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# A fundamental theorem on the structure of symplectic integrators

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**Abstract**

I show that the basic structure of symplectic integrators is governed by a theorem which states *precisely*, how symplectic integrators with positive coefficients cannot be corrected or processed beyond second order. All previous known results can now be derived quantitatively from this theorem. The theorem provided sharp bounds on second-order error coefficients explicitly in terms of factorization coefficients. By saturating these bounds, one can derive fourth-order algorithms analytically with arbitrary numbers of operators.


## 1. Introduction

Algorithms for solving diverse physical problems ranging from celestial mechanics [1–4], quantum statistical mechanics [5–9] to quantum dynamics [10–13] can all be derived from approximating the evolution operator $\mathrm{e}^{\varepsilon(T+V)}$ in the product form

$$\prod_{i=1}^{N} \mathrm{e}^{t_i \varepsilon T} \mathrm{e}^{v_i \varepsilon V} = \exp\bigl[\varepsilon\bigl(e_T T + e_V V + \varepsilon e_{TV}[T, V] + \varepsilon^2 e_{TTV}\bigl[T, [T, V]\bigr] + \varepsilon^2 e_{VTV}\bigl[V, [T, V]\bigr] + \cdots\bigr)\bigr] \quad (1)$$

with factorization coefficients $\{t_1\}$ and $\{v_i\}$. In this Letter, I prove a fundamental theorem which states that the first three error coefficients $e_{TV}$, $e_{TTV}$ and $e_{VTV}$, for arbitrary $N$, must satisfy an inequality given explicitly in terms of $t_i$ and $v_i$, if either $\{t_i\}$ or $\{v_i\}$ is assumed to be positive. The seemingly complex inequality has a surprisingly simple interpretation that for positive coefficients, the product form (1) cannot be corrected [18] or processed [19,20] beyond second-order. As we will show, many important theorems on symplectic integrators can then be deduced from this pair of inequalities.

Classically, every product of the form (1) produces a symplectic integrator for integrating classical equations of motion. For solving *time-irreversible* problems involving the diffusion operator, such as the quantum statistical trace [5–9] or the imaginary time Schrödinger equation [14–17], one must also insists that these coefficients be positive. Since $T$ and $V$ are non-commuting operators, the general problem of deriving approximations of the form (1) beyond second order, while the order-condition is known [21], regardless of the sign of the coefficients, is extremely difficult. For $N > 3$, most higher order algorithms can only be found by using symbolic algebra and numerical methods [2,13,22–24]. By saturating the inequality proved in this Letter, I also show that a large class of both *forward* and conventional fourth-order algorithm can be analytically derived for arbitrary $N$.

The error coefficients $e_T$, $e_V$, $e_{TV}$, $e_{TTV}$ and $e_{VTV}$ in (1) are related to the factorization coefficient $\{t_i\}$ and $\{v_i\}$ via [8]

$$e_T = \sum_{i=1}^{N} t_i, \qquad e_V = \sum_{i=1}^{N} v_i, \quad (2)$$

$$\frac{1}{2} + e_{TV} = \sum_{i=1}^{N} t_i u_i, \quad (3)$$

$$\frac{1}{6} + \frac{1}{2} e_{TV} + e_{TTV} = \frac{1}{2} \sum_{i=1}^{N} t_i (s_i + s_{i-1}) u_i, \quad (4)$$

$$\frac{1}{6} + \frac{1}{2} e_{TV} - e_{VTV} = \frac{1}{2} \sum_{i=1}^{N} t_i u_i^2, \quad (5)$$

