Hamiltonians for discrete dynamics

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The discrete dynamics obtained by a simple second-order map is shown to lead to an exact integration of harmonic modes with a conserved quantity: a "shadow Hamiltonian." The exact relations for "velocity" and energy are used to correct the energy obtained by the second-order algorithm commonly used in molecular dynamics simulations for complex many-body systems and lead to an improved energy conservation with a factor of 4 to 5.

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Dynamics obtained by discrete standard maps has achieved great attention in recent years [1,2] since they exhibit various types of temporal behavior including limit cycles, quasiperiodic and chaotic behavior. An example of this dynamics is the simple second-order recursion relation by Binder and Pivman [1]

$$x(n+1)=\alpha x(n)-x(n-1)\ , \tag{1}$$

where the $(n+1)$th position near a fixed point M is given by the two previous positions $x(n)$ and $x(n-1)$ and the "strength" α. They found this second-order dynamics to be useful for explaining in the collective states of discrete complex systems. The limit cycles (1) are harmonic modes, but in the more general case the system can couple with the surroundings if α depends on $x(n)$. The map can be rewritten (leap-frog) as two coupled first-order maps by introducing an auxiliary variable y, and β and γ, e.g., with $\beta\gamma=\alpha-2$ as

$$\begin{aligned} y(n+1)&=y(n)+\beta x(n)\ , \\ x(n+1)&=x(n)+\gamma y(n+1)\ . \end{aligned} \tag{2}$$

In molecular dynamics (MD) integrations of the classical mechanical equations such iterative maps or algorithms are also used instead of more refined algorithms for integrations of the coupled stiff differential equations for the analytic dynamics. The most popular MD algorithm is the time-centered difference algorithm

$$\mathbf{q}_i(t+h)=2\mathbf{q}_i(t)-\mathbf{q}_i(t-h)+h^2\ddot{\mathbf{q}}_i(t) \tag{3}$$

for the particles synchrotonous updated positions $\mathbf{q}_i$ at time t with a constant time increment h from their positions at t and $t-h$, and force or accelerations $\ddot{\mathbf{q}}_i(t)$ (mass included in the time unit). Equation (3) leads to discrete dynamics of the same kind as given by (1), but with a more complex coupling to the surroundings through the instant force field. The algorithm is widely used in computational physics and chemistry [3,4] and it is the simplest symplectic and time-reversible algorithm for MD [5]. It appears under different names in the literature, e.g., the Verlet or Stoermer algorithm, and the first known published appearance is due to Joseph Delambre (1791) [6,7]. The algorithm corresponds to Newton's formulation of classical dynamics, whereas the leap-frog algorithm corresponds to Hamilton's formulation

$$\begin{aligned} [\mathbf{p}_i(t+h/2)-\mathbf{p}_i(t-h/2)]/h&=\ddot{\mathbf{q}}_i(t)\ , \\ [\mathbf{q}_i(t+h)-\mathbf{q}_i(t)]/h&=\mathbf{p}_i(t+h/2)\ , \end{aligned} \tag{4}$$

with momentum $\mathbf{p}$ as the auxiliary variable and a timeshift between $\mathbf{q}$ and $\mathbf{p}$. By eliminating $\mathbf{p}$ in (4) one obtains (3) and for a normal mode (3)-(4) reduces to (1)-(2) with $\alpha=2-h^2\omega^2$, $\beta=-h\omega^2$ and $\gamma=h$.

It has recently been claimed [8] that, provided a mapping or algorithm is symplectic, i.e., phase space conserving, the discrete dynamical evolution generated by an algorithm describes the exact time evolution of a slightly perturbed Hamiltonian and thus processes this *shadow Hamiltonian* as a conserved quantity provided, however, that the operator expansion converges [8]. In this article the time evolution and the shadow Hamiltonian are derived for the discrete dynamics of normal modes obtained by the map, described by Eq. (1). The shadow Hamiltonian is constructed from the second moment $x(n)^2$ of the deviation from the fixed point $x=0$. This exact relation for a single harmonic mode is used to correct the energy obtained by the second-order algorithm Eq. (3) for a complex many-body system and lead to an improved energy conservation with a factor of 4 to 5.

