Comparison of Two Numerical Methods for the Integration of the Takagi-Taupin Equations

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Abstract

Two methods for the numerical resolution of the Takagi-Taupin equations are compared. It is shown that for a small integration step Taupin’s [Acta Cryst. (1967), 23, 25-35] extension to two dimensions of the one-dimensional Runge-Kutta third-order method is more accurate than the algorithm of Authier, Malgrange & Tournarie [Acta Cryst. (1968), A24, 126-136] but, for a given precision, Authier, Malgrange & Tournarie’s method is faster than Taupin’s so the former will usually be preferred for numerical calculation.

Introduction

Two methods have been used to solve numerically the Takagi-Taupin equations (Takagi, 1962, 1969; Taupin, 1964). One of them was proposed by Authier, Malgrange & Tournarie (1968), the other by Taupin (1967) and was an extension to two dimensions of the classical one-dimensional Runge-Kutta third-order method. It is therefore useful to find out which of these two methods is the better.

The Takagi-Taupin equations

These are hyperbolic equations with variable coefficients, which can be written as

\[ \frac{\lambda}{\pi} \frac{\partial D_H'}{\partial x_H} = \Psi_H D_0 + 2[\Delta \theta + \delta(\Delta \theta)] \sin 2\theta D_H' \]  
\[ \frac{\lambda}{\pi} \frac{\partial D_0'}{\partial x_0} = \Psi_{-H} D_H' , \]

where \( \delta(\Delta \theta) \) is generally a function of space coordinates, i.e., of \( x_H \) and \( x_0 \). We may shorten these equations and write

\[ \frac{\partial D_H'}{\partial x_H} = 2B' D_0 + 2W' D_H' \]
\[ = g[x_0, x_H, D_0(x_0, x_H), D_H(x_0, x_H)] \]  
\[ \frac{\partial D_0'}{\partial x_0} = 2A' D_H' = f[x_0, x_H, D_0(x_0, x_H), D_H(x_0, x_H)] , \]

where \( W' \) contains the term \( \delta(\Delta \theta) \) which depends on \( x_0 \) and \( x_H \), and where \( A' \) and \( B' \) are constant.

Analytical comparison of the precision of the two methods

Authier, Malgrange & Tournarie (1968) solve these equations by an extension of the one-dimensional half-step derivation method (Appendix 1). For one dimension, terms are neglected which are proportional to \( h^3 \), where \( h \) is the integration step. For two dimensions, the differential equations are integrated with the network shown in Fig. 1. \( D_0 \) and \( D_H \) being known at the entrance of the crystal. We shall only treat the Laue symmetrical case, where \( p = q \).

\( D_0 \) and \( D_H \) at point \( Q \) are computed with the values of \( D_0 \) and \( D_H \) at points \( M \) and \( N \) and the value of \( W' \) at the middle of \( MQ \), following the more complicated formulas (A2.13) and (A2.14) of Appendix 2. It is shown that this results in neglecting terms which are still proportional to \( p^3 \) (Appendix 2), where \( p \) is the integration step (Fig. 1).

On the other hand, it is well known that the one-dimensional Runge–Kutta third-order method neglects terms proportional to \( h^3 \), where \( h \) is the integration step (Appendix 3). One may hence hope that, if this method is extended to two dimensions, the algorithm will be more accurate than that of Authier, Malgrange & Tournarie (1968).

Taupin’s extension of the one-dimensional Runge–Kutta third-order method consists of the sequence of operations described in Appendix 4.

As in the one-dimensional Runge–Kutta calculation, it can be shown that this method neglects terms proportional to \( p^4 \), where \( p \) is the integration step (Appendix 5 and Fig. 2).

Fig. 1. Network of integration for the Takagi-Taupin equations by Authier, Malgrange & Tournarie’s (1968) method.
So, when the integration step is small enough, Taupin's method must be more accurate than Authier, Malgrange & Tournarie's method to solve numerically the Takagi–Taupin equations.