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in terms of useful variables

$$s_i = \sum_{j=1}^{i} t_j, \qquad u_i = \sum_{j=i}^{N} v_j. \tag{6}$$

Satisfying the primary constraints $e_T = 1$ and $e_V = 1$ implies that $s_N = 1$ and

$$u_1 = 1. \tag{7}$$

For $\{t_i\} > 0$, (5) is a quadratic form in $u_i$ whose minimum can be determined subject to linear constraints (3) and (4). This then leads to an inequality relating $e_{TV}$, $e_{TTV}$ and $e_{VTV}$ sufficient to prove that the general product (1) cannot be corrected (to be explained below) beyond second order with positive coefficients [8]. However, the exact minimum was not determined because the required sum, first appeared in Suzuki's work [25],

$$g = \sum_{i=1}^{N} s_i s_{i-1}(s_i - s_{i-1}) = \frac{1}{3}(1 - \delta g), \tag{8}$$

was not known in closed form. The inequality was therefore weak, excluding the possibility of being equal. Surprisingly, a closed form exists and was found in Ref. [26],

$$\delta g = \sum_{i=1}^{N} t_i^3. \tag{9}$$

The minimum was then determined, but without explicitly incorporating the constraint (7). Recently, it was realized [27] that constraint (7) can be enforced without affecting any of Eqs. (3)–(5) by simply setting $t_1 = 0$. The resulting minimum is then only true for algorithms whose first operator is $e^{v_1 \varepsilon V}$. Since classically this operator updates the velocity (momentum) variable, the constraint (7) dictates that the minimum derived in Ref. [26] only holds for *velocity*-type algorithms. By interchanging $T \leftrightarrow V$ and $\{t_i\} \leftrightarrow \{v_i\}$ in all of the above, the constraint $e_T = 1$ now dictates that $v_1 = 0$ and another minimum holds for *position* type algorithm whose first operator is $e^{t_1 \varepsilon T}$. One is finally able to state the exact relationship between $e_{TV}$, $e_{TTV}$ and $e_{VTV}$ directly in terms of *either* $\{t_i\}$ *or* $\{v_i\}$ corresponding to either velocity or position-type algorithms. By constructing integrator whose error coefficients are precisely at the quadratic minimum, the condition for being fourth-order can be directly stated, and easily solved for, in terms of $\{t_i\}$ *or* $\{v_i\}$. One is then able to construct fourth-order integrators analytically for arbitrary $N$ as it was done in Ref. [27]. The current theorem provided sound theoretical support and unified derivation of results obtained in Ref. [27].

## 2. The theorem

The constrained minimum of the quadratic form in (5) can be obtained by the method of Lagrange multiplier. Since this has been worked out in details in Ref. [8] (but for a much weaker goal), we will just summarize the results. For $t_1 = 0$ and $\{t_{i>1}\} > 0$, minimize

$$F = \frac{1}{2}\sum_{i=1}^{N} t_i u_i^2 - \lambda_1\left(\sum_{i=1}^{N} t_i u_i\right) - \lambda_2\left(\sum_{i=1}^{N} t_i(s_i + s_{i-1})u_i\right) \tag{10}$$

with respect to $u_i$ gives,

$$u_i = \lambda_1 + \lambda_2(s_i + s_{i-1}). \tag{11}$$

Substituting this back to satisfy constraints (3) and (4) determines $\lambda_1$ and $\lambda_2$:

$$\lambda_1 + \lambda_2 = \frac{1}{2} + e_{TV}, \tag{12}$$

$$\lambda_1 + \lambda_2 + g\lambda_2 = \frac{1}{3} + e_{TV} + 2e_{TTV}, \tag{13}$$

where $\sum_{i=1}^{N} t_i(s_i + s_{i-1})^2 = 1 + g$. The minimum of the quadratic form is then

$$F_{\min} = \frac{1}{2}\sum_{i=1}^{N} t_i\big[\lambda_1 + \lambda_2(s_i + s_{i-1})\big]^2 = \frac{1}{2}\big[(\lambda_1 + \lambda_2)^2 + g\lambda_2^2\big]$$
$$= \frac{1}{2}\left(\frac{1}{2} + e_{TV}\right)^2 + \frac{1}{2g}\left(2e_{TTV} - \frac{1}{6}\right)^2. \tag{14}$$

Setting the LHS of (5) greater or *equal* (this is the most important point, the main contribution of this Letter) to $F_{\min}$ gives,

