Forward symplectic integrators and the long-time phase error in periodic motions

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We show that when time-reversible symplectic algorithms are used to solve periodic motions, the energy error after one period is generally two orders higher than that of the algorithm. By use of correctable algorithms, we show that the phase error can also be eliminated two orders higher than that of the integrator. The use of fourth order forward time step integrators can result in sixth order accuracy for the phase error and eighth order accuracy in the periodic energy. We study the one-dimensional harmonic oscillator and the two-dimensional Kepler problem in great detail, and compare the effectiveness of some recent fourth order algorithms.

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I. INTRODUCTION

Symplectic integrators [1–5] preserve Poincaré invariants when integrating classical trajectories. For periodic motion, their energy errors are bounded and periodic, in contrast to nonsymplectic Runge-Kutta type algorithms [6] whose energy error grows linearly with the number of periods [7–9]. Energy conservation alone suggests that symplectic algorithms are a better long-time integrator of classical motions. However, for periodic motion, even symplectic algorithms are not immune from the linear growth of the phase error [7–9]. Whereas the energy error is the error of the *action* variable, the phase error is the error of the *angle* variable. Of the two, the phase error is even more important in determining the long-term accuracy of trajectories. For example, when symplectic algorithms are used to compute the Keplerian orbit, the elliptical orbit is easily seen to precess. The precession is of nearly constant radius. Since the semimajor axis of the ellipse is fixed by the initial energy, the constancy of the precession radius implies excellent energy conservation. Yet in spite of that, the precession itself implies that the trajectory is highly inaccurate. This orbital precession is a direct manifestation of phase error. Thus to preserve the long-term accuracy of periodic trajectories, despite the primacy of energy conservation [10], one must seek to reduce the phase error directly.

For periodic motion, the only error that matters is error that persists after one period [9]. A fundamental finding of this work is that, for periodic motion after one period, the energy error is at least $(\Delta t)^2$ times that of the phase error, where Δt is the time step size used. Thus at small Δt the phase error is the dominant error governing the long-term accuracy of periodic motion. Moreover, we show that the phase error of the symplectic corrector [11–15] kernel algorithm is $(\Delta t)^2$ times the phase error of other algorithms nominally of the same order. Recently, one of us [16] has made explicit the "correctability" requirement in deriving a correctable kernel algorithm. This criterion determines the optimal symplectic algorithms for solving periodic motion. The corrector algorithm has its origin in canonical perturbation theory [17]. It has been studied extensively [11–15] for its labor saving feature of only having to iterate the kernel algorithm. Here we draw the connection between symplectic corrector algorithms and the phase error in periodic motion. Much of our analysis is analytical rather than numerical, so that one can understand the result in a transparent way. We also found that *forward* time step symplectic algorithms [18–22] generally have much smaller phase errors than traditional algorithms with backward intermediate time steps [3,5,23–25].

In this work, we will analyze in detail the two fundamental prototypes of periodic motion: the one-dimensional (1D) harmonic oscillator and the two-dimensional (2D) Kepler orbit. We are not interested in solving the harmonic oscillator *per se*, but only in using it as a vehicle for understanding the phase error and the working of our algorithms. It is only with such a simple model that we can show analytically how the phase error can be reduced by fine-tuning the algorithm. To the extent that harmonic motion is the simplest periodic motion, this is clearly a necessary first step for proposing any scheme of phase error reduction. In the 2D Kepler case, we demonstrate the usefulness of forward symplectic algorithms as compared to existing negative time step algorithms. For completeness, we begin with a brief review of the operator construction of symplectic algorithms, followed by a synopsis of symplectic corrector algorithms. In Sec. V, we illustrate the basic idea of our analysis by showing how a second order algorithm can achieve fourth order accuracy in the phase error when solving the 1D harmonic oscillator. In Sec. VI, we repeat the same analysis for a class of fourth order forward algorithms. Error terms up to eighth order are computed by use of the Lie series [27] expansion. Beyond eighth order, the error terms can be determined by exactly solving the matrix model. All these are done analytically. We repeat the analysis for the Kepler problem in Sec. VII. Here, we compare the phase error numerically for a number of recent fourth order symplectic algorithms. We summarize our conclusions in Sec. VIII. For the reader's convenience, some lengthy formulas and explicit calculations are given in the Appendix.

II. OPERATOR FACTORIZATION

Symplectic algorithms can be derived most simply on the basis of operator factorization. (See the excellent review by Yoshida [2] and earlier references therein.) For any dynamical variable $W(q_i,p_i)$, its time evolution is given by the Poisson bracket, and therefore by the corresponding Lie operator $\hat{H}$ associated with the Hamiltonian function $H(q_i,p_i)$, i.e.,

$$\frac{dW}{dt} = \{W,H\} \equiv \frac{\partial W}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial W}{\partial p_i}\frac{\partial H}{\partial q_i} \tag{2.1}$$

$$= \left(\frac{\partial H}{\partial p_i}\frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial}{\partial p_i}\right)W = \hat{H}W. \tag{2.2}$$

(Repeated indices imply summation.) More generally, for any dynamical variable Q, we can define its associated Lie operator $\hat{Q}$ via the Poisson bracket

$$\hat{Q}W = \{W,Q\}. \tag{2.3}$$

As we will see, this fundamental operator mapping underpins the entire development of symplectic integrators.

The operator equation (2.2) can be formally solved via

$$W(t) = e^{t\hat{H}}W(0). \tag{2.4}$$

Symplectic algorithms are derived by approximating the evolution operator $e^{t\hat{H}}$ for a short time in a product form. For Hamiltonian function of the standard separable form,

$$H(\mathbf{q},\mathbf{p}) = T(\mathbf{p}) + V(\mathbf{q}), \quad \text{with } T(\mathbf{p}) = \frac{1}{2}p_i p_i, \tag{2.5}$$

the Hamiltonian operator (2.2) is also separable,

$$\hat{H} = \hat{T} + \hat{V}, \tag{2.6}$$

with first order differential operators $\hat{T}$ and $\hat{V}$ given by

$$\hat{T} \equiv \frac{\partial T}{\partial p_i}\frac{\partial}{\partial q_i} = p_i\frac{\partial}{\partial q_i}, \tag{2.7}$$

$$\hat{V} \equiv -\frac{\partial V}{\partial q_i}\frac{\partial}{\partial p_i} = F_i(\mathbf{q})\frac{\partial}{\partial p_i}. \tag{2.8}$$

Note that $\hat{H}$, $\hat{T}$, and $\hat{V}$ individually satisfy the defining equality (2.3).

The corresponding Lie transforms [27] $e^{\varepsilon\hat{T}}$ and $e^{\varepsilon\hat{V}}$ are then displacement operators which shift q_i and p_i forward in time via

$$\mathbf{q} \to \mathbf{q} + \varepsilon\mathbf{p} \text{ and } \mathbf{p} \to \mathbf{p} + \varepsilon\mathbf{F}. \tag{2.9}$$

Thus, if $e^{\varepsilon\hat{H}}$ can be factorized into products of Lie transforms $e^{\varepsilon\hat{T}}$ and $e^{\varepsilon\hat{V}}$, then each factorization gives rise to an integrator for evolving the system forward in time. Most of the existing literature on symplectic algorithms is concerned with decomposing $e^{\varepsilon\hat{H}}$ to arbitrarily higher order in the product form of

$$e^{\varepsilon(\hat{T}+\hat{V})} \approx \prod_{i=1}^{N} e^{t_i\varepsilon\hat{T}}e^{v_i\varepsilon\hat{V}}, \tag{2.10}$$

with a well-chosen set of factorization coefficients $\{t_i,v_i\}$. In most cases, we will consider only the left-right symmetric factorization schemes such that either $t_1=0$ and $v_i=v_{N-i+1}$, $t_{i+1}=t_{N-i+1}$, or $v_N=0$ and $v_i=v_{N-i}$, $t_i=t_{N-i+1}$. In either case, the algorithm is exactly time-reversible, and the energy error terms can only be an even function of ε. Such a symmetric factorization is then at least second order. As first proved by Sheng [29], and Suzuki [30], beyond second order, decompositions of the form (2.10) must contain some negative coefficients t_i and v_i. Goldman and Kaper [31] further proved that beyond second order, there must be at least one pair of negative coefficients (t_i,v_i). To circumvent this backward time step restriction [18,19], one must factorize the evolution operator in terms of operators $\hat{T}$, $\hat{V}$ *and* the commutator $[\hat{V},[\hat{T},\hat{V}]]$. In this work, we will further demonstrate that these forward symplectic algorithms are also effective in reducing the phase error.

