Structure of positive decompositions of exponential operators

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(Received 2 August 2004; revised manuscript received 12 October 2004; published 12 January 2005)

The solution of many physical evolution equations can be expressed as an exponential of two or more operators acting on initial data. Accurate solutions can be systematically derived by decomposing the exponential in a product form. For time-reversible equations, such as the Hamilton or the Schrödinger equation, it is immaterial whether or not the decomposition coefficients are positive. In fact, most symplectic algorithms for solving classical dynamics contain some negative coefficients. For time-irreversible systems, such as the Fokker-Planck equation or the quantum statistical propagator, only positive-coefficient decompositions, which respect the time-irreversibility of the diffusion kernel, can yield practical algorithms. These positive time steps only, forward decompositions, are a highly effective class of factorization algorithms. This work presents a framework for understanding the structure of these algorithms. By a suitable representation of the factorization coefficients, we show that specific error terms and order conditions can be solved *analytically*. Using this framework, we can go beyond the Sheng-Suzuki theorem and derive a lower bound for the error coefficient e_{VTV}. By generalizing the framework perturbatively, we can further prove that it is not possible to have a sixth-order forward algorithm by including only the commutator $[VTV]\equiv[V,[T,V]]$. The pattern of these higher-order forward algorithms is that in going from the $(2n)$th to the $(2n+2)$th order, one must include a different commutator $[VT^{2n-1}V]$ in the decomposition process.

DOI: 10.1103/PhysRevE.71.016703 PACS number(s): 02.70.Ss, 02.70.Ns, 95.10.Ce

I. INTRODUCTION

Many physical evolution equations, from classical mechanics [1–4], electrodynamics [5], statistical mechanics [6,7] to quantum mechanics [8–10], all have the form

$$\frac{\partial w}{\partial t} = (T+V)w, \tag{1.1}$$

where T and V are noncommuting operators. Such an equation can be solved iteratively via

$$w(t+\epsilon) = e^{\epsilon(T+V)}w(t), \tag{1.2}$$

provided that one has a suitable approximation for the short time evolution operator $e^{\epsilon(T+V)}$. Usually, $e^{\epsilon T}$ and $e^{\epsilon V}$ can be solved exactly. By factorizing $e^{\epsilon(T+V)}$ to higher order in the form

$$e^{\epsilon(T+V)} = \prod_{i=1}^{N} e^{t_i\epsilon T}e^{v_i\epsilon V}, \tag{1.3}$$

one can solve (1.1) accurately with excellent conservation properties. Classically, each factorization (1.3) produces a *symplectic integrator*, which exactly conserves all Poincaré invariants. A vast literature [1–3] exists on producing symplectic integrators of the form (1.3). Once a factorization scheme is derived, it can be implemented specifically to solve any particular evolution equation of the form (1.1).

However, as one examines these factorization schemes more closely, one is immediately struck by the fact that beyond second order, all such schemes contain some negative coefficients [1–3] t_i and v_i. Since the fundamental diffusion kernel cannot be simulated or integrated backward in time, none of these higher-order schemes can be applied to *time-irreversible* systems. This lack of positive-coefficient decompositions beyond second order was noted and proved by Sheng [11]. Sheng showed that equations for determining the third-order coefficients in (1.3) are incompatible if the coefficients $\{t_i,v_i\}$ are assumed to be positive. This is a valuable demonstration, but it shed no light on the cause of this incompatibility nor offered clues on how to overcome this deficiency. Suzuki [12] later proved that the incompatibility can be viewed more geometrically. His proof tracked the coefficients of the operator TTV and TVV in the product expansion of (1.3). If the expansion were correct to third order, then the coefficients for both operators must be $\frac{1}{3!}$. The coefficient condition for one corresponds to a hyperplane and the other, a hypersphere. Suzuki then went on to show that for the same set of positive coefficients, the hyperplane cannot intersect the hypersphere and, therefore, no real solution is possible.

The product form (1.3) has the general expansion

$$\prod_{i=1}^{N} e^{t_i\varepsilon T}e^{v_i\varepsilon V} = \exp\big(e_T\varepsilon T + e_V\varepsilon V + e_{TV}\varepsilon^2[T,V] + e_{TTV}\varepsilon^3[T,[T,V]] + e_{VTV}\varepsilon^3[V,[T,V]] + \cdots\big) = e^{\varepsilon H_A(\varepsilon)}, \tag{1.4}$$

where the last equality defines the approximate Hamiltonian of the product decomposition. The goal of factorization is to keep $e_T=e_V=1$ and forces all other error coefficients, such as e_{TV}, e_{TTV}, e_{VTV}, etc., to zero. By tracing the incompatibility condition to error coefficients of specific operators, one can identify which error term cannot be made to vanish. The operator TTV can only occur in $[T,[T,V]]$ and TVV only in $[V,[T,V]]$. Thus the incompatibility condition is equivalent to the fact that for positive coefficients $\{t_i,v_i\}$, e_{TTV} and e_{VTV} cannot both be reduced to zero. To circumvent this, it is sufficient to force one error coefficient to zero and keep the other commutator in the factorization process. Since in quantum mechanics $[V,[T,V]]$ corresponds to a local function, just like the potential, Suzuki [13] suggested that one should factorize $e^{\varepsilon(T+V)}$ in terms of $T, V,$ *and* $[V,[T,V]]$. Following up on this suggestion, Suzuki [14] and Chin [15] have derived fourth-order factorization algorithms with only positive coefficients. Chin [15] also showed that, classically, $[V,[T,V]]$ give rises to a force gradient exactly as first suggested by Ruth [16]. Chin and collaborators have since abundantly demonstrated the efficiency of these forward time-step algorithms in solving both time-irreversible [17–20] and time-reversible [4,9,10,15] dynamical problems. Jang *et al.* [21] have used these forward factorization schemes in doing quantum statistical calculations and Omelyan *et al.* [22,23] have produced an extensive collection of higher-order algorithms (but with negative coefficients) based on this class of fourth-order forward algorithms. Moreover, they have shown that many higher-order algorithms can be derived much more economically with the inclusion of the commutator $[V,[T,V]]$.

An important question, therefore, arises: with the inclusion of the operator $[V,[T,V]]$, can one produce forward algorithms of sixth or higher order? It has been known for some time, from our own work [10], from the extensive search of higher-order algorithms by Omelyan *et al.* [22,23] and that of Blanes and Casas [24], that the answer is probably no. If such a sixth-order algorithm existed, we would have found it by now. What is lacking is a proof similar to Suzuki's, pointing out the key impediment and explaining this lack of success. In this work, we show that for a sixth-order decomposition with positive coefficients, it is the commutator $[V,[T,[T,[T,V]]]]$ that cannot be made to vanish and must be included. In order to prove this result we have developed a formalism to analyze the structure of these forward factorization schemes. By use of a suitable representation of the factorization coefficients, we show that linear order conditions and quadratic error terms can both be solved *analytically*. The resulting error term then makes it obvious that it cannot vanish if the factorization coefficients are purely positive. By use of this formalism we can go beyond the Sheng-Suzuki theorem and derive a lower bound for the magnitude of the error coefficient e_{VTV}. By generalizing the method to sixth order, we further prove the main result as stated above. This analytical method of solving the order conditions will allow us to analyze and classify factorization algorithms in general.