**Theorem**, **Part A**: *For $t_1 = 0$ and $\{t_{i>1}\} > 0$, the error coefficients for the product of operators in (1) obey the inequality,*

$$e_{VTV} \leqslant \frac{1}{24} - \frac{1}{2}e_{TV}^2 - \frac{6}{1 - \delta g}\left(e_{TTV} - \frac{1}{12}\right)^2, \tag{15}$$

*or, after slight arrangement,*

$$e_{VTV} + \frac{1}{2}e_{TV}^2 - e_{TTV} \leqslant -\frac{1}{24}\delta g - \frac{6}{1 - \delta g}\left(e_{TTV} - \frac{1}{12}\delta g\right)^2, \tag{16}$$

*where $\delta g$ is given by (9).*

Since $0 < \delta g < 1$ for $\{t_{i>1}\} > 0$ and $e_T = 1$, the second form shows that the LHS of (16) is strictly negative. Note that $t_1 = 0$ does not prevent the algorithm from being completely general. Nothing stops us from considerating algorithms with $v_1 = 0$, in which case, the result will be a position-type algorithm. This part of the theorem simply regard $\{t_i\}$ as independent variables.

By interchanging $T \leftrightarrow V$ and $\{t_i\} \leftrightarrow \{v_i\}$ in (1), the error coefficients changes respectively, $e_{TV} \to -e_{TV}$, $e_{TTV} \to -e_{VTV}$ and $e_{VTV} \to -e_{TTV}$. Making the substitution in (15) yields,

**Theorem**, **Part B**: *For $v_1 = 0$, and $\{v_{i>1}\} > 0$, the error coefficients for the product of operators*

$$\prod_{i=1}^{N} \mathrm{e}^{v_i \varepsilon V} \mathrm{e}^{t_i \varepsilon T}$$
$$= \exp\bigl[\varepsilon\bigl(e_T T + e_V V + \varepsilon e_{TV}[T,V] + \varepsilon^2 e_{TTV}\bigl[T,[T,V]\bigr] + \varepsilon^2 e_{VTV}\bigl[V,[T,V]\bigr] + \cdots\bigr)\bigr], \tag{17}$$

*obey the inequality,*

$$e_{TTV} \geqslant -\frac{1}{24} + \frac{1}{2}e_{TV}^2 + \frac{6}{1-\delta g'}\left(e_{VTV} + \frac{1}{12}\right)^2, \tag{18}$$

*or in the form*

$$e_{TTV} - \frac{1}{2}e_{TV}^2 - e_{VTV} \geqslant \frac{1}{24}\delta g' + \frac{6}{1-\delta g'}\left(e_{VTV} + \frac{1}{12}\delta g'\right)^2, \tag{19}$$

*where the corresponding $\delta g'$ is given by*

$$\delta g' = \sum_{i=1}^{N} v_i^3. \tag{20}$$

Again (19) shows that the LHS is strictly positive. We will regard (16) and (19) as fundamental statements of our theorem. To explain this, we recall the basic idea of symplectic corrector or process algorithms [18–20].

If $\rho$ denotes an approximation to $\mathrm{e}^{\varepsilon(T+V)}$ of the product form (1), then $\rho$ is "correctable" if

$$\rho' = S\rho S^{-1} \tag{21}$$

is correct to higher-order in $\varepsilon$ for some operator $S$ also of the general form (1) but with no sign restriction on its factorization coefficients [18–20]. If $\rho$ is correctable, then its trace, equal to the trace of $\rho'$, will be correct to higher order in $\varepsilon$. This is important for calculating the quantum statistical trace of an approximate density matrix, as in path integral Monte Carlo calculations [5–9]. The criterion for $\rho$ to be correctable to at least third-order in $\varepsilon$ is [8]

$$e_{VTV} + \frac{1}{2}e_{TV}^2 - e_{TTV} = 0. \tag{22}$$

However, if $\{t_i\} \geqslant 0$, then (16) shows that this is not possible. And if $\{v_i\} \geqslant 0$, then (19) also shows that this is not possible. Our theorem states *precisely*, how forward symplectic integrator of the product form, consisting of only operators $T$ and $V$, *cannot* be corrected beyond second order.

