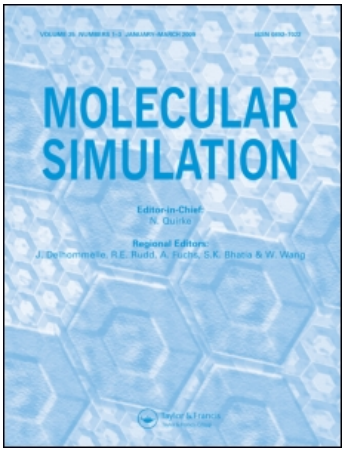

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A Sixth Order Bessel and Neurnann Fitted Method for the Numerical Solution of the Schrödinger Equation

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A SIXTH ORDER BESSEL AND NEUMANN FITTED METHOD FOR THE NUMERICAL SOLUTION OF THE SCHRÖDINGER EQUATION

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A sixth algebraic order method for the numerical solution of the Schrödinger equation is developed in this paper. The new method has free parameters which will be defined such that the method is *fitted* to spherical Bessel and Neumann functions. Based on the new method and the method of Simos and Williams [15] we have obtained a variable-step method. The results produced based on the numerical solution the radial Schrödinger equation and of coupled differential equations arising from the Schrödinger equation indicate that this new approache is more efficient than other well known methods.

Keywords: Schrödinger equation; coupled differential equations; Bessel and Neumann fitting; scattering problems

1. INTRODUCTION

Several numerical techniques exist in the literature for solving the Schrödinger equation (see [2-3, 7]).

The radial Schrödinger equation is a boundary value problem which has the form:

$$y''(x) = f(x,y) = [l(l+1)/x^2 + V(x) - k^2]y(x). \tag{1}$$

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with one boundary condition given by:

$$y(0) = 0 \tag{2}$$

and the other boundary condition, for large values of x, determined by physical considerations. Equations of this type occur very frequently in theoretical physics, in quantum physics, in nuclear physics, in theoretical chemistry, in quantum chemistry and elsewhere (see [5] and [14]) and there is a real need to be able to solve them both efficiently and reliably by numerical methods. In (1) the function $W(x) = l(l+1)/x^2 + V(x)$ denotes *the effective potential*, which satisfies $W(x) \to 0$ as $x \to \infty$, k is a constant which may be complex but in this paper we will work exclusively with the case where k is a real number, l is a given integer and V is a given function which denotes the potential.

The form of the second boundary condition depends crucially on the sign on E. Here we will investigate the case $E = k^2 > 0$. In this case, in general, the potential function $V(x)$ dies away faster than the term $l(l+1)/x^2$; Eq. (1) then effectively reduces to

$$y''(x) + \left(E - \frac{l(l+1)}{x^2}\right) y(x) = 0 \tag{3}$$

for large x. The above equation has linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l(kx)$ and $n_l(kx)$ are the spherical Bessel and Neumann functions respectively. Thus the solution of Eq. (1) has the asymptotic form:

$$\begin{aligned} y(x) &\cong_{x\to\infty} Akxj_l(kx) - Bkxn_l(kx) \\ &\cong_{x\to\infty} D\left[\sin\left(kx - \frac{l\pi}{2}\right) + \tan\delta_l \cos\left(kx - \frac{l\pi}{2}\right)\right], \end{aligned}$$

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

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)} \tag{4}$$

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

For the numerical solution of the Schrödinger type equations there are two main categories of methods. The methods with constant coefficients and the methods with coefficients which depend from the frequency of the problem. The construction of methods, which belong to any of the above mentioned categories of methods, is the subject of great activity the last years (see [3] and references there in).

One of the most well known methods for solving the molecular scattering problem of the Schrödinger equation (see [14]) is the iterative Numerov's

method of Allison [1]. Recently Raptis and Cash [9] have obtained second order Bessel and Neumann fitted methods which are more efficient than the Numerov's method or the iterative Numerov's method of Allison [1].

Another approach for developing efficient methods for the solution of (1) is exponential fitting. This approach is appropriate because for large x the solution of (1) is *periodic*. A Numerov-type exponentially fitted method has derived by Raptis and Allison [6]. Numerical results presented there indicate that these fitted methods are much more efficient than Numerov's method for the solution of (1). Many authors have investigated the idea of exponential fitting, since Raptis and Allison. The most recent and interesting contribution to these methods is the proposed by Simos [11] (see Ixaru *et al.* [4]).

In Section 2 we will develop the sixth algebraic order Bessel and Neumann fitted methods. Based on the new method and on the method developed by Simos and Williams [15] we will develop in Section 3 a variable-step method. An application of the produced variable-step method to the radial Schrödinger equation and to the coupled differential equations arising from the Schrödinger equation is presented in Section 4.