In Sec. II we introduce our notations and illustrate our method of solving the order condition analytically by giving a constructive proof of the Sheng-Suzuki theorem. In Sec. III, we discuss the conditions necessary for a sixth-order forward algorithm. In Sec. IV we introduce a perturbative approach to study the sixth-order case and show that it is not possible to have a forward sixth-order algorithm by including only the commutator $[V,[T,V]]$. In Sec. V we discuss the pattern of higher-order forward algorithms. In Sec. VI, we assess the feasibility of implementing sixth order algorithms. In Sec. VII, we summarize our conclusions and suggest directions for future research. The Appendix contains details of how to reduce a general quadratic error coefficient to a multidiagonal form.

II. A CONSTRUCTIVE PROOF OF THE SHENG-SUZUKI THEOREM

In Suzuki's proof [12], without explicitly computing e_{TTV} and e_{VTV}, he showed that both cannot be zero. Here, we show that by enforcing $e_{TV}=0$ and $e_{TTV}=0$, we can compute a lower bound for e_{VTV} analytically and show that it cannot vanish for a set of positive $\{t_i\}$. This determination of a lower bound for e_{VTV} goes beyond the Sheng-Suzuki theorem in providing a more detailed understanding of all fourth-order forward algroithms.

The first step of our approach is to compute the error coefficients e_{TV}, e_{TTV}, e_{VTV}, etc., in terms of the factorization coefficients $\{t_i, v_i\}$. This can be done as follows. The left-hand side of (1.4) can be expanded as

$$e^{\varepsilon t_1 T} e^{\varepsilon v_1 V} \cdots e^{\varepsilon t_N T} e^{\varepsilon v_N V} = 1 + \varepsilon\left(\sum_{i=1}^{N} t_i\right)T + \varepsilon\left(\sum_{i=1}^{N} v_i\right)V + \cdots . \tag{2.1}$$

Fixing $e_T = e_V = 1$, the right-hand side of (1.4) can likewise be expanded

$$\begin{aligned} e^{\varepsilon H_A(\varepsilon)} = {} & 1 + \varepsilon(T+V) + \tfrac{1}{2}\varepsilon^2(T+V)^2 + \varepsilon^2 e_{TV}[T,V] \\ & + \varepsilon^3 e_{VTV}[V,[T,V]] + \varepsilon^3 e_{TTV}[T,[T,V]] \\ & + \tfrac{1}{2}\varepsilon^3 e_{TV}\{(T+V)[T,V] + [T,V](T+V)\} \\ & + \tfrac{1}{3!}\varepsilon^3 (T+V)^3 + \cdots . \end{aligned} \tag{2.2}$$

Matching the first-order terms in ε gives the primary constraints

$$\sum_{i=1}^{N} t_i = 1 \text{ and } \sum_{i=1}^{N} v_i = 1. \tag{2.3}$$

To determine the other error coefficients, we focus on a particular operator in (2.2) whose coefficient contains e_{TV}, e_{TTV}, or e_{VTV} and match that operator's coefficients in the expansion of (2.1). For example, in the ε^2 terms of (2.2), the coefficient of the operator TV is $\left(\frac{1}{2}+e_{TV}\right)$. Equating this to the coefficients of TV from (2.1) gives

$$\frac{1}{2} + e_{TV} = \sum_{i=1}^{N} s_i v_i, \tag{2.4}$$

where we have introduced the variable

$$s_i = \sum_{j=1}^{i} t_j . \tag{2.5}$$

Alternatively, the same coefficient can also be expressed as

$$\frac{1}{2} + e_{VT} = \sum_{i=1}^{N} t_i u_i, \tag{2.6}$$

where

$$u_i = \sum_{j=i}^{N} v_j. \tag{2.7}$$

It turns out that s_i and u_i are our fundamental variables, the coefficients t_i and v_i are *backward* and *forward* finite differences of s_i and u_i,

$$t_i = s_i - s_{i-1} \equiv \nabla s_i, \quad v_i = u_i - u_{i+1} \equiv -\nabla u_i. \tag{2.8}$$

The results (2.4) and (2.6) are equivalent by virtue of the "partial summation" identity

$$\sum_{i=1}^{N} \nabla s_i u_i = -\sum_{i=1}^{N} s_i \Delta u_i. \tag{2.9}$$

(Note that $s_0=0$ and $u_{N+1}=0$.) In the following, we will use the backward finite difference operator extensively:

$$\nabla s_i^n = s_i^n - s_{i-1}^n, \tag{2.10}$$

with property

$$\sum_{i=1}^{N} \nabla s_i^n = s_N^n = 1.$$

Matching the coefficients of operators *TTV* and *TVV* gives

$$\frac{1}{3!} + \frac{1}{2}e_{TV} + e_{TTV} = \frac{1}{2}\sum_{i=1}^{N} s_i^2 v_i = \frac{1}{2}\sum_{i=1}^{N} \nabla s_i^2 u_i, \tag{2.11}$$

$$\frac{1}{3!} + \frac{1}{2}e_{TV} - e_{TVT} = \frac{1}{2}\sum_{i=1}^{N} \nabla s_i u_i^2. \tag{2.12}$$

The error coefficient e_{VTV} can be tracked directly by the operator *VTV*. The coefficient for the operator *VTV* is quadratic in v_i but not diagonal. This is more difficult to deal with than *TVV*'s coefficient. Nevertheless, we show in the Appendix that *VTV*'s coefficient can be diagonalized by a systematic procedure to yield the same constraint equation as (2.12).

In order to have a fourth-order algorithm, aside from the primary constraints (2.3), one must require $e_{TV}=0, e_{TTV}=0$, and $e_{VTV}=0$. For a symmetric product form such that $t_1=0$ and $v_i=v_{N-i+1}, t_{i+1}=t_{N-i+1}$, or $v_N=0$ and $v_i=v_{N-i}, t_i=t_{N-i+1}$, one has

$$e^{-\varepsilon H_A(-\varepsilon)} e^{\varepsilon H_A(\varepsilon)} = 1. \tag{2.13}$$

This implies that $H_A(\varepsilon)$ must be an even function of ε, and $e_{TV}=0$ is automatic. The vanishing of all odd order errors in $H_A(\varepsilon)$ implies that we must have

$$\frac{1}{(2n-1)!}\sum_{i=1}^{N} \nabla s_i^{2n-1} u_i = \frac{1}{(2n)!}, \tag{2.14}$$

ensuring that $T^{2n-1}V$ has the correct expansion coefficient. It is cumbersome to deal with symmetric coefficients directly; it is much easier to use the general form (1.3) and to invoke (2.14) when symmetric factorization is assumed.

