Shadow mass and the relationship between velocity and momentum in symplectic numerical integration

Jason Gans* and David Shalloway†
Biophysics Program, Department of Molecular Biology and Genetics, Cornell University, Ithaca, New York 14853
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It is often assumed, when interpreting the discrete trajectory computed by a symplectic numerical integrator of Hamilton's equations in Cartesian coordinates, that velocity is equal to the momentum divided by the physical mass. However, the ''shadow Hamiltonian'' which is almost exactly solved by the symplectic integrator will, in general, induce a nonlinear relationship between velocity and momentum. For the (symplectic) momentum- and midpoint-momentum-Verlet algorithms, the ''shadow mass'' that relates velocity and momentum is momentum independent only for a quadratic potential and, even in this case, differs from the physical mass. Thus, naively assuming the standard velocity-momentum relationship leads to inconsistencies and unnecessarily inaccurate estimates of velocity-dependent quantities. As examples, we calculate the shadow Hamiltonians for the momentum- and midpoint-momentum-Verlet solutions of the multidimensional harmonic oscillator, and show how their velocity-momentum relationships depend on the time step. Of practical importance is the conclusion that, to gain the full advantage of symplecticity, velocities derived from interpolated positions, rather than conventional velocity-Verlet velocities, should be used to compute physical properties.

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I. INTRODUCTION

Many physical systems of particles can be modeled using Hamilton's equations with an autonomous Hamiltonian given by

$$H(q,p)=\frac{1}{2}p^{T}m^{-1}p+U(q), \tag{1}$$

where p and q are momentum and position vectors, m is the diagonal mass tensor, and $U(q)$ is the potential energy. The dimensionality of the system is dN, where d is the number of physical dimensions (e.g., 3) and N is the number of particles. The trajectory $\{p(t),q(t)\}$ is determined by

$$\dot{q}=\nabla_{p}H, \tag{2a}$$

$$\dot{p}=-\nabla_{q}H, \tag{2b}$$

and initial conditions $\{q(0),p(0)\}$.

A numerical integrator of Eqs. (2) that produces a set of phase space points $\{q_n,p_n\}$, referring to discrete time points $t_n=nh$, is said to be *symplectic* if

$$\Psi^{T}J\Psi=J, \tag{3}$$

where Ψ is the Jacobian of the mapping from $\{q_n,p_n\}$ to $\{q_{n+1},p_{n+1}\}$:

$$\Psi\equiv\begin{bmatrix}\frac{\partial q_{n+1}}{\partial q_n} & \frac{\partial q_{n+1}}{\partial p_n}\\ \frac{\partial p_{n+1}}{\partial q_n} & \frac{\partial p_{n+1}}{\partial p_n}\end{bmatrix}, \tag{4}$$

$$J\equiv\begin{bmatrix}0 & I\\ -I & 0\end{bmatrix}, \tag{5}$$

and I is the dN-dimensional identity matrix [1]. Symplectic integrators are popular tools for simulations because of their excellent stability at large time steps and long-term approximate conservation of invariants [2]. The fact that local errors do not accumulate to grossly violate conservation of invariants is, at first glance, surprising. This global property holds because the $\{q_n,p_n\}$ computed by a symplectic integrator lie either on, or ''very approximately'' on, an exact solution trajectory $\{q(t),\ p(t)\}$ of Eqs. (2) for a *shadow Hamiltonian* $\tilde{H}$ that can be expressed as an asymptotic series in h about H [1,3]. That is,

$$q_n=q(nh), \tag{6a}$$

$$p_n=p(nh). \tag{6b}$$

Not only positions and momenta, but also their derivatives, are uniquely defined on the shadow trajectory [4,18]. In particular, the discrete symplectic velocity v_n at time point nh is uniquely defined as the derivative of the continuous position-space trajectory

$$v_n\equiv\dot{q}_n=\frac{dq(t)}{dt}\bigg|_{t=nh}=\nabla_{p}\tilde{H}\bigg|_{\substack{p=p_n\\ q=q_n}}, \tag{7}$$

and satisfies the first Hamilton's equation, Eq. (2a). As we shall discuss, by interpolating the q_n to approximate $q(t)$, Eq. (7) can be used even when, for practical reasons, $\tilde{H}$ is not known.