III. SYMPLECTIC CORRECTOR ALGORITHMS

To see the relevance of symplectic corrector algorithms to periodic motion, we recapitulate some recent results [16]. Let $\mathcal{T}_A$ be a symmetric, approximate factorization of the short time evolution operator $e^{\varepsilon(\hat{T}+\hat{V})}$,

$$\mathcal{T}_A = \prod_{i=1}^{N} e^{t_i\varepsilon\hat{T}}e^{v_i\varepsilon\hat{V}} = e^{\varepsilon\hat{H}_A}, \tag{3.1}$$

then the approximate Hamiltonian operator $\hat{H}_A$ must be even in ε, i.e.,

$$\hat{H}_A = \hat{T} + \hat{V} + \varepsilon^2(e_{TTV}[\hat{T},[\hat{T},\hat{V}]] + e_{VTV}[\hat{V},[\hat{T},\hat{V}]]) + O(\varepsilon^4), \tag{3.2}$$

with error coefficients e_{TTV}, e_{VTV} determined by factorization coefficients $\{t_i,v_i\}$. Consider the similarity transformed propagator,

$$\mathcal{T}'_A = S\mathcal{T}_A S^{-1} = Se^{\varepsilon\hat{H}_A}S^{-1} = e^{\varepsilon(S\hat{H}_A S^{-1})} = e^{\varepsilon\hat{H}'_A}, \tag{3.3}$$

where the last equality defines the transformed Hamiltonian $\hat{H}'_A$. If we now take

$$S = \exp[\varepsilon\hat{C}], \tag{3.4}$$

where $\hat{C}$ is the corrector, then the following fundamental result

$$\hat{H}'_A = e^{\varepsilon\hat{C}}\hat{H}_A e^{-\varepsilon\hat{C}} = \hat{H}_A + \varepsilon[\hat{C},\hat{H}_A] + \frac{1}{2!}\varepsilon^2[\hat{C},[\hat{C},\hat{H}_A]] + \cdots, \tag{3.5}$$

implies that

$$\hat{H}_A' = \hat{T} + \hat{V} + \varepsilon^2(e_{TTV}[\hat{T},[\hat{T},\hat{V}]] + e_{VTV}[\hat{V},[\hat{T},\hat{V}]]) + \varepsilon[\hat{C},\hat{T}+\hat{V}] + \cdots . \tag{3.6}$$

One immediately sees that the choice

$$\hat{C} = \varepsilon c_{TV}[\hat{T},\hat{V}] \tag{3.7}$$

would eliminate either second order error term with $c_{TV} = e_{TTV}$ or $c_{TV} = e_{VTV}$. More importantly, if $\hat{H}_A$ is constructed such that

$$e_{TTV} = e_{VTV}, \tag{3.8}$$

then *both* error terms can be eliminated by the corrector. Thus for such an approximate $\mathcal{T}_A$, the transformed propagator $\mathcal{T}_A'$ will be fourth order. This is the fundamental "correctability" requirement for correcting a second order $\mathcal{T}_A$ to fourth order [16]. In general, the corrector can be more complicated than the kernel algorithm $\mathcal{T}_A$. However, when one iterates $\mathcal{T}_A'$, all intermediate correctors cancel and only the initial and final corrector remains. For periodic motion, even the initial and the final corrector would have cancelled after exactly one period. Hence even if $\mathcal{T}_A$ is only second order, if it satisfies the correctability requirement (3.8), then its error after exactly one period would be fourth order. Thus among all second order algorithms, those that are "correctable," i.e., satisfy the the correctability requirement (3.8), would be two orders better. With a correctable algorithm, we will show later that the phase error is improved intrinsically even without applying the corrector. However, if the step size ε is not commensurate with the period, one may step over the minimum of the error function without knowing that it is there. In this case, it is essential to apply the corrector just prior to computing any observable. The advantage of a corrector algorithm is that for long-time integration, one usually only needs to apply the corrector sparingly at a few selected points in time.

This correctability requirement can be generalized to higher order. At higher orders, $\hat{H}_A$ will have error terms of the form $[\hat{T},\hat{Q}_i]$ and $[\hat{V},\hat{Q}_i]$, where $\hat{Q}_i$ are some higher order commutators generated by $\hat{T}$ and $\hat{V}$. If $\hat{H}_A$ is of order $2n$ in ε, then H_A' can be of order $2n+2$ if $\hat{H}_A$'s error coefficients for $[\hat{T},\hat{Q}_i]$ and $[\hat{V},\hat{Q}_i]$ are *equal* for each $\hat{Q}_i$. This is the fundamental corrector insight of [16]. In the following sections, we will demonstrate how this insight can be used to reduce the phase error in practical applications.

IV. THE MODIFIED HAMILTONIAN AND ERROR STRUCTURE

The distinct advantage of symplectic algorithms is not only that they preserve all Poincaré invariants, but that their corresponding modified Hamiltonians and error structures can be systematically determined. This is of paramount importance when one seeks to understand the fundamental cause of an algorithm's error. To illustrate the approach, we begin by analyzing the simplest, first order factorization,

$$e^{\varepsilon\hat{T}}e^{\varepsilon\hat{V}} = e^{\varepsilon\hat{H}_A}, \tag{4.1}$$

where $\hat{H}_A$ is the approximate Hamiltonian operator

$$\hat{H}_A = \hat{H} + \frac{1}{2}\varepsilon[\hat{T},\hat{V}] + \frac{1}{12}\varepsilon[\hat{T},[\hat{T},\hat{V}]] - \frac{1}{12}\varepsilon[\hat{V},[\hat{T},\hat{V}]] + \cdots \tag{4.2}$$

of the algorithm. This follows directly from the Baker-Campbell-Hausdorff (BCH) formula. Thus the algorithm evolves the system according to the modified Hamiltonian $\hat{H}_A$ rather than the original Hamiltonian $\hat{H}$. Nevertheless, the Hamiltonian structure of the system is preserved. As $\varepsilon \to 0$, one recovers the original dynamics. Moreover, knowing $\hat{H}_A$ allows us to determine the actual Hamiltonian function H_A which governs the algorithm's evolution. This can be done systematically by use of the Lie-Poisson bracket correspondence. To make this part of the discussion self-contained, we briefly summarize some pertinent results.

From the fundamental defining equality (2.3), we can deduce H_A via

$$\hat{H}_A W = \{W, H_A\}, \tag{4.3}$$

if we know how commutators of $\hat{T}$ and $\hat{V}$ transform back into functions under the operator mapping (2.3). By repeated applications of Eq. (2.3), we have

$$[\hat{T},\hat{V}]W = \hat{T}\{W,V\} - \hat{V}\{W,T\} = \{\{W,V\},T\} - \{\{W,T\},V\} = \{W,\{V,T\}\}, \tag{4.4}$$

where the last equality follows from the Jacobi identity

$$\{\{W,V\},T\} + \{\{T,W\},V\} + \{\{V,T\},W\} = 0.$$

Equality (4.4) implies the following correspondence between commutators of Lie operators and Poisson brackets of dynamical variables:

$$[\hat{T},\hat{V}] \to \{V,T\} = -\{T,V\}. \tag{4.5}$$

There is thus an order reversal, or a simple sign change, in going from Lie commutators to Poisson brackets. (There is no such order reversal in the usual correspondence between quantum mechanical commutators and Poisson brackets.) This order reversal will only change the sign of odd-order brackets, as illustrated in the following examples:

$$[\hat{V},[\hat{T},\hat{V}]] \to \{\{V,T\},V\} = \{V,\{T,V\}\},$$

$$[\hat{T},[\hat{V},[\hat{T},\hat{V}]]] \to \{\{\{V,T\},V\},T\} = -\{T,\{V,\{T,V\}\}\}. \tag{4.6}$$

Applying this to Eq. (4.3) gives, term by term,

$$\hat{H}_A W = \hat{H}W + \frac{1}{2}\varepsilon[\hat{T},\hat{V}]W + \frac{1}{12}\varepsilon^2[\hat{T},[\hat{T},\hat{V}]]W - \frac{1}{12}\varepsilon^2[\hat{V},[\hat{T},\hat{V}]]W + \cdots ,$$

$$\{W,H_A\} = \{W,H\} + \{W,\frac{1}{2}\varepsilon\{V,T\}\} + \{W,\frac{1}{12}\varepsilon^2\{\{V,T\},T\}\} - \cdots, \tag{4.7}$$

from which we can identify

$$H_A = H - \frac{1}{2}\varepsilon\{T,V\} + \frac{1}{12}\varepsilon^2\{T,\{T,V\}\} - \frac{1}{12}\varepsilon^2\{V,\{T,V\}\} + \cdots. \tag{4.8}$$

