Explicit symplectic integrators for solving nonseparable Hamiltonians

Siu A. Chin
Department of Physics, Texas A&M University, College Station, Texas 77843, USA
(Received 3 June 2009; published 21 September 2009)

By exploiting the error functions of explicit symplectic integrators for solving separable Hamiltonians, I show that it is possible to develop explicit time-reversible symplectic integrators for solving nonseparable Hamiltonians of the product form. The algorithms are unusual in that they are of fractional orders.

DOI: 10.1103/PhysRevE.80.037701 PACS number(s): 02.70.−c, 02.60.−x, 05.45.−a

I. INTRODUCTION

Symplectic integrators [1–4] are the methods of choice for solving diverse physical problems in classical [1,5–7], quantum [8–15], and statistical [16–19] mechanics. For separable Hamiltonians, the problem is well understood and many explicit integrators are available [1–4]. However, for nonseparable Hamiltonians, only implicit algorithms are known [1–4]. It is generally believed that no explicit algorithms can be developed for solving nonseparable Hamiltonians [1,2]. In this work, I show that this is not the case. Explicit time-reversible algorithms can be developed to solve a selected class of nonseparable Hamiltonians. The idea is to model nonseparable Hamiltonians by the error terms of explicit algorithms when solving separable Hamiltonians. By a suitable choice of factorization (or split) coefficients, the explicit algorithm can be made to solve error Hamiltonians, which are generally nonseparable.

In the usual study of symplectic integrations, one seeks to eliminate error terms in order to produce higher-order algorithms. These error terms are therefore not of direct interest and are rarely studied in their own right. In this work, these error terms are the nonseparable Hamiltonians we seek to solve. The method can solve nonseparable Hamiltonians of the product form (sum over repeated indices)

$$H = T_i(\mathbf{p}) V_{ij}(\mathbf{q}) T_i(\mathbf{p}), \tag{1}$$

provided that

$$T_i(\mathbf{p}) = \frac{\partial}{\partial p_i} T(\mathbf{p}) \tag{2}$$

and

$$V_{ij}(\mathbf{q}) = \frac{\partial^2}{\partial q_i \partial q_j} V(\mathbf{q}). \tag{3}$$

For one degree of freedom, given $T'(p)$ and $V''(q)$, $T(p)$ and $V(q)$ can always be obtained by integration.

In the next section we will briefly summarize essential aspects of symplectic integrators and their error functions, followed by our explicit integrator for solving the above nonseparable Hamiltonian. Higher-order algorithms are discussed in Section IV.

II. SYMPLECTIC INTEGRATORS

Given a dynamical variable $W(q_i,p_i)$ and a Hamiltonian function $H(q_i,p_i)$, the former is evolved by the latter via the Poisson bracket, and therefore by the corresponding Lie operator [20] $\hat{H}$ associated with the function $H(q_i,p_i)$,

$$\frac{dW}{dt} = \{W,H\} = \left(\frac{\partial H}{\partial p_i}\frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial}{\partial p_i} \right) W = \hat{H} W, \tag{4}$$

via exponentiation

$$W(t+\varepsilon) = e^{\varepsilon \hat{H}} W(t). \tag{5}$$

For a separable Hamiltonian

$$H(\mathbf{q},\mathbf{p}) = T(\mathbf{p}) + V(\mathbf{q}), \tag{6}$$

the corresponding Hamiltonian operator is also separable, $\hat{H}=\hat{T}+\hat{V}$, with $\hat{T}$ and $\hat{V}$ given by

$$\hat{T} \equiv \{\cdot, T\} = \frac{\partial T}{\partial p_i}\frac{\partial}{\partial q_i}, \tag{7}$$

$$\hat{V} \equiv \{\cdot, V\} = -\frac{\partial V}{\partial q_i}\frac{\partial}{\partial p_i}. \tag{8}$$

