Dissipative high phase-lag order Numerov-type methods for the numerical solution of the Schrödinger equation

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A generator of families of explicit hybrid methods with minimal phase lag is developed in this paper. The methods of the generator have algebraic order six. The main characteristic of the new methods is that they are dissipative, i.e., they are not symmetric and they have not an interval of periodicity. The generator is of dissipation order eight. Numerical results indicate that these new methods are more efficient than older ones, i.e., the property of the phase lag is more crucial than the nonempty interval of periodicity for the construction of the numerical methods for the numerical solution of the Schrödinger-type equations.

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I. INTRODUCTION

The radial Schrödinger equation has the form

$$y''(x)+f(x)y(x)=0, \tag{1.1}$$

where x is the radius, $0\leqslant x<\infty$, and $f(x)=E-l(l+1)/x^2-V(x)$. We call the term $l(l+1)/x^2$ the centrifugal potential, and the function $V(x)$ the potential, where $V(x)\to 0$ as $x\to\infty$. Based on the sign of the energy E there are two main categories of problems for (1.1) (for details see [1]). In (1.1), E is a real number denoting *the energy*, l is a given integer, and V is a given function that denotes *the potential*. The function $W(x)=l(l+1)/x^2+V(x)$ denotes *the effective potential*, which satisfies $W(x)\to 0$ as $x\to\infty$. The boundary conditions are

$$y(0)=0 \tag{1.2}$$

and a second boundary condition, for large values of x, is determined by physical considerations. In some scientific areas such as nuclear physics, physical chemistry, theoretical physics and chemistry, quantum chemistry, and molecular physics (see [2] and [3]), there is a real need for the numerical solution of the radial Schrödinger equation.

In the last two decades there has been much activity in the area of the solution of the radial Schrödinger equation (1.1) (see [4] and [5] and references therein, [1,6–8,9–11,12,13]). The most important characteristics of an efficient method for the solution of the problem (1.1) are the accuracy and the computational efficiency. The development of methods with the above mentioned characteristics is an open problem.

We mention here that the generators that have been developed in [4] and [5] by Avdelas and Simos (which are the only generators of numerical methods in the literature of the numerical solution of the Schrödinger equation) are generators of implicit and explicit *symmetric* methods, i.e., methods with nonempty interval of periodicity.

The purpose of this paper is to develop a generator of families of explicit sixth algebraic order hybrid methods with minimal phase lag. The methods are dissipative since they are not symmetric. The dissipation order of the methods is equal to eight. In Sec. II we develop the basic theory of the phase-lag analysis of two-step nonsymmetric finite difference methods. In Sec. III we develop the new generator of methods. An embedded variable-step algorithm is developed in Sec. IV and in Sec. V numerical results are presented.

II. PHASE-LAG ANALYSIS FOR NONSYMMETRIC TWO-STEP METHODS

We investigate the numerical integration of the problem

$$y''=f(x,y),y(x_0)=y_0,y'(x_0)=y_0'. \tag{2.1}$$

To examine the numerical properties of methods for solving the initial-value problem (2.1) Lambert and Watson [14] introduce the scalar test equation

$$y''=-w^2y. \tag{2.2}$$

When we apply a nonsymmetric two-step method to the scalar test equation (2.2) we obtain a difference equation of the form

$$y_{n+1}+Q(H)y_n+C(H)y_{n-1}=0, \tag{2.3}$$

where $H=wh$, h is the step length, $Q(H)$ and $C(H)$ are polynomials in H, and y_n is the computed approximation to $y(nh),n=0,1,2,\ldots$. The characteristic equation associated with (2.3) is

$$z^2+Q(H)z+C(H)=0. \tag{2.4}$$

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Theorem 1. A method that has the characteristic equation (2.4) has an interval of periodicity $(0,H_0^2)$, if for all $H^2 \in (0,H_0^2)$, $|Q(H)|<1$ and $C(H)\equiv 1$.

Definition 1. The method (2.3) is *P* stable if its interval of periodicity is $(0,\infty)$ [14].