This general result merely transcribes expressions of Lie commutators into Poisson brackets. It is valid regardless of the form of the Hamiltonian. For the separable Hamiltonian (2.5), we have specific results

$$\{T,V\} = -\frac{\partial T}{\partial p_j}\frac{\partial V}{\partial q_j} \equiv -p_j V_j, \tag{4.9}$$

$$\{T,\{T,V\}\} = -\frac{\partial T}{\partial p_i}\frac{\partial\{T,V\}}{\partial q_i} = p_i V_{ij} p_j, \tag{4.10}$$

$$\{V,\{T,V\}\} = \frac{\partial V}{\partial q_i}\frac{\partial\{T,V\}}{\partial p_i} = -V_i V_i. \tag{4.11}$$

Since $T=T(\{p_i\})$ and $V=V(\{q_i\})$, there is no ambiguity about the meaning of subscripts on T_i or V_j. Also, since $T_{ij}=\delta_{ij}$, we therefore have

$$H_A = H + \frac{1}{2}\varepsilon p_i V_i + \frac{1}{12}\varepsilon^2 p_i V_{ij} p_j + \frac{1}{12}\varepsilon^2 V_i V_i + \cdots. \tag{4.12}$$

In general, the algorithm's approximate Hamiltonian is nonseparable and more complicated than the original Hamiltonian. A similar expression has been given by Yoshida [2] in terms of H_{p_i}, $H_{q_iq_j}$, etc. For a separable Hamiltonian of the form (2.5), one can certainly write $T_i=H_{p_i}$, and $V_{ij}=H_{q_iq_j}$, etc., but the latter is not more general than the former. If the Hamiltonian is not separable, Yoshida's expression suggests a degree of generality beyond that of the formalism. It is best to leave the form of the approximate Hamiltonian function in terms of Poisson brackets, which is then valid for all Hamiltonians.

For higher order algorithms, the Hamiltonian operator corresponding to any left-right symmetric factorization is

$$\begin{aligned}\hat{H}_A = {} & \hat{T} + \hat{V} + \varepsilon^2(e_{TTV}[\hat{T}^2\hat{V}] + e_{VTV}[\hat{V}\hat{T}\hat{V}]) \\ & + \varepsilon^4(e_{TTTTV}[\hat{T}\hat{T}^3\hat{V}] + e_{VTTTV}[\hat{V}\hat{T}^3\hat{V}]) + (e_{TTVTV}[\hat{T}(\hat{T}\hat{V})^2] \\ & + e_{VTVTV}[\hat{V}(\hat{T}\hat{V})^2]) + \cdots,\end{aligned} \tag{4.13}$$

where e_{TTV}, e_{VTTTV}, etc. are coefficients specific to a particular algorithm and where we have used the condensed commutator notation $[\hat{T}^2\hat{V}]\equiv[\hat{T},[\hat{T},\hat{V}]]$. Note that for symmetric decompositions, one has only even order commutators and the Lie-Poisson correspondence is trivial. In terms of similarly condensed Poisson brackets, $\{T^2V\}\equiv\{T,\{T,V\}\}$, the Hamiltonian function can be read off by inspection,

$$\begin{aligned}H_A = {} & T + V + \varepsilon^2(e_{TTV}\{T^2V\} + e_{VTV}\{VTV\}) \\ & + \varepsilon^4(e_{TTTTV}\{TT^3V\} + e_{VTTTV}\{VT^3V\} \\ & + e_{TTVTV}\{T(TV)^2\} + e_{VTVTV}\{V(TV)^2\}) + \cdots.\end{aligned} \tag{4.14}$$

For the separable Hamiltonian (2.5), these higher brackets are

$$\begin{aligned}\{TT^3V\} &= p_i p_j p_k p_l V ijkl, \\ \{VT^3V\} &= -3p_i p_j V_{ijk} V_k, \\ \{T(TV)^2\} &= -2p_i(V_{ikj}V_k + V_{ik}V_{kj})p_j, \\ \{V(TV)^2\} &= 2V_i V_{ij} V_j.\end{aligned} \tag{4.15}$$

The results in this section will allow us to analyze any symplectic algorithm from second to sixth order. Beyond sixth order, the number of Lie and Poisson brackets proliferates and other means of determining the Hamiltonian error terms may be more efficient.

V. HARMONIC OSCILLATOR: SECOND ORDER INTEGRATOR

To illustrate some of our key ideas in the simplest context, we will begin our study of the phase error with the second order factorization scheme

$$\mathcal{T}_2(\varepsilon,\alpha) \equiv e^{1/2\varepsilon\hat{T}}e^{\varepsilon\hat{V}_1}e^{1/2\varepsilon\hat{T}}, \tag{5.1}$$

with $\hat{V}_1$ given by

$$\hat{V}_1 = \hat{V} + \alpha\varepsilon^2[\hat{V},[\hat{T},\hat{V}]]. \tag{5.2}$$

Classically, this Lie commutator produces a modified force [19]

$$[V,[T,V]] = 2F_j\frac{\partial F_i}{\partial q_j}\frac{\partial}{\partial p_i} = \nabla_i|\mathbf{F}|^2\frac{\partial}{\partial p_i}, \tag{5.3}$$

resulting in the following more general second order symplectic integrator:

$$\begin{aligned}\mathbf{q}_1 &= \mathbf{q}_0 + \frac{1}{2}\varepsilon\mathbf{p}_0, \\ \mathbf{p}_1 &= \mathbf{p}_0 + \varepsilon[\mathbf{F}(\mathbf{q}_1) + \alpha\varepsilon^2\nabla|\mathbf{F}(\mathbf{q}_1)|^2], \\ \mathbf{q}_2 &= \mathbf{q}_1 + \frac{1}{2}\varepsilon\mathbf{p}_1.\end{aligned} \tag{5.4}$$

Here, $(\mathbf{q}_0,\mathbf{p}_0)$ and $(\mathbf{q}_2,\mathbf{p}_1)$ are the initial and final states of the algorithm, respectively. The introduction of the gradient term with parameter α will allow us to satisfy the correctability criterion in its simplest setting. When applied to the 1D harmonic oscillator with Hamiltonian

$$H(q,p) = \frac{p^2}{2} + \frac{1}{2}\omega^2 q^2, \tag{5.5}$$

the force gradient is just

$$F(q) = -\omega^2 q \rightarrow \nabla_q |F(q)|^2 = 2\omega^4 q. \tag{5.6}$$

For the standard Hamiltonian, the approximation Hamiltonian operator for any symmetric factorization is given by Eq. (4.14). The nonvanishing error coefficients corresponding to algorithm (5.1) are just

$$e_{TTV} = -\frac{1}{24}, \quad e_{VTV} = \alpha - \frac{1}{12}, \tag{5.7}$$

$$e_{TTVTV} = \frac{1}{480} - \frac{1}{24}\alpha, \quad e_{VTVTV} = \frac{1}{120} - \frac{1}{6}\alpha. \tag{5.8}$$

The Hamiltonian function is then as given by Eq. (4.15). For the harmonic oscillator as defined by Eq. (5.5), we have $V_{ij} = \omega^2 \delta_{ij}$, $V_{ijk} = 0$, $\{TT^3V\} = 0$, $\{VT^3V\} = 0$, and nonvanishing brackets,

$$\{T,\{T,V\}\} = \omega^2 p^2,$$

$$\{V,\{T,V\}\} = -\omega^4 q^2,$$

$$\{T(TV)^2\} = -2\omega^4 p^2,$$

$$\{V(TV)^2\} = 2\omega^6 q^2. \tag{5.9}$$

Notice the clear separation between the contributions of the algorithm, which are the error coefficients, and that of the physical system, which are the Poisson brackets. The final form of the Hamiltonian function due to algorithm (5.4) is therefore

$$H_A(q,p) = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2 + \omega^2 \varepsilon^2 (e_{TTV} p^2 - e_{VTV}\omega^2 q^2) - 2\omega^4 \varepsilon^4 (e_{TTVTV} p^2 - e_{VTVTV}\omega^2 q^2) + \cdots \tag{5.10}$$

$$= \frac{1}{2m^*}p^2 + \frac{1}{2}k^* q^2. \tag{5.11}$$

Thus the oscillator being evolved by the algorithm is one with an effective mass and spring constant,

$$m^* = m^*(\varepsilon) \equiv (1 + 2\varepsilon^2\omega^2 e_{TTV} - 4\varepsilon^4\omega^4 e_{TTVTV} + \cdots)^{-1}, \tag{5.12}$$

$$k^* = k^*(\varepsilon) \equiv (1 - 2\varepsilon^2\omega^2 e_{VTV} + 4\varepsilon^4\omega^4 e_{VTVTV} + \cdots)\omega^2, \tag{5.13}$$

from which one can deduce the approximate angular frequency

$$\omega_A(\varepsilon) = \sqrt{\frac{k^*}{m^*}}. \tag{5.14}$$

The phase error is simply related to the fractional deviation of the approximate angular frequency from the exact frequency:

$$\Delta\phi = (\omega_A - \omega)T = 2\pi\left(\frac{\omega_A}{\omega} - 1\right). \tag{5.15}$$