2. A SIXTH ALGEBRAIC ORDER BESSEL AND NEUMANN FITTED METHOD

Consider, now, the two parameter family of two-step sixth order methods $M_6(a_i)$, $i = 0, 1$

$$\begin{aligned}
\bar{y}_{n+1} &= y_{n+1} - a_0 h^2 (f_{n+1} - f_n) \\
\bar{\bar{y}}_{n+1} &= 2y_n - y_{n-1} + \frac{h^2}{12}(\bar{f}_{n+1} + 10f_n + f_{n-1}) \\
\bar{y}_{n+\frac{1}{2}} &= \frac{1}{104}(5y_{n+1} + 146y_n - 47y_{n-1}) \\
&\quad + \frac{h^2}{4992}(-59\bar{\bar{f}}_{n+1} + 1438f_n + 253f_{n-1}) \\
\bar{y}_{n-\frac{1}{2}} &= \frac{1}{52}(3y_{n+1} + 20y_n + 29y_{n-1}) \\
&\quad + \frac{h^2}{4992}(41\bar{\bar{f}}_{n+1} - 682f_n - 271f_{n-1}) \\
\bar{y}_n &= y_n - a_1 h^2 [(f_{n+1} - 2f_n + f_{n-1}) \\
&\quad - 4(\bar{f}_{n+\frac{1}{2}} - 2f_n + \bar{f}_{n-\frac{1}{2}})] \\
y_{n+1} - 2y_n + y_{n-1} &= \frac{h^2}{60}[f_{n+1} + 26\bar{f}_n + f_{n-1} + 16(\bar{f}_{n+\frac{1}{2}} + \bar{f}_{n-\frac{1}{2}})] \qquad (5)
\end{aligned}$$

where $f_p = f(x_p, y_p)$, $p = n-1(1)n+1$, $\bar{f}_q = f(x_q, \bar{y}_q)$, $q = n,\ n+1$, $\bar{\bar{f}}_q = f(x_q, \bar{\bar{y}}_q)$, $q = n+1$, $\bar{f}_{n\pm\frac{1}{2}} = f(x_{n\pm\frac{1}{2}}, \bar{y}_{n\pm\frac{1}{2}})$.

The corresponding local truncation error is given by

$$LTE = -\frac{h^8}{4717440}\left(39y_n^{(8)} + 63y_n^{(6)} + 127764a_1 y_n^{(6)}\right) + O(h^{10}) \tag{6}$$

Demanding now that the family of methods $M_6(a_i), i = 0,\ 1$ integrate exactly the functions $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l(kx)$ and $n_l(kx)$ are the spherical Bessel and Neumann functions respectively, we have the following equations

$$\begin{aligned}
\bar{J}_{n+1} &= J_{n+1} - a_0(F_{n+1}J_{n+1} - F_nJ_n)\\
\bar{\bar{J}}_{n+1} &= 2J_n - J_{n-1} + \frac{1}{12}(F_{n+1}\bar{J}_{n+1} + 10F_nJ_n + F_{n-1}J_{n-1})\\
\bar{J}_{n+\frac{1}{2}} &= \frac{1}{104}(5J_{n+1} + 146J_n - 47J_{n-1})\\
&\quad + \frac{1}{4992}(-59F_{n+1}\bar{\bar{J}}_{n+1} + 1438F_nJ_n + 253F_{n-1}J_{n-1})\\
\bar{J}_{n-\frac{1}{2}} &= \frac{1}{52}(3J_{n+1} + 20J_n + 29J_{n-1})\\
&\quad + \frac{1}{4992}(41F_{n+1}\bar{\bar{J}}_{n+1} - 682F_nJ_n - 271F_{n-1}J_{n-1})\\
\bar{J}_n &= J_n - a_1[(F_{n+1}J_{n+1} - 2F_nJ_n + F_{n-1}J_{n-1})\\
&\quad - 4(F_{n+\frac{1}{2}}\bar{J}_{n+\frac{1}{2}} - 2F_nJ_n + F_{n-\frac{1}{2}}\bar{J}_{n-\frac{1}{2}})]\\
J_{n+1} - 2J_n + J_{n-1} &= \frac{1}{60}[F_{n+1}J_{n+1} + 26F_n\bar{J}_n + F_{n-1}J_{n-1}\\
&\quad + 16(F_{n+\frac{1}{2}}\bar{J}_{n+\frac{1}{2}} + F_{n-\frac{1}{2}}\bar{J}_{n-\frac{1}{2}})]
\end{aligned} \tag{7}$$

and the equations

$$\begin{aligned}
\bar{Y}_{n+1} &= Y_{n+1} - a_0(F_{n+1}Y_{n+1} - F_nY_n)\\
\bar{\bar{Y}}_{n+1} &= 2Y_n - Y_{n-1} + \frac{1}{12}(F_{n+1}\bar{Y}_{n+1} + 10F_nY_n + F_{n-1}Y_{n-1})\\
\bar{Y}_{n+\frac{1}{2}} &= \frac{1}{104}(5Y_{n+1} + 146Y_n - 47Y_{n-1})\\
&\quad + \frac{1}{4992}(-59F_{n+1}\bar{\bar{Y}}_{n+1} + 1438F_nY_n + 253F_{n-1}Y_{n-1})\\
\bar{Y}_{n-\frac{1}{2}} &= \frac{1}{52}(3Y_{n+1} + 20Y_n + 29Y_{n-1})
\end{aligned}$$

$$+\frac{1}{4992}\left(41F_{n+1}\bar{\bar{Y}}_{n+1}-682F_nY_n-271F_{n-1}Y_{n-1}\right)$$