A point that has frequently been overlooked is that, unlike H, $\tilde{H}$ need not be separable into the simple form of Eq. (1). As we show in Sec. II A (using one form of the Verlet algo-

*Electronic address: jdg9@cornell.edu
†Electronic address: dis2@cornell.edu

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rithm as an example), $\tilde{H}$ will in general be a nonquadratic function of p. Thus, the shadow mass

$$\tilde{m} \equiv \left(\frac{\partial^2 \tilde{H}}{\partial p^2} \right)^{-1} = \left(\frac{\partial v}{\partial p} \right)^{-1}, \tag{8}$$

will depend on both q and p, and velocity and momentum will *not* be linearly related. The multidimensional harmonic oscillator is a special case in which the shadow mass is a constant. But even in this case, it does not equal the physical mass. Moreover, the tensor structure of $\tilde{m}$ may not preserve the physical-particle structure of m, where each particle has the same mass in each of the d physical directions. In summary, for both harmonic and anharmonic potentials

$$p_n \neq m v_n, \tag{9}$$

the numerically computed symplectic momenta and velocities are not simply related by the physical mass.

The altered relationship between momenta and velocities has important ramifications. For example, the *velocity-Verlet* algorithm [5] is

$$q_{n+1} = q_n + h\, v_n^{\mathrm{v}} - \frac{h^2}{2} m^{-1} \nabla U(q_n), \tag{10a}$$

$$v_{n+1}^{\mathrm{v}} = v_n^{\mathrm{v}} - \frac{h}{2} m^{-1} [\nabla U(q_n) + \nabla U(q_{n+1})], \tag{10b}$$

where v_n^{v} is the velocity-Verlet ''velocity.'' This is transformed to an integrator for q_n and p_n by the replacement

$$v_n^{\mathrm{v}} \to m^{-1} p_n, \tag{11}$$

which gives the momentum-Verlet algorithm

$$q_{n+1} = q_n + h\; m^{-1} p_n - \frac{h^2}{2} m^{-1} \nabla U(q_n), \tag{12a}$$

$$p_{n+1} = p_n - \frac{h}{2} [\nabla U(q_n) + \nabla U(q_{n+1})]. \tag{12b}$$

Equations (12) satisfy Eq. (3), and are thus symplectic.

Equations (10) and (12), with substitution (11) are completely equivalent. However, because of inequality (9), the velocity-Verlet ''velocities'' do not equal the symplectic velocities and do not gain the full benefit of symplecticity. As we will see, the difference between the v_n^{v} and the derivatives of a smooth global interpolation of the q_n can significantly degrade computed results. We regard the name ''velocity-Verlet'' as a misnomer that may lead to unwary to use the v^{v} as velocities when computing physical observables. We suggest that it be replaced with the name ''momentum-Verlet'' algorithm, since momenta *are* correctly computed.

Similar considerations apply to other symplectic integrators as well. For example, the ''midpoint'' form of the velocity-Verlet integrator presented by Tuckerman *et al.* [6] is

$$v_{n+1}^{\mathrm{v}} = v_n^{\mathrm{v}} - h m^{-1} \nabla U\left(q_n + \frac{h}{2} v_n^{\mathrm{v}} \right), \tag{13a}$$

$$q_{n+1} = q_n + \frac{h}{2} (v_{n+1}^{\mathrm{v}} + v_n^{\mathrm{v}}). \tag{13b}$$

Here the gradient of the potential is evaluated at the midpoint, rather than at the beginning, of the time interval. Skeel *et al.* [2] have shown that the midpoint-momentum-Verlet integrator [7], which results from substituting Eq. (11) into Eqs. (13), satisfies Eq. (3) and thus is symplectic:

$$p_{n+1} = p_n - h \nabla U\left(q_n + \frac{h}{2} m^{-1} p_n \right), \tag{14a}$$

$$q_{n+1} = q_n + \frac{h}{2} m^{-1} (p_{n+1} + p_n). \tag{14b}$$

However, as with the velocity-Verlet algorithm, the velocities given by Eqs. (13) are inconsistent with the symplectic solution.