This is the fundamental thrust of our analysis: tracking the phase error of the algorithm back to its factorization coefficients. Observe now that from Eqs. (5.12) and (5.13), we have

$$\omega_A(\varepsilon) = \omega\sqrt{(1 + 2\varepsilon^2\omega^2 e_{TTV} + \cdots)(1 - 2\varepsilon^2\omega^2 e_{VTV} + \cdots)} \tag{5.16}$$

$$= \omega[1 + \varepsilon^2\omega^2(e_{TTV} - e_{VTV}) + O(\varepsilon^4)]. \tag{5.17}$$

In general, the approximate frequency is second order in error, as befitting a second order algorithm. However, if the correctability criterion $e_{TTV} = e_{VTV}$ is satisfied, then ω_A is fourth order. Moreover, if the algorithm is originally fourth order with $e_{TTV} = e_{VTV} = 0$ then satisfying $e_{TTVTV} = e_{VTVTV}$ would make ω_A sixth order. Thus an nth algorithm can have an $(n+2)$th order phase error if its error coefficient satisfies the correctability criterion. This is the key connection linking the phase error with correctable algorithms. [Note that by making $e_{TTV} = e_{VTV}$ (but not zero) and $e_{TTVTV} = e_{VTVTV}$ would not make the phase error sixth order.]

With only one free parameter presently available, we can only set $e_{TTV} = e_{VTV} = -\frac{1}{24}$ with the choice

$$\alpha = \frac{1}{24}, \tag{5.18}$$

thus making ω_A fourth order. This particular value corresponds to the well-known propagator first derived by Takahashi and Imada [26] for computing the quantum statistical trace [26] to fourth order. The same factorization scheme, interpreted as symplectic corrector algorithm (5.4), has also been used by Lopez-Marcos *et al.* [13,14] and Wisdom *et al.* [11] for solving classical and celestial dynamical problems. With this choice of α, the coefficient of the fourth order frequency error is, from Eqs. (5.12), (5.13), and (5.8),

$$\frac{\omega^{(4)}}{\omega} = \lim_{\varepsilon\to 0}\left[\frac{1}{\varepsilon^4}\left(\frac{\omega_A}{\omega} - 1\right)\right] = 2\omega^4(e_{VTVTV} - e_{TTV}^2 - e_{TTVTV}) = -\frac{\omega^4}{720}. \tag{5.19}$$

To gauge the relative importance of this phase error, let us compare it to the energy error after one period. Since it is the modified, or approximate Hamiltonian that is conserved by the algorithm, i.e.,

$$H_A(q,p) = H_A(q_0,p_0), \tag{5.20}$$

the energy after one period $T = 2\pi/\omega$ can be expressed as

$$H(q_T,p_T) = H(q_0,p_0) + \varepsilon^2\Delta H_T^{(2)}(\varepsilon^2) + \varepsilon^4\Delta H_T^{(4)}(\varepsilon^2) + \varepsilon^6\Delta H_T^{(6)}(\varepsilon^2) + O(\varepsilon^8). \tag{5.21}$$

From Eq. (5.10), we have in particular,

$$\Delta H_T^{(2)}(\varepsilon^2) = -\omega^2\,(e_{TTV}(p^2 - p_0^2) - e_{VTV}\omega^2(q^2 - q_0^2))|_{t=T}, \tag{5.22}$$

$$\Delta H_{\mathrm{T}}^{(4)}(\varepsilon^2) = 2\omega^4 \left(e_{TTVTV}(p^2 - p_0^2) - e_{VTVTV}\omega^2(q^2 - q_0^2)\right)\big|_{t=\mathrm{T}}. \tag{5.23}$$

In order to compute these energy deviation errors, we must solve for $p(t)$ and $q(t)$ according to Hamiltonian H_A:

$$\begin{pmatrix} q(t;\varepsilon) \\ p(t;\varepsilon) \end{pmatrix} = \begin{pmatrix} \cos(\omega_A t) & (m^*\omega_A)^{-1}\sin(\omega_A t) \\ -(m^*\omega_A)\sin(\omega_A t) & \cos(\omega_A t) \end{pmatrix} \begin{pmatrix} q_0 \\ p_0 \end{pmatrix}. \tag{5.24}$$

Since m^* and ω_A are ε^2-dependent, each function $\Delta H^{(n)}(\varepsilon^2)$ contains further dependence on ε^2. We now define the constant energy error coefficients $E_T^{(n)}$ via

$$H(q_{\mathrm{T}},p_{\mathrm{T}}) - H(q_0,p_0) \equiv \Delta E_{\mathrm{T}} = \varepsilon^2 E_{\mathrm{T}}^{(2)} + \varepsilon^4 E_{\mathrm{T}}^{(4)} + \varepsilon^6 E_{\mathrm{T}}^{(6)} + O(\varepsilon^8), \tag{5.25}$$

where, for example, we have

$$E_{\mathrm{T}}^{(2)} = \Delta H_{\mathrm{T}}^{(2)}(0),$$

$$E_{\mathrm{T}}^{(4)} = \Delta H_{\mathrm{T}}^{(4)}(0) + \Delta H_{\mathrm{T}}^{(2)\prime}(0),$$

$$E_{\mathrm{T}}^{(6)} = \Delta H_{\mathrm{T}}^{(6)}(0) + \Delta H_{\mathrm{T}}^{(4)\prime}(0) + \frac{1}{2!}\Delta H_{\mathrm{T}}^{(2)\prime\prime}(0),$$

$$E_{\mathrm{T}}^{(8)} = \Delta H_{\mathrm{T}}^{(8)}(0) + \Delta H_{\mathrm{T}}^{(6)\prime}(0) + \frac{1}{2!}\Delta H_{\mathrm{T}}^{(4)\prime\prime}(0) + \frac{1}{3!}\Delta H_{\mathrm{T}}^{(2)\prime\prime\prime}(0). \tag{5.26}$$

Here, *the prime denotes derivative with respect to* ε^2. From the form of each $\Delta H_T^{(n)}(\varepsilon^2)$, since $\varepsilon=0$ implies that $\omega_A=\omega$, $p(T)=p_0$, and $q(T)=q_0$, we must have

$$\Delta H_{\mathrm{T}}^{(n)}(0) = 0, \tag{5.27}$$

and therefore

$$E_{\mathrm{T}}^{(2)} = 0. \tag{5.28}$$

Thus for periodic motion, despite the fact the algorithm is only second order, the energy error is actually fourth order after one period.

The fourth order energy error is given by

$$E_T^{(4)} = \Delta H_{\mathrm{T}}^{(2)\prime}(0) = -2\omega^2 \left(e_{TTV}p_{\mathrm{T}}p_{\mathrm{T}}' - e_{VTV}\omega^2 q_{\mathrm{T}}q_{\mathrm{T}}'\right)\big|_{\varepsilon=0} = 4\pi\omega^5 p_0 q_0 (e_{TTV} - e_{VTV})(e_{TTV} + e_{VTV}), \tag{5.29}$$

where we have used

$$q'(T;0) = \frac{1}{\omega}p_0\omega_A'(0)T \text{ and } p'(T;0) = -\omega q_0\omega_A'(0)T, \tag{5.30}$$

and from Eq. (5.17),

$$\omega_A'(0)T = 2\pi\omega^2(e_{TTV} - e_{VTV}). \tag{5.31}$$

The fourth order error now vanishes if the algorithm satisfies the correctability criterion $e_{TTV}=e_{VTV}$. Thus for a *correctable* second order algorithm, after each period, the phase error is fourth order and the energy error is sixth order.