Their corresponding evolution operators $e^{\varepsilon \hat{T}}$ and $e^{\varepsilon \hat{V}}$ then shift q_i and p_i forward in time via

$$q_i(\varepsilon) = e^{\varepsilon \hat{T}} q_i = q_i + \varepsilon \frac{\partial T}{\partial p_i},$$

$$p_i(\varepsilon) = e^{\varepsilon \hat{V}} p_i = p_i - \varepsilon \frac{\partial V}{\partial q_i}. \tag{9}$$

Conventional symplectic integrators correspond to approximating the short-time evolution operator $e^{\varepsilon \hat{H}}$ in the product form

$$e^{\varepsilon(\hat{T}+\hat{V})} \approx \prod_{i=1}^{N} e^{t_i \varepsilon \hat{T}} e^{v_i \varepsilon \hat{V}}, \tag{10}$$

resulting in an ordered sequence of displacements (9) which defines the resulting algorithm. Here, we will consider only time-reversible 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 $v_i=v_{N-i}$, $t_i=t_{N-i+1}$.

The product of operators in Eq. (10) can be combined by use of the Baker-Campbell-Hausdorff formula to give

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$$\prod_{i=1}^{N} e^{t_i \varepsilon \hat{T}} e^{v_i \varepsilon \hat{V}} = e^{\varepsilon \hat{H}_A}, \tag{11}$$

where the approximate Hamiltonian operator $\hat{H}_A$ has the general form

$$\hat{H}_A = e_T \hat{T} + e_V \hat{V} + \varepsilon^2 e_{TTV}[\hat{T}\hat{T}\hat{V}] + \varepsilon^2 e_{VTV}[\hat{V}\hat{T}\hat{V}] + O(\varepsilon^4), \tag{12}$$

where e_T, e_{TV}, e_{TTV}, etc., are functions of $\{t_i\}$ and $\{v_i\}$ and where condensed commutator brackets, $[\hat{T}\hat{T}\hat{V}]=[\hat{T},[\hat{T},\hat{V}]]$, $[\hat{T}\hat{V}\hat{T}\hat{V}]=[\hat{T},[\hat{V},[\hat{T},\hat{V}]]]$, etc., are used. From the way Lie operators are defined via Eq. (4), one can convert operators back to functions [1,7] via $[T,V]\rightarrow\{V,T\}=-\{T,V\}$, yielding

$$H_A = e_T T + e_V V + \varepsilon^2 e_{TTV}\{TTV\} + \varepsilon^2 e_{VTV}\{VTV\} + O(\varepsilon^4), \tag{13}$$

where, again, condensed Poisson brackets, $\{TTV\}=\{T,\{T,V\}\}$, etc., are used. For a separable Hamiltonian of form (6), we have

$$\{TV\} = -\frac{\partial T}{\partial p_j}\frac{\partial V}{\partial q_j} = -T_j V_j,$$

$$\{TTV\} = -\frac{\partial T}{\partial p_i}\frac{\partial \{T,V\}}{\partial q_i} = T_i V_{ij} T_j, \tag{14}$$

$$\{VTV\} = \frac{\partial V}{\partial q_i}\frac{\partial \{T,V\}}{\partial p_i} = -V_i T_{ij} V_j. \tag{15}$$

By choosing $\{t_i\}$ and $\{v_i\}$ such that

$$e_T = e_V = 0, \tag{16}$$

and either $e_{VTV}=0$ or $e_{TTV}=0$, the algorithm would then be solving the nonseparable Hamiltonian, either

$$H_{TTV} = T_i V_{ij} T_j \quad \text{or} \quad H_{VVT} = V_i T_{ij} V_j. \tag{17}$$