$$\bar{Y}_n = Y_n - a_1[(F_{n+1}Y_{n+1}-2F_nY_n+F_{n-1}Y_{n-1})$$
$$-4(F_{n+\frac{1}{2}}\bar{Y}_{n+\frac{1}{2}}-2F_nY_n+F_{n-\frac{1}{2}}\bar{Y}_{n-\frac{1}{2}})]$$

$$Y_{n+1}-2Y_n+Y_{n-1}=\frac{1}{60}[F_{n+1}Y_{n+1}+26F_n\bar{Y}_n+F_{n-1}Y_{n-1}$$
$$+16(F_{n+\frac{1}{2}}\bar{Y}_{n+\frac{1}{2}}+F_{n-\frac{1}{2}}\bar{Y}_{n-\frac{1}{2}})] \tag{8}$$

where

$$\dot{F}_q=\left[\frac{l(l+1)}{x_q}-k^2\right]h^2$$

$$J_q=kx_qj_l(kx_q),\quad Y_q=kx_qy_l(kx_q),\quad q=n-1(1)n+1$$

In Appendix A we present the values of the parameters a_i, $i=0,\ 1$ produced solving the above system of equations.

3. ERROR ESTIMATION

It is known from the literature (see for example [8–10]) that there are many methods for the estimation of the local truncation error (LTE) in the integration of systems of initial-value problems.

In this paper we base our local error estimation technique on an embedded pair of integration methods and on the fact that when the order is maximal then the approximation of the solution for the problems with oscillatory or periodical solution is better.

The new variable-step procedure consists the following parts.

(1) We divide the integration range into two distinct parts.
(2) The first part of the integration runs from $r=0$ to r_c, where r_c is a point such that $|V(r)|$ is small. In practice we consider that $V(r)$ is small when $|V(r)|<1/8$. In the range $0\leq r<r_c$ the variable-step method is exactly described in [8].
(3) For $r\geq r_c$ we use the following variable-step procedure.

We use as lower order solution y_{n+1}^L, for the purpose of local error estimation, the fifth order Bessel and Neumann fitted method developed in [15]. As higher order solution y_{n+1}^H we use the sixth order Bessel and Neumann fitted method obtained above. Now, the local truncation error

in y_{n+1}^{L} is estimated by

$$LTE = |y_{n+1}^{H} - y_{n+1}^{L}| \tag{9}$$

We illustrate the new variable-step procedure described above by applying them to the solution of (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:

$$V(x) = m(1/x^{12} - 1/x^{6}) \quad \text{where } m = 500. \tag{10}$$

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.*, $y_1 (= y(h))$. It is well known that, for values of x close to the origin, the solution of (1) behaves like

$$y(x) \simeq Cx^{l+1} \quad \text{as } x \to 0. \tag{11}$$

In view of this we use $y_1 = h^{l+1}$ as our extra initial condition.

The problem we consider is the computation of the relevant phase shifts correct to 4 decimal places for energies $k = 1$, $k = 5$ and $k = 10$ and for $l = 0(1)\ 10$. We will consider four approaches:

Method MI: The iterative Numerov's method developed by Allison [1].
Method MII: based on the well known variable-step method of Raptis and Cash [8],
Method MIII: based on the well known variable-step method of Raptis and Cash [9],
Method MIV: based on the variable-step procedure developed by Simos [12],
Method MV: based on the variable-step procedure developed by Simos and Mousadis [13],
Method MVI: based on the variable-step procedure developed by Avdelas and Simos [3],
Method MVII: based on the variable-step method developed above.

In Table I we present the average time of computation of the phase shifts correct to four decimal places.

3.1. Coupled Differential Equations

There are many problems in quantum chemistry, theoretical physics, atomic physics, physical chemistry and chemical physics which can be transformed to the solution of coupled differential equations of the Schrödinger type.

TABLE I Phase shift problem. Average time of computation for the calculation of the phase shifts correct to 4 decimal places for energies $k = 1$, $k = 5$ and $k = 10$ and for $l = 0(1)10$

Method	*Average time of computation (in seconds)*
MI	2.750
MII	2.144
MIII	1.716
MIV	1.623
MV	1.543
MVI	1.204
MVII	0.734

The close-coupling differential equations of the Schrödinger type may be written in the form

$$\left[\frac{d^2}{dx^2} + k_i^2 - \frac{l_i(l_i+1)}{x^2} - V_{ii}\right] y_{ij} = \sum_{m=1}^{n} V_{im} y_{mj} \tag{12}$$

for $1 \leq i \leq N$ and $m \neq i$.

We have investigated the case in which all channels are open. So we have the following boundary conditions (see for details [1]):

$$y_{ij} = 0 \text{ at } x = 0 \tag{13}$$

$$y_{ij} \sim k_i x j_{l_i}(k_i x)\delta_{ij} + \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij} k_i x n_{l_i}(k_i x) \tag{14}$$

where $j_l(x)$ and $n_l(x)$ are the spherical Bessel and Neumann functions, respectively. We can also use the present method to problems involving closed channels.