Theorem 2. For a nonsymmetric two-step method we can write

$$\cos(H) = -\frac{Q(H)}{1+C(H)}. \tag{2.5}$$

Proof. The difference equation (2.3) must be satisfied for the analytical solution of (2.2) (which is equal to e^{iwx}). So we have

$$y_{n+1}+Q(H)y_n+C(H)y_{n-1}=0 \Rightarrow$$
$$e^{iw(x+h)}+Q(H)e^{iwx}+C(H)e^{iwx(x-h)}=0 \Rightarrow$$
$$e^{iwh}+Q(H)+C(H)e^{-iwh}=0 \Rightarrow$$
$$\cos(H) = -\frac{Q(H)}{1+C(H)}, \quad H=wh \square.$$

Based on the above theorem we have the following definition.

Definition 2. For any method corresponding to the characteristic equation (2.4) the quantity

$$t = H - \cos^{-1}\left[\frac{Q(H)}{1+C(H)}\right] \tag{2.6}$$

is called the dispersion or the phase error or the phase lag of the method. If $t=O(H^{q+1})$ as $H\to 0$ the order of phase lag is q. The quantity

$$u = 1 - C(H) \tag{2.7}$$

is called dissipation. If $u=O(H^p)$, the order of dissipation is p. From Definition 2 and based on an analogous remark of Coleman [15], we have the following remark.

Remark 1. If the order of dispersion is $2r$, then

$$t = cH^{2r+1}+O(H^{2r+3}) \Rightarrow \cos(H) - \frac{Q(H)}{1+C(H)}$$
$$= \cos(H)-\cos(H-t) = cH^{2r+2}+O(H^{2r+4}), \tag{2.8}$$

where t is the phase lag of the method.

III. THE GENERATOR OF SIXTH ALGEBRAIC ORDER METHODS

Consider the following family of explicit sixth algebraic order methods

$$\overline{y}_{n+1} = 2y_n - y_{n-1} + h^2 f_n, \tag{3.1}$$

$$\bar{\bar{y}}_{n+1} = 2y_n - y_{n-1} + \frac{h^2}{12}(\overline{f}_{n+1}+10f_n+f_{n-1}), \tag{3.2}$$

$$\overline{y}_{n,k} = y_n - a_{b-k+1}(\bar{\bar{f}}_{n+1}-2\overline{f}_{n,k-1}+f_{n-1}), \quad k=1(1)b, \tag{3.3}$$

$$\hat{y}_{n-1/2} = \frac{1}{2}(y_n+y_{n-1}) + \frac{h^2}{384}(5\overline{f}_{n+1}-34\overline{f}_{n,b}-19f_{n-1}), \tag{3.4}$$

$$\hat{y}_{n+1/2} = \frac{1}{2}(3y_n-y_{n-1}) + \frac{h^2}{128}[-\overline{f}_{n+1}+42\overline{f}_{n,b}+7f_{n-1}], \tag{3.5}$$

$$\hat{\bar{y}}_{n-1/2} = \frac{1}{2}(y_n+y_{n-1}) + \frac{h^2}{192}[(-5-48q)\overline{f}_{n+1} + (-32-288q)f_n + (-7-48q)f_{n-1} + (20+192q)\hat{f}_{n+1/2} + 192q\hat{f}_{n-1/2}], \tag{3.6}$$

$$\hat{\bar{y}}_{n+1/2} = \frac{1}{2}(3y_n-y_{n-1}) + \frac{h^2}{192}[\overline{f}_{n+1}+48f_n + 3f_{n-1}+20\hat{\bar{f}}_{n-1/2}], \tag{3.7}$$

$$y_{n+1}-2y_n+y_{n-1} = \frac{h^2}{60}[(\bar{\bar{f}}_{n+1}+f_{n-1})+26f_n+f_{n-1} + 16(\hat{\bar{f}}_{n+1/2}+\hat{\bar{f}}_{n-1/2})]. \tag{3.8}$$

b is the number of the family and $\overline{y}_{n,0}=y_n$. We note that $a_{b-k+1}|k=1(1)b$ are free parameters of the group of families to be chosen in order for the phase lag of the group of methods to be minimal. One can easily see that in each family, say b, the total number of stages N is given by