III. SOLVING NONSEPARABLE HAMILTONIANS

The following factorization scheme gives,

$$\mathcal{T}(\varepsilon) \equiv e^{\varepsilon v_2 \hat{V}} e^{\varepsilon t_2 \hat{T}} e^{\varepsilon v_1 \hat{V}} e^{\varepsilon t_1 \hat{T}} e^{\varepsilon v_0 \hat{V}} e^{\varepsilon t_1 \hat{T}} e^{\varepsilon v_1 \hat{V}} e^{\varepsilon t_2 \hat{T}} e^{\varepsilon v_2 \hat{V}}$$

$$= \exp(\varepsilon^3[\hat{T}\hat{T}\hat{V}] + \varepsilon^5 E_5 + \varepsilon^7 E_7 + \varepsilon^9 E_9 \cdots), \tag{18}$$

with $v_0=-2(v_1+v_2)$, $t_1=-t_2$, $v_2=-v_1/2$, and $v_1=1/t_2^2$. There is one free parameter t_2 that one can choose to minimize the resulting error, but not be set to zero. As exemplified by Eqs. (14) and (15), for a separable Hamiltonian $H=T+V$, higher-order brackets of the form $\{T,Q\}$, $\{V,Q\}$ have opposite signs. Thus, one should choose algorithms with $e_{TQ}=e_{VQ}$ to maximize error cancellations [19]. This is the basis for symplectic corrector [21] or processed [22,23] algorithms. The choice of $t_2=-6^{1/3}\approx -1.82$ forces $e_{TTTV}=e_{VTTV}$ and would be a good starting value. The right-hand side (RHS) of Eq. (18) is the evolution operator for the nonseparable Hamiltonian H_{TTV} with time step $\Delta t=\varepsilon^3$ and leading error terms $O(\varepsilon^5)$. Thus, the parameter ε used by the integrator is $\varepsilon=\sqrt[3]{\Delta t}$. Since $\varepsilon^5=\Delta t^{5/3}$, the basic algorithm (18) in terms of Δt reads

$$\mathcal{T}(\Delta t) = \exp \Delta t([\hat{T}\hat{T}\hat{V}] + \Delta t^{2/3} E_5 + \Delta t^{4/3} E_7 + \Delta t^{6/3} E_9 \cdots). \tag{19}$$

The order of the algorithm $\mathcal{T}(\Delta t)$ (the leading error in the Hamiltonian) is therefore only 2/3. We will discuss this and higher-order algorithms in the next section.

By interchange $\hat{T}\leftrightarrow\hat{V}$ everywhere, but keeping the coefficients intact, the RHS of Eq. (18) goes over to

$$e^{\varepsilon^3[\hat{T}\hat{T}\hat{V}]} \rightarrow e^{\varepsilon^3[\hat{V}\hat{V}\hat{T}]}, \tag{20}$$

and the basic algorithm $\mathcal{T}(\Delta t)$ solves the nonseparable Hamiltonian H_{VVT}. In both cases, the final force or velocity can be reused at the start of the next iteration. Thus, both algorithms require four-force and four-velocity evaluations.

For one degree of freedom, any Hamiltonian of the form

$$H = f(p)g(q) \tag{21}$$

can be solved. To test the algorithm, we solve the nonseparable Hamiltonian

$$H_{TTV} = \left(1 + \frac{p^2}{2}\right)^2 (1 + q^2), \tag{22}$$

where the phase trajectory is harmonic near the origin, but highly distorted at larger values of (p,q). The algorithm's separable Hamiltonian is

$$H = p + \tfrac{1}{6}p^3 + \tfrac{1}{2}q^2 + \tfrac{1}{12}q^4. \tag{23}$$

In Fig. 1 we compare the phase trajectories produced by algorithm (18) with exact trajectories deduced from Eq. (22). We set $t_2=-2$ and use a relatively large value of $\Delta t=0.005$, so that discrepancies can be seen. The four trajectories are started at $p_0=0$ and $q_0=0.5$, 1.0, 1.5, and 2.0, respectively. The error is largest at the positive maximum of p and next largest at the negative maximum of p. In each case, the error can be further reduced by making t_2 more negative than -2. We did not bother with this refinement here, but this will be important in the two-dimensional case discussed below.

