algorithm, we can estimate from $\Delta I(t)/I_0$ the error tolerance integrating the equations of motion (2).

Figure 5 displays two examples of curves of relative deviations $\Delta I/I_0$ from the invariant (43) for numerical simula-

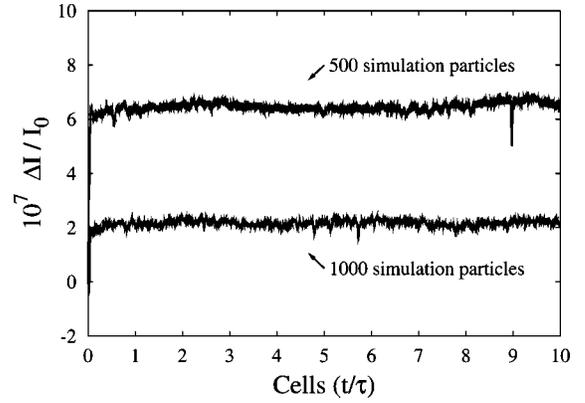


FIG. 5. Relative invariant error $\Delta I/I_0$ for three-dimensional simulations of a charged particle beam with different numbers of macroparticles.

tions of a charged particle beam. The function $f_2(t)$ and its derivatives that were used to calculate I were obtained from a numerical integration of Eq. (42) — or equivalently from the coupled set (44) and (45). The time-dependent coefficients of Eq. (42), namely the second beam moments and the field energy $W(t)$, had been determined before from three-dimensional simulations of charged particle beams propagating through a linear focusing lattice with non-negligible Coulomb interaction, as described by the potential function (40). As expected, the residual deviation $\Delta I/I_0$ depends on the number of macroparticles used in the simulation.

For a comparison, the corresponding deviation is plotted in Fig. 6 for a simulation with a systematic 5% error in the space charge force calculations. We now find a relative deviation $\Delta I/I_0$ in the order of 10^{-3} , hence three orders of magnitude larger than the previous case with no artificial space charge force error.

By comparing simulation runs with different parameters, such as the number of macroparticles, the time step size, and details of the numerical algorithm used to integrate the equations of motion, we may straightforwardly check whether the overall accuracy of our particular simulation has been improved.

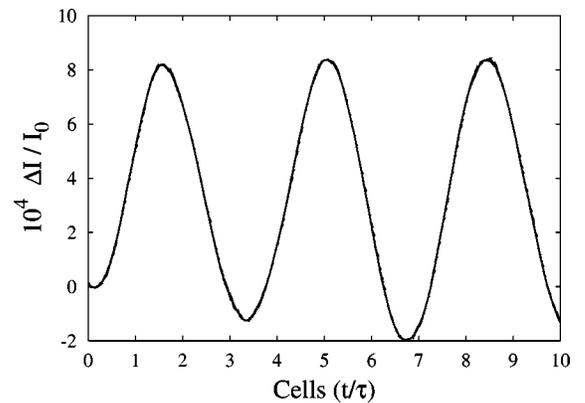


FIG. 6. Relative invariant error $\Delta I/I_0$ for a three-dimensional simulation of a charged particle beam with 5% error in the space charge force calculations.

VI. CONCLUSIONS

A fairly general result has been found: a conserved quantity can straightforwardly be deduced for explicitly time-dependent Hamiltonian systems. The invariant contains an unknown function $f_2(t)$ and its first and second time derivatives, which is determined by a linear homogeneous third-order auxiliary differential equation. In general, this auxiliary equation depends on the system's spatial degrees of freedom. Under these circumstances, the solution $f_2(t)$ can only be determined integrating the auxiliary equation *simultaneously* with the equations of motion. The invariant can be regarded as the conserved global energy for nonautonomous systems, which is obtained if we add to the time-varying energy represented by the Hamiltonian H the energies fed into or detracted from the system.

The invariant has been found to agree with the known conserved quantity of the one-dimensional time-dependent harmonic oscillator [4,6]. For this particular one-dimensional linear case, the dependence of the auxiliary equation on the particle position cancels. Then the third-order auxiliary equation can directly be integrated to yield a nonlinear second-order equation for $f_2(t)$ that applies to all particle trajectories. Furthermore, the second invariant for the time-independent harmonic oscillator could straightforwardly be reproduced [10]. All these invariants follow as special cases from the general expressions of our invariant and the associated auxiliary equation.

The existence of an invariant has been shown to be useful to check the accuracy of numerical simulations of explicitly

time-dependent Hamiltonian systems. Having numerically integrated the equations of motion, the system's third-order auxiliary differential equation can be integrated, and the numerical value of the "invariant" I can be calculated subsequently. The relative deviation $\Delta I/I_0$ of I from the exact invariant I_0 can then be used as a measure for the accuracy of the respective simulation.

The physical implications that are associated with an unstable behavior of $f_2(t)$ of the auxiliary differential equation remain to be investigated. Furthermore, the physical meaning of solutions of the auxiliary equation with $f_2(t)$ turning negative must be clarified. In that case, the elements of coordinate transformation matrix (18) become imaginary, which means that the equivalent autonomous system ceases to exist as a physical system. This indicates that the explicitly time-dependent Hamiltonian system evolves in a way that can no longer be correlated to the evolution of a time-independent system by a linear mapping. Nevertheless, the invariant I of the explicitly time-dependent system exists independently of the sign of $f_2(t)$.

We finally note that the invariant (14) together with the related auxiliary equation (13) can be derived equivalently performing an infinitesimal canonical transformation in the extended phase-space. Furthermore, the invariant and the auxiliary equation may be worked out as well on the basis of Noether's theorem [1]. Our invariant thus embodies exactly the conserved quantity that emerges as the result of Noether's symmetry transformation. We will report these results in a forthcoming paper [12].

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