Based on the detailed analysis developed in [1] and defining a matrix K' and diagonal matrices M, N by:

$$K'_{ij} = \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij}$$
$$M_{ij} = k_i x j_{l_i}(k_i x)\delta_{ij}$$
$$N_{ij} = k_i x n_{l_i}(k_i x)\delta_{ij}$$

we find that the asymptotic condition (14) may be written as:

$$\mathbf{y} \sim \mathbf{M} + \mathbf{N}\mathbf{K}' \tag{15}$$

One of the most well-known methods for the numerical solution of the coupled differential equations arising from the Schrödinger equation is the Iterative Numerov method of Allison [1].

A real problem in quantum chemistry, theoretical physics, atomic physics and molecular physics which can be transformed to close-coupling differential equations of the Schrödinger type is the rotational excitation of a diatomic molecule by neutral particle impact. Denoting, as in [1], the entrace channel by the quantum numbers $(j, 1)$, the exit channels by (j', l'), and the total angular momentum by $J = j + l = j' + l'$, we find that

$$\left[\frac{d^2}{dx^2} + k_{j'j}^2 - \frac{l'(l'+1)}{x^2}\right] y_{j'l'}^{Jjl}(x) = \frac{2\mu}{\hbar^2} \sum_{j''} \sum_{l''} \langle j'l'; J|V|j''l''; J\rangle y_{j''l''}^{Jjl}(x) \quad (16)$$

where

$$k_{j'j} = \frac{2\mu}{\hbar^2}\left[E + \frac{\hbar^2}{2I}\left\{j(j+1) - (j'+1)\right\}\right] \quad (17)$$

E is the kinetic energy of the incident particle in the center-of-mass system, I is the moment of inertia of the rotator, and μ is the reduced mass of the system.

Following the analysis of [1], the potential V can be expanded as

$$V(x, \hat{\mathbf{k}}_{j'j}\, \hat{\mathbf{k}}_{jj}) = V_0(x)P_0(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}) + V_2(x)P_2(\hat{\mathbf{k}}_{j'j}\, \hat{\mathbf{k}}_{jj}), \quad (18)$$

and the coupling matrix element may then be written as

$$\langle j'l'; J|V|j''l''; J\rangle = \delta_{j'j''}\delta_{l'l''}V_0(x) + f_2(j'l', j''l''; J)V_2(x) \quad (19)$$

where the f_2 coefficients can be obtained from formulas given by Bernstein *et al.* [16] and $\hat{\mathbf{k}}_{j'j}$ is a unit vector parallel to the wave vector $\mathbf{k}_{j'j}$ and P_i, $i = 0, 2$ are Legendre polynomials (see for details [17]). The boundary conditions are

$$y_{j'l'}^{Jjl}(x) = 0 \text{ at } x = 0 \quad (20)$$

$$y_{j'l'}^{Jjl}(x) \sim \delta_{jj'}\delta_{ll'} \exp[-i(k_{jj}x - 1/2l\pi)] - \left(\frac{k_i}{k_j}\right)^{1/2} S^J(jl; j'l') \exp[i(k_{j'j}x - 1/2l'\pi)] \quad (21)$$

where the scattering S matrix is related to the K matrix of (14) by the relation

$$\mathbf{S} = (\mathbf{I} + \mathbf{iK})(\mathbf{I} - \mathbf{iK})^{-1} \tag{22}$$

To calculate the cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles a computer program has been obtained. In this program the numerical method for step-by-step integration from the initial value to matching points is included. We must note here that this program is also based on an analogous program which has been written for the numerical applications of [1].

For numerical purposes we choose the S matrix which is calculated using the following parameters

$$\frac{2\mu}{\hbar^2} = 1000.0, \quad \frac{\mu}{I} = 2.351, \quad E = 1.1,$$
$$V_0(x) = \frac{1}{x^{12}} - 2\frac{1}{x^6}, \quad V_2(x) = 0.2283 V_0(x).$$

As is described in [1], we take $J = 6$ and consider excitation of the rotator from the $j = 0$ state to levels up to $j' = 2, 4$ and 6 giving sets of **four, nine and sixteen coupled differential equations**, respectively. Following the procedure obtained by Bernstein [17] and Allison [1] the potential infinite is considered for values of x less than some x_0. The wavefunctions are then vanished in this region and effectively the boundary condition (20) may be written as

$$y^{Jjl}_{j'l'}(x_0) = 0 \tag{23}$$

For the numerical solution of this problem we have used the most well known methods for the above problem: (i) the Iterative Numerov method of Allison [1], (ii) the variable-step method of Raptis and Cash [8] and (iii) the new variable-step method. In Table II we present the real time of computation required by the methods mentioned above to calculate the square of the modulus of the S matrix for sets of 4, 9 and 16 coupled differential equations. In Table II N indicates the number of equations of the set of coupled differential equations.

In all cases the embedded variable-step method developed in this paper is more accurate than other well known finite difference ones for a given value of *hmax* so that the new variable-step method can use a larger value of *hmax* and still gets converged results.