$$N = b+7. \tag{3.9}$$

Using the Taylor series expansions of $y_{n\pm1}, y_{n\pm1/2}, f_{n\pm1}, f_{n\pm1/2}$ about x_n in (3.1)–(3.8) we have the following result for the local truncation error $\mathcal{E}_{\mathrm{LT}}$ of the group of families (3.1)–(3.8):

$$\mathcal{E}_{\mathrm{LT}} = h^8\left[-\frac{1}{120960}y_n^{(8)} - \frac{1}{3840}(1+16q)y_n^{(6)}F_n - \frac{1}{2880}(1+16q-192qa_{b-k+1})y_n^{(4)}F_nF_n'\right], \tag{3.10}$$

where $F_n=\partial f/\partial x$, $F_n'=dF/dx$. We apply this group of families to the scalar test equation (2.2). Setting $H=wh$, we get a difference equation of the form (2.3).

Theorem 3. For the method given by (3.1)–(3.8) the polynomials $Q(H)$ and $C(H)$ in (2.3) are given by

$$Q(H) = -2+H^2-\frac{H^4}{12}+\frac{H^6}{360}+\left(\frac{1}{27648}-\frac{q}{720}\right)H^8 + \left[-\frac{5}{221184}+\frac{q}{6912}-\left(\frac{7}{768}+\frac{23q}{360}\right)\Delta_b\right]H^{10} + \left(\frac{35}{36864}+\frac{23q}{3456}\right)\Delta_b H^{12}, \tag{3.11}$$

$$C(H)=1-\frac{5}{27648}H^8, \tag{3.12}$$

where

$$\Delta_b=\left(1-\frac{H^2}{12}\right)\sum_{i=1}^{b}(-2H^2)^{i-1}\prod_{j=1}^{i}a_j \tag{3.13}$$

with a_k, $|k=1(1)b$, and $b=1,2,...$ real numbers. For the proof see Appendix A.

Based on definition 2 and (3.12), it is obvious that the dissipative order of the group of methods is equal to

$$u=1-C(H)=\frac{5}{27648}H^8, \tag{3.14}$$

i.e., the group of methods is of dissipative order eight. With the help of theorem 2 and remark 1 of Sec. II we have the following theorem.

Theorem 4. In order to maximize the attainable order of the phase lag of the group of methods defined by (3.1)–(3.8) the free parameters q and a_k, $k=1(1)b$, $b=1,2,...$ must have the following optimum values:

$$q=-\frac{23}{336}, \tag{3.15}$$

$$a_i=-\frac{s_{i-1}}{2s_{i-2}},\quad i=1(1)b, \tag{3.16}$$

where $s_{-1}=-1/2$, and s_i, $|i=0,1,...$ are the coefficients of the Taylor series expansion of a known function. For the proof see Appendix B.

Then, it is easy that for a specific value of $b=1,2,...$ and for the corresponding values of q and a_k, $k=1(1)b$, which are given from relationships (3.15) and (3.16), the phase lag of the method (3.1)–(3.8) is $O(H^{2N})=O(H^{2b+14})$, where $N=b+7$.

IV. ERROR ESTIMATION—LOCAL PHASE-LAG ERROR

The estimation of the the local truncation error (LTE) for the integration of systems of initial-value problems is obtained using several methods (see, for example, [16]).

In this paper the local error estimation technique is based on an embedded pair of integration methods and on the fact that when the phase-lag order is maximal then the approximation of the solution for the problems with an oscillatory or periodic solution is better. We have the following definition:

Definition 3. We define the local phase-lag error estimate in the lower order solution y_{n+1}^{PLL} by the quantity

$$\mathcal{E}_{LPL}=|y_{n+1}^{PLH}-y_{n+1}^{PLL}|. \tag{4.1}$$

where y_{n+1}^{PLH} is the solution obtained with higher phase-lag order method using the family $b+1$ and y_{n+1}^{PLL} is the solution obtained with lower phase-lag order method using the family b. Under the assumption that h is sufficiently small, the local phase-lag error in y_{n+1}^{PLH} can be neglected compared with that in y_{n+1}^{PLL}.

