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Spontaneous reversal of irreversible processes in a many-body Hamiltonian evolution

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Abstract. Recently a technique has been introduced to $\Omega$-modify a Hamiltonian so that the $\Omega$-modified Hamiltonian thereby produced is \textit{isochronous}: all its solutions are periodic in all degrees of freedom with the same period $\tilde{T} = 2\pi/\Omega$. In this paper—after briefly reviewing this approach—we focus in particular on the $\Omega$-modified version of the most general realistic many-body problem whose behavior, over time intervals much shorter than the \textit{isochrony} period $\tilde{T}$, differs only marginally from the thermodynamically irreversible evolution of the corresponding, unmodified and realistic many-body system. We discuss the (apparently paradoxical) periodic recurrence of the irreversible processes occurring in this $\Omega$-modified model, implying a periodic reversal of its irreversible behavior. We then discuss the equilibrium statistical mechanics of this $\Omega$-modified model, including the compatibility of standard thermodynamic notions such as entropy with the peculiar phenomenology featured by its time evolution. The theoretical discussion is complemented by numerically simulated examples of the molecular dynamics yielded by the (standard and classical) Hamiltonian describing (many) particles interacting pairwise via potentials of Lennard–Jones type and via harmonic potentials in two-dimensional space, and by its $\Omega$-modified version. In the latter case, the simulation displays (approximate) returns to configurations \textit{away} from thermodynamic equilibrium \textit{after} relaxation to equilibrium had occurred.
1. Introduction

Recently, various techniques have been introduced to modify a Hamiltonian so that the Hamiltonian thereby produced is isochronous (for a review see [1]). In this introductory section—also in order to make this paper self-contained—we review (actually via a slightly generalized treatment) the essential aspects of the most recent and effective version of this approach [1, 2], leading to an isochronous $\Omega$-modified Hamiltonian yielding motions that are all completely periodic (i.e. periodic in all degrees of freedom) with the same period $\tilde{T} = 2\pi/\Omega$.

Consider the $\Omega$-modified Hamiltonian

$$\tilde{H}\left(\tilde{p}, \tilde{q}; \Omega\right) \equiv H\left(\tilde{P}, \tilde{Q}; \tilde{\eta}, \tilde{\xi}; \Omega\right) = \frac{1}{2} \left[ \tilde{P} + \frac{h(\tilde{\eta}, \tilde{\xi})}{b} \right]^2 + \frac{1}{2} \Omega^2 \tilde{Q}^2. \tag{1}$$

Notation. Here and hereafter $\Omega$ is a positive constant ($\Omega > 0$) to which the basic isochrony period

$$\tilde{T} = \frac{2\pi}{\Omega} \tag{2}$$

is associated (in previous publications, see for instance [1, 2], we used the notation $T$ for the period associated to the circular frequency $\Omega$; the change introduced here is necessitated by the preference to reserve the standard notation $T$ to denote the temperature, see below); the $N$ components $\tilde{p}_n$ and $\tilde{q}_n$ of the $N$-vectors $\tilde{p}$ and $\tilde{q}$ are canonically conjugated variables, and likewise the $N-1$ components $\tilde{\eta}_m$ and $\tilde{\xi}_m$ of the $(N-1)$-vectors $\tilde{\eta}$ and $\tilde{\xi}$ are canonically conjugated variables, and so are the two variables $\tilde{P}$ and $\tilde{Q}$. Hence, the variables $\{\tilde{p}_n; \tilde{q}_n; n = 1, \ldots, N\}$ and $\{\tilde{P}, \tilde{\eta}_m; \tilde{Q}, \tilde{\xi}_m; m = 1, \ldots, N-1\}$ are two equivalent sets of canonical variables: a simple relation among these two sets will eventually be established, see below, when discussing specifically the many-body problem. As a general rule we superimpose a tilde on all variables that are eventually meant to evolve according to the $\Omega$-modified Hamiltonian. The function $h(\tilde{\eta}, \tilde{\xi})$, depending on the $(N-1)$ canonical momenta $\tilde{\eta}_m$ and on the $N-1$ corresponding canonical coordinates $\tilde{\xi}_m$, can of course be considered a Hamiltonian in its own right, indeed the constant $b$ (having the dimensionality of a momentum) is introduced in the right-hand side of (1) merely to provide a dimensional renormalization as we like all Hamiltonians to have the dimensions of energy (i.e. momentum squared, see (1).
and below). Note that we are assuming the canonical variables \( \tilde{P} \) and \( \tilde{Q} \) to be independent of the canonical variables \( \tilde{\eta}_m \) and \( \tilde{\xi}_m \); this of course entails that, under the time evolution yielded by the \( \Omega \)-modified Hamiltonian \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega) \)—on which our consideration is hereafter mainly focused—the function \( h(\tilde{\eta}, \tilde{\xi}) \) is a constant of the motion (since it Poisson-commutes with \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega) \)),

\[
h \left( \tilde{\eta}, \tilde{\xi} \right) = E. \tag{3}
\]

It is plain that the \( \Omega \)-modified Hamiltonian \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega) \) yields for the two canonical variables \( \tilde{P} \) and \( \tilde{Q} \), also thanks to (3), the ‘harmonic’ equations of motion

\[
\dot{\tilde{Q}} = \frac{\partial \tilde{H}}{\partial \tilde{P}} = \tilde{P} + \frac{E}{b}, \tag{4a}
\]

\[
\dot{\tilde{P}} = -\frac{\partial \tilde{H}}{\partial \tilde{Q}} = -\Omega^2 \tilde{Q}, \tag{4b}
\]

where superimposed dots denote of course—here and throughout—differentiations with respect to the independent variable \( t \), timing the evolution determined by the Hamiltonian \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega) \). Clearly these equations of motion entail the following periodic evolution (with period \( \tilde{T} \), see (2)):

\[
\tilde{Q}(t) = \tilde{Q}(0) \cos (\Omega t) + \frac{\dot{\tilde{Q}}(0)}{\Omega} \frac{\sin (\Omega t)}{b}, \tag{5a}
\]

\[
\tilde{P}(t) = \tilde{P}(0) \cos (\Omega t) + \frac{\dot{\tilde{P}}(0)}{\Omega} \frac{\sin (\Omega t)}{b} - \frac{E}{b} \left[ 1 - \cos (\Omega t) \right], \tag{5b}
\]

Likewise, the \( \Omega \)-modified Hamiltonian \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega) \) yields, via (3) and (4a), for the remaining canonical variables \( \tilde{\eta}_m \) and \( \tilde{\xi}_m \), the Hamiltonian equations of motion

\[
\dot{\tilde{\xi}}_m = \frac{\partial \tilde{H}}{\partial \tilde{\eta}_m} = \frac{b P + E}{b^2} \frac{\partial h}{\partial \tilde{\eta}_m}, \quad m = 1, \ldots, N - 1, \tag{6a}
\]

\[
\dot{\tilde{\eta}}_m = -\frac{\partial \tilde{H}}{\partial \tilde{\xi}_m} = -\frac{b P + E}{b^2} \frac{\partial h}{\partial \tilde{\xi}_m} = -\frac{\dot{\tilde{Q}}}{b} \frac{\partial h}{\partial \tilde{\xi}_m}, \quad m = 1, \ldots, N - 1. \tag{6b}
\]

These equations of motion clearly entail

\[
\frac{d \tilde{\xi}_m}{d\tau} = \frac{\partial h}{\partial \tilde{\eta}_m}, \quad m = 1, \ldots, N - 1, \tag{7a}
\]

\[
\frac{d \tilde{\eta}_m}{d\tau} = -\frac{\partial h}{\partial \tilde{\xi}_m}, \quad m = 1, \ldots, N - 1. \tag{7b}
\]
namely just the Hamiltonian equations of motion yielded by the Hamiltonian \( h(\tilde{\eta}, \tilde{\xi}) \), but with the proviso that the independent variable be, instead of \( t \),

\[
\tau \equiv \tau (t) = \frac{\tilde{Q}(t) - \tilde{Q}(0)}{b},
\]

where we have set the arbitrary additive constant in this definition so that \( \tau (0) = 0 \). Since \( \tilde{Q}(t) \)
hence \( \tau (t) \) are periodic in \( t \) with period \( \tilde{T} \) (see (2)),

\[
\tau (t) = A \{ \cos \left[ \Omega \left( t - t_0 \right) \right] - \cos \left( \Omega t_0 \right) \},
\]

\[
A^2 = \left[ \frac{\dot{\tilde{Q}}(0)}{b} \right]^2 + \left[ \frac{\dot{\tilde{Q}}(0)}{b \Omega} \right]^2, \quad \tan (\Omega t_0) = \frac{\dot{\tilde{Q}}(0)}{\Omega \dot{\tilde{Q}}(0)},
\]

(see (8) and (5a)), clearly implying

\[
\tau \left( t + \tilde{T} \right) = \tau \left( \tilde{T} - t \right) = \tau (t), \mod \left( \tilde{T} \right),
\]

this same property carries over to all the canonical variables,

\[
\tilde{\xi}_m \left( t + \tilde{T} \right) = \tilde{\xi}_m \left( \tilde{T} - t \right) = \tilde{\xi}_m (t), \quad m = 1, \ldots, N - 1, \mod \left( \tilde{T} \right),
\]

\[
\tilde{\eta}_m \left( t + \tilde{T} \right) = \tilde{\eta}_m \left( \tilde{T} - t \right) = \tilde{\eta}_m (t), \quad m = 1, \ldots, N - 1, \mod \left( \tilde{T} \right).
\]

Likewise the explicit expressions (5) of the time evolution of the variables \( \tilde{Q} \) and \( \tilde{P} \) clearly implies as well that

\[
\tilde{Q} \left( t + \tilde{T} \right) = \tilde{Q} \left( \tilde{T} - t \right) = \tilde{Q} (t), \quad \tilde{P} \left( t + \tilde{T} \right) = \tilde{P} \left( \tilde{T} - t \right) = \tilde{P} (t), \mod \left( \tilde{T} \right).
\]

Hence, the isochrony with period \( \tilde{T} \) of the time evolution yielded by the \( \Omega \)-modified Hamiltonian \( \tilde{H}(\tilde{P}, \tilde{Q}; \Omega) \),

\[
\tilde{q}_n \left( t + \tilde{T} \right) = \tilde{q}_n \left( \tilde{T} - t \right) = \tilde{q}_n (t), \quad n = 1, \ldots, N, \mod \left( \tilde{T} \right),
\]

\[
\tilde{p}_n \left( t + \tilde{T} \right) = \tilde{p}_n \left( \tilde{T} - t \right) = \tilde{p}_n (t), \quad n = 1, \ldots, N, \mod \left( \tilde{T} \right),
\]

entailing that the \( \Omega \)-modified system goes through the same dynamical configuration twice within every time period \( \tilde{T} \) (just as the circular functions \( \cos(x) \) and \( \sin(x) \), periodic with period \( 2\pi \) as a function of \( x \), take twice the same value within every interval \( 2\pi \)).