TABLE II RTC = Real time of computation (in seconds) to calculate $|S|^2$ for the variable-step methods (1)–(3). $acc = 10^{-6} \cdot hmax$ is the maximum stepsize

Method	*N*	*hmax*	*RTC*
Iterative Numerov [1]	4	0.014	3.25
	9	0.014	23.51
	16	0.014	99.15
Variable-step Method	4	0.056	1.65
of Rapits and Cash [8]	9	0.056	8.68
	16	0.056	45.21
New Variable-step	4	0.448	0.14
method	9	0.448	0.85
	16	0.224	4.90

4. CONCLUSIONS

In the present paper a sixth algebraic order Bessel and Neumann fitted method for the numerical solution of the phase shift problem of the radial Schrödinger equation and of the coupled differential equations arising from the Schrödinger equation is introduced. Based on this new method and on the fifth algebraic order method developed by Simos and Williams [15], we introduce a new variable-step method for the solution of the Schrödinger equation (radial and coupled differential equations). The numerical results given by this new variable-step method are better than those of the most well known variable-step method of Raptis and Cash [8] and of the well known iterative Numerov method of Allison [1].

It can be seen from the theoretical and numerical results that the new method is more efficient than the other variable-step procedures, which are the most recent and well-known methods in the literature.

All computations were carried out on a PC i586 using double precision arithmetic (16 significant digits accuracy).

APPENDIX A

$$
\begin{aligned}
a_0 = 1872(&-192J_nF_{n+1}Y_{n+1} - 576F_nJ_nY_{n-1} + 96J_{n+1}F_{n-1}Y_{n-1} \\
&- 7F_{n+1}J_{n+1}F_{n-\frac{1}{2}}F_nY_n + 2F_{n+1}J_{n+1}F_{n+\frac{1}{2}}F_{n-1}Y_{n-1} \\
&+ 13F_{n+1}J_{n+1}F_{n+\frac{1}{2}}F_nY_n - 2F_{n+1}J_{n+1}F_{n-\frac{1}{2}}F_{n-1}Y_{n-1} \\
&+ 54F_{n+1}J_{n+1}F_{n+\frac{1}{2}}Y_n - 19F_{n+1}J_{n+1}F_{n+\frac{1}{2}}Y_{n-1} + 32F_{n+1}J_{n+1}F_nY_n \\
&- 34F_nJ_nF_{n+\frac{1}{2}}Y_{n-1} - 34F_nJ_nF_{n-\frac{1}{2}}Y_{n+1} + 126F_nJ_nF_{n-\frac{1}{2}}Y_{n-1}
\end{aligned}
$$