A much weaker form of this theorem, that the LHS of (22) cannot be zero, has been proved previously by Chin [8], and by Blanes and Casas [28] using a very different method. The current theorem is much sharper, stating the precise amount by which the correctability condition (22) is being missed, when $\{t_i\} \geqslant 0$, and when $\{v_i\} \geqslant 0$.

Two main corollaries: **(1)** It is easy to force $e_{TV} = 0$; all odd-order error terms will vanish if we simply choose factorization coefficients that are left–right symmetric in (1) or (17). If $e_{TV} = 0$, then the correctability criterion is just $e_{TTV} = e_{VTV}$. However, (16) and (19) both show that there is an unbridgeable gap between the two coefficients; they can never be equal. In particular, they can never *both* equal to zero. This corollary is the Sheng–Suzuki theorem [25,29]: there cannot be factorization algorithms of the form (1) with positive coefficients beyond second order. Again our current theorem is more quantitative in showing that if $\{t_i\} > 0$, then the gap is given by (16) and if $\{v_i\} > 0$, then the gap is given by (19). **(2)** If both $e_{TV}$ and $e_{TTV}$ are zero, then (16) implies that

$$e_{VTV} \leqslant -\frac{1}{24}\frac{\delta g}{1-\delta g}, \tag{23}$$

and can only vanish if $\delta g = 0$, requiring at least one $t_i$ to be negative. If both $e_{TV}$ and $e_{VTV}$ are zero, then (19) implies that

$$e_{TTV} \geqslant \frac{1}{24}\frac{\delta g'}{1-\delta g'}, \tag{24}$$

and can only vanish if $\delta g' = 0$, requiring at least one $v_i$ to be negative. This corollary is the Goldman–Kaper theorem [30]: beyond second order, factorization algorithms with only operators $T$ and $V$ must have at least a pair of negative coefficients $(t_k, v_k)$. Our current theorem is again much more quantitative with symmetric forms (23) and (24).

## 3. Constructing fourth-order algorithms

Since all odd-order error terms vanish with left–right symmetric coefficients, fourth-order algorithms can be obtained by forcing both $e_{TTV}$ and $e_{VTV}$ to zero. Let us consider first velocity-type algorithms described by Part A of the theorem. When $e_{TV}$ and $e_{TTV}$ are both zero, the bound for $e_{VTV}$ (23) is the actual error coefficient for algorithms with $u_i$ given by (11), corresponding to

$$v_i = -\lambda_2(t_i + t_{i+1}), \tag{25}$$
$$v_1 = \frac{1}{2} + \lambda_2(1 - t_2) \quad \text{and} \quad v_N = \frac{1}{2} + \lambda_2(1 - t_N), \tag{26}$$

with $\lambda_2$ given by (12) and (13),

$$\lambda_2 = -\frac{1}{2}\frac{1}{1-\delta g}. \tag{27}$$

Eq. (25) is true for all algorithms whose quadratic form is *stationary* with respect to $u_i$. Thus the equal sign in (23) holds even for negative $t_i$. A fourth-order algorithm results if we choose a left–right symmetric set of $\{t_i\}$ with $t_1 = 0$ such that $e_T = 1$ and $\delta g = 0$. For example, for $N = 6$, we can choose $t_6 = t_2$, $t_5 = t_3$. The constraints

$$2t_2 + 2t_3 + t_4 = 1,$$
$$2t_2^3 + 2t_3^3 + t_4^3 = 0 \tag{28}$$

can be solved by setting $t_2 = \alpha t_3$, giving

$$t_4 = -2^{1/3}\bigl(1+\alpha^3\bigr)^{1/3} t_3, \tag{29}$$
$$t_3 = \frac{1}{2(1+\alpha) - 2^{1/3}(1+\alpha^3)^{1/3}}. \tag{30}$$

The case of $\alpha = 0$ reduces back to the well-known Forest–Ruth integrator [31]. For $\delta g = 0$, coefficients $v_i$ given by (25), (26) are *linearly* related to $\{t_i\}$. For position-type algorithms, one can simply exchange operators $T \leftrightarrow V$ and their coefficients

$\{t_i\} \leftrightarrow \{v_i\}$. For further examples of constructing this type of algorithms, see Ref. [27].