For a single decoupled mode with amplitude A_0 and frequency ω_0 (in one dimension) the classical mechanical dynamical equation is $\ddot{x}=-\omega_0^2 x$ with the Hamiltonian $H_0=(A_0\omega_0)^2/2$ for analytic dynamics. The map needs two consecutive points to start with and it is convenient (but not necessary [9]) to start the computation from the points $x(0)=0$ at $t=0$ and $x(1)=\delta$ at $t=h$. The iterative map (1) with $\alpha=2-\omega_0^2h^2$ gives $x(2)=\alpha\delta$, $x(3)=(\alpha^2-1)\delta$, $x(4)=(\alpha^3-2\alpha)\delta$, $x(5)=(\alpha^4-3\alpha^2+1)\delta$, $x(6)=(\alpha^5-4\alpha^3+3\alpha)\delta$. In general the $(n+1)$th position can be written as

$$x(n+1)=\delta\mathcal{U}_n(\alpha)=\delta\sum_{i=0}^{[n/2]}(-1)^i\begin{bmatrix} n-i \\ i \end{bmatrix}\alpha^{n-2i}\ , \tag{5}$$

where the upper summation limit in (5) is for even numbers of i smaller or equal to $n/2$. These polynomials $\mathcal{U}_n(\alpha)$ are the Tschebyscheff polynomials of second kind

[10] with argument $\alpha/2$ and with the recursion relation

$$\mathcal{U}_n(\alpha/2)=\mathcal{U}_n(\cos\Theta)=\frac{\sin[(n+1)\Theta]}{\sin\Theta} \tag{6}$$

with $\Theta=\cos^{-1}(\alpha/2)=\cos^{-1}(1-\omega_0^2h^2/2)$ so the nth position generated by the algorithm can be written as

$$x(n)=x(nh)=\delta\sin(n\Theta)/\sin\Theta=A\sin(\omega t) \tag{7}$$

with time $t=nh$ and the frequency ω and the amplitude A:

$$\omega=\frac{\Theta}{h}=\sin^{-1}(\omega_0h/2)/(h/2)$$
$$\simeq\omega_0\left[1+\frac{1}{2^33}\omega_0^2h^2+\frac{3}{2^75}\omega_0^4h^4+O(h^6)\right] \tag{8}$$

and

$$A=\frac{\delta}{\sin(\Theta)}\simeq A_0\left[1-\frac{1}{2^33}\omega_0^2h^2+\frac{7}{2^75}\omega_0^4h^4+O(h^6)\right], \tag{9}$$

so by integration with the algorithm (1) one generates points on a harmonic trajectory. The frequency ω and amplitude A are shifted from ω_0 and A_0 for the corresponding analytic dynamics. (The solution is basically the same for unstable modes $\ddot{x}=\omega_0^2x$. In this case, and for discrete dynamics, the particle is exponentially repelled from $x=0$ by the second-order map at discrete points given by (5) with $\alpha=2+h^2\omega_0^2$ and the solution and other Tschebyscheff relations are given by (6)–(9) by replacing the trigonometric functions by the corresponding hyperbolic functions.)

The discrete propagator in the **q** space has no prescription for the velocity or higher order derivatives of a corresponding analytic trajectory. These derivatives for a coherent space and time have no impact on the dynamics which is given solely by the development in the **q** space as in quantum dynamics. The generated points contain, however, a conserved quantity, a shadow Hamiltonian, which can be obtained directly from the discrete values without any analytic differentiation or *ad hoc* definition of velocity for discrete dynamics. The shadow Hamiltonian is constructed from the second moment $x(n)^2$ of the deviation from the fixed point:

$$x(n)^2=\delta^2\mathcal{U}_{n-1}(\alpha/2)^2=\frac{\delta^2(1-\mathcal{T}_n^2(\alpha/2))}{1-(\alpha/2)^2} \tag{10}$$

using standard formulas for Tschebyscheff polynomials [10], and where $\mathcal{T}_n$ is the nth polynomial of first kind, which is related with the polynomials of second kind by

$$\mathcal{T}_n(\alpha/2)=\mathcal{U}_n-\frac{\alpha}{2}\mathcal{U}_{n-1}=\delta^{-1}\frac{x(n+1)-x(n-1)}{2}. \tag{11}$$

By inserting (11) in (10), one obtains the following relation for the identity of the second moment of the discrete positions, obtained by the second-order map (1):

$$x(n)^2+\left[\frac{x(n+1)-x(n-1)}{2}\right]^2[1-(\alpha/2)^2]^{-1}=\frac{\delta^2}{1-(\alpha/2)^2}. \tag{12}$$