This might be considered an uninteresting finding: the \( \Omega \)-modified Hamiltonian \( \tilde{H}(\tilde{P}, \tilde{Q}; \Omega) \) entails the de facto introduction of a periodic external forcing causing the time evolution to be completely periodic with period \( \tilde{T} \). Yet, by specifying this Hamiltonian \( \tilde{H}(\tilde{P}, \tilde{Q}; \Omega) \) to be the \( \Omega \)-modified version of the Hamiltonian describing the (standard and quite general) many-body problem, we will see below that this \( \Omega \)-modified Hamiltonian \( \tilde{H}(\tilde{P}, \tilde{Q}; \Omega) \) might itself qualify as a rather reasonable Hamiltonian describing many-body dynamics, raising interesting issues.
Indeed in the next section 2, we focus on the Hamiltonian describing the standard nonrelativistic many-body problem and its $\Omega$-modified isochronous variant, and we outline in this context the remarkable coexistence of the irreversible and periodic aspects of the behavior of this isochronous model.

Then, in section 3, we briefly discuss the equilibrium thermodynamics of our $\Omega$-modified model and we show that in such a context the, correctly defined, equilibrium entropy of this system remains constant. It is thus seen that, even for our $\Omega$-modified model, the behavior at thermodynamic equilibrium corresponds to standard expectations (see for instance [3]). On the other hand for our model it is clearly impossible to define for nonequilibrium thermodynamic states a generalized entropy having the property always to grow over time, as happens for the Boltzmann entropy of an ideal gas evolving in the standard manner (see for instance [3]).

Finally, in section 4 and the appendix, we show that the phenomenology described above can be actually reproduced in a specific ‘realistic’ example involving many particles interacting via Lennard–Jones potentials. Although the emergence of this phenomenology (including the reversal of irreversible processes!) is implied beyond doubt by our treatment, it is remarkable that this fact can actually be reproduced in a numerical simulation.

A brief section 5 entitled ‘Outlook’ completes our paper.

2. $\Omega$-modified version of the standard many-body problem

Let us take as starting point of our treatment the standard Hamiltonian describing a many-body problem:

$$H(p, q) = \frac{1}{2} \sum_{n=1}^{N} p_n^2 + V(q). \quad (11)$$

This is the most general Hamiltonian describing such a system—with the canonical coordinates $q_n$ identifying the position of the (pointlike) moving particles—except for the two restrictions to limit consideration to one-dimensional unit-mass particles, introduced here merely for simplicity (lifting both these restrictions would be a trivial task and would entail no significant change in the following treatment; in fact the first one shall be eliminated below, see section 4).

We moreover assume validity of the (physically very natural) requirement that the potential $V(q) \equiv V(q_1, \ldots, q_N)$ be translation invariant,

$$V(q_1 + a, \ldots, q_N + a) = V(q_1, \ldots, q_N), \quad (12)$$

where $a$ denotes an arbitrary constant. It is then natural to introduce the center-of-mass momentum and coordinate,

$$P = \sum_{n=1}^{N} p_n, \quad Q = \frac{1}{N} \sum_{n=1}^{N} q_n, \quad (13)$$

the first of which is, of course, a constant of motion, $P(\tau) = P(0)$, while the second behaves linearly, $Q(\tau) = Q(0) + Q'(0) \tau$, under the evolution yielded by the Hamiltonian $H(p, q)$; note that the independent variable corresponding to this evolution is here and hereafter denoted as $\tau$, emphasizing its difference from the independent variable $t$ characterizing the time-evolution implied by the $\Omega$-modified Hamiltonian $H(\vec{p}, \vec{q}; \Omega)$, see above and below. And it is correspondingly natural to separate the Hamiltonian $H(\vec{p}, \vec{q})$ into a (trivial) part describing
the (trivial) evolution of the center-of-mass variables and a remaining part describing motions in the center-of-mass frame, via the standard position

\[
H \left( p, q \right) = \frac{p^2}{2N} + h \left( \eta, \xi \right),
\]

\[ \tag{14a} \]

\[
h \left( \eta, \xi \right) = \frac{1}{2} \sum_{m=1}^{N-1} \eta_m^2 + V \left( \xi \right) = \frac{1}{4N} \sum_{n,m=1}^{N} \left( p_n - p_m \right)^2 + V \left( q \right), \]

\[ \tag{14b} \]

\[
V \left( \xi \right) = V \left( q \right), \]

\[ \tag{14c} \]

where the last equation is justified by (12) (see also below). We have thereby introduced a new set of canonical variables \( \{ P, \eta_m; Q, \xi_m; m = 1, \ldots, N - 1 \} \) (see (13)); we hereafter refer to the \( 2(N-1) \) canonical momenta and coordinates \( \eta_m \) and \( \xi_m \) as ‘internal’ canonical variables; in the case of equal particles they can be chosen so as to maintain the invariance of the Hamiltonian under their permutation, a specific choice being the well-known Jacobi coordinates. These variables are related to the original ‘particle variables’ \( \{ p_n; q_n; n = 1, \ldots, N \} \) by a well-known linear constant-coefficient transformation that need not be explicitly displayed here. Indeed, it is often more convenient—as we did in our previous paper [2] and will do hereafter—to use the following ‘natural’ definition of the internal variables:

\[
x_n = q_n - Q, \quad y_n = p_n - \frac{P}{N}, \quad n = 1, \ldots, N. \]

\[ \tag{15a} \]

Note that we thereby introduce \( 2N \) rather than \( 2(N-1) \) variables, obviously constrained (see (13)) by the conditions

\[
\sum_{n=1}^{N} x_n = 0, \quad \sum_{n=1}^{N} y_n = 0. \]

\[ \tag{15b} \]

These variables are not quite canonical, because their Poisson bracket reads

\[
[y_n, x_{n'}] = \left[ p_n - \frac{P}{N}, q_{n'} - Q \right] = \delta_{nn'} - \frac{1}{N}, \quad n, n' = 1, \ldots, N. \]

\[ \tag{15c} \]

But this can be appropriately taken care of. So, for completeness and future reference, let us now also display the version of the many-body Hamiltonian (14) in terms of these internal variables:

\[
H \left( p, q \right) = \frac{p^2}{2N} + h \left( y, x \right),
\]

\[ \tag{16a} \]

\[
h \left( y, x \right) = \frac{1}{2} \sum_{n=1}^{N} y_n^2 + V \left( x \right) = \frac{1}{4N} \sum_{n,m=1}^{N} \left( p_n - p_m \right)^2 + V \left( q \right), \]

\[ \tag{16b} \]

\[
V \left( x \right) = V \left( q \right). \]

\[ \tag{16c} \]

This is the version we shall consider hereafter; note the standard slight abuse of notation entailed by our using the same letter \( h \) to denote the internal motion Hamiltonian as function of the \( 2(N-1) \) canonical variables \( \eta_m \) and \( \xi_m \) (see (14)) and as function of the \( 2N \) noncanonical variable \( y_n \) and \( x_n \) constrained by the identities (15b) (see (16)). Note moreover the close
similarity among the formulae (14) and (16), the only difference (other than the name of the variables) being the insertion of $N$ in place of $N - 1$ as upper limit of the first sum in the right-hand side of (16b). It can moreover be verified that, in spite of the noncanonical character of the variables $y_n$ and $x_n$, see (15c), the equations of motion yielded by this Hamiltonian (16) by firstly writing the Hamiltonian equations in terms of the proper canonical variables $p_n$ and $q_n$, and by then using the relations of these variables to the noncanonical internal variables $y_n$ and $x_n$) end up reading just as the standard canonical equations of motion which would be yielded by the Hamiltonian (16b) by treating the variables $y_n$ and $x_n$ as canonically conjugated independent variables:

\[
\frac{dx_n}{d\tau} = \frac{\partial h(y_n, x_n)}{\partial y_n}, \quad n = 1, \ldots, N, \quad (17a)
\]

\[
\frac{dy_n}{d\tau} = -\frac{\partial h(y_n, x_n)}{\partial x_n}, \quad n = 1, \ldots, N. \quad (17b)
\]

Let us re-emphasize that here we denote as $\tau$ the independent variable characterizing the evolution due to the standard many-body Hamiltonian $H(p, q)$, see (11) and (16). Of course, these equations of motion must be supplemented by the constraints (15b), whose compatibility with them is of course guaranteed by the assumed translation invariance of the potential $V(x)$, see (12), and (16c) (15a).

