Explicit symplectic integrators for solving non-separable Hamiltonians.

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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 non-separable Hamiltonians of the product form. The algorithm is unusual in that it is of fractional order.

I. INTRODUCTION

Symplectic integrators\textsuperscript{1–4} are the methods of choice for solving diverse physical problems in classical\textsuperscript{1,5–7}, quantum\textsuperscript{8–15}, and statistical\textsuperscript{16–19} mechanics. For separable Hamiltonians, the problem is well understood and many explicit integrators are available\textsuperscript{1–4}. However, for non-separable Hamiltonians, only implicit algorithms are known\textsuperscript{1–4}. It is generally believed that no explicit algorithms can be developed for solving non-separable Hamiltonians\textsuperscript{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 non-separable Hamiltonians. The idea is to model non-separable 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 non-separable.

In the usual study of symplectic integrators, 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 non-separable Hamiltonians we seek to solve. The method can solve non-separable Hamiltonians of the product form, (sum over repeated indices)

\[ H = T_i(p)V_j(q)T_i(p), \]

provided that

\[ T_i(p) = \frac{\partial}{\partial p_i}T(p). \]

and

\[ V_{ij}(q) = \frac{\partial^2}{\partial q_i \partial q_j}V(q). \]

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 non-separable Hamiltonian.

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 later via the Poisson bracket, and therefore by the corresponding Lie operator\textsuperscript{20} \( \hat{H} \) associated with the function \( H(q_i, p_i) \),

\[
\frac{dW}{dt} = \{W, H\} = \left( \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i} \right) W = \hat{H} W,
\]

via exponentiation,

\[ W(t + \varepsilon) = e^{\varepsilon \hat{H}} W(t). \]

For a separable Hamiltonian,

\[ H(q, p) = T(p) + V(q), \]
the corresponding Hamiltonian operator is also separable, \( \hat{H} = \hat{T} + \hat{V} \), with \( \hat{T} \) and \( \hat{V} \) given by

\[
\hat{T} \equiv \{ , T \} = \frac{\partial T}{\partial p_i} \frac{\partial}{\partial q_i},
\]

(2.4)

\[
\hat{V} \equiv \{ , V \} = \frac{\partial V}{\partial q_i} \frac{\partial}{\partial p_i}.
\]

(2.5)

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

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

\[
p_i(\varepsilon) = e^{\varepsilon \hat{V}} p_i = p_i - \varepsilon \frac{\partial V}{\partial q_i}.
\]

(2.6)

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

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

resulting in an ordered sequence of displacements (2.6) 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 (2.7) can be combined by use of the Baker-Campbell-Hausdorff (BCH) formula to give

\[
\prod_{i=1}^{N} e^{\varepsilon t_i \hat{T}} e^{\varepsilon v_i \hat{V}} = e^{\varepsilon \hat{H}_A},
\]

(2.8)

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

\[
\hat{H}_A = e_T \hat{T} + e_V \hat{V} + \varepsilon^2 e_{TV} [\hat{T} \hat{V}] + \varepsilon^3 e_{TTV} [\hat{T} \hat{T} \hat{V}] + O(\varepsilon^4)
\]

(2.9)

where \( e_T, e_{TV}, e_{TTV}, \) etc., are functions of \( \{ t_i \} \) and \( \{ v_i \} \) and where condensed commutator brackets, \( [\hat{T} \hat{V}] = [\hat{T}, [\hat{T}, \hat{V}]], [\hat{T} \hat{T} \hat{V}] = [\hat{T}, [\hat{T}, [\hat{T}, \hat{V}]]], \) etc., are used. From the way Lie operators are defined via (2.1), one can convert operators back to functions \( \{ t_i \} \) and \( \{ v_i \} \) via \( \{ T, V \} \rightarrow \{ T, V \} = -\{ T, V \} \), yielding

\[
H_A = e_T T + e_V V + \varepsilon^2 e_{TV} TTV + \varepsilon^3 e_{TTV} TTTV + O(\varepsilon^4),
\]

(2.10)

where again, condensed Poisson brackets, \( \{ TTV \} = \{ T, \{ T, V \} \} \), etc., are used. For a separable Hamiltonian of the form (2.3), we have

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

\[
\{ TTV \} = -\frac{\partial T}{\partial p_i} \frac{\partial V}{\partial q_j} = T_i V_{ij} T_j,
\]

(2.11)

\[
\{ VTV \} = \frac{\partial V}{\partial q_i} \frac{\partial T}{\partial p_j} = -V_i T_{ij} V_j.
\]

(2.12)

By choosing \( \{ t_i \} \) and \( \{ v_i \} \) such that

\[
e_T = e_V = 0,
\]

(2.13)

and either \( e_{TV} = 0 \), or \( e_{TTV} = 0 \), the algorithm would then be solving the non-separable Hamiltonian, either

\[
H_{TTV} = T_i V_{ij} T_j \quad \text{or} \quad H_{VVT} = V_i T_{ij} V_j.
\]

(2.14)
III. SOLVING NON-SEPARABLE HAMILTONIANS

The following factorization scheme gives,

\[ e^{\epsilon v_2 \dot{V}} e^{\epsilon v_1 \dot{V}} e^{\epsilon v_2 \dot{V}} e^{\epsilon v_1 \dot{V}} e^{\epsilon v_0 \dot{V}} e^{\epsilon v_1 \dot{V}} e^{\epsilon v_2 \dot{V}} e^{\epsilon v_0 \dot{V}} \]

\[ = e^{\epsilon^2 [\dot{V} \dot{V}]} + O(\epsilon^3), \quad (3.1) \]

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 (2.11) and (2.12), 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 \( \epsilon_{TQ} = \epsilon_{VQ} \) to maximize error cancellations\(^{19}\). This is the basis for symplectic corrector\(^{21}\) or processed\(^{22,23}\) algorithms. The choice of \( t_2 = -6t^3/5 \approx -1.82 \) forces \( \epsilon_{TQTV} = \epsilon_{VQTV} \) and would be a good starting value. The RHS of (3.1) is the evolution operator for the non-separable Hamiltonian \( H_{T+V} \) with time step \( \Delta t = \epsilon^3 \) and error terms \( O(\epsilon^5). \) Thus the parameter \( \epsilon \) used by the integrator is \( \epsilon = \sqrt{\Delta t}. \) Since \( \epsilon^5 = \Delta t^{5/3}, \) the order of the algorithm (the error in the Hamiltonian) is only 2/3.