We use the multidimensional harmonic oscillator as an example to analytically elucidate these points. In Sec. II B we analyze its velocity-Verlet solution, and show that the velocity-Verlet ''velocities'' are inconsistent with the position trajectory. In Sec. II C we derive the analytic shadow Hamiltonian for the momentum-Verlet algorithm and show how the time-step-dependent shadow mass relates velocities and momenta. We extend this analysis to the midpoint-momentum-Verlet algorithm in Sec. II D. In Sec. II E we show how naive use of the velocity-Verlet ''velocities'' leads to unnecessarily large energy fluctuations, and how this can be remedied by the use of interpolated velocities.

II. RESULTS

A. Nonlinear symplectic relationship between momentum and velocity

The shadow Hamiltonian for time-reversible algorithms, such as momentum- or midpoint-momentum-Verlet algorithms, can be expanded as an asymptotic series using even powers of h,

$$\tilde{H}(q,p) = H(q,p) + G(h^2; q,p), \tag{15}$$

where G is a functional series beginning in $O(h^2)$:

$$G(h^2; q,p) \equiv \frac{h^2}{2!} {}^{(2)}g(q,p) + \frac{h^4}{4!} {}^{(4)}g(q,p) + \cdots. \tag{16}$$

The ${}^{(i)}g(q,p)$ can be determined using the method of modified equations [3,8], which demands order-by-order (in h) consistency between Eqs. (2) (with $H \to \tilde{H}$) and Eqs. (12). Straightforward application to the momentum-Verlet algorithm yields in lowest order

$$^{(2)}g(q,p)=\frac{1}{6}p^T m^{-1}\frac{\partial^2 U(q)}{\partial q^2}m^{-1}p - \frac{1}{12}[\nabla U(q)]^T m^{-1}\nabla U(q). \tag{17}$$

When U is quadratic, this expression is quadratic in both p and q. Thus to this order the shadow mass is a constant $\tilde{m}=[m^{-1}+(h^2/6)\,m^{-1}\partial^2 U/\partial q^2 m^{-1}]^{-1}$. It is easy to show that G will contain only quadratic terms in q and p to all orders in h^2; thus the exact shadow Hamiltonian is quadratic, but has $\tilde{m}\neq m$ and $\partial^2\tilde{H}/\partial q^2 \neq \partial^2 H/\partial q^2$.

When U is anharmonic, the shadow mass will depend on q in $O(h^2)$. Furthermore, in higher orders, $G(q,p)$ will contain nonquadratic terms in p such as $(h^4/720\,m^4)\,p^4\partial^4 U(q)/\partial q^4$ and $(h^6/1680\,m^5)\,p^4[\partial^3 U(q)/\partial q^3]^2$ (for simplicity, here we ignore tensor ordering), and $\tilde{m}$ will be momentum dependent. However, for small h the momentum-dependence may be small in regions where the higher derivatives of $U(q)$ are not too large. When a harmonic approximation is appropriate, $\tilde{m}$ can be approximated as a constant tensor, though it may differ between potential catchment regions. Analogous results hold for the midpoint momentum-Verlet algorithm.

B. Velocity-Verlet solution of the multidimensional harmonic oscillator

The form of the shadow Hamiltonian can be calculated analytically (i.e., to all orders in h^2) for the multidimensional harmonic oscillator. The Hamiltonian is

$$H(q,p)=\frac{1}{2}p^T m^{-1}p+\frac{1}{2}q^T K q, \tag{18}$$

where K and m are symmetric, positive-definite matrices. The exact solutions for $q(t)$ and $p(t)$ are