If a local phase-lag error of $\mathcal{A}$ is requested and the nth step of the integration procedure is obtained using a step size equal to h_n, the estimated step size for the $(n+1)$st step, which would give a local phase-lag error of $\mathcal{A}$, must be

$$h_{n+1}=h_n\left(\frac{\mathcal{A}}{\mathcal{E}_{LPL}}\right)^{1/q}, \tag{4.2}$$

where q is the order of the phase lag.

However, for ease of programming we have restricted all step changes to halving and doubling. Thus, based on the procedure developed in [9] for the local truncation error, the step control procedure that we have actually used is

$$\begin{aligned} &If\ \mathcal{E}_{LPL}<\mathcal{A}, h_{n+1}=2h_n,\\ &If\ 100\mathcal{A}>\mathcal{E}_{LPL}\geqslant\mathcal{A}, h_{n+1}=h_n,\\ &if\ \mathcal{E}_{LPL}\geqslant 100\mathcal{A},\ h_{n+1}=\frac{h_n}{2}\ \text{and repeat the step.}\end{aligned} \tag{4.3}$$

We note, here, that the local phase-lag error estimate is in the lower order solution y_{n+1}^{PLL}. However, if this error estimate is acceptable, i.e., less than $\mathcal{A}$, we adopt the widely used procedure of performing local extrapolation. Thus, although we are actually controlling an estimate of the local error in lower phase-lag order solution y_{n+1}^{PLL}, it is the higher order solution y_{n+1}^{PLH} which we actually accept at each point.

Now our method to estimate the local phase-lag error in y_{n+1}^{PLL} using the phase lag of y_{n+1}^{PLH} is clear. At every step we start with $k=1$ and go on increasing k and checking the local phase-lag error ($\mathcal{E}_{LPL}$) until $\mathcal{E}_{LPL}$ be less than the bound $\mathcal{A}$ $(1\leqslant k\leqslant b)$. If there is a k for which $\mathcal{E}_{LPL}<\mathcal{A}$ then the step size is doubled, otherwise we carry out the integration. Moreover, when we applied our method to our computer (i586 PC) we observed that if the value of b was greater than 6, then (because of the round-off errors) the phase-lag became of higher order than the precision of the computer used.

V. NUMERICAL ILLUSTRATIONS

In the present section we will illustrate the efficiency of the new proposed embedded technique by applying it to a well known problem. We consider the numerical integration of the radial Schrödinger equation (1.1) with one boundary condition $y(0)=0$, and a second boundary condition for large values of x determined by physical considerations. The form of the second boundary condition depends crucially on the sign of E. In the case where $E=k^2>0$, then, in general, the potential function $V(x)$ dies away faster than the term $l(l+1)/x^2$, Eq. (1.1) effectively reduces to $y''(x)+(k^2-[l(l+1)/x^2])y(x)=0$, for large x. The reduced equation has linearly independent solutions $krj_l(kx)$ and $krn_l(kx)$, where $j_l(kx)$ and $n_l(kx)$ are the spherical Bessel and Neumann functions, respectively. Thus the solution of equation (1.1) has the asymptotic form

$$y(x)\cong Akxj_1(kx)-Bkxn_l(kx) \quad \text{for} \quad r\to\infty$$
$$\cong A\left[\sin\left(kx-\frac{l\pi}{2}\right)+\tan\delta_l\cos\left(kx-\frac{l\pi}{2}\right)\right]$$
$$\text{for} \quad x\to\infty,$$

where δ_l is the phase shift, which may be calculated from the formula

$$\tan\delta_l=\frac{y(x_2)S(x_1)-y(x_1)S(x_2)}{y(x_1)C(x_2)-y(x_2)C(x_1)} \tag{5.1}$$

for x_1 and x_2 distinct points in the asymptotic region with $S(x)=kxj_l(kx)$ and $C(x)=-kxn_l(kx)$.