We will demonstrate that $\mathcal{T}(\Delta t)$ indeed converges as $\Delta t^{2/3}$ in the next section. For more than one degree of freedom, the generalization of Eq. (21) to

$$H = \sum_i f_i(p_i) g_i(q_i) \tag{24}$$

can always be solved. However, it is more interesting to generalize Eq. (23) to N dimension by reinterpreting p and q as radial coordinates: $p=\sqrt{\Sigma_i p_i^2}$, $q=\sqrt{\Sigma_i q_i^2}$. For any radial potential $V(q)$,

$$V_{ij} = \frac{V'}{q}\delta_{ij} + \left(V'' - \frac{V'}{q}\right)\hat{q}_i \hat{q}_j, \tag{25}$$

where here $\hat{\mathbf{q}}$ is the unit vector. Thus the nonseparable Hamiltonian H_{TTV} corresponding to the radial Hamiltonian (23) is

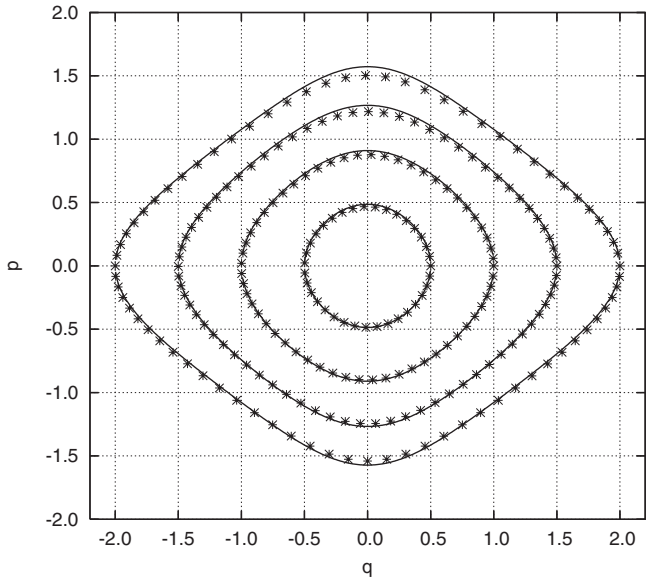

FIG. 1. The phase trajectories of the nonseparable Hamiltonian (22). The computed phase points (stars) are compared with exact trajectories (lines). The initial values are $p_0=0$ and $q_0=0.5$, 1.0, 1.5, and 2.0, corresponding to energy values of 1.25, 2.0, 3.25, and 5.0, respectively.

$$H_{TTV} = \left(1 + \frac{p^2}{2}\right)^2 \left[1 + \frac{1}{3}q^2 + \frac{2}{3}q^2(\hat{\mathbf{p}} \cdot \hat{\mathbf{q}})^2\right]. \tag{26}$$

This can again be solved by our explicit integrator (18). In two dimensions, most trajectories are not closed and are likely to be chaotic. However, for some special initial configurations, a rich variety of closed orbits can be found. Figure 2 shows a sample of three such closed orbits. For this calculation, since the order of the algorithm is only 2/3, reducing the step size is not efficient in achieving higher accuracy. Instead, we find that the error can be substantially reduced by changing t_2 to ≈ -3. For the circle, triangle, and the twisted orbits of Fig. 3, the step sizes used were $\Delta t=0.0012$, 0.001, and 0.0005, respectively.

Finally, the standard kinetic-energy term

$$T(\mathbf{p}) = \tfrac{1}{2} p_i p_i \tag{27}$$

produces

$$H_{TTV} = \{TTV\} = p_i V_{ij} p_j, \tag{28}$$

$$H_{VTV} = \{VTV\} = -V_i V_i, \tag{29}$$

and only H_{TTV} is nonseparable. Here, V_{ij} can be viewed as a position-dependent inverse mass matrix. This work shows that if V_{ij} can be derived from a potential function $V(\mathbf{q})$, then this nonseparable Hamiltonian can also be solved by our explicit algorithm. Also, by itself, this quadratic Hamiltonian does not possess closed orbits for most $V(\mathbf{q})$, thus explaining why this error term would disrupt closed orbit of the original Hamiltonian at large ε.