$$q(t)=\mu^{-1}[\cos(\omega t)\mu A+\sin(\omega t)\mu B] \tag{19}$$

and

$$p(t)=\mu^T\omega[-\sin(\omega t)\mu A+\cos(\omega t)\mu B], \tag{20}$$

where

$$\omega\equiv[(\mu^{-1})^T K\mu^{-1}]^{1/2}, \tag{21}$$

A and B are constant vectors determined by the initial conditions

$$A=q(0), \tag{22a}$$

$$B=\mu^{-1}\omega^{-1}(\mu^{-1})^T p(0) \tag{22b}$$

and μ is any real matrix that satisfies

$$m=\mu^T\mu. \tag{23}$$

μ is arbitrary up to an orthogonal or pseudo-orthogonal transformation Q, i.e.,

$$\mu=Qm^{1/2}, \tag{24}$$

where $m^{1/2}$ is the (unique up to eigenvector degeneracy) symmetric matrix that satisfies $m=m^{1/2}m^{1/2}$. The choice of Q determines the vector basis in which ω is represented.

The Störmer form of the Verlet algorithm [9] is

$$q_{n+1}=2q_n-q_{n-1}-h^2 m^{-1}\nabla U(q_n). \tag{25}$$

It has been shown [10,11] that in one dimension it produces positions q_n that can be interpolated by a sinusoid having the modified frequency

$$\tilde{\omega}=\frac{1}{h}\arccos\left(1-\frac{(\omega h)^2}{2}\right). \tag{26}$$

We generalize to higher dimensions by seeking an interpolation having the form of Eq. (19):

$$q(t)=\tilde{\mu}^{-1}[\cos(\tilde{\omega}t)\tilde{\mu}A+\sin(\tilde{\omega}t)\tilde{\mu}B], \tag{27}$$

where $\tilde{\omega}$ is given by Eq. (26) as a matrix equation

$$\tilde{\omega}=\frac{1}{h}\arccos\left(I-\frac{(\omega h)^2}{2}\right). \tag{28}$$

Each eigenvalue of $\tilde{\omega}$ is greater than the corresponding eigenvalue of ω for $h>0$, and $\lim_{h\to 0}\tilde{\omega}=\omega$. Equation (27) will satisfy

$$q(nh)=q_n \tag{29}$$

if

$$\tilde{\mu}=\eta(\omega)\,m^{1/2}, \tag{30}$$

where η is any real, invertible function of ω. Because η is not yet fixed, $\tilde{\mu}$ and the shadow mass cannot be determined from the position trajectory alone.

The second-order discrete derivative of the Störmer-Verlet trajectory defines ''velocities''

$$v_n^{\mathrm{v}}=\frac{q_{n+1}-q_{n-1}}{2h} \tag{31}$$

which are the same as those produced by the velocity-Verlet algorithm. As illustrated for the one-dimensional harmonic oscillator in Fig. 1, they do *not* equal the derivative of the position trajectory Eq. (27): $v_n^{\mathrm{v}}\neq dq(t)/dt|_{t=nh}$. The inconsistency is evident whether we use the interpolation of Eq. (27) (which we will soon see is an exact symplectic trajectory) or a simple cubic-spline interpolation (which is visually almost identical). In fact, any globally smooth trajectory that matches both the velocity-Verlet positions and velocities will necessarily have kinks, such as those in the dotted interpolation in Fig. 1. In summary, Eqs. (27) and (31) are not consistent components of a solution to a shadow Hamiltonian.

C. Momentum-Verlet solution of the multidimensional harmonic oscillator

Contrast this dilemma with the outcome when the same interpolation procedure is applied to the position-momentum output of the momentum-Verlet algorithm: The q_n are identical to those produced by the Störmer-Verlet and velocity-

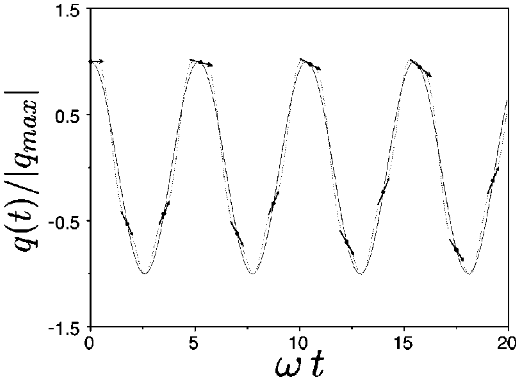

FIG. 1. Interpolation of a velocity-Verlet solution of the one dimensional harmonic oscillator. The dots are at the q_n; the vectors have slope given by v_n^{v}. The solid line is the sinusoidal interpolation of Eq. (27), which corresponds to the symplectic trajectory. The dotted line is a simple harmonic interpolation that matches both the q_n and v_n^{v}.