(These changes of notation are described in detail here for the sake of completeness and precision; they are of particularly little relevance when investigating, as we shall do below, properties of our system in the framework of statistical mechanics and thermodynamics, when, of course, $N$ is assumed to be very large: indeed in the limit $N \to \infty$ the noncanonical Poisson bracket (15c) becomes canonical, and the difference between $N - 1$ and $N$ becomes negligible.)

Let us finally introduce our $\Omega$-modified version $\tilde{H}(\tilde{p}, \tilde{q}; \Omega)$ of the standard many-body Hamiltonian (16) via our basic formula (1), now reading

\[
\tilde{H}(\tilde{p}, \tilde{q}; \Omega) \equiv \tilde{H}(\tilde{p}, \tilde{q}; \tilde{y}, \tilde{x}; \Omega) = \frac{1}{2} \left[ \tilde{P} + \frac{h(\tilde{y}, \tilde{x})}{b} \right]^2 + \frac{1}{2} \Omega^2 \tilde{Q}^2. \quad (18)
\]

Here, we trust the notation to be self-explanatory; recall that the decoration of the variables with a superimposed tilde is merely a reminder that their time evolution is now determined by this $\Omega$-modified Hamiltonian $\tilde{H}(\tilde{p}, \tilde{q}; \Omega)$. This entails of course that the center-of-mass variables $\tilde{P}$ and $\tilde{Q}$ are defined by the analogs of (13),

\[
\tilde{P} = \sum_{n=1}^{N} \tilde{p}_n, \quad \tilde{Q} = \frac{1}{N} \sum_{n=1}^{N} \tilde{q}_n, \quad (19)
\]

that the internal coordinates $\tilde{y}_n$ and $\tilde{x}_n$ are related to the coordinates $\tilde{p}_n$ and $\tilde{q}_n$ by the analogs of (15a),

\[
\tilde{y}_n = \tilde{q}_n - \tilde{Q}, \quad \tilde{x}_n = \tilde{p}_n - \frac{\tilde{P}}{N}, \quad n = 1, \ldots, N. \quad (20a)
\]
and of course satisfy the constraints
\[\sum_{n=1}^{N} \tilde{x}_n = 0, \quad \sum_{n=1}^{N} \tilde{y}_n = 0.\]  
(20b)

This Hamiltonian \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega) \)—whose isochronous character has been demonstrated in the preceding section 1—is of course somewhat different from the standard many-body Hamiltonian \( H(p, q), \) compare (18) with (16); and it is not normal, not just the sum of the standard, quadratic, kinetic energy part plus a momentum-independent potential energy. But it is not too different, indeed it might be considered an alternative, legitimate, Hamiltonian describing an alternative, perhaps somewhat unusual, many-body system; the more so since, as we now show, over time intervals much shorter than the isochrony period \( \bar{T} \) the motions yielded by this \( \Omega \)-modified Hamiltonian \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega), \) see (18) with (16) and (19), generally differ only marginally from those yielded by the standard many-body Hamiltonian \( H(p, q), \) see (16).

Indeed, the treatment given in the preceding section 1 implies that the time evolution yielded by this \( \Omega \)-modified Hamiltonian \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega) \) for the \( 2N \) momenta and coordinates \( \tilde{p}_n \) and \( \tilde{q}_n \) is that entailed (via (19) and (20a)) by the formulae (5) for the center-of-mass variables \( \tilde{Q}(t) \) and \( \tilde{P}(t) \) and by the analogs of the equations of motion (17) for the internal variables \( \tilde{x}_n(t) \) and \( \tilde{y}_n(t), \) reading
\[\frac{d\tilde{x}_n}{d\tau} = \frac{\partial h(\tilde{y}, \tilde{x})}{\partial \tilde{y}_n}, \quad n = 1, \ldots, N,\]  
(21a)
\[\frac{d\tilde{y}_n}{d\tau} = -\frac{\partial h(\tilde{y}, \tilde{x})}{\partial \tilde{x}_n}, \quad n = 1, \ldots, N,\]  
(21b)
but now with \( \tau \) related to \( t \) by the formulae (8) and (9) (compare with (7)). Hence,
\[\tilde{x}_n(t) = x_n(\tau), \quad \tilde{y}_n(t) = y_n(\tau), \quad n = 1, \ldots, N,\]  
(22)
as implied by the identity of the equations of motion (17) and (21) (of course with an appropriate setting of the initial conditions, entailing the validity of these relations (22) at the initial time \( t = \tau = 0 \)). Let us re-emphasize that the equations of motion (17) correspond to the fact that the \( N \) internal coordinates \( y_n(\tau) \) and \( x_n(\tau) \) evolve in \( \tau \) according to the unmodified internal-motion Hamiltonian \( h(y, x), \) see (16); hence these formulae (22) show that, in order to obtain the evolution yielded, for the \( N \) analogous internal variables \( \tilde{y}_n(t) \) and \( \tilde{x}_n(t), \) by the \( \Omega \)-modified Hamiltonian \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega), \) all one must do is take account of the fact that \( \tau \equiv \tau(t) \) evolves in \( t \) according to (9).

These results obviously confirm the isochronous character of the evolution yielded by the \( \Omega \)-modified Hamiltonian \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega), \) as entailed by the periodic character of \( \tau(t), \) see (10a), (10e), (10f) and (10d). But the explicit formula (9) with (2) implies as well (by Taylor expansion) that, in the neighborhood of a generic time \( \bar{t}, \)
\[\tau(t) = \tau(\bar{t}) + \frac{\dot{\tau}(\bar{t})}{b} (t - \bar{t}) + O \left( \left( \frac{t - \bar{t}}{T} \right)^2 \right).\]  
(23)
Hence, in the neighborhood of any time \( \bar{t} \) such that \( \dot{\tau}(\bar{t}) \neq 0 \)—the neighborhood being defined by the condition that \( |t - \bar{t}| \ll \bar{T}, \) see (2)—the time evolution yielded, for the internal variables,
by the $\Omega$-modified Hamiltonian $\tilde{H}(\tilde{p}, \tilde{q}; \Omega)$, see (18), differs marginally—only by a constant translation and rescaling of the time variable—from the time evolution yielded by the original many-body Hamiltonian $H(p, q)$, see (11) and (16): this justifies the conclusion that, over such time scales, the dynamics yielded by the $\Omega$-modified Hamiltonian $\tilde{H}(\tilde{p}, \tilde{q}; \Omega)$ essentially coincides with that yielded by the original many-body Hamiltonian $H(p, q)$.

Let us assume that the original many-body problem is of the standard ‘physical’ type, nonintegrable and characterized by short-range two-body potentials. Its typical dynamics shall then be macroscopically irreversible, characterized—even if it starts from a simple ordered state—by a transition, in its center-of-mass frame, to a disordered state with energy equipartition. Such a transition is characteristic of a thermodynamically irreversible process. It generally occurs in a time $\Delta$ which is a relatively small multiple of the typical ‘collision time’—or rather, ‘close encounter time’—between the particles. If the irreversible process takes place at a time $\bar{t}$ such that $\dot{\bar{t}} \neq 0$ and if $|b/\dot{\bar{t}}| \ll \bar{T}$, the same ‘irreversible’ behavior shall be displayed, over time intervals much shorter than $\bar{T}$—as implied by the previous discussion—by the dynamics yielded by our $\Omega$-modified Hamiltonian $\tilde{H}(\tilde{p}, \tilde{q}; \Omega)$ (with an appropriate, constant, time rescaling). Yet, somewhat paradoxically, the isochronous dynamics yielded by the $\Omega$-modified Hamiltonian $\tilde{H}(\tilde{p}, \tilde{q}; \Omega)$ must also cause the system to return twice to its initial state within the time $\bar{T}$: the irreversible transition to thermodynamic equilibrium must therefore be eventually undone—and this shall of course happen again and again, as implied by the isochronous character of the time evolution yielded by the $\Omega$-modified Hamiltonian $\tilde{H}(\tilde{p}, \tilde{q}; \Omega)$.

The paradoxical behavior described above might be attributed to the fact that the time-rescaling factor $b/\dot{\bar{t}}$, see (23), can have either sign. This is of course highly relevant (see below), but does not provide by itself an explanation. Let us take again as prototype of irreversible process the transition, in the context of both the unmodified dynamics yielded by the Hamiltonian $H(p, q)$ (see (16)) and of the $\Omega$-modified dynamics yielded by our $\Omega$-modified Hamiltonian $\tilde{H}(\tilde{p}, \tilde{q}; \Omega)$ (see (18) with (16)), from an ordered configuration to a disordered state of thermodynamic equilibrium, the latter taking place in a time $|\tilde{\Delta}|$ much shorter than $\bar{T}$, $|\tilde{\Delta}| \ll \bar{T}$, where