We illustrate the performance of the new method derived in Sec. III by applying it to the solution of (1.1), where $V(x)$ is the Lennard-Jones potential, which has been widely discussed in the literature. For this problem the potential $V(x)$ is given by

$$V(x)=m(1/x^{12}-1/x^6), \quad \text{where} \quad m=500. \tag{5.2}$$

We solve this problem as an initial-value one and, in order to be able to use a two-step method, we need an extra initial condition to be specified, e.g., $y_1[=y(h)]$. This value is computed using the Runge-Kutta-Nyström method of Dormand *et al.* [17].

The problem we consider is the computation of the relevant phase shifts correct to six decimal places. We will consider the following variable-step approaches:

(1) Method M I: based on the sixth algebraic order embedded method of Avdelas and Simos [4];

(2) Method M II: based on the variable step method of Simos [12];

(3) Method M III: based on the variable step method of Simos and Mousadis [13];

(4) Method M IV: based on the generator of *P*-stable methods of Avdelas and Simos [5];

(5) Method M V: The Runge-Kutta-Nyström method developed by Dormand and Prince (see Table 13.4 of [18])

(6) Method M VI: The extrapolation method described in [18] (see Chapter II.13 of [18], pp. 271–273 and code ODEX2);

(7) Method M VII: The Runge-Kutta Dormand-El-Mikkawy-Prince 12(10) [19];

(8) Method M VIII: based on the new group of families of methods developed in Sec. III.

The procedures (1)–(7) are described in [4], [13], [5], [12], [18], [19], respectively and are used without modification. The method used in (8) is developed in Sec. III and the error control procedure is described in Sec. IV.

In Tables I–III we present the real time of computation of the phase shifts correct to six decimal places. We note that, based on [9], the $\mathcal{A}$ we take for the application of the new methods is equal to 10^{-2M}, where M is the number of the required correct decimal digits.

TABLE I. Real time of computation (in seconds) of the phase shifts correct to seven decimal places for $E=1$ obtained using the Methods M I–M VIII.

1	Exact phase shift	Method M I	Method M II
0	0.1544208	0.14	0.10
1	1.2328816	0.34	0.26
2	−1.4296847	0.46	0.38
3	0.7832088	0.34	0.26
4	0.1258708	0.14	0.10
5	0.0366527	0.24	0.16
6	0.0147209	0.34	0.26
7	0.0068469	0.10	0.08
8	0.0035729	0.34	0.26
9	0.0020165	0.50	0.42
10	0.0012091	0.66	0.58

Method M III	Method M IV	Method M V
0.07	0.04	0.28
0.22	0.16	0.50
0.34	0.26	0.59
0.22	0.16	0.52
0.08	0.04	0.30
0.12	0.06	0.41
0.23	0.16	0.53
0.08	0.04	0.27
0.23	0.16	0.53
0.39	0.30	1.22
0.55	0.40	1.30

Method M VI	Method M VII	Method M VIII
0.24	0.20	0.02
0.44	0.39	0.03
0.54	0.50	0.07
0.46	0.42	0.03
0.25	0.22	0.02
0.28	0.25	0.02
0.49	0.43	0.03
0.23	0.20	0.03
0.45	0.41	0.03
1.11	1.06	0.06
1.23	1.14	0.08

VI. CONCLUSIONS

We have constructed a new group of families of methods with an embedded automatic error control procedure. We note that the methods of this group of families of methods are nonsymmetric (dissipative). We note also that for this group of families of methods we have proposed procedures to define the parameters of the methods of the families in order that the phase lag of the methods be minimal (until the phase lag becomes of the order of the precision of the computer used). The numerical results show that the crucial property for a method for the solution of the Schrödinger-type equations is the phase lag. It can be seen from the theoretical and numerical results that the new methods are considerably more efficient than the other numerical methods we have considered for the numerical solution of the Schrödinger equation.

All computations were carried out on a PCi586 computer using double precision arithmetic (16 significant digits accuracy).

TABLE II. Real time of computation (in seconds) of the phase shifts correct to seven decimal places for $E=5$ obtained using the Methods M I–MVIII.