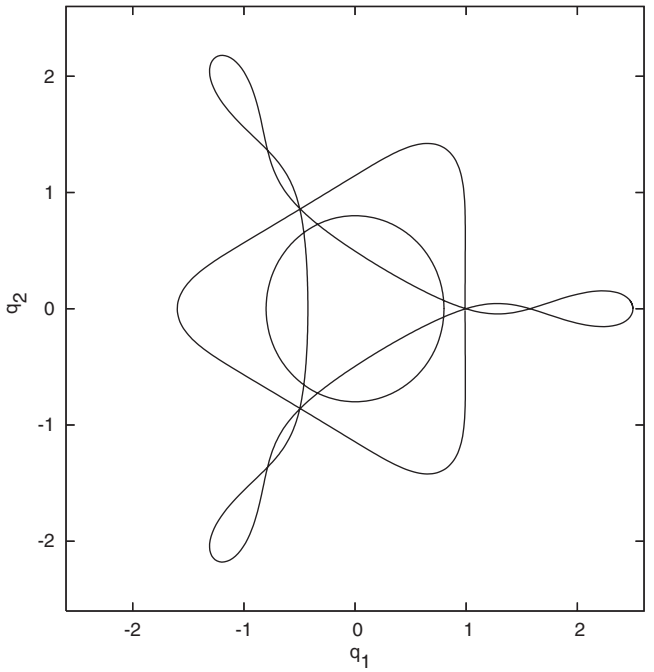

FIG. 2. Some two-dimensional orbits of the nonseparable Hamiltonian (26). Most trajectory are not closed and only very special initial conditions can result in closed orbits. The initial conditions (q_1,q_2,p_1,p_2) that produce the circle, the triangle and the twisted orbits are, respectively, (0.8,0,0,0.425), (0.99,0,0,0.789), and (2.5,0,0,0.1884).

IV. HIGHER-ORDER ALGORITHMS

In the previous section, we have shown that the primitive algorithm $\mathcal{T}(\Delta t)$ does work and reproduces the correct phase

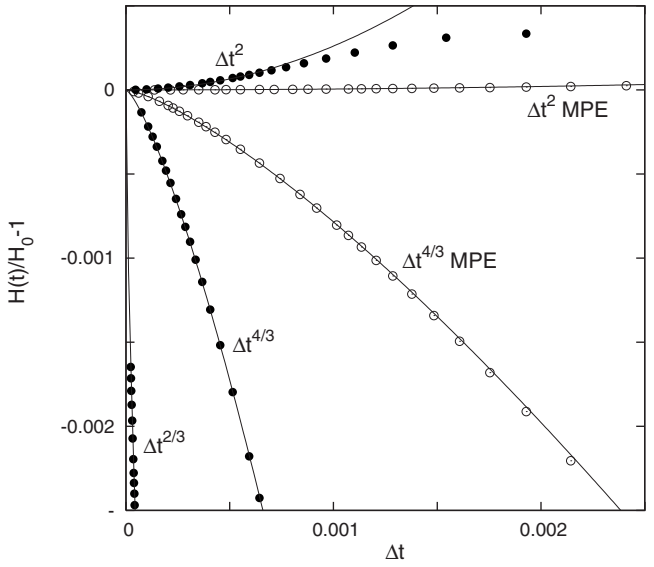

FIG. 3. The fractional power convergence of various explicit algorithms. The relative energy error is evaluated at the first quarter period $t=0.385\,841$, for the outermost trajectory of Fig. 1. The solid circles denote results of symplectic algorithms (18), (30), and (31). The hallow circles give results of MPE algorithms (32) and (33). The lines are fitted curves of the form $c\Delta t^n$, with $n=2/3$, 4/3, or 2 as indicated.