Since the factor (5.31) is common to all first derivatives (in ε^2), we conclude that for $e_{TTV}=e_{VTV}$

$$\Delta H_{\mathrm{T}}^{(n)\prime}(0) = 0. \tag{5.32}$$

Hence for $e_{TTV}=e_{VTV}$, the sixth order energy error can be now computed as

$$E_{\mathrm{T}}^{(6)} = \frac{1}{2}\Delta H_{\mathrm{T}}^{(2)\prime\prime}(0) \tag{5.33}$$

$$= 2\pi\omega^6[2\pi(p_0^2 - \omega^2 q_0^2) - p_0 q_0 \omega](e_{TTV} + e_{VTV}) \times (e_{TTV} - e_{VTV})^2 - 4\pi p_0 q_0 \omega^7 (e_{TTV} + e_{VTV}) \times [2(e_{TTVTV} - e_{VTVTV}) + e_{TTV}^2 + e_{VTV}^2] = \frac{\pi\omega^7}{2160}p_0 q_0. \tag{5.34}$$

The above calculation demonstrates the general property of the energy deviation error after one period. For correctable algorithms, the first two terms in the error expansion (5.26) vanish identically, which means that to compute $E_T^{(6)}$, one need not know the explicit form $\Delta H_T^{(6)}(\varepsilon^2)$. However, in order to compute $\Delta H_T^{(2)\prime\prime}(0)$, one must know $m^*(\varepsilon^2)$ and $\omega_A(\varepsilon^2)$ accurately to $O(\varepsilon^4)$, which means knowing the fourth order Hamiltonian error function, or $\Delta H_T^{(4)}(\varepsilon^2)$. Thus although Eq. (5.33) makes no reference to $\Delta H_T^{(4)}(\varepsilon^2)$, one must know it implicitly. Similarly, $E_T^{(8)}$ can be computed from $\Delta H_T^{(2)}(\varepsilon^2)$ and $\Delta H_T^{(4)}(\varepsilon^2)$ via

$$E_{\mathrm{T}}^{(8)} = \frac{1}{2!}\Delta H_{\mathrm{T}}^{(4)\prime\prime}(0) + \frac{1}{3!}\Delta H_{\mathrm{T}}^{(2)\prime\prime\prime}(0). \tag{5.35}$$

However, in order to compute $\Delta H_T^{(2)\prime\prime\prime}(0)$ one must know $\Delta H^{(2)}(\varepsilon^2)$ correctly to $O(\varepsilon^6)$. This would again require knowing the sixth order error Hamiltonian or $\Delta H^{(6)}(\varepsilon^2)$. In general, $E_T^{(n)}$ can be computed two orders beyond the accuracy of knowing the Hamiltonian.

To summarize, for a second order algorithm, the energy after one period is automatically fourth order in ε $(=\Delta t)$. If the algorithm is correctable, then the energy error is sixth order. For special initial conditions $p_0=0$ or $q_0=0$, by solving the algorithm exactly in the case of the harmonic oscillator [28], one can show that the energy error is actually tenth order. This last error reduction only occurs for the harmonic oscillator. Nevertheless this further emphasizes that the energy error after one period is not a very good gauge of any integrator's accuracy. On the other hand, the phase error, as reflected in the fractional change of the oscillator's angular frequency, can at most be fourth order and is a much more stringent and discriminating benchmark.

VI. HARMONIC OSCILLATOR: FOURTH ORDER FORWARD INTEGRATORS

Beyond second order, all symplectic algorithms of the form (2.10) must have some negative intermediate time steps [29–31]. This means that at some intermediate time, the algorithm is moving the phase trajectory backward in time. For

classical mechanics, which is time-reversible, these negative time steps are harmless. However, for solving time-irreversible problems, such as the diffusion or Fokker-Planck equation, backward time step evolution is not possible. These systems can only be solved by *forward* decomposition algorithms, with all positive, even intermediary, time steps. Some fourth order forward algorithms have been derived recently for solving a variety of time-irreversible [32,33] and time-reversible [19,21,22] equations, both with excellent results. Beyond second order, purely forward time steps are possible only if one includes the commutator $[\hat{V},[\hat{T},\hat{T}]]$ in addition to operators $\hat{T}$ and $\hat{V}$ in the factorization process. In this work we will apply these fourth order forward algorithms to study the phase problem of periodic motion. In this section, we further generalize our study of the harmonic oscillator by use of these fourth order forward algorithms.

Chin and Chen [21,22] have introduced a family of fourth order forward algorithms 4*ACB* parametrized by a parameter t_0. We use here a slightly generalized form by multiplying the central commutator by $1-\alpha$ and adding $\alpha/2$ times the commutator to each potential operator on each side. The resulting algorithm has the operator form

$$\mathcal{T}^{(4)}_{ACB}(\varepsilon,\alpha) \equiv e^{t_0\varepsilon\hat{T}} e^{v_1\varepsilon\hat{V}_1} e^{t_1\varepsilon\hat{T}} e^{v_2\varepsilon\hat{V}_2} e^{t_1\varepsilon\hat{T}} e^{v_1\varepsilon\hat{V}_1} e^{t_0\varepsilon\hat{T}}, \quad (6.1)$$

where

$$\hat{V}_1 = \hat{V} + \frac{\alpha}{2}\frac{u_0}{v_1}\varepsilon^2[\hat{V},[\hat{T},\hat{V}]],$$

$$\hat{V}_2 = \hat{V} + (1-\alpha)\frac{u_0}{v_2}\varepsilon^2[\hat{V},[\hat{T},\hat{V}]], \quad (6.2)$$

$$u_0 = \frac{1}{12}\left[1 - \frac{1}{1-2t_0} + \frac{1}{6(1-2t_0)^3}\right], \quad (6.3)$$

and

$$t_1 = \frac{1}{2} - t_0, \quad v_1 = \frac{1}{6}\frac{1}{(1-2t_0)^2}, \quad v_2 = 1 - 2v_1. \quad (6.4)$$

The corresponding forward symplectic integrator can be read off directly as

$$\mathbf{q}_1 = \mathbf{q}_0 + \varepsilon t_0 \mathbf{p}_0,$$

$$\mathbf{p}_1 = \mathbf{p}_0 + \varepsilon\left[v_1\mathbf{F}(\mathbf{q}_1) + \frac{\alpha}{2}u_0\varepsilon^2\nabla|\mathbf{F}(\mathbf{q}_1)|^2\right],$$

$$\mathbf{q}_2 = \mathbf{q}_1 + \varepsilon t_1 \mathbf{p}_1,$$

$$\mathbf{p}_2 = \mathbf{p}_1 + \varepsilon[v_2\mathbf{F}(\mathbf{q}_2) + (1-\alpha)u_0\varepsilon^2\nabla|\mathbf{F}(\mathbf{q}_2)|^2],$$

$$\mathbf{q}_3 = \mathbf{q}_2 + \varepsilon t_1 \mathbf{p}_2,$$

$$\mathbf{p}_3 = \mathbf{p}_2 + \varepsilon\left[v_1\mathbf{F}(\mathbf{q}_3) + \frac{\alpha}{2}u_0\varepsilon^2\nabla|\mathbf{F}(\mathbf{q}_3)|^2\right],$$

$$\mathbf{q}_4 = \mathbf{q}_3 + \varepsilon t_0 \mathbf{p}_3, \quad (6.5)$$

where $(\mathbf{q}_0,\mathbf{p}_0)$ and $(\mathbf{q}_4,\mathbf{p}_3)$ are the initial and final states of the algorithm, respectively. The parameter α can be changed from 0 to 1, but there is really no restriction on its range. When applied to the harmonic oscillator, the parameter α can be used to correct the algorithm to sixth order. The parameter t_0 can be varied from 0 to $t_c=\frac{1}{2}(1-1/\sqrt{3})\approx 0.21$. For $t_0=0$, the final force evaluation can be reused at the next iteration, thus eliminating one force evaluation. At the upper limit of $t_0=t_c$, $v_2=0$ also eliminates one force evaluation. For $t_0>t_c$, v_2 becomes negative, and the algorithm ceases to be a forward algorithm.

Our analysis of the second order algorithm can now be repeated verbatim for the fourth order case. The approximate Hamiltonian operator corresponding to any symmetric fourth order algorithm is of the form

$$\hat{H}_A = \hat{T} + \hat{V} + \varepsilon^4(e_{TTTTV}[\hat{T}\hat{T}^3\hat{V}] + e_{VTTTV}[\hat{V}\hat{T}^3\hat{V}] + e_{TTVTV}[\hat{T}(\hat{T}\hat{V})^2] + e_{VTVTV}[\hat{V}(\hat{T}\hat{V})^2]) + O(\varepsilon^6). \quad (6.6)$$

For the harmonic oscillator, $[\hat{T}^3\hat{V}]=0$, and the first two error terms vanish identically. The evaluation of the last two error coefficients for the family of fourth order algorithm (6.5) is nontrivial and is given in the Appendix. The corresponding Hamiltonian function, after recalling the Poisson form (4.15) and brackets (5.9), is

$$H_A(q,p) = \frac{p^2}{2} + \frac{1}{2}\omega^2q^2 - 2\omega^4\varepsilon^4(e_{TTVTV}p^2 - e_{VTVTV}\omega^2q^2) + \cdots, \quad (6.7)$$

$$= \frac{1}{2m^*}p^2 + \frac{1}{2}k^*q^2, \quad (6.8)$$

with

$$m^* = m^*(\varepsilon) \equiv (1 - 4\varepsilon^4\omega^4 e_{TTVTV} + \cdots)^{-1}, \quad (6.9)$$

$$k^* = k^*(\varepsilon) \equiv \omega^2(1 + 4\varepsilon^4\omega^4 e_{VTVTV} + \cdots), \quad (6.10)$$

and approximate frequency

$$\omega_A(\varepsilon) = \omega\sqrt{(1 + 4\varepsilon^4\omega^4 e_{VTVTV} + \cdots)(1 - 4\varepsilon^4\omega^4 e_{TTVTV} + \cdots)} \quad (6.11)$$

$$= \omega[1 + 2\varepsilon^4\omega^4(e_{VTVTV} - e_{TTVTV}) + O(\varepsilon^6)]. \quad (6.12)$$