The identity can be rewritten as a conserved shadow Hamiltonian $H(\omega_0,A_0)$, i.e., independent of n. It consists of a sum of potential and "kinetic energy" which deviates asymptotically from the Hamiltonian H_0 as

$$H=\tfrac{1}{2}\omega_0^2x(n)^2+\tfrac{1}{2}v(n)^2=\frac{\delta^2}{2h^2(1-\omega_0^2h^2/4)}$$
$$\simeq H_0-\frac{A_0^2\omega_0^4h^2}{24}+O(h^4) \tag{13}$$

with a definition of the velocity $v(n)$ for discrete dynamics, where $v_0(n)$ is the usual time-centered expression for the velocity (and used in MD):

$$v(n)\equiv v_0(n)(1-\omega_0^2h^2/4)^{-1/2}$$
$$=\left[\frac{x(n+1)-x(n-1)}{2h}\right](1-\omega_0^2h^2/4)^{-1/2}. \tag{14}$$

But as pointed out, $v(n)$ is an auxiliary parameter with no impact on the dynamics, and the classical mechanical energy conservation here is an identity for the second moment of the iterative map near a fixed point. [In the case of unstable modes, where the particle is repelled at a concave energy surface, the identities (12)-(13) and (14) are the same; but the corresponding potential energy is $-\omega_0^2x(n)^2/2$ and the denominator in (13) and (14) is $1+\omega_0^2h^2/4$.]

The next example is a string of one dimensional particles with harmonic forces. In the case of a continuous time one obtains the usual elementary solid state result for waves in a harmonic lattice. In the present case the force on particle s is obtained from its displacement from its equilibrium position as

$$F_s(nh)=-\omega_0^2x_s(nh)=\kappa^2[x_{s+1}(nh)-x_s(nh)]$$
$$-\kappa^2[x_s(nh)-x_{s-1}(nh)]. \tag{15}$$

This is just another second-order map $x_{s+1}(nh)=\alpha'x_s(nh)-x_{s-1}(nh)$ with $\alpha'=2-(\omega_0/\kappa)^2$. The map (15) generates a discrete representation of lattice oscillations given by

$$x_s(nh)=\frac{\delta}{\sin\Phi}\sin(s\Phi) \tag{16}$$

with the (Brillouin) dispersion relation between κ, k, and ω_0 for a wave with wave vector k and traveling on a lattice with a lattice constant a:

$$\Phi=ka=\cos^{-1}(\alpha'/2)=\cos^{-1}\{1-[\omega_0/(2\kappa)]^2\}. \tag{17}$$

Since it is ω_0 which enters into the Brillouin relation (17), the group velocity of a wave packet on the lattice is not affected by the discreteness of the dynamics.

The last example is a complex system of many particles N. In this case it is not possible to directly evaluate the

conserved shadow Hamiltonian because the potential energy $U(\mathbf{r}^N)$ is in general strongly anharmonic. Even though it is possible to associate an instant set of frequencies (the power spectrum) to the dynamics, the individual particles change their frequency at the collisions. It is, however, possible to apply the derived expressions for harmonic modes, and to arrive at the probability that a shadow Hamiltonian also exists for these systems. This is done by making harmonic corrections, using the relations derived for a single mode. The system considered contains $N=1024$ Lennard-Jones particles in a volume with periodical boundaries, at a density and temperature, $(\rho\sigma^3, kT/\epsilon)=(0.8,1)$ and $(1,0.8)$ which corresponds to a liquid and solid, respectively (argon) [11]. This system was one of the first to be simulated [12,13]. The time increment h used in the simulations is $h=0.005(\sim 10^{-14}$ s; time unit in units of $\sigma(\epsilon/m)^{1/2})$. From the set of instant positions $\mathbf{r}_i(t-h)$, $\mathbf{r}_i(t)$, $\mathbf{r}_i(t+h)$ for the ith particle and the corresponding set for the forces $\mathbf{f}_i$ one can determine the frequency a particle would have if it moves harmonically as

$$\omega_{0,i}^2(t)=\frac{|\mathbf{f}_i(t+h)-\mathbf{f}_i(t-h)|}{\mathbf{r}_i(t+h)-\mathbf{r}_i(t-h)} . \tag{18}$$