$$
\begin{aligned}
&- 32F_nJ_nF_{n+1}Y_{n+1} - 32F_nJ_nF_{n-1}Y_{n-1} + 126F_nJ_nF_{n+\frac{1}{2}}Y_{n+1}\\
&+ 7F_nJ_nF_{n+\frac{1}{2}}F_{n-1}Y_{n-1} - 13F_nJ_nF_{n-\frac{1}{2}}F_{n-1}Y_{n-1} - 576F_nJ_nY_{n+1}\\
&+ 19F_{n+\frac{1}{2}}J_{n-1}F_{n+1}Y_{n+1} + 34F_{n+\frac{1}{2}}J_{n-1}F_nY_n - 54F_{n+\frac{1}{2}}J_nF_{n+1}Y_{n+1}\\
&+ 32F_{n-1}J_{n-1}F_nY_n + 192F_{n+1}J_{n+1}Y_n - 96F_{n+1}J_{n+1}Y_{n-1}\\
&+ 6F_{n+1}J_{n+1}F_{n-\frac{1}{2}}Y_n + 21F_{n+1}J_{n+1}F_{n-\frac{1}{2}}Y_{n-1} - 126F_{n+\frac{1}{2}}J_{n+1}F_nY_n\\
&+ 34F_{n-\frac{1}{2}}J_{n+1}F_nY_n - 13F_{n+\frac{1}{2}}F_nJ_nF_{n+1}Y_{n+1}\\
&- 2F_{n+\frac{1}{2}}F_{n-1}J_{n-1}F_{n+1}Y_{n+1} - 7F_{n+\frac{1}{2}}F_{n-1}J_{n-1}F_nY_n\\
&- 6F_{n-\frac{1}{2}}J_nF_{n+1}Y_{n+1} + 576J_{n+1}F_nY_n + 2F_{n-\frac{1}{2}}F_{n-1}J_{n-1}F_{n+1}Y_{n+1}\\
&+ 96J_{n-1}F_{n+1}Y_{n+1} + 576J_{n-1}F_nY_n + 192F_{n-\frac{1}{2}}J_nY_{n+1} + 576F_{n-\frac{1}{2}}J_nY_{n-1}\\
&+ 13F_{n-\frac{1}{2}}F_{n-1}J_{n-1}F_nY_n + 7F_{n-\frac{1}{2}}F_nJ_nF_{n+1}Y_{n+1}\\
&- 19Y_{n+1}F_{n-\frac{1}{2}}F_{n-1}J_{n-1} - 21F_{n+\frac{1}{2}}F_{n-1}Y_{n-1}J_{n+1} - 192Y_nF_{n+\frac{1}{2}}J_{n-1}\\
&- 576Y_nF_{n-\frac{1}{2}}J_{n-1} - 576Y_nF_{n+\frac{1}{2}}J_{n+1} + 6Y_nF_{n+\frac{1}{2}}F_{n-1}J_{n-1}\\
&+ 54Y_nF_{n-\frac{1}{2}}F_{n-1}J_{n-1} + 576F_{n+\frac{1}{2}}J_nY_{n+1} - 192Y_nF_{n-\frac{1}{2}}J_{n+1}\\
&- 192J_nF_{n-1}Y_{n-1} + 192F_{n+\frac{1}{2}}J_nY_{n-1} - 96F_{n-1}J_{n-1}Y_{n+1}\\
&- 6F_{n+\frac{1}{2}}J_nF_{n-1}Y_{n-1} - 54F_{n-\frac{1}{2}}J_nF_{n-1}Y_{n-1} + 19F_{n-\frac{1}{2}}F_{n-1}Y_{n-1}J_{n+1}\\
&- 192Y_{n+1}F_{n+\frac{1}{2}}J_{n-1} - 21F_{n-\frac{1}{2}}J_{n-1}F_{n+1}Y_{n+1} - 126F_{n-\frac{1}{2}}J_{n-1}F_nY_n\\
&+ 192F_{n-1}J_{n-1}Y_n + 192Y_{n+1}F_{n-\frac{1}{2}}J_{n-1} - 192Y_{n-1}F_{n-\frac{1}{2}}J_{n+1}\\
&+ 192F_{n+\frac{1}{2}}Y_{n-1}J_{n+1} + 21Y_{n+1}F_{n+\frac{1}{2}}F_{n-1}J_{n-1})/((24J_nF_{n+1}Y_{n+1}\\
&- 12F_nJ_nY_{n-1} - F_{n+1}J_{n+1}F_{n-1}Y_{n-1} - 11F_{n+1}J_{n+1}F_nY_n\\
&+ 11F_nJ_nF_{n+1}Y_{n+1} + F_nJ_nF_{n-1}Y_{n-1} - 12F_nJ_nY_{n+1} + F_{n-1}J_{n-1}F_{n+1}Y_{n+1}\\
&- F_{n-1}J_{n-1}F_nY_n - 24F_{n+1}J_{n+1}Y_n + 12F_{n+1}J_{n+1}Y_{n-1} + 12J_{n+1}F_nY_n\\
&- 12J_{n-1}F_{n+1}Y_{n+1} + 12J_{n-1}F_nY_n)(-59F_{n+\frac{1}{2}} + 41F_{n-\frac{1}{2}})F_{n+1}^2). \qquad (24)
\end{aligned}
$$

$$
\begin{aligned}
a_1 = &-\frac{2}{13}(449280J_nF_{n+1}Y_{n+1} + 59F_{n+1}^2J_{n+1}F_{n+\frac{1}{2}}F_{n-1}Y_{n-1} - 224640F_nJ_nY_{n-1}\\
&- 3744F_{n+1}J_{n+1}F_{n-1}Y_{n-1} + 8184F_{n+1}J_{n+1}F_{n-\frac{1}{2}}F_nY_n\\
&+ 492F_{n+1}^2J_{n+1}F_{n-\frac{1}{2}}Y_{n-1} - 984F_{n+1}^2J_{n+1}F_{n-\frac{1}{2}}Y_n\\
&- 3036F_{n+1}J_{n+1}F_{n+\frac{1}{2}}F_{n-1}Y_{n-1} - 17256F_{n+1}J_{n+1}F_{n+\frac{1}{2}}F_nY_n\\
&- 708F_{n+1}^2J_{n+1}F_{n+\frac{1}{2}}Y_{n-1} + 1416F_{n+1}^2J_{n+1}F_{n+\frac{1}{2}}Y_n\\
&+ 3252F_{n+1}J_{n+1}F_{n-\frac{1}{2}}F_{n-1}Y_{n-1} - 84096F_{n+1}J_{n+1}F_{n+\frac{1}{2}}Y_n\\
&+ 27072F_{n+1}J_{n+1}F_{n+\frac{1}{2}}Y_{n-1} + 41F_nJ_nF_{n-\frac{1}{2}}F_{n+1}F_{n-1}Y_{n-1}
\end{aligned}
$$