$$\tilde{\Delta} = \frac{b \Delta}{\dot{Q}(\bar{t})}. \tag{24}$$

Note that this can always be achieved since the assignment of $\Omega$, hence of $\tilde{T}$, is our privilege when manufacturing our $\Omega$-modified Hamiltonian $\tilde{H}(\tilde{p}, \tilde{q}; \Omega)$. Then the transition to thermodynamic equilibrium occurs after a time of order $\Delta$, both in the direction of increasing time and in the direction of decreasing time, for the system defined by the standard Hamiltonian $H(p, q)$—whose dynamics is indeed generally invariant under microscopic time reversal, as is the case for all Hamiltonians invariant under the change of sign of all momenta, hence in particular for normal Hamiltonians. Likewise, it occurs in a time of order $|\tilde{\Delta}|$ in the direction of increasing or decreasing time for the system defined by the $\Omega$-modified Hamiltonian $\tilde{H}(\tilde{p}, \tilde{q}; \Omega)$ if one looks at the behavior of this system in the neighborhood of a time $\bar{t}$ such that the time-rescaling factor $b/\dot{\bar{t}}$ (hence $\tilde{\Delta}$ as well, see (24)) is positive, and in the direction of decreasing or increasing time if the time-rescaling factor $b/\dot{\bar{t}}$ (hence $\tilde{\Delta}$ as well) is negative.
Hardly a difference: in any case one would witness an approach to thermodynamic equilibrium, namely a typically irreversible evolution. Note incidentally that for the above argument to work, it is not necessary to assume that the unmodified Hamiltonian \( H(p, q) \), or equivalently \( h(y, x) \), be invariant under time reversal: the dynamics yielded by \( H(\tilde{p}, \tilde{q}; \Omega) \) for \( t \) in the neighborhood of a time \( \tilde{t} \) such that \( \left| \Omega \Delta \right| \ll 1 \) (see (24)) will be similar to the dynamics yielded by \( H(p, q) \) if \( b/\dot{Q}(\tilde{t}) \) is positive and to the corresponding time-reversed dynamics if \( b/\dot{Q}(\tilde{t}) \) is negative. But in the following, we generally assume time-reversal invariance of the unmodified Hamiltonian, as is indeed the case for the standard many-body problem characterized by the unmodified Hamiltonian \( H(p, q) \), see (16).

To understand what really happens to the system whose time evolution is determined by the \( \Omega \)-modified Hamiltonian \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega) \) it is rather useful to focus on the special times \( t_s \) when the time-rescaling factor diverges, \( \dot{Q}(t_s) = 0 \), (25) see (24). There are clearly two such times \( t_s \) within every period \( \tilde{T} \) (see (5a)). At such times all the velocities of the particles—in the center-of-mass frame—vanish (\( \dot{x}_{\alpha} = 0 \), see (22), (8) and (25)). Immediately before and after these times, all these velocities have opposite signs; and after such times, the system retraces its steps, going backward through its previous dynamical configurations, as implied by (22) with (9) (and note again that this happens irrespective of the time-reversibility of the unmodified dynamics).

Incidentally: this development is more peculiar than the ‘timequake’ envisaged by the extravagant imagination of Kurt Vonnegut [4], in as much as the repetition of all previous happenings characterizing a Vonnegut timequake is preceded in our phenomenology by a phase when they occur in reverse order, and by a phase when they mimic, first in reverse order and then in the proper order, the dynamics that occurred before the timequake. The first part of this phenomenology is actually familiar to whoever has watched a celluloid film as it was shown, and then rewound back, with the projector always on; indeed it gets accurately reproduced when the speed of this projection is varied periodically, coinciding with \( \tau(t) \), see (9). But this analogy only extends to the first part of the evolution of our \( \Omega \)-modified system, until the moment when the initial configuration is reproduced for the first time; the following evolution, to complete the periodic cycle, corresponds instead to the dynamics of the unmodified system before it arrived at its initial configuration.

It is thus seen that, for the \( \Omega \)-modified system, at the special times \( t_s \) a kind of time reversal is performed by the dynamics itself. This clarifies the main characteristic of the \( \Omega \)-modification approach. The fact that performing such time-reversal transformations—specifically, changing the sign of all velocities without changing the positions of the particles—causes a system to reverse its time evolution—if the dynamics of the system in question is microscopically reversible—was of course well known. But it was generally argued that performing such a reversal is operationally impossible for a realistic system: as famously emphasized in the debate between Boltzmann, on one side, and Loschmidt and Zermelo on the other, when the latter debaters pointed out that this fact seemed to contradict the irreversibility of macroscopic evolutions and the reply by Boltzmann was the challenge to actually perform the feat of reversing the speeds of all the molecules of a gas (see for instance [5]). Our \( \Omega \)-modification technique shows that it is indeed possible to envisage a dynamics—both Hamiltonian and autonomous—which realizes such reversals, as it were, spontaneously, without affecting
significantly the time evolution over times much shorter than the period $\tilde{T}$—whose assignment remains our privilege, hence it can be set to be much larger than the timescale characterizing the behavior of the original, unmodified system. These questions are of course intimately related to the much debated issue of the ‘thermodynamical arrow of time’, see for instance [6] and the literature quoted there.

In conclusion it is clear that, over times of the order or larger than $\tilde{T}$, the behavior of the many-body system described by the $\Omega$-modified Hamiltonian (18) with (16) is quite different from that of the related many-body system described by the Hamiltonian (11) characterizing standard molecular dynamics. The former behavior, yielded by the $\Omega$-modified Hamiltonian (18) with (16), is isochronous, an even more constraining requirement than being integrable or even maximally superintegrable (i.e. possessing the maximal number of constants of motion, $2N - 1$ of them for the systems treated herein); indeed, all confined motions yielded by maximally superintegrable systems are completely periodic because all their degrees of freedom are slave to a single time evolution [7], but the periods of the motions generally depend on the initial data, which is not the case for isochronous systems (hence, while isochronous systems are clearly maximally superintegrable, the converse is not generally true). The latter behavior, yielded by the unmodified Hamiltonian (11), is instead generally chaotic, leading to energy equipartition and thermodynamic equilibrium with the eventual applicability of statistical mechanics and thermodynamics. On the other hand, let us reiterate that if the isochrony period $\tilde{T}$ of the $\Omega$-modified Hamiltonian (18) with (16) is chosen to be very much larger than the collision times characterizing the related, standard many-body Hamiltonian (11), the dynamics yielded by these two Hamiltonians are generally only marginally different over times long in terms of the intrinsic features of the dynamics associated with the unmodified Hamiltonian (11), but short with respect to the isochrony period $\tilde{T}$. Hence, from the experimental point of view, if $\tilde{T}$ is very large the differences among these two systems might be difficult to notice. This may be interpreted as a warning that systems behaving similarly over times characterizing key aspects of their dynamics—for instance, their approach to thermodynamic equilibrium—might nevertheless behave quite differently over longer times.

And let us end this discussion by airing the amusing eschatological conjecture that the time evolution characterizing our Universe—assuming it is simply determined in the classical context by a standard many-body Hamiltonian of type (11)—should be in truth replaced by a corresponding $\Omega$-modified Hamiltonian of type (18) with (16) and an associated value of $\tilde{T}$ sufficiently large to have defied observation so far; thereby providing a ‘scientific’ basis for the expectation of a recurring cosmological evolution, as envisaged by some religions, catering—as many religions, according to some nonbelievers, do—to the fear entertained by many humans that their death is the end of it all.

3. Entropy

As a first step towards unraveling the macroscopic behavior of the many-body model characterized by the isochronous $\Omega$-modified Hamiltonian (18) with (16)—with

$$\left| \Delta \right| \ll \tilde{T},$$

(26)

see previous discussion—we need to evaluate the entropy of the system it describes, in order to understand its thermodynamics. Let us first of all point out that the two macroscopic center-of-mass degrees of freedom $\tilde{P}$ and $\tilde{Q}$ should not be treated like the others: they move much more
slowly. Indeed, in order to obtain the specific effects to be discussed here, their rate of change must be slow compared to all system relaxation times (see (5) and (26)). They are therefore to be treated, in a thermodynamic context, as external parameters. Another hint that this must be done comes from the fact that any attempt to compute the full partition function including the \( \tilde{P} \) and \( \tilde{Q} \) variables leads to a divergent result, due to the infinite range of integration for these variables.

Let us therefore evaluate the ‘internal entropy’ of our \( \Omega \)-modified system as defined by the following expression:

\[
\delta \left( \tilde{E}; \tilde{P}, \tilde{Q}; \Omega \right) = \frac{1}{N} \ln \left\{ \int d\tilde{\gamma} \, d\tilde{x} \, \delta \left[ \tilde{E} - \tilde{\mathcal{H}} \left( \tilde{P}, \tilde{Q}; \tilde{\gamma}, \tilde{x}; \Omega \right) \right] \right\},
\]

(27)
of course with \( \tilde{\mathcal{H}}(\tilde{P}, \tilde{Q}; \tilde{\gamma}, \tilde{x}; \Omega) \) defined by (18) with (16). To this end we introduce the two quantities

\[
\mathcal{E}_{\pm} \left( \tilde{E}; \tilde{P}, \tilde{Q}; \Omega \right) = -\tilde{P} \pm \sqrt{2\tilde{E} - \Omega^2 \tilde{Q}^2},
\]

(28a)
so that (see (18) with (16))

\[
\tilde{\mathcal{H}} \left( \tilde{P}, \tilde{Q}; \tilde{\gamma}, \tilde{x}; \Omega \right) - \tilde{E} = \frac{1}{2} \left\{ \frac{h \left( \tilde{\gamma}, \tilde{x} \right)}{b} - \mathcal{E}_+ \left( \tilde{E}; \tilde{P}, \tilde{Q}; \Omega \right) \right\} \left[ \frac{h \left( \tilde{\gamma}, \tilde{x} \right)}{b} - \mathcal{E}_- \left( \tilde{E}; \tilde{P}, \tilde{Q}; \Omega \right) \right].
\]

(28b)
From this there follows (via standard properties of the delta-function) the formula

\[
\delta(\tilde{E} - \tilde{\mathcal{H}}) = 2b \left\{ \mathcal{E}_+ \left( \tilde{E}; \tilde{P}, \tilde{Q}; \Omega \right) - \mathcal{E}_- \left( \tilde{E}; \tilde{P}, \tilde{Q}; \Omega \right) \right\}.
\]