Instead of forcing $e_{VTV}$ to vanish on the RHS of (1), one can simply move the entire operator

$$\exp\bigl(\varepsilon^3 e_{VTV}\bigl[V,[T,V]\bigr]\bigr)$$

back to the LHS, and combine the commutator $\varepsilon^3 e_{VTV}[V,[T,V]]$ symmetrically with one or more operator $\varepsilon v_i V$. For $T = p^2/2$, both classically [32] and quantum mechanically [33], $[V,[T,V]]$ corresponds to an additional *gradient* force or potential similar to $V$. By doing this, one gets around the Sheng–Suzuki theorem in producing fourth-order *forward* ($t_{i>1} > 0$) symplectic integrator by factorizing $e^{\varepsilon(T+V)}$ through an additional operator $[V,[T,V]]$. This results in a far richer family of algorithms since any set of symmetric coefficient $\{t_{i>1}\}$ (regardless of sign) satisfying $e_T = 1$ will now yield a fourth-order algorithm. For example, for $N = 4$, taking $t_2 = t_3 = t_4 = 1/3$ produces

$$v_1 = v_4 = \frac{1}{8}, \qquad v_2 = v_3 = \frac{3}{8}, \qquad e_{VTV} = -\frac{1}{192}, \tag{31}$$

which is forward algorithm 4D [12]. But one can also take $t_2 = t_4 = 2/3$, $t_3 = -1/3$, giving

$$v_1 = v_4 = \frac{1}{8}, \qquad v_2 = v_3 = \frac{3}{8}, \qquad e_{VTV} = -\frac{5}{96}. \tag{32}$$

This also illustrates that the Goldman–Kaper theorem no longer holds if one includes $[V,[T,V]]$ in the factorization process. More examples of deriving velocity-type gradient algorithms are given in Ref. [27].

To construct position-type algorithms, we invoke Part B of the theorem. Since we have a preference for keeping the commutator $[V,[T,V]]$, we must set $e_{TV} = e_{TTV} = 0$ in (18) and solve for $e_{VTV}$,

$$e_{VTV} = -\frac{1}{12}\bigl(1 - \sqrt{1-\delta g'}\bigr), \tag{33}$$

where we have picked the solution which vanishes with $\delta g'$. Under the interchange $T \leftrightarrow V$ and $\{t_i\} \leftrightarrow \{v_i\}$, the corresponding Eq. (13) for $\lambda_2$ reads

$$\frac{1}{2} + g'\lambda_2 = \frac{1}{3} - 2e_{VTV}, \tag{34}$$

from which one deduces

$$\lambda_2 = -\frac{1}{2}\frac{1}{\sqrt{1-\delta g'}}. \tag{35}$$

Thus any set of symmetric $\{v_i\}$ with $v_1 = 0$ and $e_V = 1$ will produce a fourth-order algorithm via

$$t_i = -\lambda_2(v_i + v_{i+1}), \tag{36}$$

$$t_1 = \frac{1}{2} + \lambda_2(1 - v_2) \quad \text{and} \quad t_N = \frac{1}{2} + \lambda_2(1 - v_N), \tag{37}$$

with $\lambda_2$ and $e_{VTV}$ given by (35) and (33). For $N = 4$, $v_2 = v_3 = v_4 = 1/3$, this gives

$$t_1 = t_4 = \frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\right), \qquad t_2 = t_3 = \frac{1}{2\sqrt{2}} \tag{38}$$

and

$$e_{VTV} = -\frac{1}{12}\left(1 - \frac{2}{3}\sqrt{2}\right). \tag{39}$$

More examples of deriving position-type forward algorithms can be found in Ref. [27].

In conclusion, I have presented a fundamental theorem on symplectic integrators from which fourth-order algorithms of arbitrary length can be constructed for solving diverse physical problems. Other important properties of symplectic integrators can also be deduced from this theorem.

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