Verlet algorithms and, as before, can be interpolated by Eq. (27). Following the same procedure, we look for an interpolation of the p_n having the form of Eq. (20):

$$p(t)=\tilde{\mu}^T\tilde{\omega}[-\sin(\tilde{\omega}t)\tilde{\mu}A+\cos(\tilde{\omega}t)\tilde{\mu}B]. \tag{32}$$

Satisfaction of Eq. (29) again requires that $\tilde{\mu}$ have the form given by Eq. (30). In addition, substituting Eqs. (28), (27), and (30) into Eq. (12a) implies that

$$\eta^2=\tilde{\omega}^{-1}\omega\left[I-\frac{(\omega h)^2}{4}\right]^{1/2}. \tag{33}$$

[Equation (28) implies that the magnitude of the eigenvalues of η are all less than 1.] It is easy to verify that Eq. (32), along with the auxiliary conditions of Eqs. (28), (30), and (33), satisfies

$$p(nh)=p_n, \tag{34}$$

so we have consistent interpolations for both the q_n and p_n.

Referring to the exact quadratic solution specified by Eqs. (18)–(24), we recognize that the interpolated phase-space trajectory specified by Eqs. (27) and (32) is an exact solution of the modified Hamiltonian

$$\tilde{H}(p,q)=\frac{1}{2}p^T\tilde{m}^{-1}p+\frac{1}{2}q^T\tilde{K}q, \tag{35}$$

where

$$\tilde{K}=\tilde{\mu}^T\tilde{\omega}^2\tilde{\mu}, \tag{36}$$

$$\tilde{m}=\tilde{\mu}^T\tilde{\mu}, \tag{37}$$

and $\tilde{\mu}$ is specified by Eqs. (30) and (33). Thus, $\tilde{H}$ is the shadow Hamiltonian for the symplectic momentum-Verlet solution of the multidimensional harmonic oscillator. Similarly, $\tilde{m}$ is the shadow mass tensor satisfying Eq. (8), $\tilde{K}$ is the shadow spring-constant tensor, and $\tilde{\omega}$ is the shadow angular-

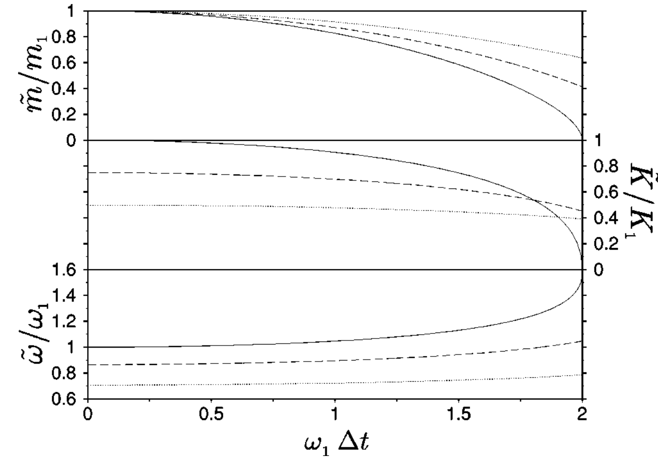

FIG. 2. The normalized shadow mass, spring-constant and angular-frequency eigenvalues for the momentum-Verlet solution of a particle in a three-dimensional, anisotropic harmonic potential. The eigenvalues of ω, $\{\omega_1, \omega_2, \omega_3\}$, are $\{1.0, \sqrt{0.75}, \sqrt{0.5}\}$. The solid, dashed, and dotted lines are the corresponding eigenvalues of $\tilde{\omega}$, $\tilde{m}$, and $\tilde{K}$ as a function of $\omega_1 h$. The plots terminate at the instability limit [see Eq. (28)].

frequency tensor. As expected, Eq. (35) is consistent with the $O(h^2)$ expansion obtained from the method of modified equations in Sec. II A.