(28c)
Now for the typical many-body Hamiltonian, see (11) with stable potentials [8], one has

\[
\left| \mathcal{E}_+ \left( \tilde{E}; \tilde{P}, \tilde{Q}; \Omega \right) - \mathcal{E}_- \left( \tilde{E}; \tilde{P}, \tilde{Q}; \Omega \right) \right| \leq c \, N,
\]

(29)
where \( N \) is the total number of particles and \( c \) is an \( N \)-independent constant. In the limit of large \( N \)—to which all considerations in this section of course refer—we may therefore ignore the contribution of these terms in the evaluation (27) of the entropy and we obtain

\[
\delta \left( \tilde{E}; \tilde{P}, \tilde{Q}; \Omega \right) = \frac{1}{N} \ln \left\{ \max \left\{ \mathcal{Z}_+ \left( \tilde{E}; \tilde{P}, \tilde{Q}; \Omega \right), \mathcal{Z}_- \left( \tilde{E}; \tilde{P}, \tilde{Q}; \Omega \right) \right\} \right\},
\]

(30)
where the quantities \( \mathcal{Z}_\pm(\tilde{E}; \tilde{P}, \tilde{Q}; \Omega) \) are defined as follows:

\[
\mathcal{Z}_\pm \left( \tilde{E}; \tilde{P}, \tilde{Q}; \Omega \right) = \int d\tilde{\gamma} \, d\tilde{x} \, \delta \left[ b\mathcal{E}_\pm \left( \tilde{E}; \tilde{P}, \tilde{Q}; \Omega \right) - h \left( \tilde{\gamma}, \tilde{x} \right) \right].
\]

(31)
Hence, \( \mathcal{Z}_\pm(\tilde{E}; \tilde{P}, \tilde{Q}; \Omega) \) is the center-of-mass partition function of the unmodified system, at an energy defined by \( b\mathcal{E}_\pm(\tilde{E}; \tilde{P}, \tilde{Q}; \Omega) \). However, as it is readily verified, when \( \tilde{P} \) and \( \tilde{Q} \) evolve according to the dynamics defined by the \( \Omega \)-modified Hamiltonian \( \tilde{\mathcal{H}}(\tilde{P}, \tilde{Q}; \Omega) \), see (18) with (16), the quantities \( \mathcal{E}_\pm(\tilde{E}; \tilde{P}, \tilde{Q}) \) are time independent. One can therefore introduce the time independent quantity

\[
\mathcal{E}_\pm \left( \tilde{E}; \Omega \right) \equiv b\mathcal{E}_\pm \left( \tilde{E}; \tilde{P}(0), \tilde{Q}(0); \Omega \right) = b\mathcal{E}_\pm \left( \tilde{E}; \tilde{P}(t), \tilde{Q}(t); \Omega \right),
\]

(32)
and then write
\[
\tilde{S}(E; \tilde{P}, \tilde{Q}; \Omega) = \max \left\{ S_+(E; \tilde{\Omega}), \quad S_-(E; \tilde{\Omega}) \right\},
\]
where \( S(E) \) is the internal entropy of the unmodified system (in its center-of-mass frame), as defined by
\[
S(E) = \frac{1}{N} \ln \left\{ \int d\tilde{y} \, d\tilde{x} \delta \left( E - h(\tilde{y}, \tilde{x}) \right) \right\}. 
\]

From this result several interesting consequences follow. First and foremost, the entropy remains constant over time. Moreover, one sees that the internal entropy \( \tilde{S}(E; \tilde{P}, \tilde{Q}; \Omega) \) of the \( \Omega \)-modified system characterized by the \( \Omega \)-modified Hamiltonian \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega) \), see (18) with (16), is given by the same expression as the center-of-mass entropy \( S \) of the unmodified system characterized by the center-of-mass Hamiltonian \( h(\tilde{y}, \tilde{x}) \), see (16), except for a rescaling of the energy amounting to replacing \( E \) by \( E_+(E; \tilde{\Omega}) \) or \( E_-(E; \tilde{\Omega}) \), see (32). Since all thermodynamic quantities can be evaluated from knowledge of the entropy as a function of the energy \( E \), of the volume \( V \) and of the number of particles \( N \), it follows that all thermodynamic quantities associated with the \( \Omega \)-modified Hamiltonian \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega) \) can be straightforwardly computed from the corresponding quantities associated with the unmodified center-of-mass Hamiltonian \( h(\tilde{y}, \tilde{x}) \). Hence, all thermodynamic properties (temperature, specific heat, etc) of the \( \Omega \)-modified system are time-independent, that is they depend on the values of the (slowly evolving) ‘external parameters’ \( \tilde{P}(t) \) and \( \tilde{Q}(t) \) only through their initial values. These external parameters vary in such a way that the entropy remains constant (adiabatic variation) and also the temperature remains constant (isothermal variation). The fact that such a variation is both adiabatic and isothermal is indeed anomalous: for standard thermodynamically stable systems these two types of variations are generally different. This is presumably intimately linked to the conservation of the Hamiltonian \( h(\tilde{y}, \tilde{x}) \) in the dynamics defined by \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega) \).

At the qualitative level, the time independence of the thermodynamic quantities can be understood as follows. As explained in section 2, the periodic dynamics and the unmodified one differ only by a (constant) time rescaling over short timescales. However, it is clear that equilibrium thermodynamics does not depend on the rate at which the underlying dynamics proceeds, so that we indeed do not expect any dependence at all (not even a slow dependence) of the thermodynamic properties on time, that is, on \( \tilde{P}(t) \) and \( \tilde{Q}(t) \).

In elementary thermodynamics, as applied to normal (kinetic plus potential energy) Hamiltonians, the temperature is often defined as the so-called ‘kinetic temperature’, which is proportional to the mean kinetic energy per particle (the proportionality constant depends on the number of degrees of freedom for each particle and does not concern us here). Since in our isochronous \( \Omega \)-modified model the particle velocities vary periodically over time, vanishing twice in every period, this definition might appear to be inconsistent with the claim made above, that the temperature remains constant. However, the kinetic temperature is defined via the kinetic energy, which is defined in terms of the momenta, not the velocities. Furthermore, since the Hamiltonian \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega) \) is not normal, there is no reason to expect the identity of thermodynamic and kinetic temperatures. On the other hand, if the unmodified Hamiltonian \( H(p, q) \) is normal, as we indeed assumed, see (11), then, using standard results concerning the value of the thermodynamic temperature in the microcanonical ensemble \( [9] \) as well as results
concerning ensemble equivalence [8], one obtains

\[ T = \left( \frac{\partial S(E)}{\partial E} \right)^{-1} = T_{\text{Kin}} + O \left( \frac{1}{N} \right), \]  

(35)

where \( T \) denotes the thermodynamic temperature and \( T_{\text{Kin}} \) the kinetic temperature of the dynamics defined by \( H(p, q) \). This follows from the standard result for normal Hamiltonians that the thermodynamic temperature defined through the microcanonical entropy is the same as the kinetic temperature up to corrections of order \( 1/N \) [8].

The above holds, of course, only if the system is in thermodynamic equilibrium. The description of standard systems far from thermodynamic equilibrium is well known to be fraught with conceptual difficulties [10]. In many practically important circumstances, however, one may describe a system out of equilibrium by describing it as being locally in equilibrium [11]. The spatially varying thermodynamic parameters then reach a common value as the system relaxes to thermodynamic equilibrium in a characteristic time. Clearly, if the initial conditions are such that this happens in the unmodified dynamics (with a characteristic time \( \Delta \)), and if moreover the modified dynamics is such that \( \tilde{\Delta} \ll \tilde{T} \), see (24) and (26), then something similar happens over short times in the dynamics defined by the \( \Omega \)-modified Hamiltonian \( \tilde{H}(\tilde{p}, \tilde{q}; \Omega) \). The peculiarity, however, arises when the \( \Omega \)-modified system returns spontaneously to the out-of-equilibrium state (reversing a typically irreversible process!), to then decay to thermodynamic equilibrium again, repeating the process over and over (with period \( \tilde{T} \): see (10e) and (10f)).

4. Numerical simulations

To verify whether this somewhat peculiar phenomenology could in fact be observed numerically, we attempted a simulation using a limited but not too small number of particles, \( N = 40 \), interacting via ‘realistic’ two-body potentials (but, for simplicity, in two-dimensional (2D) space; there is no reason to expect any qualitative difference in three-dimensional space). The unmodified system we consider is characterized by the following standard Hamiltonian:

\[
H(\tilde{p}, \tilde{q}) = \sum_{n=1}^{N} \frac{\tilde{p}_n^2}{2} + \sum_{n,m=1,n>m}^{N} \left[ V_{\text{HO}} (|\tilde{q}_n - \tilde{q}_m|) + V_{\text{LJ}} (|\tilde{q}_n - \tilde{q}_m|) \right]
\]

(36a)

\[
= \frac{\tilde{P}^2}{2N} + \frac{1}{2} \sum_{n=1}^{N} \tilde{y}_n^2 + \sum_{n,m=1,n>m}^{N} \left[ V_{\text{HO}} (|\tilde{x}_n - \tilde{x}_m|) + V_{\text{LJ}} (|\tilde{x}_n - \tilde{x}_m|) \right]
\]

\[
= \frac{\tilde{P}^2}{2N} + h \left( \tilde{y}, \tilde{x} \right).
\]

Here, the canonical variables \( \tilde{p}_n \) and \( \tilde{q}_n \) are two-dimensional vectors, and the notation in the second version of this definition of \( H(\tilde{p}, \tilde{q}) \) is, we trust, self-evident on the basis of the notation introduced and discussed in section 2—but let us re-emphasize that \( \tilde{P}, \tilde{y}_n \) and \( \tilde{x}_n \) are now two-vectors in the plane, for which if need be we shall use the self-evident notation.
readily deduces the following expressions for $x_n$ and $y_n$ entailing of course $P^2 \equiv \vec{P} \cdot \vec{P} = P_x^2 + P_y^2$ and $y_n^2 \equiv \vec{y}_n \cdot \vec{y}_n = y_{nx}^2 + y_{ny}^2$. The two potentials $V_{HO}(r)$ and $V_{LJ}(r)$ are defined as follows:

$$V_{HO}(r) = \frac{kr^2}{2N^2}$$  \hspace{1cm} (36b)

is a standard harmonic oscillator potential (introduced to confine the system, in its center-of-mass frame), while the short-range Lennard–Jones potential

$$V_{LJ}(r) = r^{-12} - r^{-6}$$  \hspace{1cm} (36c)

is introduced as an interaction between the particles (of a standard type in molecular dynamics). Note that, via this potential, we have introduced adimensional units of length and energy: since this fixes the scales of energy and of length, and the scale of mass was already fixed by setting those of the particles to unity, our unit system is thereby completely fixed. Finally, the $N$-dependence of the harmonic potential $V_{HO}(r)$ has been chosen so that, as $N \to \infty$, both the area and the energy per particle tend to finite values.