By interchange \( \dot{T} \leftrightarrow \dot{V} \) everywhere, but keeping the coefficients intact, the RHS of (3.1) goes over to

\[ e^{\epsilon^2 [\dot{V} \dot{V}]} \rightarrow e^{\epsilon^2 [\dot{V} \dot{V}]} , \]

and the algorithm solves the non-separable Hamiltonian \( H_{VT} \). In both cases, the final force or velocity can be re-used 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

\[ H = f(p)g(q) \]

(3.3)

can be solved. To test the algorithm, we solve the non-separable Hamiltonian

\[ H_{T+V} = (1 + p^2/2)(1 + q^2), \]

(3.4)

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

\[ H = p + 1/6 p^3 + 1/2 q^2 + 1/12 q^4. \]

(3.5)

In Fig.1 we compare the phase trajectories produced by algorithm (3.1) with exact trajectories deduced from (3.4). 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 \( p. \) (Since the algorithm is time-reversible, it is surprising that the errors at these two points are not identical.) 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 will be important in the 2D case discussed below. Notice that the velocity of the algorithm’s Hamiltonian (3.5) is always positive, regardless of the sign of \( p. \) The fact that the final \( p \) can change sign is due entirely to the negative coefficient \( t_2. \)

In Fig.2, we demonstrate that the algorithm indeed converges as \( \Delta t^{2/3} \). The case of \( p_0 = 0 \) and \( q_0 = 2.0 \) is computed with four time step sizes \( \Delta t = 0.005, 0.002, 0.001 \) and \( 0.0005. \) For each \( \Delta t, \) the normalized energy error, after being divided by \( \Delta t^{2/3}, \) is plotted as a function of \( t \) for one period (\( \approx 1.53. \)) If the power were truly \( \Delta t^{2/3}, \) then one should approach a constant function as \( \Delta t \to 0. \) This is indeed the case, although the convergence seemed rather slow. The phase point is moving clock-wise; the two big error dips occur at the negative and the positive maximum of \( p \) respectively and account for the greater trajectory discrepancy near the positive maximum of \( p \) as seen in Fig.1.

For more than one degree of freedom, the generalization of (3.3) to

\[ H = \sum_i f_i(p_i)g_i(q_i) \]

(3.6)

can always be solved. However, it is more interesting to generalize (3.5) to N-dimension by reinterpreting \( p \) and \( q \) as radial coordinates: \( p = \sqrt{\sum_i p_i^2}, q = \sqrt{\sum_i q_i^2}. \) For any radial potential \( V(q), \)

\[ V_{ij} = \frac{V'}{q} \delta_{ij} + \left(V'' - \frac{V'}{q}\right)q_iq_j, \]

(3.7)
where here \( \hat{q} \) is the unit vector. Thus the non-separable Hamiltonian \( H_{TTV} \) corresponding to the radial Hamiltonian (3.5) is
\[
H_{TTV} = (1 + \frac{p^2}{2})^2 \left[ 1 + \frac{1}{3}q^2 + \frac{2}{3}q^2(\hat{p} \cdot \hat{q})^2 \right].
\]
(3.8)

This can again be solved by our explicit integrator (3.1). In two-dimension, 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. Fig. 3 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 \( \approx -3 \). 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
\[
T(p) = \frac{1}{2}p_ip_i
\]
produces
\[
H_{TTV} = \{TTV\} = p_iV_{ij}p_j,
\]
(3.10)
\[
H_{VT} = \{VT\} = -V_iV_i,
\]
(3.11)
and only \( H_{TTV} \) is non-separable. 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 \( V(q) \), then this non-separable Hamiltonian can also be solved by our explicit algorithm. Also, by itself, this quadratic Hamiltonian does not possess closed orbits for most \( V(q) \), thus explaining why this error term would disrupt closed orbit of the original Hamiltonian at large \( \varepsilon \).

IV. CONCLUDING SUMMARY

In this work, we have demonstrated that explicit symplectic integrators can be devised to solve a selected class of non-separable Hamiltonians. Any non-separable Hamiltonian which can be modelled by the error terms of an explicit integrator can be solved by the same integrator with changed split coefficients. The algorithm, however, only converges as \( \Delta t^{2/3} \), which makes it essential to reduce the error first by adjusting any free parameter of the algorithm.

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FIG. 1: The phase trajectories of the non-separable Hamiltonian (3.4). 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.
FIG. 2: The fractional power convergence of the explicit algorithm (3.1). The energy error over one period, for the outermost trajectory of Fig.1, is divided by $\Delta t^{2/3}$ for four values of $\Delta t$ (top to bottom curves). The fractional power convergence is clear but rather slow, specially beyond the second error dip.
FIG. 3: Some two dimensional orbits of the non-separable Hamiltonian (3.8). 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 \((2.5,0,0,0.1884)\).