1	Exact phase shift	Method M I	Method M II
0	0.4830254	0.33	0.24
1	0.9282463	1.13	1.04
2	−0.9635401	1.27	1.18
3	0.1207370	1.20	1.10
4	1.0329037	1.00	0.90
5	−1.3784055	1.27	1.18
6	−0.8439898	1.27	1.18
7	−0.5254397	0.33	0.26
8	−0.4574379	0.33	0.30
9	−0.7570240	0.33	0.30
10	1.4148608	0.33	0.27

Method M III	Method M IV	Method M V
0.22	0.13	1.04
1.00	0.88	1.45
1.14	1.01	1.57
1.07	0.92	1.52
0.87	0.73	1.40
1.16	1.02	1.58
1.14	1.01	2.00
0.24	0.13	1.05
0.27	0.18	1.10
0.26	0.18	1.08
1.12	0.90	1.10

Method M VI	Method M VII	Method M VIII
0.57	0.51	0.02
1.30	1.21	0.18
1.41	1.33	0.25
1.40	1.31	0.12
1.31	1.22	0.06
1.40	1.33	0.15
1.45	1.37	0.11
0.55	0.50	0.02
0.56	0.49	0.03
0.57	0.50	0.03
0.55	0.50	0.03

TABLE III. Real time of computation (in seconds) of the phase shifts correct to seven decimal places for $E=10$ obtained using the Methods M I–M VIII.

1	Exact phase shift	Method M I	Method M II
0	0.4310044	0.80	0.70
1	1.0450084	1.20	1.10
2	−0.7158077	1.20	1.10
3	0.5688067	1.60	1.50
4	−1.3857667	1.40	1.30
5	0.2983425	1.40	1.32
6	0.6868290	1.40	1.32
7	1.5663027	1.60	1.52
8	0.8594020	1.60	1.52
9	−0.1524079	1.40	1.31
10	0.3778998	1.20	1.13

Method M III	Method M IV	Method M V
0.68	0.54	1.55
1.09	0.95	2.30
1.09	0.93	2.30
1.49	1.28	2.71
1.29	1.10	2.42
1.31	1.10	2.43
1.30	1.10	2.40
1.48	1.28	2.73
1.50	1.28	2.75
1.27	1.07	2.45
1.12	0.90	2.31

Method M VI	Method M VII	Method M VIII
1.48	1.32	0.25
1.81	1.65	0.50
1.82	1.67	0.50
2.21	2.02	0.53
2.05	1.76	0.43
2.05	1.81	0.41
2.10	1.76	0.35
2.27	2.05	0.43
2.25	2.03	0.41
2.08	1.83	0.30
1.86	1.68	0.30

APPENDIX A

(a) *Proof of the Theorem 3*. To calculate the coefficients q and a_k of the family b of the group of methods (3.1)–(3.8) we have applied the above mentioned algorithm to the test Eq. (2.2). So, we have the following formulas:

$$\overline{y}_{n+1}=(2-H^2)y_n-y_{n-1},$$

$$\bar{\bar{y}}_{n+1}=\left(2-H^2+\frac{H^4}{12}\right)y_n-y_{n-1},$$

$$\overline{y}_{n,k}=y_n+a_{b-k+1}H^2\left[\left(2-H^2+\frac{H^4}{12}\right)y_n-2\overline{y}_{n,k-1}\right]|k=1(1)b,\overline{y}_{n,0,b}=y_n. \quad \text{(A1)}$$

The above relationships give

$$\overline{y}_{n,b}=\left[1-a_1H^4\left(1-\frac{H^2}{12}\right)(1-2a_2H^2\times\{1-2a_3H^2[\cdots(1-2a_bH^2)]\cdots\}\right)y_n, \quad \text{(A2)}$$

or

$$\overline{y}_{n,b}=1-a_1H^4\left(1-\frac{H^2}{12}\right)\Bigg[1-2a_2H^2+2^2a_2a_3H^4-2^3a_2a_3a_4H^6+\ldots+(-2H^2)^{b-1}\prod_{j=1}^{b}a_j\Bigg]y_n, \tag{A3}$$

or

$$\overline{y}_{n,b}=(1-H^4\Delta_b)y_n, \tag{A4}$$

where

$$\Delta_b=\left(1-\frac{H^2}{12}\right)\sum_{i=1}^{b}(-2H^2)^{i-1}\prod_{j=1}^{i}a_j. \tag{A5}$$