The corresponding $\Omega$-modified Hamiltonian $\vec{H}(\vec{p}, \vec{q}; \Omega)$ is given by the following variant of our basic formula (18), valid for 2D:

$$\vec{H}(\vec{p}, \vec{q}; \Omega) = \frac{1}{2} \left[ \vec{P}_x + \frac{h \left( \frac{\vec{y}_x, \vec{y}_y}{2b} \right)}{b} \right]^2 + \frac{1}{2} \Omega^2 \vec{Q}_x^2.$$  \hspace{1cm} (37)

Note that we replaced $\vec{P}$ with the component $\vec{P}_x$ of the two-vector $\vec{P}$, and correspondingly $\vec{Q}$ with the component $\vec{Q}_x$ of the two-vector $\vec{Q}$ (compare (18) with the first version of (37)); this is of course consistent with our treatment, since $\vec{P}_x$ and $\vec{Q}_x$ are canonically conjugate variables. But let us also emphasize that there is an element of arbitrariness in this choice: we might just as well choose $\alpha \vec{P}_x + \beta \vec{P}_y$ in place of $\vec{P}_x$ and $\gamma \vec{Q}_x + \delta \vec{Q}_y$ in place of $\vec{Q}_x$ with the four constants $\alpha$, $\beta$, $\gamma$ and $\delta$ arbitrarily assigned except for the condition $a\gamma + b\delta = 1$. Such choices would yield different $\Omega$-modified Hamiltonians, of course characterized by analogous phenomenologies to the one discussed above and displayed below.

We report here the findings arrived at by our numerical study of the molecular dynamics of this system and of its $\Omega$-modified version, confining to the appendix an outline of the (not entirely trivial) methodology used to integrate numerically the relevant equations of motion.

The various parameters of this model are fixed as follows: $T = 60$ hence $\Omega = \pi/30$, $N = 40$ and $b = 1$. The values of $\vec{P}_x(0)$ and $\vec{Q}_x(0)$ were chosen as follows: from formulae (9) one readily deduces the following expressions for $\vec{Q}_x(0)$ and $\vec{P}_x(0)$:

$$\vec{P}_x(0) = b\tau(0) - \frac{E}{b}, \quad \vec{Q}_x(0) = \frac{b\tau(0)}{\Omega} \cot \Omega t_0,$$  \hspace{1cm} (38a)

where

$$\tau(0) = -A\Omega \sin \Omega(t - t_0)$$  \hspace{1cm} (38b)

is the time rescaling connecting the modified and the unmodified systems at the initial time. For ease of comparison between the two systems, we always set it equal to unity,

$$\tau(0) = 1.$$  \hspace{1cm} (38c)
We moreover always assigned to $t_0$ the value such that $\Omega t_0 = -\arccot(0.8)$. Then $\tilde{Q}_x(t_0)$ is uniquely assigned, $\tilde{Q}_x(t_0) = -24/\pi$ and $P_x(t_0) = 1 - E$, where the value of $E$ will depend on the initial conditions, see (45) below.

To minimize arbitrariness in the choice of the initial conditions of the unmodified system, we chose the initial positions of the particles from an equilibrium ensemble at a given temperature $T$ generated by a standard Monte Carlo simulation [12]. We checked that if the momenta—or, in the unmodified system, equivalently the velocities—are chosen from the corresponding Maxwell distribution, the unmodified system remains in thermodynamic equilibrium, that is, the temperature and the volume (or rather the area, see below) remain constant up to fluctuations. Since, however, we wish to observe irreversible behavior caused by an initial condition that is out of equilibrium, we chose initial velocities to be quite different from the equilibrium Maxwell distribution. Specifically, we considered two possibilities. Firstly, we set all velocities to zero, except for that of one randomly chosen particle, which was given a velocity of magnitude $\sqrt{2NT}$ pointing toward the center-of-mass of the system. Such an initial condition, corresponding to an ‘individual excitation’, relaxes to the same equilibrium from which the initial configuration was chosen (because the temperature $T$ coincides with the kinetic temperature, see (39) below). Secondly, we looked at the situation in which all velocities were set to zero. In this case, the system collapses and rearranges itself to a new thermal equilibrium at a lower temperature: we shall say these initial conditions correspond to a ‘global cooling’.

We then proceeded to simulate the modified and the unmodified systems using the fourth-order symplectic algorithm described in the appendix. All computations were made in double precision. The step size $\delta t$ was assigned values between $1.2 \times 10^{-4}$ and $6 \times 10^{-4}$. The conservation of both components of linear momentum as well as of angular momentum was found to be of the size of the round-off error, since the algorithm in fact preserves these quantities exactly. Energy was conserved with a relative error of approximately $10^{-11}$.

We then monitored the three following quantities: the kinetic temperature $T_{\text{Kin}}$, the volume (or rather area) $A$ and the kurtosis $K$ of the momenta. (Note in passing that all definitions below are given for the $\Omega$-modified system, but that they all have exact equivalents for the unmodified system.) They are defined as follows:

$$T_{\text{Kin}} = \frac{1}{2N} \sum_{n=1}^{n} \tilde{\gamma}_n^2 = \frac{1}{2N} \sum_{n=1}^{n} (\tilde{\gamma}_{nx}^2 + \tilde{\gamma}_{ny}^2),$$

$$A \equiv R_g^2 = \frac{1}{N} \sum_{n=1}^{N} \tilde{x}_n^2 = \frac{1}{N} \sum_{n=1}^{N} (\tilde{x}_{nx}^2 + \tilde{x}_{ny}^2)$$

(39)

$$K = \frac{2N \sum_{n=1}^{N} (\tilde{\gamma}_{nx}^4 + \tilde{\gamma}_{nx}^4)}{\left[\sum_{n=1}^{N} (\tilde{\gamma}_{nx}^2 + \tilde{\gamma}_{nx}^2)^2\right]} - 3.$$  

(40)

(41)

Note that, if the momenta $\tilde{\gamma}_n$ in this formula are taken from a Gaussian distribution, $K$ vanishes when averaged over that distribution; hence its value over time is an (inverse) measure of the extent to which the momenta have equilibrated.

We have looked at two temperatures, $T = 1$ and $T = 1/3$, as well as at two different values of the parameter $\kappa$ (which can be viewed as a substitute for the pressure, see (36b)): $\kappa = 10$.
Figure 1. Initial spatial configuration of the particles corresponding to thermal equilibrium at $T = 1/3$ with $\kappa = 10$. The circles, which have unit diameter, are meant to indicate the effective size of the particles, so that two overlapping circles indicate particles which have a positive value of their Lennard–Jones potential, see (36c). Note the presence of an incipient crystalline order, indicating a state between the liquid and solid phases. The particle to which all the kinetic energy was given in the individual excitation is identified by a cross.

and $\kappa = 40$. All of these were considered both for initial conditions corresponding to individual excitation and to global cooling, as defined above. Here, we only display the results for $T = 1/3$ and $\kappa = 10$, both for individual excitation and global cooling. The initial configuration we used is shown in figure 1. The other cases were quite similar, apart from sometimes showing slower decay to equilibrium, due to the excitation of some collective oscillation. In the case we report, however, such effects are rather small and the thermodynamic variables relax rapidly to their equilibrium values.

Below we display the time dependence of the volume, temperature and kurtosis for the initial conditions just described, for both the ‘individual excitation’ and the ‘global cooling’ initial conditions. In figures 2 and 3 we display the numerical results for initial conditions corresponding to individual excitation, whereas in figures 4 and 5 we show the case of initial conditions corresponding to global cooling. Figures 2 and 4 show the kinetic temperature (see (35) and the preceding discussion) as a function of time, whereas figures 3 and 5 show the volume and the kurtosis as functions of time.

We chose a period, $\tilde{T} = 60$, considerably larger than the typical collision time, which is of order unity. However, since—especially for the initial conditions corresponding to individual excitation—there seem to be a significant amount of collective relaxation, this period $\tilde{T}$ turns out to be comparable to—though clearly still somewhat larger than—the time over which the relaxation to thermodynamic equilibrium actually takes place. We see approximate returns of the thermodynamic variables to their initial out-of-equilibrium values. It should be pointed out that, although the returns after one period, and at the intermediate time $2t_0$, are quite clear and sometimes relatively accurate, this is not the case at all at the singular times $t_s = t_0 + k\tilde{T}/2$, where $k$ is an arbitrary integer. There deviations from periodicity of the order of 10% or more.
**Figure 2.** Temperature versus time in the isochronous Ω-modified model (left) and in the unmodified model (right). The initial condition corresponds to *individual excitation*. Note the approximate periodicity in the Ω-modified system, as well as the fact that the initial value is not quite attained in the first period.