However, Taupin's algorithm is more complicated than that of Authier, Malgrange & Tournarie, and so the computation time must be longer. We shall determine, for a given precision, which of the two methods gives the shorter computation time.

### Numerical comparison of the precision and of the computation time of the two methods

We studied a Mo 220 reflexion on a perfect silicon-iron crystal. The incident wave was chosen to be of the form

\[ D_0 = A \exp\left(-\frac{\pi}{R_w} x^2\right), \]  

where \( x \) is the coordinate along the entrance surface of the crystal and \( R_w = 20 \mu m \). The physical input pencil width is then about 20 \( \mu m \), but we took into account a non-zero intensity 100 \( \mu m \) from the mid-point of the incident wave.

We then calculated the diffracted intensity at the exit surface of a perfect crystal (101.76 \( \mu m \) thick) for an integration step \( \text{ELEM} \) (Fig. 1) (0.1325 \( \mu m \)) very small when compared with the Pendellösung distance (14.6 \( \mu m \)). The results are nearly the same by both methods: the root of the mean-square difference between the two methods is \( \text{CQM} = 0.17 \times 10^{-5} \) (the intensity at the centre of the Borrmann fan is 0.1221 \( \times 10^{-1} \) by both methods). We took as a reference the results obtained for \( \text{ELEM} = 0.1325 \mu m \). We then made the computation for increasing integration steps \( \text{ELEM} \) and calculated the root \( \text{RQM} \) of the mean-square deviation between the intensities \( I_{\text{calc}} \) calculated for each step and the intensities of reference \( I_{\text{ref}} \).

\[
\text{RQM} = \left[ \frac{\sum (I_{\text{calc}} - I_{\text{ref}})^2}{N} \right]^{1/2}.
\]

The results are indicated in Table 1. It can be seen that, when integration steps are small, Taupin's method is more accurate than Authier, Malgrange & Tournarie's, but its computation time for a given integration step is slightly longer.

### Comparison of the computation times of each method for a given precision. Conclusion

To know which of the two methods is faster for a given precision, we have plotted on log log paper (Fig. 3) the

* We chose such an incident wave to avoid the problem of an infinite derivative of \( D_0 \) at the edges of the slit. If we had chosen \( D_0 \) constant at the entrance of the slit and zero elsewhere, Taupin's method would have given worse results on the edges of the Borrmann triangle than that of Authier, Malgrange & Tournarie, because the former uses higher-order derivatives. We verified this by computing the intensity at the exit surface of the crystal by the two methods (Nourtier, 1979).

### Table 1. Root RQM of the mean-square deviation between the intensities \( I_{\text{calc}} \) and the reference intensities \( I_{\text{ref}} \) and time of computation for both integration methods as a function of the integration step

<table>
<thead>
<tr>
<th>Integration step (( \mu m ))</th>
<th>AMT: Authier, Malgrange &amp; Tournarie (1968); T: Taupin (1967)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intensity at the centre of the Borrmann triangle</td>
<td>RQM</td>
</tr>
<tr>
<td>0.265</td>
<td>(0.1218 \times 10^{-1})</td>
</tr>
<tr>
<td>0.530</td>
<td>(0.1208 \times 10^{-1})</td>
</tr>
<tr>
<td>1.060</td>
<td>(0.1169 \times 10^{-1})</td>
</tr>
<tr>
<td>2.12</td>
<td>(0.1049 \times 10^{-1})</td>
</tr>
<tr>
<td>4.24</td>
<td>(0.8348 \times 10^{-2})</td>
</tr>
<tr>
<td>8.48</td>
<td>(0.3369 \times 10^{-2})</td>
</tr>
<tr>
<td>Time of computation (s)</td>
<td>(52.2)</td>
</tr>
<tr>
<td>(0.3956 \times 10^{-2})</td>
<td>(0.39 \times 10^{-4})</td>
</tr>
</tbody>
</table>
root RQM of the mean-square deviation as a function of the computation time. For a given RQM, the computation time is always a little longer by Taupin's method than by Authier, Malgrange & Tournarie's (1.15 times longer for RQM ≈ 10^{-3}, which gives a good precision). Since Authier, Malgrange & Tournarie's algorithm is easier than Taupin's one, the first of these methods seems preferable to integrate the Takagi-Taupin equations.