Based on the above we have

$$\hat{y}_{n-1/2}=\left(\frac{1}{2}+\frac{H^2}{16}+\frac{5H^4}{384}-\frac{17H^6}{192}\Delta_b\right)y_n+\left(\frac{1}{2}+\frac{H^6}{16}\right)y_{n-1},$$

$$\hat{y}_{n+1/2}=\left(\frac{3}{2}-\frac{5H^2}{16}-\frac{H^4}{128}+\frac{21H^6}{64}\Delta_b\right)y_n-\left(\frac{1}{2}+\frac{H^6}{16}\right)y_{n-1},$$

$$\begin{aligned}\hat{\hat{y}}_{n-1/2}=&\Bigg(\frac{1}{2}-H^2\Bigg[\left(-\frac{5}{192}-\frac{q}{4}\right)(2-H^2)-\frac{1}{6}-\frac{3q}{2}\\&+\left(\frac{5}{48}+q\right)\left(\frac{3}{2}-\frac{5H^2}{16}-\frac{H^4}{128}+\frac{21H^6}{64}\Delta_b\right)\\&+q\left\{\frac{1}{2}-H^2\left(-\frac{1}{16}-\frac{5H^2}{384}+\frac{17H^6}{192}\Delta_b\right)\right\}\Bigg]\Bigg)y_n\\&+\Bigg[\frac{1}{2}-H^2\left\{-\frac{1}{96}+\left(\frac{5}{48}+q\right)\left(-\frac{1}{2}-\frac{H^2}{16}\right)\right.\\&\left.+q\left(\frac{1}{2}+\frac{H^2}{16}\right)\right\}\Bigg]y_{n-1},\end{aligned}$$

$$\begin{aligned}\hat{\hat{y}}_{n+1/2}=&\Bigg[\frac{3}{2}-H^2\Bigg\{\frac{5}{16}-\frac{H^2}{192}-\frac{5H^2}{48}\Bigg[\left(-\frac{5}{192}-\frac{q}{4}\right)(2-H^2)\\&-\frac{1}{6}-\frac{3q}{2}+\left(\frac{5}{48}+q\right)\left(\frac{3}{2}-\frac{5H^2}{16}-\frac{H^4}{128}+\frac{21H^6}{64}\Delta_b\right)\\&+q\left\{\frac{1}{2}-H^2\left(-\frac{1}{16}-\frac{5H^2}{384}+\frac{17H^6}{192}\Delta_b\right)\right\}\Bigg]\Bigg\}\Bigg]y_n\\&+\Bigg[\frac{1}{2}-H^2\Bigg\{\frac{1}{16}-\frac{5H^2}{48}\Bigg[-\frac{1}{96}+\left(\frac{5}{48}+q\right)\left(-\frac{1}{2}-\frac{H^2}{16}\right)\\&+q\left(\frac{1}{2}+\frac{H^2}{16}\right)\Bigg]\Bigg\}\Bigg]y_{n-1}.\end{aligned}$$

Using the above relations in (3.8) and based on (2.3) it can be seen, after straightforward manipulations, that $Q(H)$ is given by (3.11) and $C(H)$ is given by (3.12).