**Figure 3.** Kurtosis (left) and volume (right) versus time for the isochronous Ω-modified model (full line) as well as for the unmodified model (dotted line). The initial condition corresponds to *individual excitation*.

can be seen. Since, according to our results, the periodicity should be exact everywhere, the deviations from it must be attributed to the amplification, by the chaotic dynamics of \( h(\vec{y}, \vec{\lambda}) \), of errors generated by round-off and by the slight systematic differences between the integration algorithm and the true dynamics. That the periodicity should be spoiled by such effects is, of course, no surprise. It is instead remarkable that the approximate returns of the thermodynamic variables are not destroyed thereby. With exponential instability occurring on the timescale of the collision time \( \Delta \) (or \( \tilde{\Delta} \) in the Ω-modified evolution) one would expect such deviations to wash out any memory of the initial conditions over a few collision times. Repeated returns (albeit approximate) to the original out of equilibrium values are therefore surprising.
Figure 4. Temperature versus time in the isochronous $\Omega$-modified model (left) as well as in the unmodified model (right). The initial condition corresponds to global cooling. Note the remarkable approximate periodicity in the $\Omega$-modified model in spite of the occurrence of significant deviations from periodicity at intermediate times. Note also the fast decay to thermodynamic equilibrium in the unmodified system.

Figure 5. Kurtosis (left) and volume (right) versus time for the isochronous $\Omega$-modified model (full line) as well as for the unmodified model (dotted line). The initial condition corresponds to global cooling. Note the remarkable periodicity of both the kurtosis and volume graphs in the $\Omega$-modified case.

To better appreciate the deviations from ideal behavior that arise due to inaccuracies of the numerical simulation, we also performed an explicit reparametrization of the numerically obtained behavior of the unmodified system by using the transformations (23) and (8). This should, in the absence of any numerical error, coincide with the solution obtained by simulating the $\Omega$-modified system. In figure 6, we display the difference between the two curves, both for temperature and volume (for an initial condition obtained by global cooling). One sees that the size of the differences is indeed appreciable, even though the periodicity of temperature and volume are both rather good in this case. We therefore confirm in this way that rather sizable errors in the thermodynamic variables do not automatically destroy the return to previous values nor the reversal of the irreversible relaxation to equilibrium.
Figure 6. Difference between the value of the temperature (left figure) and the volume (right figure) obtained by simulation of the $\Omega$-modified system and the value obtained by reparametrizing the calculated values of the unmodified system according to (22) with (8). Note the relatively large size of these differences as well as the sharp increase at the times for which the out of equilibrium state is reattained.

5. Outlook

In a previous paper [2], we showed how to $\Omega$-modify the standard many-body Hamiltonian so as to obtain thereby an autonomous Hamiltonian system having the isochrony property: all its solutions are completely periodic (i.e. periodic in all their degrees of freedom) with a fixed period $\tilde{T} = 2\pi/\Omega$. Remarkably, the dynamics produced by our $\Omega$-modified Hamiltonian has moreover the property to yield motions which, over generic time intervals very much shorter than the period $\tilde{T}$ (whose magnitude can be set arbitrarily, since the value of the parameter $\Omega$ can be freely chosen), differ marginally—only by a constant rescaling of the time variable—from the motions entailed by the standard many-body Hamiltonian. In this paper, we focused on the paradoxical aspects entailed by this finding, in view of the fact that the standard many-body dynamics underpins the validity of statistical mechanics and macroscopic thermodynamics, with the ordinary occurrence in that context of irreversible processes; while the occurrence of irreversible processes in the context of an isochronous dynamics obviously entails that such processes must eventually be reversed, in order for the system to return periodically to its previous configurations. But let us now note that the use of isochronous systems to illustrate this paradox has an element of overkill. Indeed, suppose the system we manufactured was not isochronous but just periodic, namely such that, in an open (hence fully dimensional) region of its phase space, all its solutions are completely periodic: but with periods which may be different, namely they may depend on the initial conditions characterizing each solution. Then the paradox connected with the reversal of irreversible processes would equally emerge, as long as relaxation in the modified system, which occurs on a time scale $\Delta$, remains much more rapid than the periods involved.

This suggests that it shall be of interest to investigate also periodic variants of the standard many-body Hamiltonian, provided they possess the property to yield dynamics which, over finite time intervals, differ only marginally from those of the original, unmodified, standard
many-body problem. An \(\Omega\)-modified model of this kind is provided by the following \(\Omega\)-modified Hamiltonian,

\[
\tilde{H} \left( \tilde{\vec{p}}, \tilde{\vec{q}}; \Omega \right) = \tilde{\tilde{H}} \left( \tilde{\vec{P}}, \tilde{\vec{Q}}; \tilde{\vec{y}}, \tilde{\vec{x}}; \Omega \right) = \frac{1}{2} \left[ \tilde{\vec{P}}^2 + \Omega^2 \tilde{\vec{Q}}^2 + \left( \alpha \tilde{\vec{P}}^2 + 2\beta \Omega \tilde{\vec{P}} \tilde{\vec{Q}} + \gamma \Omega^2 \tilde{\vec{Q}}^2 \right) h \left( \tilde{\vec{y}}, \tilde{\vec{x}} \right) \right],
\]

with \(\alpha, \beta\) and \(\gamma\), three arbitrary real constants (with the dimensions of inverse energy, or equivalently inverse square momenta, and not all vanishing; while we trust the remaining notation to be self-evident, see (18)). Note that this should be considered a simpler Hamiltonian than (18), since it is linear rather than quadratic in the internal-variables Hamiltonian \(h\). It is indeed easy to convince oneself that this Hamiltonian has the property to only yield periodic solutions, with period

\[
\tilde{T} = \frac{2\pi}{\Omega} \left[ 1 + (\alpha + \gamma) E + (\alpha \gamma - \beta^2) E^2 \right]^{-1/2},
\]

in the region of phase space where this quantity is real (and then chosen to be positive). Here, of course \(E\) is the constant of motion corresponding to the energy of the internal motion (see for instance (3), or (A.2) below). But we defer a treatment of this Hamiltonian problem to a separate paper.

And it is presumably also possible to manufacture other \(\Omega\)-modified variants of the standard many-body problem whose dynamical evolutions yield the paradoxical phenomenology discussed above, without this being necessarily associated with periodic solutions. But also this issue is postponed to future treatments, as well as additional clarifications—possibly also including more sophisticated numerical simulations—of the phenomenology associated with the Hamiltonian (18) treated herein.

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**Appendix. Numerical techniques**

In this appendix, we outline the scheme we used for the numerical solution of the dynamics yielded by the Hamiltonian \(H(\vec{p}, \vec{q})\), see (36), and its \(\Omega\)-modified version \(\tilde{H}(\tilde{\vec{p}}, \tilde{\vec{q}}; \Omega)\), see (37): in fact, we describe below in some detail only the way we treat the second of these two evolutions, since the treatment of the first is clearly analogous and simpler.

We now re-write our \(\Omega\)-modified Hamiltonian as follows:

\[
\tilde{H}(\tilde{\vec{p}}, \tilde{\vec{q}}; \Omega) = \frac{1}{2} \left( \tilde{\tilde{P}} x + \frac{E}{b} \right)^2 + \frac{1}{b} \left( \tilde{\tilde{P}} x + \frac{E}{b} \right) \left[ h \left( \tilde{\tilde{y}}, \tilde{\tilde{x}} \right) - E \right] + \frac{1}{2b^2} \left[ \frac{h \left( \tilde{\tilde{y}}, \tilde{\tilde{x}} \right) - E}{2} \right]^2 + \frac{1}{2} \Omega^2 \tilde{\tilde{Q}}^2.
\]
The right-hand side of this formula corresponds to our previous definition, see (37), indeed it is a matter of trivial algebra to verify that the presence here of the constant $E$ is only apparent. We will thus be free to assign to this constant a value at our convenience; eventually we will assign to it the value

$$E = h\left(\vec{y}(t), \vec{x}(t)\right) = h\left(\vec{y}(0), \vec{x}(0)\right),$$

(A.2)
a permitted choice since this quantity is indeed a constant of motion under the flow induced by the Hamiltonian $\tilde{H}(\vec{p}, \vec{q}; \Omega)$ (as evidenced by the second equality in (A.2)). But it is then easily seen that the third (quadratic) term in the right-hand side of (A.1) gives no contribution to the Hamiltonian equations of motion and can therefore be altogether eliminated. So we hereafter work with the Hamiltonian

$$\tilde{H}(\vec{p}, \vec{q}; \Omega) = \frac{1}{2} \left(\vec{P}_x + \frac{E}{b}\right)^2 + \frac{1}{b} \left(\vec{P}_x + \frac{E}{b}\right) \left[h\left(\vec{y}, \vec{x}\right) - E\right] + \frac{1}{2} \Omega^2 \dot{\vec{Q}}_x^2,$$

(A.3)
of course without forgetting that, in the equations of motion and in the formulae derived from them, the constant $E$ must be assigned the value (A.2).