The next step in our strategy is to compute a lower bound for the magnitude of e_{VTV}, after satisfying constraints $e_{TV}=0$ and $e_{TTV}=0$. We view the latter two constraints

$$\sum_{i=1}^{N} \nabla s_i u_i = \frac{1}{2}, \tag{2.15}$$

$$\sum_{i=1}^{N} \nabla s_i^2 u_i = \frac{1}{3}, \tag{2.16}$$

as constraints on $\{u_i\}$ for given a set of $\{t_i\}$ coefficients. For positive $\{t_i\}$, the right-hand side of (2.12) is a positive-definite quadratic form in u_i. Its lower bound can be determined by the method of constrained minimization using Lagrange multipliers. Minimizing

$$F = \frac{1}{2}\sum_{i=1}^{N} \nabla s_i u_i^2 - \lambda_1\left(\sum_{i=1}^{N} \nabla s_i u_i - \frac{1}{2}\right) - \lambda_2\left(\sum_{i=1}^{N} \nabla s_i^2 u_i - \frac{1}{3}\right) \tag{2.17}$$

gives

$$u_i = \lambda_1 \frac{\nabla s_i}{\nabla s_i} + \lambda_2 \frac{\nabla s_i^2}{\nabla s_i} = \lambda_1 + \lambda_2(s_i + s_{i-1}). \tag{2.18}$$

Imposing (2.15) and (2.16) determines λ_1 and λ_2,

$$\lambda_1 + \lambda_2 = \tfrac{1}{2}, \tag{2.19}$$

$$\lambda_1 + \lambda_2 + g\lambda_2 = \tfrac{1}{3}, \tag{2.20}$$

where g defined by

$$\sum_{i=1}^{N} \frac{\nabla s_i^2 \nabla s_i^2}{\nabla s_i} = 1 + g, \tag{2.21}$$

is given by

$$g = \sum_{i=1}^{N} s_i s_{i-1}(s_i - s_{i-1}). \tag{2.22}$$

By substituting in $s_i s_{i-1} = [s_i^2 + s_{i-1}^2 - (s_i - s_{i-1})^2]/2$, one discovers that

$$g = -\tfrac{1}{2}g + \tfrac{1}{2}(1 - \delta g),$$

and therefore

$$g = \frac{1}{3}(1 - \delta g), \text{ where } \delta g = \sum_{i=1}^{N} t_i^3. \tag{2.23}$$

The factor $\frac{1}{3}$ is the continuum limit $(N \to \infty)$ of g when the sum is replaced by the integral $\int_0^1 s^2 ds$. The evaluation of general sums of the form (2.22) will be further discussed below. This exact form for g obviated the need to determine g's upper bound as it is done originally in the work of Suzuki [12], and in the more recent work on symplectic correctors [7]. With λ_1 and λ_2 known, the minimum of F is given by

$$F = \frac{1}{2}(\lambda_1 + \lambda_2)^2 + \frac{1}{2}g\lambda_2^2 = \frac{1}{4} + \frac{1}{72g} = \frac{1}{6} + \frac{1}{24}\frac{\delta g}{(1 - \delta g)}, \tag{2.24}$$

and therefore

$$e_{VTV} \leqslant -\frac{1}{24}\frac{\delta g}{(1-\delta g)}. \tag{2.25}$$

This implies that, first, e_{VTV} must be negative. Second, its magnitude is

$$|e_{VTV}| \geqslant \frac{1}{24}\frac{\delta g}{(1-\delta g)}. \tag{2.26}$$

The Sheng-Suzuki theorem now follows as a simple corollary. If all the t_i's are positive, then e_{VTV} cannot vanish because its lower bound (2.26), which depends on δg as given by (2.23), cannot vanish. The only way to achieve a fourth-order forward algorithm is to keep the commutator $[V,[T,V]]$ with coefficient e_{VTV}, but move it to the left-hand side of (1.4). This means that for all such fourth-order algorithms, the sum of factorization coefficients of all the $[V,[T,V]]$ terms must be positive. All such fourth-order algorithms are characterized by their respective values of e_{VTV} and how well they saturate the lower bound (2.26). Note that in deriving this lower bound, we did not need to incorporate the primary constraints $u_1=1$.

A very different "elementary" proof of the Sheng-Suzuki result has been offered by Blanes and Casa [24]. Our work is more precise in demonstrating that, not only can e_{VTV} not vanish, it has a lower bound (2.26) determined only by $\{t_i\}$.

Note also that $v_i=u_i-u_{i+1}$ and (2.18) implies that

$$v_i = \lambda_2(s_{i-1}-s_{i+1}) = \frac{1}{2}\frac{(t_i+t_{i+1})}{(1-\delta g)}. \tag{2.27}$$

Thus, if one insists that e_{VTV} be zero, then δg can be zero only if at least one t_i is negative such that (t_i+t_{i+1}) or (t_i+t_{i-1}) remains negative. Equation (2.27) then implies that its adjacent values of v_i or v_{i-1} must also be negative. Thus a fourth-order factorization without keeping any additional operator, such as $[V,[T,V]]$, must have at least one pair of negative t_i, v_i coefficients. This result was first proved by Goldman and Kaper [25]. This simpler proof follows the idea of Blanes and Casa [24].

III. THE SIXTH-ORDER CASE

By incorporating the potential-like operator $[V,[T,V]]$, many families [10,22,23] of fourth-order forward algorithms have been found. They are not only indispensable for solving time-irreversible problems [17–20]; but they are also superior to existing fourth-order algorithms in solving time-reversible classical [4,15,22,23] and quantum [9,10] dynamical problems. It is therefore of great interest to determine whether there exist practical forward algorithms of even higher order. We show in this section that sixth-order forward algorithms requires the inclusion of the commutator $[V,[T,[T,[T,V]]]]$. The inclusion of $[V,[T,V]]$, which makes possible fourth-order forward algorithms, is insufficient to guarantee a sixth-order forward algorithm. In general, if $F_{2n}(\varepsilon)$ is a $2n$th order forward decomposition of $e^{\varepsilon(T+V)}$, then $F_{2n+2}(\varepsilon)$ would require the inclusion of a new operator not previously included in the construction of $F_{2n}(\varepsilon)$. We have proved the case of $n=1$ in Sec. II. The new operator is

$$V_1 \equiv [V,[T,V]]. \tag{3.1}$$

Consider now the case $n=2$. In the following discussion, we will use the condensed bracket notation: $[V^2T^3V] \equiv [V,[V,[T,[T,[T,V]]]]]$, etc. We have shown in Sec. II that, for positive t_i, with u_i satisfying constraints (2.15) and (2.16), we can factorize $e^{\varepsilon(T+V)}$ up to the form

$$\prod_{i=1}^{N} e^{t_i\varepsilon T}e^{v_i\varepsilon V} = \exp\left[\varepsilon\left(T+V+e_{VTV}\varepsilon^2[VTV]+\varepsilon^4\sum_{i=1}^{4} e_iQ_i + O(\varepsilon^6)\right)\right], \tag{3.2}$$

where e_{VTV} cannot be made to vanish, and Q_i are four independent operators described below. There is one error operator $[TV]$ in first order; two error operators, $[TTV]$ and $[VTV]$, in second order; four operators, $[TTTV],[VTTV],[TVTV]$, and $[VVTV]$, in third order; and eight operators, $[TTTTV],[VTTTV],[TVTTV],[VVTTV],[TTVTV],[VTVTV],[TVVTV]$, and $[VVVTV]$, in fourth order. These error operators are results of concatenating T and V with lower-order operators on the left. In each order, not all the operators are independent. For example, setting $C=[AB]$ in the Jacobi identity

$$[ABC]+[BCA]+[CAB]=0,$$

gives $[ABC]=[BAC]$ and therefore

$$[ABAB]=[BAAB].$$

For the case where $[VTV]$ commutes with V we also have $[V^nVTV]=0$. Hence there are only two independent operators $[TTTV],[TVTV]$ in third order and four operators $[TTTTV],[VTTTV],[TTVTV],[VTVTV]$ in fourth order. The last two are just $[TTV_1]$ and $[VTV_1]$, which resemble second-order errors for a new potential V_1. To have a sixth-order algorithm, one must eliminate these four error terms. Since $[TTV_1]$ and $[VTV_1]$ are linear in V_1, they can always be eliminated by including a sufficient number of V_1 operators in the factorization process. The remaining error terms $[T^4V]$ and $[VT^3V]$ are unaffected by V_1 and can *only be eliminated by the choice of coefficients* $\{t_i,v_i\}$. Thus we can apply our previous strategy of dealing *only* with coefficients $\{t_i,v_i\}$ but now computing the error coefficient e_{VT^3V} explicitly.