Again, one immediately sees that if the sixth order correctability criterion

$$e_{VTVTV} = e_{TTVTV} \quad (6.13)$$

is satisfied, then ω_A will be sixth order. Note that we now have

$$\omega_A' T|_{\varepsilon=0} = 0,$$

$$\omega_A'' T|_{\varepsilon=0} = 4\pi\omega^4(e_{TTVTV} - e_{VTVTV}), \tag{6.14}$$

where primes still denote derivative with respect to ε^2. The conservation of $H_A(q,p)$ again implies that the energy deviation after one period can be expressed as

$$H(q_T,p_T) = H(q_0,p_0) + \varepsilon^4 \Delta H_T^{(4)}(\varepsilon^2) + \varepsilon^6 \Delta H_T^{(6)}(\varepsilon^2) + \varepsilon^8 \Delta H_T^{(8)}(\varepsilon^2) + O(\varepsilon^{10}), \tag{6.15}$$

with

$$\Delta H_T^{(4)}(\varepsilon^2) = 2\omega^4 \left(e_{TTVTV}(p^2 - p_0^2) - e_{VTVTV}\omega^2(q^2 - q_0^2)\right)|_{t=T}. \tag{6.16}$$

The constant energy error coefficients $E_T^{(n)}$ defined by

$$H(q_T,p_T) - H(q_0,p_0) \equiv \Delta E_T = \varepsilon^4 E_T^{(4)} + \varepsilon^6 E_T^{(6)} + \varepsilon^8 E_T^{(8)} + \varepsilon^{10} E_T^{(10)} + O(\varepsilon^{12}) \tag{6.17}$$

are now of the form

$$E_T^{(4)} = \Delta H_T^{(4)}(0),$$

$$E_T^{(6)} = \Delta H_T^{(6)}(0) + \Delta H_T^{(4)\prime}(0),$$

$$E_T^{(8)} = \Delta H_T^{(8)}(0) + \Delta H_T^{(6)\prime}(0) + \frac{1}{2!}\Delta H_T^{(4)\prime\prime}(0),$$

$$E_T^{10} = \Delta H_T^{(10)}(0) + \Delta H_T^{(8)\prime}(0) + \frac{1}{2!}\Delta H_T^{(6)\prime\prime}(0) + \frac{1}{3!}\Delta H_T^{(4)\prime\prime\prime}(0). \tag{6.18}$$

Now, because of Eq. (6.14), for $e_{TTVTV}=e_{VTVTV}$, not only do we have $\Delta H_T^{(n)}(0)=0$, but also

$$\Delta H_T^{(n)\prime}(0) = 0 \text{ and } \Delta H_T^{(n)\prime\prime}(0) = 0. \tag{6.19}$$

This implies that

$$E_T^{(4)} = E_T^{(6)} = E_T^{(8)} = 0, \tag{6.20}$$

and the first nonvanishing energy error is tenth order,

$$E_T^{10} = \frac{1}{3!}\Delta H_T^{(4)\prime\prime\prime}(0). \tag{6.21}$$

However, as noted in the last section, in order to compute this, one must determine the sixth order error Hamiltonian.

Due to the complexity of the algorithm, these higher error terms are difficult to compute by Lie series. However, they can always be computed using the matrix method [28]. For brevity, we will skip over the details and just report the final results.

We have shown earlier that the fourth order phase error term will vanish if $e_{TTVTV}=e_{VTVTV}$. For a given value of t_0, this criterion can now be satisfied by a specific choice of α given by $\alpha=\alpha(t_0)$ in Eq. (A12). Using this functional form to eliminate α in terms of t_0, the sixth order error term $\omega^{(6)}/\omega=f(t_0)$ scaled such that $\omega=1$, is plotted in Fig. 1.

Within the forward range of $0 \leqslant t_0 \leqslant 0.21$, the sixth order frequency error has a minimum of value

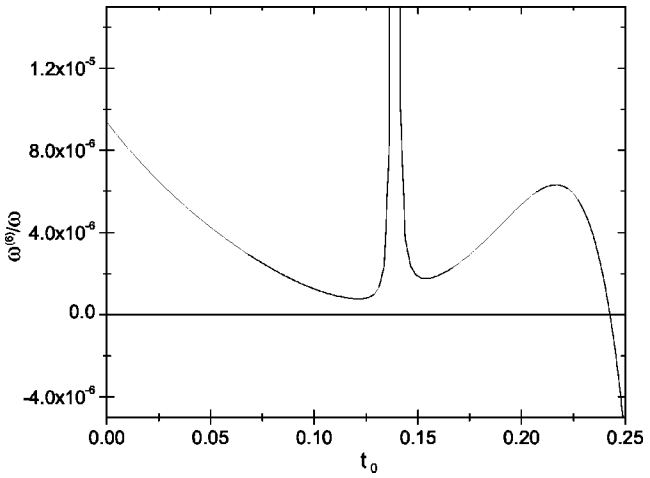

FIG. 1. The sixth order angular frequency error as a function of the algorithm's parameter t_0.

$$\left.\frac{\omega^{(6)}}{\omega}\right|_{min} = 7.718621317057857 \times 10^{-7}\omega^6, \tag{6.22}$$

at $t_0=0.12129085056575276$, and a pole at

$$t_0 = 0.13882413776781183.$$

Note that outside of the forward range, the error can actually vanish at $t_0=0.24265927253055103$.

The eighth order energy deviation error after one period is

$$\Delta E_T^{(8)} = 16\pi\omega^9(e_{TTVTV}^2 - e_{VTVTV}^2)q_0 p_0, \tag{6.23}$$

which again vanishes for $e_{TTVTV}=e_{VTVTV}$ or $e_{TTVTV}=-e_{VTVTV}$, analogous to the second order case.

Thus for a corrected fourth order algorithm, the first nonzero energy deviation error is tenth order. This is plotted in Fig. 2 scaled such that $\omega=q_0=p_0=1$.

Within the forward range of $0 \leqslant t_0 \leqslant 0.21$, the tenth order energy deviation error has a minimum of value

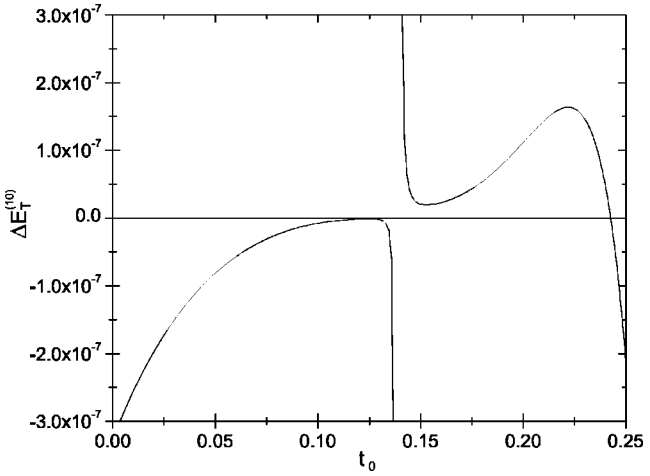

FIG. 2. The tenth order energy deviation error after one period as a function of the algorithm's parameter t_0.

$$\Delta E_{\mathrm{T}}^{(10)}|_{min} = -1.3398713813012635 \times 10^{-9}\omega^{11}q_0p_0, \tag{6.24}$$

at $t_0=0.12482248354859667$ and a pole at $t_0=0.13882413776781183$, (same as in the frequency case). In both cases the error term vanishes at the same value, i.e., $t_0=0.24265927253055103$, outside of the forward range. (Note also that this error term vanishes for a special starting value of $p_0=0$ or $q_0=0$. It can be shown that for either $p_0=0$ or $q_0=0$, the first nonvanishing energy error term is 16th order, again demonstrating that the phase error dominates overwhelmingly over the energy error.)