[In (18) we have taken the absolute values of the force differences; but the unstable modes play no role for the thermodynamical stable states [14].] The corresponding amplitude A_0 is obtained as

$$A_i^2=\left[\frac{\mathbf{f}_i(t)}{\omega_{0,i}^2}\right]^2+\left[\frac{\mathbf{v}_i(t)}{\omega_{0,i}}\right]^2 \tag{19}$$

with $\mathbf{v}_i$ given by (14). The traditional energy E_0 is corrected in two steps using (13) and (14). The kinetic energy is adjusted using (14) and (18), and the contribution to the discrete dynamics from the harmonic corrections is subtracted using (13). The conserved energy for discrete dynamics is finally obtained as

$$E=U(\mathbf{r}^N)+\tfrac{1}{2}\sum_i^N\left[\frac{\mathbf{r}_i(t+h)-\mathbf{r}_i(t-h)}{2h}\right]^2(1-\omega_{0,i}^2h^2/4)^{-1} - \sum_i^N A_i^2\omega_{0,i}^4h^2/24 . \tag{20}$$

Figure 1 shows a typical variation of the energy as a function of time (steps). The energy is for the solid state (*fcc*) and the lower curve is the traditional energy E_0. It has a mean deviation of energy $\delta|E|$ of 0.000 027 per time step and an rms deviation from the mean energy of 0.000 081. The upper curve is $E_0(t)$, when correcting the velocity from a fifth-order difference fit to the discrete values of the positions in a traditional way [15]. It

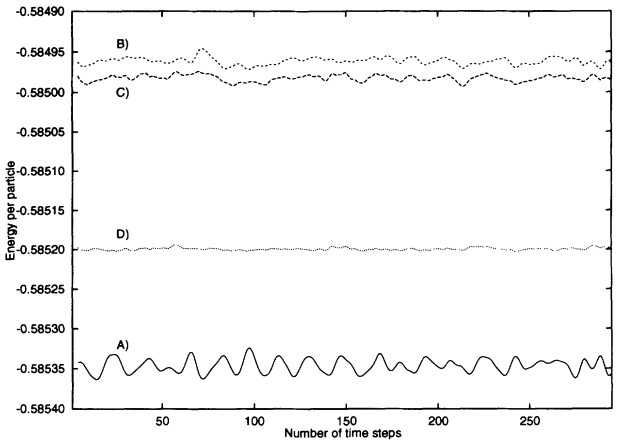

FIG. 1. Energy per particle as a function of time steps for 1024 Lennard-Jones particles at a solid state. *A* is the traditional MD energy E_0; *B* is the energy obtained after a fifth-order fit to the discrete positions; *C* is the energy E by only correcting the discrete dynamics "velocities" by $\omega_{0,i}$ in (20); and *D* is $E(n)$ given by (20).

reduces $\delta|E|$ to the half, but the rms is unchanged. By only correcting the velocities by the $\omega_{0,i}$ and using expression (14) instead, one obtains a corrected $E(t)$ which is very similar. Hence the correction to the *ad hoc* central difference expression for the velocity by $(1-\omega_{0,i}^2h^2/4)^{1/2}$ results in a correction to the energy which is very similar to the correction obtained by fitting an analytic curve to sets of discrete positions. The middle curve is the energy $E(t)$ using (20). The energy variation $\delta|E|$ and the rms deviation from the mean energy is now reduced by a factor of 5 for the solid state and about a factor of 4 for the liquid state. The small variation in E, which remain after the two corrections, is interpreted as being due to the anharmonic energy in $U(\mathbf{r}^N)$. The system was followed by more than 200 000 steps and with no detectable energy drift, as one should expect for a symplectic and time-reversible algorithm [5,6].

Conclusion. The discrete dynamics for a harmonic mode, obtained by the second-order map (1) leads to a "shadow Hamiltonian" for which the generated points are the exact solution. For a complex system with strong anharmonic potentials it is not possible to drive an expression for a conserved Hamiltonian; but adjustment of the energy using the expressions for harmonic modes improves the energy conservation with a factor of 4 (liquid) to 5 (solid).

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$$x_{n+m}-x_{n-m}=\alpha(x_{n+m-1}-x_{n-m+1})-(x_{n+m-2}-x_{n-m+2})$$

from any point x_n with $\delta\equiv x_{n+1}-x_{n-1}$.
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