A careful reexamination of our proof for the Sheng-Suzuki theorem shows that we have proved more than that is required. The minimization procedure produces a lower bound for e_{VTV}, whereas the Sheng-Suzuki theorem only requires that e_{VTV} not be zero. The expansion (2.18) merely served as a vehicle for demonstrating that, for any $\{u_i\}$ satisfying (2.15) and (2.16), e_{VTV} cannot vanish for positive $\{t_i\}$. We do not really need to minimize anything or to determine an actual lower bound. This suggests a simple strategy for proving the sixth-order case. It is sufficient to show that e_{VT^3V} cannot vanish for any set of $\{u_i\}$, satisfying higher-order constraints.

IV. PROVING THE SIXTH-ORDER CASE

As discussed in Sec. III, for a sixth-order algorithm, a symmetric factorization must satisfy, in addition to (2.15) and (2.16), the constraint (2.14) for $n=2$,

$$\sum_{i=1}^{N} \nabla s_i^3 u_i = \frac{1}{4}. \tag{4.1}$$

Also, since the operator T^4V uniquely tracks the commutator $[T^4V]$, the error coefficient e_{T^4V} will vanish if the expansion coefficient of T^4V is $\frac{1}{5!}$. This means that factorization coefficients $\{t_i, v_i\}$ must also obey

$$\sum_{i=1}^{N} \nabla s_i^4 u_i = \frac{1}{5}. \tag{4.2}$$

These four constraints (2.15), (2.16), (4.1), and (4.2) can be satisfied by the expansion,

$$u_i = \lambda_1 + \lambda_2 \frac{\nabla s_i^2}{\nabla s_i} + \lambda_3 \frac{\nabla s_i^3}{\nabla s_i} + \lambda_4 \frac{\nabla s_i^4}{\nabla s_i}. \tag{4.3}$$

We must now demonstrate that in this case, e_{VT^3V} cannot vanish if $\{t_i\}$ are all positive. When u_i is expanded via (4.3), the four constraints (2.15), (2.16), (4.1), and (4.2) produce the following set of four linear equations for $m=1$ to 4,

$$\sum_{n=1}^{4} G_{mn}\lambda_n = \frac{1}{m+1}. \tag{4.4}$$

The matrix G_{mn} is given by

$$G_{mn} = \sum_{i=1}^{N} \frac{\nabla s_i^m \nabla s_i^n}{\nabla s_i} = 1 + \sum_{i=1}^{N} s_i s_{i-1} \frac{\nabla s_i^{m-1} \nabla s_i^{n-1}}{\nabla s_i} \equiv 1 + g_{mn}, \tag{4.5}$$

where we have used the identity

$$\frac{\nabla s_i^m \nabla s_i^n}{\nabla s_i} = \nabla s_i^{m+n-1} + s_i s_{i-1} \frac{\nabla s_i^{m-1} \nabla s_i^{n-1}}{\nabla s_i} \tag{4.6}$$

to define the reduced symmetric matrix g_{mn}. Since $G_{1n} = G_{n1} = 1$ (and, hence, $g_{1n} = g_{n1} = 0$), we can subtract the first constraint equation

$$\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = \tfrac{1}{2} \tag{4.7}$$

from the other three and reduce the system down to three equations for $m=2$ to 4,

$$\sum_{n=2}^{4} g_{mn}\lambda_n = \frac{1}{m+1} - \frac{1}{2}. \tag{4.8}$$

By writing $s_i = s_{i-1/2} + \frac{1}{2}\nabla s_i$ and $s_{i-1} = s_{i-1/2} - \frac{1}{2}\nabla s_i$ where $s_{i-1/2} = \frac{1}{2}(s_i + s_{i-1})$, we can systematically expand

$$\nabla s_i^n = \left(s_{i-1/2} + \frac{1}{2}\nabla s_i\right)^n - \left(s_{i-1/2} - \frac{1}{2}\nabla s_i\right)^n$$
$$= \frac{n!}{1!\,(n-1)!} s_{i-1/2}^{n-1}(\nabla s_i) + \frac{n!}{3!\,(n-3)!\,2^2} s_{i-1/2}^{n-3}(\nabla s_i)^3 + \cdots.$$

When each summant $\nabla s_i^m \nabla s_i^n / \nabla s_i$ is expanded and compared with the similarly expanded integral

$$\int_{s_{i-1}}^{s_i} mns^{m+n-2} ds = \frac{mn}{m+n-1} \nabla s_i^{m+n-1},$$

we deduce that

$$G_{mn} = \frac{mn}{m+n-1} - \frac{1}{12} mn(m-1)(n-1) \times \left\{ \sum_{i=1}^{N} s_{i-1/2}^{m+n-4} (\nabla s_i)^3 + A_5 \sum_{i=1}^{N} s_{i-1/2}^{m+n-6} (\nabla s_i)^5 + \cdots \right\}, \tag{4.9}$$

with

$$A_5 = \tfrac{1}{120}[(m+n-4)^2 + (m-2)(2m-7) + (n-2)(2n-7)].$$

The constant part of the matrix is the continuum limit ($N \to \infty$) of the sum, which is the integral

$$\int_0^1 mns^{m+n-2} ds = \frac{mn}{m+n-1}.$$

We will denote this constant part of the matrix as G_{mn}^0. The corresponding continuum part of g_{mn} is $g_{mn}^0 = G_{mn}^0 - 1$. The remaining finite parts of G_{mn} in (4.9), which depends explicitly on s_i, will be denoted as δG_{mn}. Since g_{mn} differs from G_{mn} only by a constant, its finite part δg_{mn} is the same as that of G_{mn}, i.e., $\delta g_{mn} = \delta G_{mn}$. By repeated applications of the identity (4.6), one can reduce g_{mn} to a sum of terms of the form

$$\kappa(l,n) = \sum_{i=1}^{N} (s_i s_{i-1})^l \nabla s_i^n. \tag{4.10}$$

Since the explicit form of g_{mn} is known via (4.9), these functions are not particularly useful as calculational tools. However, they are very useful in quickly identifying the matrix element of g_{mn} when doing analytical calculations. For later reference, we list some g_{mn}'s in terms of $\kappa(l,n)$ as follows:

$$g_{22} = \kappa(1,1),$$

$$g_{23} = \kappa(1,2),$$

$$g_{24} = \kappa(1,3),$$

$$g_{32} = \kappa(1,3) + \kappa(2,1),$$

$$g_{33} = \kappa(1,4) + \kappa(2,2),$$

$$g_{34} = \kappa(1,5) + \kappa(2,3) + \kappa(1,3). \qquad (4.11)$$

Note that g_{22} is the g function of the last section. From the general formula (4.9), one finds indeed that $g_{22}^0 = \frac{1}{3}$ and

$$\delta g_{22} = -\frac{1}{3}\sum_{i=1}^{N} (\nabla s_i)^3 = -\frac{1}{3}\delta g. \qquad (4.12)$$