As required for a physical interpretation, $\tilde{m}$, $\tilde{K}$, and $\tilde{\omega}$ are all symmetric. However, degenerate eigenvalues of m will not be degenerate in $\tilde{m}$ unless ω has the same degeneracies. For example, if H represents, in physical three space, a single particle of mass m (i.e., a triply degenerate mass tensor) in an anisotropic harmonic oscillator potential having three different eigenvalues, $\tilde{m}$ will also have three different eigenvalues. Thus, while the computed trajectory is an exact solution of the shadow Hamiltonian $\tilde{H}$, this Hamiltonian does not describe the same type of physical system.

As noted above, the eigenvalues of $\tilde{\omega}$ are larger than the corresponding eigenvalues of ω. Rearranging Eq. (36) to express $\tilde{\omega}$ as a function of $\tilde{K}$ and $\tilde{m}$ [i.e., analogously to Eq. (21)], we can understand the frequency shifts as the combined result of changes in both the mass and spring-constant tensors. Interestingly, Eqs. (28), (30), (33), (36), and (37) imply that, for momentum-Verlet, the eigenvalues of both $\tilde{K}$ and $\tilde{m}$ are smaller than their physical counterparts, and these changes have opposing effects on the shadow frequencies. However, the mass eigenvalues decrease faster than the spring-constant eigenvalues (with increasing h), resulting in frequency increases. Figure 2 plots the normalized eigenvalues of the momentum-Verlet $\tilde{K}$, $\tilde{m}$, and $\tilde{\omega}$ for a single particle in an anisotropic three-dimensional quadratic well.

The analytic relationship between the momenta and velocities on the shadow trajectory is given by Eq. (7):

$$v_n=\tilde{m}^{-1}p_n(\text{valid only for the harmonic oscillator}), \tag{38a}$$

$$=\tilde{m}^{-1}mv_n^{\mathrm{v}}. \tag{38b}$$

The second line provides the h-dependent relationship between the velocity-Verlet and the symplectic velocities for the multidimensional harmonic oscillator, and shows that former are smaller than the latter beginning in $O(h^2)$ [12]. Since the position trajectory is accurate in $O(h^2)$, ignoring this difference degrades the overall accuracy of the algorithm. We will see a manifestation of this when we consider energy fluctuations in Sec. II E.

D. Midpoint-momentum-Verlet solution of the multidimensional harmonic oscillator

Following the derivation used for the momentum-Verlet algorithm, we find that the continuous trajectory that interpolates that midpoint-momentum-Verlet solution of the multidimensional harmonic oscillator is given by Eqs. (27), (30), and (32), but with the altered expression

$$\eta^2=\tilde{\omega}^{-1}\omega\left[I-\frac{(\omega h)^2}{4}\right]^{-1/2}. \tag{39}$$

(In contrast with the momentum-Verlet form for η, η now has eigenvalues of magnitude greater than 1.) The shadow Hamiltonian [13] is again given by Eqs. (35)–(37), but because η is different, $\tilde{m}$ and $\tilde{K}$ will differ from their momentum-Verlet counterparts. In contrast with the momentum-Verlet case, the eigenvalues of these $\tilde{m}$ and $\tilde{K}$ are both *larger* than their physical values. The eigenvalues of $\tilde{K}$ increase faster than those of $\tilde{m}$ with increasing h, resulting in the same shadow frequency increases as observed with the momentum-Verlet algorithm.

The midpoint-velocity-Verlet ''velocities'' for the multidimensional harmonic oscillator are related to the symplectic velocities by Eq. (38b) using the appropriate $\tilde{m}$ [12]. In this case the Verlet ''velocities'' are larger than the symplectic velocities.