APPENDIX B

(b) *Proof of the Theorem 4*. From the relation (requirement) (2.5) we have that

$$-\frac{Q(H)}{1+C(H)}\equiv\cos(H). \tag{B1}$$

If we substitute $\cos(H)\equiv\Sigma_{i=0}^{2N+2}H^{2i}/2i!$ and $C(H)$, which is given by (3.12), into (B1), we obtain

$$\begin{aligned}Q(H)\equiv&-2+H^2-\frac{H^4}{12}+\frac{H^6}{360}+\frac{127H^8}{967680}-\frac{2609H^{10}}{29030400}\\&+\frac{28859H^{12}}{3832012800}-\frac{175159H^{14}}{697426329600}\\&+\frac{375367H^{16}}{83691159552000}-\frac{1276267H^{18}}{25609494822912000}\\&+\frac{367411H^{20}}{9731608032706560000}\\&-\frac{9326617H^{22}}{4496002911110430720000}+\cdots.\end{aligned} \tag{B2}$$

$Q(H)$, however, is given by (3.11). Therefore, from (3.11) and (B2) we get explicitly the value

$$q=-\frac{23}{336}. \tag{B3}$$

If we substitute (B3) into (3.11), we obtain

$$\begin{aligned}Q(H)\equiv&-2+H^2-\frac{H^4}{12}+\frac{H^6}{360}+\frac{127H^8}{967680}-\frac{151H^{10}}{4644864}\\&-\frac{1147H^{10}}{241920}\Delta_b+\frac{1147H^{12}}{2322432}\Delta_b.\end{aligned} \tag{B4}$$

Based on (B4), the requirement (B2) gives

$$\begin{aligned}&\left(\frac{1147}{241920}-\frac{1147H^2}{2322432}\right)H^{10}\Delta_b\\&\quad\equiv\frac{6661H^{10}}{116121600}-\frac{28859H^{12}}{3832012800}+\frac{175159H^{14}}{697426329600}\\&\qquad-\frac{375367H^{16}}{83691159552000}+\frac{1276267H^{18}}{25609494822912000}\\&\qquad-\frac{3674117H^{20}}{9731608032706560000}\\&\qquad+\frac{9326617H^{22}}{4496002911110430720000}+\cdots\end{aligned} \tag{B5}$$

or the equivalent relation [using the formula (3.13)]

$$\sum_{i=1}^{b}(-2H^2)^{i-1}\prod_{j=1}^{i}a_j\equiv s_0+s_1H^2+s_2H^4+\cdots, \tag{B6}$$

TABLE IV. Initial five values of parameters s_j, $j=0(1)4$, defined in theorem 4 and the coefficients of the group of method a_i, $i=1(1)b$.

$s_j\ j=0(1)4$	a_i, $i=1(1)5$
$s_0=\frac{6661}{550650}$	$a_1=\frac{6661}{550650}$
$s_1=\frac{39539}{58139136}$	$a_2=-\frac{197695}{7034016}$
$s_2=\frac{95820041}{1269758730240}$	$a_3=-\frac{95820041}{1727063520}$
$s_3=\frac{2224595489}{304742095257600}$	$a_3=-\frac{2224595489}{45993619680}$
$s_4=\frac{180082834933}{248669549730201600}$	$a_3=-\frac{180082834933}{3630539838048}$

where s_i, $|i=0,1,2,...$ are the coefficients of the Taylor series expansion which is obtained by dividing the right-hand side of the relation (requirement) (B5) by $(1147/241920-1147H^2/2322432)(1-H^2/12)H^{10}$.

Obtaining successively $b=1,2,...$, the requirement (B6) gives

$$a_1=s_0,$$

$$a_2=\frac{s_1}{-2a_1}=-\frac{s_1}{2s_0},$$

$$a_3=\frac{s_2}{(-2)^2a_2a_1}=\frac{s_2}{(-2)^2s_0}\frac{-2s_0}{s_1}=\frac{s_2}{-2s_1}$$

and generally

$$a_b=\frac{s_{b-1}}{(-2)^{b-1}a_{b-1}a_{b-2}\cdots a_1}=\frac{s_{b-1}}{(-2)^{b-1}}\frac{-2s_{b-2}}{s_{b-3}}\cdots\frac{-2s_0}{s_1}$$

$$=-\frac{s_{b-1}}{2s_{b-2}} \tag{B7}$$

and the theorem is proved.

Presumptively, in Table IV we present the initial five values of s_j, $j=0(1)4$ and a_i, $i=1(1)5$.

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