APPENDIX 1
If we want to solve the one-dimensional differential equation dy/dx = f(x, y), we can calculate y(x_0 + h) - y(x_0) by the formula

\[ y(x_0 + h) - y(x_0) = pf X_0 + -\frac{1}{2}y(x_0) + \frac{1}{2}y(x_0 + h) + O(h^3). \]

APPENDIX 2
The Takagi-Taupin equations are (Fig. 1)

\[ \frac{\partial D_0}{\partial x_0} = 2A'D'_H \]  
\[ \frac{\partial D_H}{\partial x_H} = 2B'D'_0 + 2W'D'_H. \]  

To solve these equations, Authier, Malgrange & Tournarie use the following method: multiply (A2.1) by \( p \) and (A2.2) by \( q \). One gets

\[ p \frac{\partial D'_0}{\partial x_0} = 2AD'_H \]  
\[ q \frac{\partial D'_H}{\partial x_H} = 2BD'_0 + 2WD'_H. \]  

where \( A = pA' \), \( B = qB' \), \( W = qW' \).

By neglecting terms proportional to the cube of the integration step, one may write

\[ p \frac{\partial}{\partial x} f(x + \frac{p}{2}) = p \left( \frac{\partial f}{\partial x} \right) \left( x + \frac{p}{2} \right); \]

If we introduce this formula into (A2.3) and (A2.4), we get

\[ p \frac{\partial}{\partial x_0} D'_0 \left( x_0 - \frac{p}{2}, x_H \right) = D'_0(x_0, x_H) - D'_0(x_0 - p, x_H) + O(p^3) \]  
\[ q \frac{\partial}{\partial x_H} D'_H \left( x_0, x_H - \frac{q}{2} \right) = D'_H(x_0, x_H) - D'_H(x_0, x_H - q) + O(q^3). \]

Moreover, (A2.3) and (A2.4) imply that

\[ p \frac{\partial}{\partial x_0} D'_0 \left( x_0 - \frac{p}{2}, x_H \right) = 2AD'_H \left( x_0 - \frac{p}{2}, x_H \right) \]  
\[ q \frac{\partial}{\partial x_H} D'_H \left( x_0, x_H - \frac{q}{2} \right) = 2BD'_0 \left( x_0, x_H - \frac{q}{2} \right) + 2W \left( x_0, x_H - \frac{q}{2} \right) D'_H \left( x_0, x_H - \frac{q}{2} \right). \]

If we compare (A2.5), (A2.6) with (A2.7), (A2.8), we get

\[ D'_0(x_0, x_H) = D'_0(x_0 - p, x_H) + 2AD'_H \left( x_0 - \frac{p}{2}, x_H \right) + O(p^3) \]  
\[ D'_H(x_0, x_H) = D'_H(x_0, x_H - q) + 2BD'_0 \left( x_0, x_H - \frac{q}{2} \right) + 2W \left( x_0, x_H - \frac{q}{2} \right) D'_H \left( x_0, x_H - \frac{q}{2} \right) + O(q^3). \]

To eliminate

\[ D'_H \left( x_0 - \frac{p}{2}, x_H \right), D'_0 \left( x_0, x_H - \frac{q}{2} \right) \]

and

\[ D'_H \left( x_0, x_H - \frac{q}{2} \right), \]
we make the approximation
\[ 2f \left( x + \frac{p}{2} \right) = f(x) + f(x + p). \]