$$
\begin{aligned}
&- 101088F_{n+1}J_{n+1}F_nY_n - 27072F_nJ_nF_{n+\frac{1}{2}}Y_{n-1} + 3456F_nJ_nF_{n-\frac{1}{2}}Y_{n+1}\\
&+ 33408F_nJ_nF_{n-\frac{1}{2}}Y_{n-1} - 59F_nJ_nF_{n+\frac{1}{2}}F_{n+1}F_{n-1}Y_{n-1}\\
&+ 101088F_nJ_nF_{n+1}Y_{n+1} + 3744F_nJ_nF_{n-1}Y_{n-1} + 2880F_nJ_nF_{n+\frac{1}{2}}Y_{n+1}\\
&+ 451F_nJ_nF_{n-\frac{1}{2}}F_{n+1}^2Y_{n+1} - 492F_nJ_nF_{n-\frac{1}{2}}F_{n+1}Y_{n-1}\\
&+ 3036F_nJ_nF_{n+\frac{1}{2}}F_{n-1}Y_{n-1} - 649F_nJ_nF_{n+\frac{1}{2}}F_{n+1}^2Y_{n+1}\\
&+ 708F_nJ_nF_{n+\frac{1}{2}}F_{n+1}Y_{n-1} - 3252F_nJ_nF_{n-\frac{1}{2}}F_{n-1}Y_{n-1} - 224640F_nJ_nY_{n+1}\\
&+ 708F_{n+\frac{1}{2}}F_{n+1}^2J_{n-1}Y_{n+1} - 27072F_{n+\frac{1}{2}}J_{n-1}F_{n+1}Y_{n+1}\\
&+ 27072F_{n+\frac{1}{2}}J_{n-1}F_nY_n + 84096F_{n+\frac{1}{2}}J_nF_{n+1}Y_{n+1}\\
&+ 3744F_{n-1}J_{n-1}F_{n+1}Y_{n+1} - 3744F_{n-1}J_{n-1}F_nY_n - 449280F_{n+1}J_{n+1}Y_n\\
&+ 224640F_{n+1}J_{n+1}Y_{n-1} - 451F_{n+1}^2J_{n+1}F_{n-\frac{1}{2}}F_nY_n\\
&- 41F_{n+1}^2J_{n+1}F_{n-\frac{1}{2}}F_{n-1}Y_{n-1} - 23040F_{n+1}J_{n+1}F_{n-\frac{1}{2}}Y_n\\
&- 33408F_{n+1}J_{n+1}F_{n-\frac{1}{2}}Y_{n-1} + 649F_{n+1}^2J_{n+1}F_{n+\frac{1}{2}}F_nY_n\\
&- 2880F_{n+\frac{1}{2}}J_{n+1}F_nY_n - 3456F_{n-\frac{1}{2}}J_{n+1}F_nY_n + 17256F_{n+\frac{1}{2}}F_nJ_nF_{n+1}Y_{n+1}\\
&+ 3036F_{n+\frac{1}{2}}F_{n-1}J_{n-1}F_{n+1}Y_{n+1} - 3036F_{n+\frac{1}{2}}F_{n-1}J_{n-1}F_nY_n\\
&+ 984F_{n-\frac{1}{2}}F_{n+1}^2J_nY_{n+1} + 23040F_{n-\frac{1}{2}}J_nF_{n+1}Y_{n+1}\\
&- 708F_{n+\frac{1}{2}}F_{n+1}J_{n-1}F_nY_n - 1416F_{n+\frac{1}{2}}F_{n+1}^2J_nY_{n+1} + 224640J_{n+1}F_nY_n\\
&- 492F_{n-\frac{1}{2}}F_{n+1}^2J_{n-1}Y_{n+1} + 492F_{n-\frac{1}{2}}F_{n+1}J_{n-1}F_nY_n\\
&- 3252F_{n-\frac{1}{2}}F_{n-1}J_{n-1}F_{n+1}Y_{n+1} - 224640J_{n-1}F_{n+1}Y_{n+1}\\
&+ 224640J_{n-1}F_nY_n + 3252F_{n-\frac{1}{2}}F_{n-1}J_{n-1}F_nY_n\\
&- 8184F_{n-\frac{1}{2}}F_nJ_nF_{n+1}Y_{n+1} + 41F_{n-\frac{1}{2}}F_{n+1}^2F_{n-1}J_{n-1}Y_{n+1}\\
&- 41F_{n-\frac{1}{2}}F_{n+1}F_{n-1}J_{n-1}F_nY_n + 33408F_{n-\frac{1}{2}}J_{n-1}F_{n+1}Y_{n+1}\\
&- 33408F_{n-\frac{1}{2}}J_{n-1}F_nY_n + 59F_{n+\frac{1}{2}}F_{n+1}F_{n-1}J_{n-1}F_nY_n\\
&- 59F_{n+\frac{1}{2}}F_{n+1}^2F_{n-1}J_{n-1}Y_{n+1})/(F_n(59F_{n+1}^2J_{n+1}F_{n+\frac{1}{2}}F_{n-1}Y_{n-1}\\
&+ 14976F_{n+1}J_{n+1}F_{n-1}Y_{n-1} + 8184F_{n+1}J_{n+1}F_{n-\frac{1}{2}}F_nY_n\\
&+ 492F_{n+1}^2J_{n+1}F_{n-\frac{1}{2}}Y_{n-1} - 984F_{n+1}^2J_{n+1}F_{n-\frac{1}{2}}Y_n\\
&- 3036F_{n+1}J_{n+1}F_{n+\frac{1}{2}}F_{n-1}Y_{n-1} - 17256F_{n+1}J_{n+1}F_{n+\frac{1}{2}}F_nY_n\\
&- 708F_{n+1}^2J_{n+1}F_{n+\frac{1}{2}}Y_{n-1} + 1416F_{n+1}^2J_{n+1}F_{n+\frac{1}{2}}Y_n\\
&+ 3252F_{n+1}J_{n+1}F_{n-\frac{1}{2}}F_{n-1}Y_{n-1} - 84096F_{n+1}J_{n+1}F_{n+\frac{1}{2}}Y_n\\
&+ 27072F_{n+1}J_{n+1}F_{n+\frac{1}{2}}Y_{n-1} + 41F_nJ_nF_{n-\frac{1}{2}}F_{n+1}F_{n-1}Y_{n-1}
\end{aligned}
$$