If we only keep the continuum matrix g_{mn}^0 in (4.8)

$$\begin{pmatrix} \frac{1}{3} & \frac{1}{2} & \frac{3}{5} \\ \frac{1}{2} & \frac{4}{5} & 1 \\ \frac{3}{5} & 1 & \frac{9}{7} \end{pmatrix}\begin{pmatrix} \lambda_2 \\ \lambda_3 \\ \lambda_4 \end{pmatrix} = \begin{pmatrix} -\frac{1}{6} \\ -\frac{1}{4} \\ -\frac{3}{10} \end{pmatrix},$$

the solution is trivial: $\lambda_2 = -\frac{1}{2}, \lambda_3 = 0, \lambda_4 = 0$. This suggests that we should also expand each λ_i into its continuum and finite part: $\lambda_2 = -\frac{1}{2} + \delta\lambda_2, \lambda_3 = \delta\lambda_3, \lambda_4 = \delta\lambda_4$. For our purpose, it is enough to keep the leading finite-size correction term, i.e., we can neglect the terms of the form $\delta g_{mn}\delta\lambda_k$. In this case, we just have

$$\begin{pmatrix} \frac{1}{3} & \frac{1}{2} & \frac{3}{5} \\ \frac{1}{2} & \frac{4}{5} & 1 \\ \frac{3}{5} & 1 & \frac{9}{7} \end{pmatrix}\begin{pmatrix} \delta\lambda_2 \\ \delta\lambda_3 \\ \delta\lambda_4 \end{pmatrix} = \begin{pmatrix} \frac{1}{2}\delta g_{22} \\ \frac{1}{2}\delta g_{23} \\ \frac{1}{2}\delta g_{24} \end{pmatrix}. \qquad (4.13)$$

We do not need to solve each $\delta\lambda_k$ explicitly; we only need to know that they are proportional to δg_{2n}. Since $\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = \frac{1}{2}$, this also implies that $\lambda_1 = 1 + \delta\lambda_1$ with

$$\delta\lambda_1 + \delta\lambda_2 + \delta\lambda_3 + \delta\lambda_4 = 0. \qquad (4.14)$$

The above discussion suggests that one should also separate u_i into its continuum and finite parts,

$$u_i = \left(1 - \frac{1}{2}\frac{\nabla s_i^2}{\nabla s_i}\right) + \delta u_i. \qquad (4.15)$$

The constraints on u_i now translate into constraints on δu_i

$$\sum_{i=1}^{N} \nabla s_i^n \delta u_i = \frac{1}{n+1} - \sum_{i=1}^{N} \nabla s_i^n \left(1 - \frac{1}{2}\frac{\nabla s_i^2}{\nabla s_i}\right) = \frac{1}{n+1} - \left(1 - \frac{1}{2}G_{2n}\right) = \frac{1}{2}\delta g_{2n}. \qquad (4.16)$$

Recall that since $g_{1n} = g_{n1} = 0$, we also have $\delta g_{n1} = \delta g_{1n} = 0$. The above constraints for δu_i are exact. We have not yet invoked any particular representation for δu_i.

To illustrate how this formalism will be used, let us recompute the quadratic form of the last section

$$\sum_{i=1}^{N} \nabla s_i u_i^2 = \sum_{i=1}^{N} \nabla s_i \left[\left(1 - \frac{1}{2}\frac{\nabla s_i^2}{\nabla s_i}\right) + \delta u_i\right]^2 = \frac{1}{4}\sum_{i=1}^{N} \frac{\nabla s_i^2 \nabla s_i^2}{\nabla s_i} + 2\sum_{i=1}^{N} \nabla s_i \delta u_i - \sum_{i=1}^{N} \nabla s_i^2 \delta u_i + O(\delta u_i^2) \qquad (4.17)$$

$$= \frac{1}{4}G_{22} - \frac{1}{2}\delta g_{22} = \frac{1}{3} - \frac{1}{4}\delta g_{22} = \frac{1}{3} + \frac{1}{12}\delta g. \qquad (4.18)$$

This then implies that

$$e_{VTV} = -\frac{1}{24}\sum_{i=1}^{N} t_i^3. \qquad (4.19)$$

The first key observation is Eq. (4.17); to leading order in δg_{2n}, this quadratic form only depends on the first two constraints on δu_i. Its leading finite part is unchanged by additional, higher-order constraints on δu_i; that is, δu_i can be very general. By inspection, e_{VTV} above cannot vanish for positive $\{t_i\}$. Thus this leading-order calculation, while not sufficient to determine the exact lower bound for e_{VTV}, is sufficient to show that e_{VTV} cannot vanish, and thus proves the Sheng-Suzuki theorem.

Second, if δu_i were to be represented as

$$\delta u_i = \delta\lambda_2\left(\frac{\nabla s_i^2}{\nabla s_i} - 1\right) + \delta\lambda_3\left(\frac{\nabla s_i^3}{\nabla s_i} - 1\right) + \delta\lambda_4\left(\frac{\nabla s_i^4}{\nabla s_i} - 1\right), \qquad (4.20)$$

then in order for the constraints (4.16) to determine $\delta\lambda_k$ to the same leading order in δg_{2n} as in (4.13), it is enough to compute only the constant (continuum) part of any sums multiplying $\delta\lambda_k$. This implies that we may replace any such sum by its integral or by any other sum having the same integral. *Thus for any sum multiplying δu_i, we may replace it by another sum having the same integral*. This crucial simplification makes it unnecessary to solve for each λ_k explicitly.

To compute the error coefficient e_{VT^3V}, one must use an operator that tracks the commutator $[VT^3V]$ uniquely. The analogous operator T^3V^2, whose expansion coefficient is easy to compute, is no longer suitable. Let $C_{T^3V^2}$ denote its expansion coefficient in terms of $\{t_i, v_i\}$ from the left-hand side of (3.2). By matching the same operator's expansion coefficient from the right-hand side, one finds [26]

$$C_{T^3V^2} = \tfrac{1}{5!} - \tfrac{1}{3!}e_{VTV} - e_{T^2VTV} - e_{VT^3V}. \qquad (4.21)$$

It is difficult to disentangle e_{VT^3V} from the contaminating effects of e_{VTV} and e_{T^2VTV}. The three operators that track $[VT^3V]$ uniquely are VT^3V, VT^2VT, and TVT^2V. We choose the symmetric choice VT^3V, whose coefficient is related to e_{VT^3V} by

$$C_{VT^3V} = \tfrac{1}{5!} + 2e_{VT^3V}. \qquad (4.22)$$

From the left-hand side of (3.2), one deduces

$$C_{VT^3V} = \frac{1}{3!}\sum_{i=1}^{N-1} v_i \sum_{j=i+1}^{N} (s_j - s_i)^3 v_j. \qquad (4.23)$$