E. The symplectic energy fluctuation

Since the v_n^{v} do not equal the v_n, they do not correspond to a trajectory that remains on a fixed shadow energy surface. Thus, they are not fully constrained by symplecticity and the energies computed using them can fluctuate excessively. This agrees with Mazur [14], who has previously noted that the energy fluctuations computed using the velocity-Verlet velocities overestimate the algorithmic error.

Mazur has gone on to suggest that energy fluctuations are therefore not a good measure of algorithmic accuracy [14]. However, we can now show that the energy fluctuations computed using the appropriate velocities [i.e., the v_n defined by Eq. (7)] can be related to the microcanonical ensemble average of the mean-square deviation between the physical and shadow Hamiltonians, which *is* a good measure of accuracy. Since we know that $\tilde{H}$ is invariant on the symplectic trajectory, the ergodic hypothesis implies that an equal-time-weighted trajectory average approaches (in the long-trajectory limit) the microcanonical ensemble average for a fixed value $\tilde{E}$ of $\tilde{H}$. Thus, the microcanonical ensemble mean-square average of the deviation between H and $\tilde{H}$, adjusted for the difference between their means [15], is

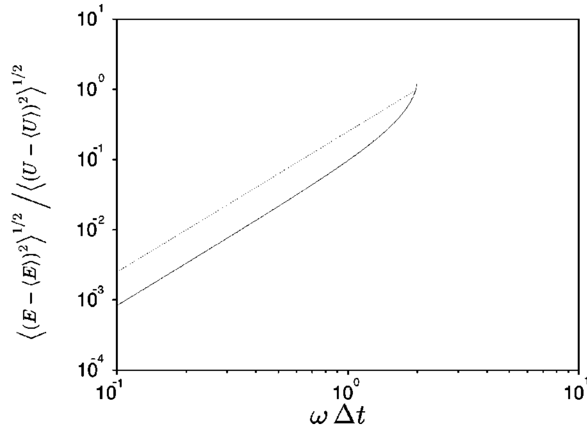

FIG. 3. Root-mean-square (rms) total energy E fluctuation (normalized by the rms potential energy fluctuation) of the Verlet trajectory of a one-dimensional harmonic oscillator computed using $E_n=\frac{1}{2}v_n^{\mathrm{v}T}mv_n^{\mathrm{v}}+\frac{1}{2}q_n^TKq_n$ (using the velocity-Verlet velocities; dotted line) and $E_n=\frac{1}{2}\dot{q}_n^Tm\dot{q}_n+\frac{1}{2}q_n^TKq_n$ (using the momentum-Verlet velocities; solid line).

$$\langle[(\tilde{H}-H)-\langle(\tilde{H}-H)\rangle_{\tilde{E}}]^2\rangle_{\tilde{E}} = \lim_{N\to\infty}N^{-1}\sum_{n=1}^{N}\left[(\tilde{E}_n-E_n)-N^{-1}\sum_{n=1}^{N}(\tilde{E}_n-E_n)\right]^2 \tag{40a}$$

$$=\lim_{N\to\infty}N^{-1}\sum_{n=1}^{N}\left(E_n-N^{-1}\sum_{n=1}^{N}E_n\right)^2, \tag{40b}$$

where E_n and $\tilde{E}_n$ are the values of H and $\tilde{H}$, respectively, at corresponding phase-space points. (The $\tilde{E}_n$ terms cancel since $\tilde{E}_n=\tilde{E}$ at all points.)

Because H and $\tilde{H}$ induce different explicit relationships between momenta and velocities through Eq. (2a), the momenta that are used in evaluating them at the same point differ and some care is needed when evaluating E. Since there is no ambiguity in $q(t)$ and its derivative $v(t)$, we can express E as a function of these variables. In particular,

$$E_n=\frac{1}{2}\dot{q}_n^Tm\dot{q}_n+U(q_n). \tag{41}$$

When this form is used, the magnitude of the energy fluctuations defined by Eq. (40b) *does* provide a useful measure of accuracy. The incorrect method—evaluating E as a function of $q(t)$ and $p(t)$—corresponds to using velocity-Verlet velocities to compute the energy.