$$
\begin{aligned}
&+ 104832F_{n+1}J_{n+1}F_nY_n - 27072F_nJ_nF_{n+\frac{1}{2}}Y_{n-1} + 3456F_nJ_nF_{n-\frac{1}{2}}Y_{n+1}\\
&+ 33408F_nJ_nF_{n-\frac{1}{2}}Y_{n-1} - 59F_nJ_nF_{n+\frac{1}{2}}F_{n+1}F_{n-1}Y_{n-1}\\
&- 104832F_nJ_nF_{n+1}Y_{n+1} - 14976F_nJ_nF_{n-1}Y_{n-1} + 2880F_nJ_nF_{n+\frac{1}{2}}Y_{n+1}\\
&+ 451F_nJ_nF_{n-\frac{1}{2}}F_{n+1}^2Y_{n+1} - 492F_nJ_nF_{n-\frac{1}{2}}F_{n+1}Y_{n-1}\\
&+ 3036F_nJ_nF_{n+\frac{1}{2}}F_{n-1}Y_{n-1} - 649F_nJ_nF_{n+\frac{1}{2}}F_{n+1}^2Y_{n+1}\\
&+ 708F_nJ_nF_{n+\frac{1}{2}}F_{n+1}Y_{n-1} - 3252F_nJ_nF_{n-\frac{1}{2}}F_{n-1}Y_{n-1}\\
&+ 708F_{n+\frac{1}{2}}F_{n+1}^2J_{n-1}Y_{n+1} - 27072F_{n+\frac{1}{2}}J_{n-1}F_{n+1}Y_{n+1}\\
&+ 27072F_{n+\frac{1}{2}}J_{n-1}F_nY_n + 84096F_{n+\frac{1}{2}}J_nF_{n+1}Y_{n+1}\\
&- 14976F_{n-1}J_{n-1}F_{n+1}Y_{n+1} + 14976F_{n-1}J_{n-1}F_nY_n\\
&- 451F_{n+1}^2J_{n+1}F_{n-\frac{1}{2}}F_nY_n - 41F_{n+1}^2J_{n+1}F_{n-\frac{1}{2}}F_{n-1}Y_{n-1}\\
&- 23040F_{n+1}J_{n+1}F_{n-\frac{1}{2}}Y_n - 33408F_{n+1}J_{n+1}F_{n-\frac{1}{2}}Y_{n-1}\\
&+ 649F_{n+1}^2J_{n+1}F_{n+\frac{1}{2}}F_nY_n - 2880F_{n+\frac{1}{2}}J_{n+1}F_nY_n - 3456F_{n-\frac{1}{2}}J_{n+1}F_nY_n\\
&+ 17256F_{n+\frac{1}{2}}F_nJ_nF_{n+1}Y_{n+1} + 3036F_{n+\frac{1}{2}}F_{n-1}J_{n-1}F_{n+1}Y_{n+1}\\
&- 3036F_{n+\frac{1}{2}}F_{n-1}J_{n-1}F_nY_n + 984F_{n-\frac{1}{2}}F_{n+1}^2J_nY_{n+1}\\
&+ 23040F_{n-\frac{1}{2}}J_nF_{n+1}Y_{n+1} - 708F_{n+\frac{1}{2}}F_{n+1}J_{n-1}F_nY_n\\
&- 1416F_{n+\frac{1}{2}}F_{n+1}^2J_nY_{n+1} - 492F_{n-\frac{1}{2}}F_{n+1}^2J_{n-1}Y_{n+1}\\
&+ 492F_{n-\frac{1}{2}}F_{n+1}J_{n-1}F_nY_n - 3252F_{n-\frac{1}{2}}F_{n-1}J_{n-1}F_{n+1}Y_{n+1}\\
&+ 3252F_{n-\frac{1}{2}}F_{n-1}J_{n-1}F_nY_n - 8184F_{n-\frac{1}{2}}F_nJ_nF_{n+1}Y_{n+1}\\
&+ 41F_{n-\frac{1}{2}}F_{n+1}^2F_{n-1}J_{n-1}Y_{n+1} - 41F_{n-\frac{1}{2}}F_{n+1}F_{n-1}J_{n-1}F_nY_n\\
&+ 33408F_{n-\frac{1}{2}}J_{n-1}F_{n+1}Y_{n+1} - 33408F_{n-\frac{1}{2}}J_{n-1}F_nY_n\\
&+ 59F_{n+\frac{1}{2}}F_{n+1}F_{n-1}J_{n-1}F_nY_n - 59F_{n+\frac{1}{2}}F_{n+1}^2F_{n-1}J_{n-1}Y_{n+1})). \qquad (25)
\end{aligned}
$$

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