VII. THE 2D KEPLER PROBLEM

In light of our previous discussion, for long-term trajectory simulation, one must judge all symplectic algorithms on how well they minimize the phase errors rather than the energy error. In this section, we will examine Keplerian motions in 2D defined by the Hamiltonian

$$H = \frac{1}{2}\mathbf{p}^2 - \frac{1}{|\mathbf{q}|}. \tag{7.1}$$

Here, our analysis of fourth order algorithms will not be as extensive as in the harmonic oscillator case because the approximate Hamiltonian

$$\hat{H}_A = \hat{T} + \hat{V} + \varepsilon^4(e_{TTTTV}[\hat{T}\hat{T}^3\hat{V}] + e_{VTTTV}[\hat{V}\hat{T}^3\hat{V}] + e_{TTVTV}[\hat{T}(\hat{T}\hat{V})^2] + e_{VTVTV}[\hat{V}(\hat{T}\hat{V})^2]) + O(\varepsilon^6) \tag{7.2}$$

can no longer be solved analytically. The operator $[\hat{T}^3\hat{V}] \neq 0$ and while we can still force $e_{TTVTV}=e_{VTVTV}$ as in the harmonic oscillator case, we have no way of ensuring that $e_{TTTTV}=e_{VTTTV}$. Currently, there are no known fourth order forward symplectic algorithms that can be corrected to sixth order. Nevertheless, identical analysis as in the harmonic oscillator case shows that

$$E_T^{(4)} = \Delta H_{\mathrm{T}}^{(4)}(0) = 0, \tag{7.3}$$

and the energy error after one period must be at least sixth order. Thus if fourth order algorithms are used to solve Keplerian orbits, it is more fitting to examine their fourth order phase errors instead.

For two-dimensional motion, there are two basic phase angles associated with the two sets of canonical variables (q_1,p_1) and (q_2,p_2). A convenient measure of these phase errors is the precession error of the orbit in the (q_1,q_2) plane, which can be tracked [20] by the rotation of the Laplace-Runge-Lenz (LRL) vector

$$\mathbf{A} = \mathbf{p} \times \mathbf{L} - \hat{\mathbf{q}}. \tag{7.4}$$

In the above definition, $\mathbf{L}=\mathbf{q}\times\mathbf{p}$ is the angular momentum vector.

To see how various algorithms compare, we first plot the fourth order energy error function defined by

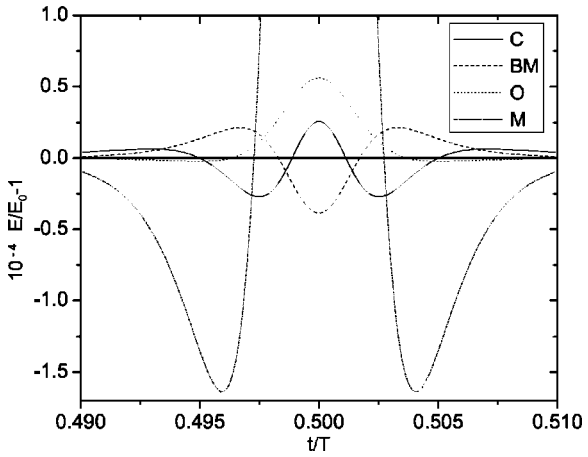

FIG. 3. The energy error at half a period for an eccentricity of 0.9.

$$H_4(\mathbf{q}(t),\mathbf{p}(t)) = \lim_{\varepsilon\to 0}\frac{1}{\varepsilon^4 E_0}[E(\mathbf{q}(t),\mathbf{p}(t)) - E_0] \tag{7.5}$$

in Fig. 3.

Note that this is an intrinsic function characteristic of each algorithm independent of the step size. We compute this function by finding the energy deviation from the initial energy along the orbit and then dividing it by ε^4. As ε gets smaller and smaller, this function converges to its limiting form. The functional form is basically unchanged for $\varepsilon \leqslant T/3000$, where T is the period of the Keplerian orbit. All results shown in Fig. 3 are computed with $\varepsilon=T/5000$.

Since we have shown that $E(\mathbf{q}(T),\mathbf{p}(T))-E_0=O(\varepsilon^6)$, H_4 vanishes exactly after one period. Thus each energy error curve of Fig. 3 reverts back to zero at $t=T$. This is a characteristic behavior of all symplectic algorithms. Nonsymplectic Runge-Kutta algorithms do not have this property and their energy deviation error accumulates rather than vanishing after each period. However, even for symplectic algorithms, the energy deviation error is nonvanishing at other times. Here, due to the high eccentricity ($e=0.9$) of the orbit, the energy error is at a maximum near midperiod. Algorithm Chin-C (C), is the forward algorithm (6.1) with $t_0=1/6$ and $\alpha=0$, first derived in [19]; Blanes-Moan (BM) is an algorithm recommended in McLachlan and Quispel's review [5]; Omelyan *et al.* [25] (O) is a recent alternative forward algorithm that uses the same force gradient defined by Eq. (5.6); McLachlan [3] (M) is a greatly improved version of the first fourth order Ruth-Forest [23] algorithm. With the exception of M, all algorithms have comparable error height at midperiod. Note, however, that BM requires six force evaluations, M uses four force evaluations, O uses four force plus four force-gradient evaluations, but C uses only three force and one force-gradient evaluation. Algorithm M's error height reaches up to 14, which is more than 20 times higher. This is rather surprising, since algorithm M works very well in solving quantum mechanical [21,34] and three-body [22] problems.

In Fig. 4 we track the rotation of the LRL vector during orbital motion. If the orbit is exact, the LRL vector is a

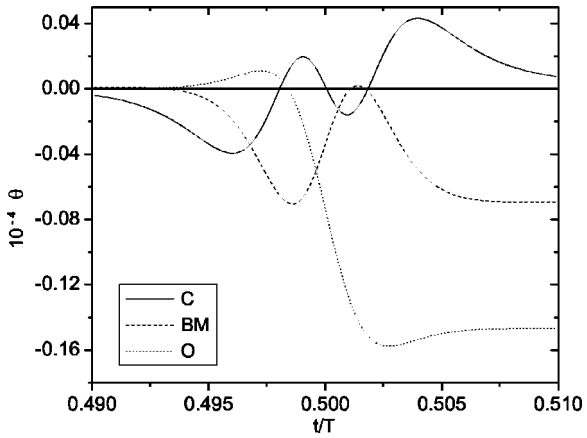

FIG. 4. The precession deviation error after half a period for eccentricity 0.9 with starting point $q=(10,0)$ and $p=(0,0.1)$.

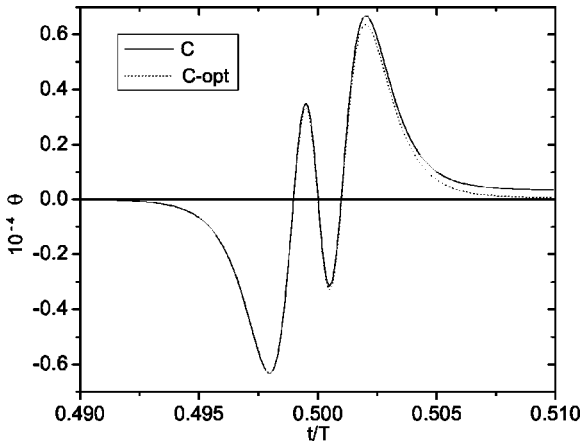

FIG. 5. The precession deviation error after half a period for eccentricity 0.936 with starting point $q=(10,0)$ and $p=(0,0.08)$.

constant vector pointing along the semimajor axis of the orbit. If the orbit precesses, then the LRL vector rotates accordingly. At any point in the orbit, the angle of the LRL vector is given by

$$\theta(t) = \tan^{-1}\left[\frac{A_y(t)}{A_x(t)}\right] = \epsilon^4\theta_4(t) + \varepsilon^6\theta_6(t) + \cdots, \quad (7.6)$$

from which one can extract the fourth order angle error function via

$$\theta_4(t) = \lim_{\epsilon\to 0}\frac{1}{\epsilon^4}\theta(t). \quad (7.7)$$

Again, this intrinsic function is computed in the limit of small ε. We have checked that it has indeed converged to its limiting form for $\varepsilon = T/5000$. Since the orbit precesses the most when the particle is closest to the attractor, the LRL vector rotates measurably only during midperiod. It is constant before, and remained constant after, the midperiod. Thus the rotation after one period is essentially the same as the rotation shortly after midperiod. Note that this (phase) angle error *does not* revert back to zero after each period, but accumulates after each period even for symplectic algorithms regardless of order. Thus the only way to minimize this phase error is to make it as small as possible. From Fig. 4 we see that algorithm C's rotation angle after midperiod in nearly an order of magnitude smaller that that of either BM or O. The actual values after one period are 0.0076, −0.0692, and −0.1466, respectively. Algorithm M's rotation function reaches down to ≈ -2.5, which is an order of magnitude greater than that of BM and O and two orders of magnitude greater than that of C. We did not bother to plot it.

Since parameters t_0 and α are at our disposal, we can further optimize the family of algorithm (6.1) to reduce the rotation error. The resulting optimal choice is shown in Fig. 5, with $t_0=0.166160$ and $\alpha=0$. The angle error after one period is further reduced by a factor of 5 from 0.0360 to 0.0077.