For illustration, Fig. 3 compares the energy fluctuations of the numerical solution for a one-dimensional harmonic oscillator as a function of h when the energy E is computed using either momentum- or velocity-Verlet velocities. The root-mean-square energy fluctuation computed using the momentum-Verlet velocities is about a factor of 3 smaller than that computed with the velocity-Verlet velocities (except as h approaches the instability limit, $\omega h=2$). The precise interpolation given by Eq. (19) is not needed for this result: essentially the same fluctuations are computed (except very close to the instability limit) using a cubic-spline interpolation. The main requirement is that the interpolation should be globally consistent and adequately smooth.

In both cases, the energy fluctuations are $O(h^2)$. As pointed out by Mazur [14], most of the velocity-Verlet energy fluctuation results from velocity error. This error is removed when the symplectic velocities are used. The smaller symplectic $O(h^2)$ fluctuation is a true measure of the microcanonical average of the deviation of $\tilde{H}$ from H; in the case of the harmonic oscillator, this mirrors the $O(h^2)$ deviation of $\tilde{\omega}$ from ω. The situation is similar when the energy fluctuations of the midpoint-velocity-Verlet and midpoint-momentum-Verlet algorithms are compared.

III. CONCLUSION

Ignoring the difference between the shadow and physical mass in symplectic numerical integration, and the related error of assuming that the velocity-Verlet velocities are consistent with the symplectic shadow trajectory, has caused some confusion. We have examined this explicitly for the multidimensional harmonic oscillator by examining the relationship between the standard and midpoint-velocity-Verlet velocities and the corresponding symplectic velocities. The differences are of $O(h^2)$ and globally bounded, so the symplectic global stability properties, though impaired, are retained in weakened form even when the velocity-Verlet velocities are assumed to be correct. But since more accurate results are obtained when it is recognized that only momenta, and not velocities, are correctly computed by the algorithms, we suggest that it is more appropriate to use the term ''momentum Verlet'' in describing them.

Even without the symplectic analysis, it is evident that something is wrong with velocity-Verlet velocities, since they do not match derivatives of smooth interpolations of the discrete position trajectory and they yield unnecessarily large energy fluctuations [14]. The correct symplectic relationship between the numerically computed momenta and velocities, and the shadow Hamiltonian that generates them, cannot be obtained without accounting for the difference between the physical and shadow masses. For example, Toxvaerd [16], in an effort to improve energy conservation, rescaled the velocity-Verlet velocities and constructed, for the one-dimensional harmonic oscillator, a ''shadow Hamiltonian,'' that is, to $O(h^2)$, a multiple of the shadow Hamiltonian given by Eq. (35). Although (to low order), it conserves energy to the same extent as $\tilde{H}$ does, it does not satisfy Hamilton's equations, and so can not be considered to be a true shadow Hamiltonian.

Our main practical conclusion is that derivatives of interpolated position trajectories, rather than velocity-Verlet ''velocities,'' should be used for computing energy fluctuations and physical velocity-dependent observables (e.g., diffusion constants [17]). For the simple case of the multidimensional harmonic oscillator, we were able to calculate the symplectic interpolation. However, for general anharmonic problems, the N computed phase-space points and the knowledge that they have been generated by a symplectic integrator will not be adequate to uniquely specify an interpolation, the shadow mass, or the shadow Hamiltonian. However, when physical considerations imply that an upper limit can be placed on the rate of variation of the position trajectory, we expect that velocities computed by differentiating a sufficiently smooth interpolation will give more accurate results than the velocity-Verlet velocities. Similar considerations apply to the midpoint form of the velocity-Verlet algorithm and probably to symplectic numerical integrators in general.

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[4] Since, in general, $\tilde{H}$, and hence the shadow trajectory, is only defined as an asymptotic series, the definition is not formally unique. However, it appears that in most practical cases asymptotic convergence will be to high accuracy, so this is not a practical concern [1,18].

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