We now take advantage of the standard subdivision of the Hamiltonian $h(\vec{y}, \vec{x})$ in kinetic and potential energy (see (36a)):

$$h(\vec{y}, \vec{x}) = \tilde{T}(\vec{y}) + V(\vec{x}),$$

(A.4a)
where of course (see (36))

$$\tilde{T}(\vec{y}) = \frac{1}{2} \sum_{n=1}^{N} \vec{y}_n^2,$$

(A.4b)

$$V(\vec{x}) = \sum_{n,m=1; n \neq m}^{N} \left[V_{HO}\left(|\vec{x}_n - \vec{x}_m|\right) + V_{LJ}\left(|\vec{x}_n - \vec{x}_m|\right)\right].$$

(A.4c)

This allows us to introduce the following convenient subdivision of the Hamiltonian $\tilde{H}(\vec{p}, \vec{q}; \Omega)$ into three components:

$$\tilde{H}(\vec{p}, \vec{q}; \Omega) = \tilde{H}_1\left(\vec{p}_x, \vec{Q}_x; E\right) + \tilde{H}_2\left(\vec{P}_x; \vec{y}; E\right) + \tilde{H}_3\left(\vec{P}_x; \vec{x}; E\right)$$

(A.5a)
with the 3 Hamiltonians $\tilde{H}_i$ defined as follows:

$$\tilde{H}_1 = \frac{1}{2} \left(\vec{P}_x + \frac{E}{b}\right)^2 + \frac{\Omega^2 \dot{\vec{Q}}_x^2}{2},$$

(A.5b)

$$\tilde{H}_2 = \frac{1}{b} \left(\vec{P}_x + \frac{E}{b}\right) \left[\tilde{T}(\vec{y}) - \frac{E}{2}\right],$$

(A.5c)

$$\tilde{H}_3 = \frac{1}{b} \left(\vec{P}_x + \frac{E}{b}\right) \left[V(\vec{x}) - \frac{E}{2}\right].$$

(A.5d)

The advantage of this subdivision is that the dynamics yielded by each of these 3 Hamiltonians is explicitly solvable (see below), opening thereby the way to the numerical integration of the evolution yielded by the Hamiltonian $\tilde{H}(\vec{p}, \vec{q}; \Omega)$ via a technique that we shall now outline.
Note that the term $E/2$ in the right-hand side of (A.5c) could be replaced by $\alpha E$ with $\alpha$ an arbitrary constant, provided the analogous term $E/2$ in the right-hand side of (A.5d) were correspondingly replaced by $(1 - \alpha)E$; the assignment $\alpha = 1/2$ we made was motivated by the general principle to make ‘symmetrical choices’ whenever possible (although the validity of this principle in this case is hardly cogent . . .).

Let us now define the Liouville operators—acting on phase space functions $\rho(\vec{p}, \vec{q})$—corresponding to these Hamiltonians as follows:

$$
\mathcal{L}(\rho) = \left[ \vec{H}, \rho \right], \quad \mathcal{L}_\ell(\rho) = \left[ \vec{H}_\ell, \rho \right], \quad \ell = 1, 2, 3, \quad (A.6a)
$$

so that

$$
\mathcal{L}(\rho) = \mathcal{L}_1(\rho) + \mathcal{L}_2(\rho) + \mathcal{L}_3(\rho). \quad (A.6b)
$$

It is then clear that the action of the propagators

$$
\Pi_\ell(t) \equiv \exp(t \mathcal{L}_\ell), \quad \ell = 1, 2, 3 \quad (A.7)
$$

can be evaluated exactly for all times, that is, the corresponding Hamiltonian equations can be integrated exactly (see below). We may use this fact to evaluate approximately the complete propagator $\Pi(\delta t) \equiv \exp(\delta t \mathcal{L})$ for $\delta t$ small compared to the time over which the particles move a distance sufficient to cause a significant change in the interaction $V$. Indeed, it is easy to verify that (A.6b) implies

$$
\Pi(\delta t) \equiv \exp(\delta t \mathcal{L}) = \exp[\delta t \left( \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3 \right)]
\quad = \exp\left( \frac{\delta t \mathcal{L}_1}{2} \right) \exp\left( \frac{\delta t \mathcal{L}_2}{2} \right) \exp\left( \frac{\delta t \mathcal{L}_3}{2} \right) \exp\left( \frac{\delta t \mathcal{L}_1}{2} \right)
\quad \times \left\{ 1 + O\left[ (\delta t)^3 \right] \right\}
\quad = \Pi^{(2)}(\delta t) \left\{ 1 + O\left[ (\delta t)^3 \right] \right\} \quad (A.8)
$$

where of course

$$
\Pi^{(2)}(t) = \Pi_1\left( \frac{t}{2} \right) \Pi_2\left( \frac{t}{2} \right) \Pi_3(t) \Pi_2\left( \frac{t}{2} \right) \Pi_1\left( \frac{t}{2} \right). \quad (A.9)
$$

From this formula, it is straightforward to obtain an explicit symplectic integration scheme. This is a second-order method (i.e. exact to second order in $\delta t$; as evidenced by the number 2 appended to $\Pi^{(2)}(t)$) and it therefore requires a fairly small time step $\delta t$. On the other hand, it is presumably robust, as similar algorithms are known to be [13]. We preferred (after some experimentation) to improve this algorithm by using the following elementary remark inspired by the Romberg integration method [14]: instead of using $\Pi^{(2)}(\delta t)$ as the approximate propagator, we use

$$
\Pi^{(4)}(\delta t) = \left[ \Pi^{(2)}\left( \frac{\delta t}{6} \right) \right]^4 \Pi^{(2)}\left( -\frac{\delta t}{3} \right) \left[ \Pi^{(2)}\left( \frac{\delta t}{6} \right) \right]^4. \quad (A.10)
$$

which coincides with $\Pi^{(2)}(\delta t)$ in leading order and in which the cubic error terms manifestly cancel exactly, yielding thereby a result correct to third order in $\delta t$. In fact, a more careful examination shows that $\Pi^{(4)}(\delta t)$ is exact to fourth order in $\delta t$, thanks to its symmetrical form, see [15, 16] for details, as well as for further information on a very similar algorithm. It is moreover easy to program and seems sufficiently reliable (on the basis of standard tests) to give us confidence that the results reported in section 4 are valid, as discussed there.

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The unmodified system is treated in the same way by dividing the Hamiltonian \( h(\vec{y}, \vec{x}) \) into kinetic and potential energy (see (A.4a)). The second order algorithm then reduces to the standard leapfrog method, which is in turn improved to fourth order as explained just above.

To complete this appendix, let us report without further comments the explicit formulae corresponding to the implementation of the three solvable propagators (A.7) with (A.6a) and (A.5), namely their effect on the dynamical variables \( \tilde{P}(t), \tilde{\dot{Q}}(t) \) and \( \tilde{\dot{y}}_n(t), \tilde{x}_n(t) \). With the convention that when the effect on one of these variables is not reported this simply means that the relevant propagator does not modify that variable at all, they read:

\[
\Pi_1 (\delta t) \tilde{\dot{Q}}_s(t) = \tilde{\dot{Q}}_s(t) \cos (\Omega \delta t) + \left[ \tilde{P}_s(t) + \frac{E}{b} \right] \sin (\Omega \delta t), \quad (A.11a)
\]

\[
\Pi_1 (\delta t) \tilde{P}_s(t) = \tilde{P}_s(t) \cos (\Omega \delta t) - \Omega \tilde{\dot{Q}}_s(t) \sin (\Omega \delta t) - \frac{E}{b} [1 - \cos (\Omega \delta t)], \quad (A.11b)
\]

\[
\Pi_2 (\delta t) \tilde{\dot{Q}}_s(t) = \tilde{\dot{Q}}_s(t) + \frac{\delta t}{b} \left[ \tilde{T} \left( \tilde{\dot{y}}_n(t) \right) - \frac{E}{2} \right], \quad (A.12a)
\]

\[
\Pi_2 (\delta t) \tilde{\dot{x}}_n(t) = \tilde{x}_n(t) + \frac{\delta t}{b} \left[ \tilde{P}_s(t) + \frac{E}{b} \right] \tilde{y}_n, \quad n = 1, \ldots, N, \quad (A.12b)
\]

\[
\Pi_3 (\delta t) \tilde{\dot{x}}_n(t) = \tilde{x}_n(t) + \frac{\delta t}{b} \left[ \tilde{V} \left( \tilde{x}_n(t) \right) - \frac{E}{2} \right], \quad (A.13a)
\]

\[
\Pi_3 (\delta t) \tilde{\dot{y}}_n(t) = \tilde{y}_n(t) + \frac{\delta t}{b} \left[ \tilde{P}_s(t) + \frac{E}{b} \right] \tilde{F}_n \left( \tilde{x}_n(t) \right), \quad n = 1, \ldots, N \quad (A.13b)
\]

with the ‘force’ \( \tilde{F}_n(\tilde{x}(t)) \) defined by the formula

\[
\tilde{F}_n \left( \tilde{x} \right) = -\frac{\partial V \left( \tilde{x} \right)}{\partial \tilde{x}_n}, \quad n = 1, \ldots, N, \quad (A.13c)
\]

where of course \( V \left( \tilde{x} \right) \) is defined by (A.4c) with (36b) and (36c). The diligent reader will have no difficulty in writing the explicit version—used in our numerical computations—of the right-hand side of this last formula.

Let us finally emphasize that our numerical computations of the solutions \( \tilde{\dot{y}}_n(t) \) and \( \tilde{x}_n(t) \) of our \( \Omega \)-modified dynamics have been performed by integrating the Hamiltonian equations of motion implied by the Hamiltonian (A.3). These yield exactly the same dynamics as our original Hamiltonian (37), as explained at the beginning of this appendix. This equivalence rests, however, on the conservation of \( h(\vec{y}, \vec{x}) \), which is not exact in the integration scheme we used. The procedure may therefore appear inconsistent. A moment’s thought shows, however, that this is not any worse than any other discrepancy between two different algorithms used to simulate the same system.

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