This quadratic form in $\{v_i\}$ is difficult to work with because it is not diagonal in u_i or some other variable. In the Appendix, we show that it can be simplified to the following bidiagonal form,

$$C_{VT^3V}=\frac{1}{3!}\left(3\sum_{i=1}^{N}\nabla s_i z_i^2-\sum_{i=1}^{N}\nabla s_i^3 u_i^2-\frac{1}{4}\right), \qquad (4.24)$$

where z_i is defined by

$$z_i=\sum_{j=i}^{N} v_j s_j. \qquad (4.25)$$

The required coefficient e_{VT^3V} can now be computed from

$$e_{VT^3V}=\frac{1}{12}\left(3\sum_{i=1}^{N}\nabla s_i z_i^2-\sum_{i=1}^{N}\nabla s_i^3 u_i^2-\frac{3}{10}\right). \qquad (4.26)$$

The quadratic form involving u_i^2 is

$$\sum_{i=1}^{N}\nabla s_i^3 u_i^2=\sum_{i=1}^{N}\nabla s_i^3\left(1-\frac{1}{2}\frac{\nabla s_i^2}{\nabla s_i}\right)^2+2\sum_{i=1}^{N}\nabla s_i^3\delta u_i-\frac{3}{2}\sum_{i=1}^{N}\nabla s_i^4\delta u_i + O(\delta u_i^2) \qquad (4.27)$$

$$=\frac{3}{4}-G_{32}+\frac{1}{4}(G_{33}+G_{24})+\delta g_{23}-\frac{3}{4}\delta g_{24}$$

$$=\frac{1}{10}+\frac{1}{4}\delta g_{33}-\frac{1}{2}\delta g_{24}. \qquad (4.28)$$

In (4.27), we have replaced the sum involving $\nabla s_i^3\nabla s_i^2/\nabla s_i$ by its integral equivalent $\frac{3}{2}\nabla s_i^4$. Also, we have used the identity

$$\frac{\nabla s_i^3}{\nabla s_i}\left(\frac{\nabla s_i^2\nabla s_i^2}{\nabla s_i}\right)=\frac{\nabla s_i^3\nabla s_i^3}{\nabla s_i}+\frac{\nabla s_i^4\nabla s_i^2}{\nabla s_i}-\nabla s_i^5.$$

Given the expansion (4.3) for u_i, we can deduce the corresponding expansion for z_i. From (4.25), we can rewrite z_i as

$$z_i=u_i s_i+\sum_{j=i+1}^{N} u_j\nabla s_j. \qquad (4.29)$$

For $u_i=\lambda_n\nabla s_i^n/\nabla s_i$, we have

$$z_i=\lambda_n\left[\frac{\nabla s_i^n}{\nabla s_i}s_i+\left(1-s_i^n\right)\right],$$

$$=\lambda_n\left[\left(s_i^{n-1}+s_{i-1}\frac{\nabla s_i^{n-1}}{\nabla s_i}\right)s_i+\left(1-s_i^n\right)\right],$$

$$=\lambda_n\left[1+s_i s_{i-1}\frac{\nabla s_i^{n-1}}{\nabla s_i}\right]. \qquad (4.30)$$

Hence corresponding to (4.3), z_i has the expansion

$$z_i=\lambda_1+\lambda_2(1+s_i s_{i-1})+\lambda_3\left(1+s_i s_{i-1}\frac{\nabla s_i^2}{\nabla s_i}\right) + \lambda_4\left(1+s_i s_{i-1}\frac{\nabla s_i^3}{\nabla s_i}\right). \qquad (4.31)$$

One can check that this form for z_i satisfies the four constraints (2.15), (2.16), (4.1), and (4.2) when they are expressed in terms of z_i

$$z_1=\lambda_1+\lambda_2+\lambda_3+\lambda_4=\tfrac{1}{2},$$

and for $m=1$ to 3,

$$\sum_{i=1}^{N}\nabla s_i^m z_i=\frac{1}{m+2}. \qquad (4.32)$$

The identity (4.6) is needed to show that (4.32) is equivalent to the last three constraint equations for u_i. As in the case of u_i, we can write z_i in the form

$$z_i=\tfrac{1}{2}(1-s_i s_{i-1})+\delta z_i \qquad (4.33)$$

and transfer the last three constraints on z_i to δz_i,

$$\sum_{i=1}^{N}\nabla s_i^{n-1}\delta z_i=\frac{1}{2}\delta g_{2n}. \qquad (4.34)$$

The quadratic form for z_i is then

$$\sum_{i=1}^{N}\nabla s_i z_i^2=\frac{1}{4}\sum_{i=1}^{N}\nabla s_i(1-s_i s_{i-1})^2+\sum_{i=1}^{N}\nabla s_i\delta z_i - \sum_{i=1}^{N}\nabla s_i(s_i s_{i-1})\delta z_i+O(\delta z_i^2)$$

$$=\frac{1}{4}-\frac{1}{2}\kappa(1,1)+\frac{1}{4}\kappa(2,1)+\frac{1}{2}\delta g_{22}-\frac{1}{3}\sum_{i=1}^{N}\nabla s_i^3\delta z_i$$

$$=\frac{1}{4}-\frac{1}{2}g_{22}+\frac{1}{4}(g_{33}-g_{24})+\frac{1}{2}\delta g_{22}-\frac{1}{6}\delta g_{24}$$

$$=\frac{2}{15}+\frac{1}{4}\delta g_{33}-\frac{5}{12}\delta g_{24}. \qquad (4.35)$$

We have again replaced the sum involving $\nabla s_i(s_i s_{i-1})$ by its integral equivalent $\frac{1}{3}\nabla s_i^3$ and used (4.11) to express the required sum in terms of g_{mn}'s. Thus the bidiagonal form is

$$3\sum_{i=1}^{N}\nabla s_i z_i^2-\sum_{i=1}^{N}\nabla s_i^3 u_i^2=\frac{3}{10}+\frac{1}{4}(2\,\delta g_{33}-3\,\delta g_{24}).$$

From (4.9) we find

$$\delta g_{33}=-3\sum_{i=1}^{N}s_{i-1/2}^2(\nabla s_i)^3-\frac{1}{20}\sum_{i=1}^{N}(\nabla s_i)^5,$$

$$\delta g_{24}=-2\sum_{i=1}^{N}s_{i-1/2}^2(\nabla s_i)^3-\frac{1}{10}\sum_{i=1}^{N}(\nabla s_i)^5, \qquad (4.36)$$

and therefore, finally,

$$e_{VT^3V}=\frac{1}{240}\sum_{i=1}^{N}(\nabla s_i)^5=\frac{1}{240}\sum_{i=1}^{N}t_i^5. \qquad (4.37)$$

This is remarkably similar to (4.19). Thus if $\{t_i\}$ are all positive, then e_{VT^3V} cannot vanish. No sixth-order positive factorization scheme is possible without including the commutator $V_3=[VT^3V]$.