trajectory. However, its 2/3-order convergence is very poor and requires extremely small Δt to produce accurate results. To demonstrate its fractional order convergence, we return to the one-dimensional case (22) and integrate from $t=0$, $p_0=0$, $q_0=2$ to $t=T_{1/4}\equiv 0.385\,841$, $p(t)=-1.569\,196$, $q(t)=0$, corresponding to a quarter clockwise rotation of the outermost phase trajectory of Fig. 1. In Fig. 3, the relative error of the Hamiltonian (22) at $t=T_{1/4}$ is plotted as a function of Δt. The error of $\mathcal{T}(\Delta t)$ can be perfectly fitted with the power law $-2\Delta t^{2/3}$, but due to this fractional power the convergence at small Δt is very poor. Fortunately, the error structure (19) of $\mathcal{T}(\Delta t)$ allows simple ways of generating higher-order symplectic algorithms. The triplet construction of Creutz and Gocksch [24] and Yoshida [25] can produce arbitrary high-order algorithms such as the following 4/3rd-order algorithm:

$$\mathcal{T}_{4/3}(\Delta t)=\mathcal{T}\left(\frac{\Delta t}{2-s}\right)\mathcal{T}\left(-\frac{s\Delta t}{2-s}\right)\mathcal{T}\left(\frac{\Delta t}{2-s}\right) \tag{30}$$

with $s=2^{3/5}$ and the following (6/3)rd=second-order algorithm:

$$\mathcal{T}_{2}(\Delta t)=\mathcal{T}_{4/3}\left(\frac{\Delta t}{2-s}\right)\mathcal{T}_{4/3}\left(-\frac{s\Delta t}{2-s}\right)\mathcal{T}_{4/3}\left(\frac{\Delta t}{2-s}\right) \tag{31}$$

with $s=2^{3/7}$. As can be seen in Fig. 3, these higher-order symplectic algorithms are orders of magnitude better than the basic algorithm $\mathcal{T}(\Delta t)$. The disadvantage of the triplet construction is that the computational effort triples in going from order $k/3$ to $(k+2)/3$. For example, the second-order algorithm $\mathcal{T}_2(\Delta t)$ requires three evaluations of $\mathcal{T}_{4/3}(\Delta t)$, or nine evaluations of $\mathcal{T}(\Delta t)$. Alternatively, arbitrary high-order algorithms can also be obtained via the multiproduct expansion (MPE) [26], with only quadratically growing computational efforts. For example, by replacing $k_i^2\rightarrow k_i^{2/3}$ in [26], one obtains

$$\mathcal{T}_{4/3}^{MPE}(\Delta t)=\frac{1^n}{1^n-2^n}\mathcal{T}(\Delta t)+\frac{2^n}{2^n-1^n}\mathcal{T}^2\left(\frac{\Delta t}{2}\right), \tag{32}$$

$$\begin{aligned}\mathcal{T}_{2}^{MPE}(\Delta t)=&\frac{(1^n)^2}{(1^n-2^n)(1^n-3^n)}\mathcal{T}(\Delta t)\\&+\frac{(2^n)^2}{(2^n-1^n)(2^n-3^n)}\mathcal{T}^2\left(\frac{\Delta t}{2}\right)\\&+\frac{(3^n)^2}{(3^n-1^n)(3^n-2^n)}\mathcal{T}^3\left(\frac{\Delta t}{3}\right)\end{aligned} \tag{33}$$

with $n=2/3$ in both cases. Here, $\mathcal{T}_2^{MPE}(\Delta t)$ only requires six evaluations of $\mathcal{T}(\Delta t)$. The disadvantage of MPE is that it is no longer symplectic, but it is like Runge-Kutta-Nyström-type algorithms. However, as shown in Fig. 3, their energy error can be much smaller than the triplet symplectic algorithms.

V. CONCLUDING SUMMARY

In this work, I have shown that explicit symplectic integrators can be devised to solve a selected class of nonseparable Hamiltonians. Any nonseparable Hamiltonian that can be modeled by the error terms of an explicit integrator can be solved by the same integrator with changed splitting coefficients. The initial explicit algorithm is only of fractional order $\Delta t^{2/3}$, but higher-order algorithms can be easily obtained by the use of the triplet construction or the multiproduct expansion.

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