While one can optimize the family of algorithm (6.1) for any one specific problem, or at one eccentricity, it is of greater value to devise an optimal algorithm for solving a general class of problems. For the Kepler problem, all possible shapes of closed orbits are spanned by the eccentricity; it is thus more desirable if one can devise an optimal algorithm for all values of the eccentricity. In Fig. 6 we plot the LRL rotation angle after one period as a function of the orbit's eccentricity, as determined by different initial conditions.

Most algorithms work well for orbits of low eccentricity and the rotation angle is correspondingly small. We therefore compare algorithms at $e \geqslant 0.9$. At $e=0.95$, the angle error values for M, BM, O, and C are, respectively, −166.1870, −4.8865, −10.4470, and 0.1244. Algorithm C's angle error is orders of magnitude smaller than other algorithms.

In Fig. 7 we again show that a better algorithm can be devised from the family of algorithms (6.1). The choice of $\alpha=0$ (only one force-gradient) and $t_0=0.166160$ (only

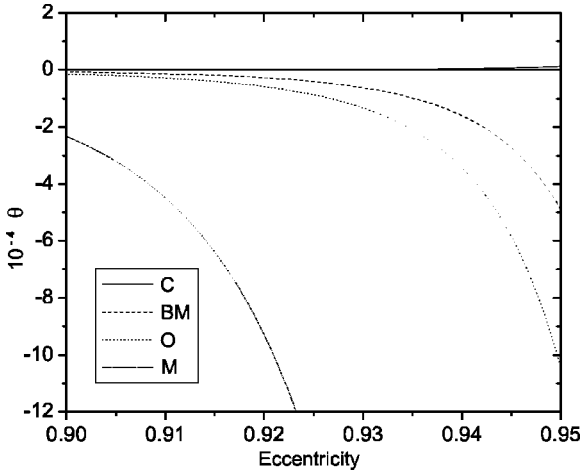

FIG. 6. The precession deviation error for highly eccentric orbits.

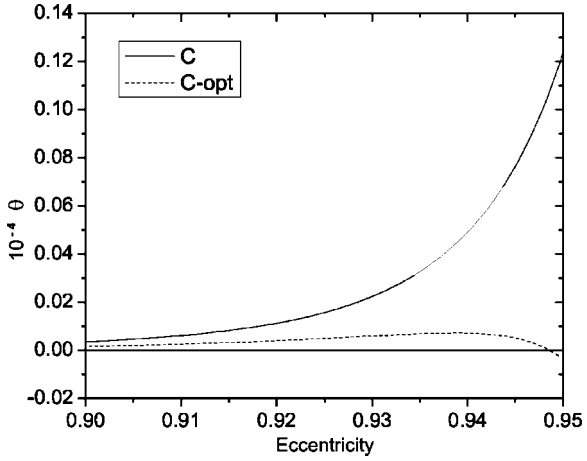

FIG. 7. The precession deviation error for highly eccentric orbits.

slightly below the canonical value of $t_0=1/6$), produces an algorithm with uniformly small phase error up to $e=0.95$. At $e=0.95$ the angle error value for Opt-C is -0.00357, compared to C's value of 0.12363.

VIII. CONCLUSION

In this work we showed that for periodic motion, the energy error after one period is generally two orders higher than that of the algorithm. If the algorithm is correctable, the phase error can also be reduced two orders higher. The use of fourth order forward time step integrators can result in sixth order accuracy for the phase error and eighth accuracy in the periodic energy. By generalizing the recently discovered one-parameter family of fourth order symplectic algorithms [21], we can minimize the energy and phase error to even higher order. The results of this study provide a direct verification of Chin's correctability criterion [16] for correcting a symplectic algorithm to higher order. In particular, we showed that the correctability criterion is superior to the conventional wisdom of minimization of the sum of squares of error coefficients. The most important conclusion of this work is that for periodic motion, the phase error is a more discriminating gauge of an algorithm's effectiveness than the energy error.

As a more important application of the phase error analysis, we track the orbital precession angle of the 2D Kepler problem by monitoring the rotation angle of the Laplace-Runge-Lenz vector [20]. By comparing with various recent fourth order algorithms, we demonstrated the uniqueness of the forward symplectic algorithm in minimizing the phase error of this important class of celestial mechanics problems.

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APPENDIX: FOURTH ORDER ERROR COEFFICIENTS

The error coefficients of the fourth order forward algorithm (6.1) can be computed in terms of algorithm's factorization coefficients via a MATHEMATICA program [32]. They are

$$e_T = 2(t_0 + t_1), \tag{A1}$$

$$e_V = (2v_1 + v_2), \tag{A2}$$

$$e_{TTV} = -\frac{1}{6}[t_1^2(-4v_1 + v_2) + t_0^2(2v_1 + v_2) + 2t_0t_1(2v_1 + v_2)], \tag{A3}$$

$$e_{VTV} = \frac{1}{6}[6u_0 - t_0(2v_1 + v_2)^2 + t_1(2v_1^2 + 2v_1v_2 - v_2^2)], \tag{A4}$$

$$e_{TTTTV} = \frac{1}{360}[7t_0^3(t_0 + 4t_1)(2v_1 + v_2) + t_1^3(4t_0 + t_1)(7v_2 - 16v_1) + 6t_0^2t_1^2(4v_1 + 7v_2)], \tag{A5}$$

$$e_{VTTTV} = \frac{1}{90}[2t_0^2(t_0 + 3t_1)(2v_1 + v_2)^2 - 6t_0t_1^2(6v_1^2 + v_1v_2 - v_2^2) + t_1^3(8v_1^2 - 7v_1v_2 + 2v_2^2)], \tag{A6}$$

$$e_{TTVTV} = \frac{1}{60}[t_0^3(2v_1 + v_2)^2 + t_1^2(10(3\alpha - 1)u_0 + t_1(-16v_1^2 + 4v_1v_2 + v_2^2)) + t_0^2(-10u_0 + t_1(2v_1^2 + 2v_1v_2 + 3v_2^2)) + t_0t_1(-20u_0 + t_1(12v_1^2 + 2v_1v_2 + 3v_2^2))], \tag{A7}$$

$$e_{VTVTV} = \frac{1}{60}[2t_0^2(2v_1 + v_2)^3 - 4t_0(2v_1 + v_2)(5u_0 + t_1(v_1^2 + v_1v_2 - v_2^2)) + t_1(10u_0[2v_1 + (3\alpha - 2)v_2] - t_1(4v_1^3 + v_1^2v_2 + 3v_1v_2^2 - 2v_2^3))]. \tag{A8}$$

In order for the algorithm to be fourth order, we must have $e_T=e_V=1$ and $e_{TTV}=e_{VTV}=0$. These four constraints can be satisfied by

$$t_1 = t_2 = \frac{1}{2} - t_0, \quad t_3 = t_0, \quad v_1 = v_3 = \frac{1}{6(1-2t_0)^2}, \tag{A9}$$

$$v_2 = 1 - (v_1 + v_3), \quad u_0 = \frac{1}{12}\left[1 - \frac{1}{1-2t_0} + \frac{1}{6(1-2t_0)^3}\right]. \tag{A10}$$

This is the family of fourth order algorithms (6.1) with parameters t_0 and α. For the harmonic oscillator, e_{TTTTV} and e_{VTTTV} vanish identically. A fourth order algorithm can be corrected to sixth order if one can set $e_{TTVTV}=e_{VTVTV}$. Substituting Eqs. (A9) and (A10) into Eqs. (A7) and (A8) gives

e_{TTVTV} and e_{VTVTV} as functions of the parameters t_0 and α, i.e.,

$$e_{TTVTV} = \frac{1 + 5\alpha - 12t_0[1 + 5\alpha + 20\alpha t_0(-1 + t_0)]}{2880(1 - 2t_0)},$$

$$e_{VTVTV} = \frac{1 + 10\alpha - 6t_0(3 + 30\alpha - t_0\{9 + 210\alpha + 8t_0[1 - 85\alpha - 3t_0(1 - 40\alpha + 20\alpha t_0)]\})}{4320(1 - 2t_0)^4}. \tag{A11}$$

Solving for $e_{TTVTV} = e_{VTVTV}$ determines α as a function of t_0:

$$\alpha = \frac{1 + 6t_0\{-3 + 4t_0[6 + t_0(-23 + 24t_0)]\}}{5[1 - 12t_0(1 - 2t_0)^2][1 - 6t_0(1 + 2t_0 - 4t_0^2)]}. \tag{A12}$$

However, there exists no real solution of the parameters for which both e_{TTVTV} and e_{VTVTV} can be set to zero, i.e., we can have an algorithm that is correctable to sixth order, but not a real sixth order algorithm.

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