V. BEYOND SIXTH ORDER

In Sec. II, we have shown that in order to have a fourth-order forward algorithm, one must include the commutator $V_1=[VTV]$ in the factorization process. In Sec. IV, we have proved that in order to have a sixth-order forward algorithm one must include, in addition to V_1, the commutator $V_3=[VT^3V]$. By repeating the same argument, it is not difficult to discern the pattern of higher-order forward algorithms. In going from the $(2n)$th to the $(2n+2)$th order, one must add a new commutator

$$V_{2n-1}=[VT^{2n-1}V]$$

to the factorization process. A proof of this general result is a straightforward generalization of our approach in Sec. IV, but technically much more involved. For example, to prove the eighth-order case, we must track e_{VT^5V} uniquely via the operator VT^5V's coefficient given by $S_5/5!$, where S_5, as shown in the Appendix, is tridiagonal in u_i, z_i, and

$$y_i=\sum_{j=i}^{N} v_j s_j^2 .$$

One then has to work out the expansion for y_i as in the case of z_i. Moreover, since e_{VT^5V} is anticipated to be $\propto\Sigma_{i=1}^{N}(\nabla s_i)^7$, one can no longer ignore the contribution of order $(\delta u_i)^2 \propto[\Sigma_{i=1}^{N}(\nabla s_i)^3]^2$. Thus the current formalism, while powerful in determining e_{VTV} variationally and e_{VT^3V} perturbatively, is too demanding for the general case. To prove such a general result, one must find a less explicit approach.

VI. SIXTH-ORDER ALGORITHMS

Now that the pattern of higher-order forward factorizations is known, we will consider the practical issue of whether a sixth-order algorithm is implementable. Just as we have denoted the factorization coefficients associated with T and V as t_i and v_i, we will denote in this section, the coefficients associated with commutator V_1 and V_3 by u_i and w_i. For a symmetric sixth-order algorithm, we must satisfy the two primary constraints (2.3), the vanishing of the error coefficients of two second-order commutators V_1 and $[TTV]$, and four fourth-order commutators $[TTTTV],[VTTTV]$, $[TTV_1]$, and $[VTV_1]$. Because the error coefficients for $V_1,[TTV_1]$, and $[VTV_1]$ are linear in u_i, they can always be forced to zero by three u_i's. Likewise, since $[TTTTV]$ is linear in v_i, its coefficient can be made zero and the primary constraint be satisfied with two v_i's. The primary constraint on t_i and the quadratic constraint on t_i due to $[TTV]$ can also be satisfied with two t_i's. Thus a minimal sixth-order forward algorithm is

$$\mathcal{T}_A^{(6)}(\epsilon)\equiv e^{\varepsilon^5 w_1 V_3} e^{\varepsilon u_2 V_1} e^{\varepsilon t_2 T} e^{\varepsilon(v_1 V+\varepsilon^2 u_1 V_1)} e^{\varepsilon t_1 T} \times e^{\varepsilon(v_0 V+\varepsilon^2 u_0 V_1)} e^{\varepsilon t_1 T} e^{\varepsilon(v_1 V+\varepsilon^2 u_1 V_1)} e^{\varepsilon t_2 T} e^{\varepsilon u_2 V_1} e^{\varepsilon^5 w_1 V_3} \tag{6.1}$$

with

$$v_0=\tfrac{4}{9},\quad v_1=\tfrac{5}{18},\quad t_1=\tfrac{1}{2}\sqrt{\tfrac{3}{5}},\quad t_2=\tfrac{1}{2}-\tfrac{1}{2}\sqrt{\tfrac{3}{5}}, \tag{6.2}$$

$$u_0=\tfrac{7}{60}-\tfrac{5}{54}\sqrt{\tfrac{5}{3}},\quad u_1=-\tfrac{1}{48}+\tfrac{5}{216}\sqrt{\tfrac{5}{3}},\quad u_2=\tfrac{1}{240}-\tfrac{1}{144}\sqrt{\tfrac{5}{3}}, \tag{6.3}$$

and

$$w_1=-\tfrac{7\sqrt{15}-27}{12960}. \tag{6.4}$$

The coefficient of $[TTV]$ can be eliminated more simply by an additional v_2. In this case, we can minimize the coefficient w_1 near $t_2=1/5$, yielding

$$\mathcal{T}_B^{(6)}(\epsilon)\equiv \cdots e^{\varepsilon(v_0 V+\varepsilon^2 u_0 V_1)} e^{\varepsilon t_1 T} e^{\varepsilon(v_1 V+\varepsilon^2 u_1 V_1)} \times e^{\varepsilon t_2 T} e^{\varepsilon(v_2 V+\varepsilon^2 u_2 V_1)} e^{\varepsilon^5 w_1 V_3}, \tag{6.5}$$

$$v_0=\tfrac{8}{27},\quad v_1=\tfrac{125}{432},\quad v_2=\tfrac{1}{16},\quad t_1=\tfrac{3}{10},\quad t_2=\tfrac{1}{5}, \tag{6.6}$$

$$u_0=\tfrac{3121}{1710720},\quad u_1=\tfrac{1145}{2737152},\quad u_2=\tfrac{409}{1520640},\quad w_1=-\tfrac{1}{414720}. \tag{6.7}$$

Since the factorization is symmetric, we only listed operators from the center to the right.

Fourth-order forward algorithms are practical because it is relatively easy to compute V_1. For the standard classical Hamiltonian

$$H=\tfrac{1}{2}p_i p_i+U(q_i),$$

the operators T and V are just

$$T=p_i\frac{\partial}{\partial q_i}\ \text{and}\ V=F_i\frac{\partial}{\partial p_i},$$

where $F_i=-U_i=-\partial U/\partial q_i$. The commutator V_1 is simply

$$V_1=[VTV]=2U_iU_{ij}\frac{\partial}{\partial p_j}=\nabla_j(F_iF_i)\frac{\partial}{\partial p_j}.$$

Since this is just like the operator V with a modified force, it can simply be combined with V. By contrast, V_3 is of the form

$$V_3=[VT^3V]=3p_ip_j(U_lU_{lijk}+U_{lij}U_{lk})\frac{\partial}{\partial p_k}-6p_iU_jU_{ijk}\frac{\partial}{\partial q_k} \tag{6.8}$$

and is more complicated than the original operator problem $T+V$ we seek to solve. Thus in most cases, it seems difficult to implement a general sixth-order forward algorithm. This would make fourth-order forward algorithms unique. There are no easy higher generalizations. However, before we dismiss sixth-order algorithms out of hand, we note that for the harmonic oscillator, $V_3=0$ and sixth-order forward algorithms certainly exist. [For the harmonic oscillator, there are many sixth-order forward algorithms much simpler than (6.1).] Second, there may be ways of constructing the commutator V_3 indirectly rather than by direct evaluation. For example, the commutator

$$[T,V] = -p_i U_{ij}\frac{\partial}{\partial p_j} + U_j\frac{\partial}{\partial q_j}$$

has the same sort of complexicity as V_3, but $e^{\varepsilon^4[T,V]}$ can be approximated by products of $e^{v_i\varepsilon^2 V}e^{t_i\varepsilon^2 T}$ (See Ref. [7]). Some coefficients t_i in this approximation must be negative, however, because they are of order ε^2 and can be combined judiciously with existing operator T of order ε such that the overall coefficient of the T operator is positive for sufficiently small ε. There may exist similar ways of approximating $e^{\varepsilon^5 w_1 V_3}$. Thus until a simpler way of evaluating V_3 is found, fourth-order algorithms are the only higher-order practical forward algorithms.

VII. CONCLUSIONS

In this work, we have presented a framework for analyzing and understanding the structure of factorized algorithms. There are three key ideas: (i) the order constraints and error coefficients can be tracked by operators and expressed directly in terms of factorization coefficients. (ii) By introducing a suitable representation for the factorization coefficients, the order constraints and error terms can be solved analytically. (iii) For many purposes, it is sufficient to determine the error coefficients perturbatively. This last point is especially important. All previous works on factorization algorithms are based on exact decompositions. Since this is difficult to do analytically, one can make little progress except numerically. This work shows that a leading-order calculation is sufficient to establish most of the important results we know about these algorithms. In particular, we have provided a constructive proof of the Shang-Suzuki theorem. Most importantly, we have shown that in order to have a sixth-order forward time-step algorithm, one must include the commutator $[VT^3V]$ in the factorization process.

This work suggests that there is regularity to the existence of forward algorithms. In order to have only positive time steps, one must continue to enlarge one's collection of constituent operators for factorizing $e^{\varepsilon(T+V)}$. For a $(2n)$th-order forward algorithm one must include all commutators of the form $[VT^{2k-1}V]$ from $k=1$ to $k=n-1$, in addition to T and V. The proof of this general result is currently beyond the scope of our perturbative approach. Moreover, the massive cancellations that produced the sixth-order result (4.37) strongly suggest that a better formulation, with these cancellations built in, must be possible. This work suggests that a more powerful way of understanding the structure of these algorithms is still waiting to be found.

The need to include $[VT^3V]$ makes it difficult to construct, but may not necessarily preclude the possibility of a sixth-order forward algorithm. One must seek clever ways of obtaining $[VT^3V]$ without computing it directly. Very recently, Sakkos, Casulleras, and Boronat [27] have reported sixth-order convergence in calculating the partition function of quantum-liquid helium by use of a family of fourth-order algorithms as described in Ref. [10]. Thus it may be difficult to derive a general sixth-order algorithm, sixth-order convergence is achievable for individual problems by fine tuning fourth-order forward algorithms.

ACKNOWLEDGMENTS

I thank Harald Forbert for pointing out the inadequacy of an earlier version of this work and for many stimulating discussions. This work was supported in part by National Science Foundation Grant No. DMS-0310580.

APPENDIX: COEFFICIENT OF VTV, VT^3V, AND VT^5V

There is a systematic way of diagonalizing the sum

$$S_m = \sum_{i=1}^{N-1}\sum_{j=i+1}^{N} v_i(s_j - s_i)^m v_j$$

needed in computing the error coefficients e_{VT^mV}. The above is a sum over the upper triangle of a $N\times N$ square matrix and can be denoted more simply as $\Sigma_{j>i}$.

The general form we need to diagonalize is

$$S(f,g) = \sum_{j>i} f_i(g_j - g_i)f_j = \sum_{i>j} f_j g_j f_i - \sum_{j>i} f_i g_i f_j, \tag{A1}$$

where we have interchanged the summation indices in the first term on the right-handside. The key point here is that if we introduce a new variable

$$h_i = \sum_{j=i}^{N} f_j,$$

such that $f_i = h_i - h_{i+1}$, then the second term on the right-hand side of (A1) is only a single sum. The first term can be eliminated by completing the "square matrix." Let $\Sigma_i f_i g_i = P$ and $\Sigma_j f_j = F$ be known sums, then

$$PF = \sum_i f_i g_i \sum_j f_j = \sum_i f_i^2 g_i + \sum_{i>j} f_i g_i f_j + \sum_{j>i} f_i g_i f_j. \tag{A2}$$

Subtracting (A1) from (A2) gives

$$\begin{aligned} PF - S(f,q) &= \sum_i f_i^2 g_i + 2\sum_{j>i} f_i g_i f_j \\ &= \sum_{i=1}^{N} g_i(h_i - h_{i+1})^2 + 2\sum_{i=1}^{N} g_i(h_i - h_{i+1})h_{i+1} \\ &= \sum_{i=1}^{N} g_i(h_i^2 - h_{i+1}^2) = \sum_{i=1}^{N} \nabla g_i h_i^2, \end{aligned} \tag{A3}$$

and hence

$$S(f,g) = PF - \sum_{i=1}^{N} \nabla g_i h_i^2. \tag{A4}$$

For the case of $m=1$, we have $f_i = v_i, g_i = s_i, h_i = u_i, F=1$ from (2.3), and $P = \left(\frac{1}{2} + e_{TV}\right)$ from (2.4). Therefore, we have

$$S_1 = \left(\frac{1}{2} + e_{TV}\right) - \sum_{i=1}^{N} \nabla s_i u_i^2.$$

Since the coefficient of VTV is just $S_1 = \frac{1}{3!} + e_{VTV}$, the above is identical to (2.12). The use of the more complicated operator VTV determines the same e_{VTV}, as it must.

For $m=3$, we have

$$S_3=\sum_{j>1} v_i(s_j^3-s_i^3)v_j-3\sum_{j>1} v_is_i(s_j-s_i)s_jv_j.$$

Assuming now that all linear constraints on v_i are satisfied up to the relevant order, we have for the first and second term on the right, respectively, $f_i=v_i, g_i=s_i^3, h_i=u_i, F=1, P=\frac{1}{4}$, and $f_i=s_iv_i, g_i=s_i, h_i=z_i, F=\frac{1}{2}$, and $P=\frac{1}{3}$. Hence we have

$$S_3=\frac{1}{4}-\sum_{i=1}^{N}\nabla s_i^3u_i^2-3\left(\frac{1}{6}-\sum_{i=1}^{N}\nabla s_iz_i^2\right),$$

where

$$z_i=\sum_{j=i}^{N} v_js_j.$$

The coefficient of VT^3V is $S_3/3!$. Since $[VT^3V]$ contains the operator VT^3V twice, we have

$$\tfrac{1}{6}S_3=\tfrac{1}{5!}+2e_{VT^3V},$$

and therefore

$$12e_{VT^3V}=S_3-\frac{1}{20}=3\sum_{i=1}^{N}\nabla s_iz_i^2-\sum_{i=1}^{N}\nabla s_i^3u_i^2-\frac{3}{10}. \quad \text{(A5)}$$

For the case $m=5$, we have

$$S_5=\sum_{j>i} v_i(s_j^5-s_i^5)v_j-5\sum_{j>i} v_is_i(s_j^3-s_i^3)s_jv_j + 10\sum_{j>i} v_is_i^2(s_j-s_i)s_j^2v_j. \quad \text{(A6)}$$

For the first term we have $f_i=v_i, g_i=s_i^5, h_i=u_i, F=1$, and $P=\frac{1}{6}$. For the second term we have $f_i=s_iv_i, g_i=s_i^3, h_i=z_i, F=\frac{1}{2}$, and $P=\frac{1}{5}$. For the third term, we have $f_i=s_i^2v_i, g_i=s_i, h_i=y_i, F=\frac{1}{3}$, and $P=\frac{1}{4}$. We, therefore, have

$$S_5=\frac{1}{6}-\sum_{i=1}^{N}\nabla s_i^5u_i^2-5\left(\frac{1}{10}-\sum_{i=1}^{N}\nabla s_i^3z_i^2\right)+10\left(\frac{1}{12}-\sum_{i=1}^{N}\nabla s_iy_i^2\right)$$
$$=\frac{1}{2}-\sum_{i=1}^{N}\nabla s_i^5u_i^2+5\sum_{i=1}^{N}\nabla s_i^3z_i^2-10\sum_{i=1}^{N}\nabla s_iy_i^2,$$

where

$$y_i=\sum_{j=i}^{N} v_js_j^2.$$

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