We then neglect terms which are proportional to \( p^2 \). But
\[ D'_H \left( x_0 - \frac{p}{2}, x_H \right), D' \left( x_0, x_H - \frac{q}{2} \right) \]
and
\[ D'_H \left( x_0, x_H - \frac{q}{2} \right) \]
are respectively multiplied by \( A, B \) and \( W \), which are proportional to \( p \) or \( q \). In equations (A2.9) and (A2.10) we then neglect terms proportional to \( p^3 \) or \( q^3 \). We obtain
\[ D'(X_0, X_n) = D'(X_0 - p, X_H) + AD'(X_0, X_H) \]
\[ + BD'(X_0, X_H - q) + O(p^3) \]  
\[ \text{and} \]
\[ D''(X_0, X_n) = D''(X_0, X_H - q) + BD'(X_0, X_H) + W \left( x_0, x_H - \frac{q}{2} \right) D'(x_0, x_H) \]
\[ + W \left( x_0, x_H - \frac{q}{2} \right) D'(x_0, x_H - q) + O(q^3). \]  
(A2.12)

By solving this system of two equations with two unknowns \( D'(x_0, x_H) \) and \( D''(x_0, x_H) \), we obtain the result
\[ dD'(x_0, x_H) = AD'(x_0 - p, x_H) + AC'D'(x_0, x_H) \]
\[ + BD'(x_0, x_H - q) + AC'BD'(x_0, x_H - q) \]  
\[ \text{and} \]
\[ dD''(x_0, x_H) = BD'(x_0 - p, x_H) + CD'D'(x_0, x_H) \]
\[ + C'D'(x_0, x_H - q) + BD'(x_0, x_H - q), \]  
(A2.13)

where
\[
C_1 = 1 + W \left( x_0, x_H - \frac{q}{2} \right) \\
C_2 = 1 - W \left( x_0, x_H - \frac{q}{2} \right) \\
d = C_2 - AB.
\]

One can easily verify that the neglected terms are proportional to the cube of the integration step.

One may easily see by another way that the neglected terms are proportional to \( p^3 \) to calculate \( D'_0 \) and \( D''_H \) in \( Q \) (Fig. 1), one only uses the values of \( D'_0 \) and \( D''_H \) in \( M \) and \( N \) (and the value of \( W \) at the middle of \( M \), \( Q \)). So one can approximate the values of \( \partial D'_0 / \partial t \) and \( \partial D''_H / \partial t \), but not the values of \( \partial^2 D'_0 / \partial t^2 \) and \( \partial^2 D''_H / \partial t^2 \). If we wanted to calculate \( D'_0 \) and \( D''_H \) in \( Q \) to third order, we should know \( \partial^3 D'_0 / \partial t^2 \partial z \) and \( \partial^3 D''_H / \partial t^2 \partial z \), which we cannot find by the method used [two points \( M \) and \( N \) only along \( Ot \) (Fig. 1)]. So we can only calculate \( D'_0 \) and \( D''_H \) in \( Q \) to second order, and we neglect terms which are proportional to \( p^3 \).

### APPENDIX 3

We find in the book written by Mineur (1966) a description of a one-dimensional Runge–Kutta third-order method.

If we want to solve the equation \( dy/dx = f(x, y) \), we can calculate \( y(x_0 + h) - y(x_0) \) by the formula
\[ y(x_0 + h) - y(x_0) = \frac{h}{6} \left( k_1 + 4k_2 + k_3 \right) + O(h^4), \]
where
\[
k_1 = hf(x_0, y_0) \\
k_2 = hf \left( x_0 + \frac{h}{2}; \; y_0 + \frac{1}{2}k_1 \right) \\
k_3 = hf(x_0 + h; \; y_0 - k_1 + 2k_2). \]

### APPENDIX 4

We shall extend to two dimensions the one-dimensional Runge–Kutta third-order method described in Appendix 3. We wish to solve equations (3) and (4) of the main paper. To outline the fact that \( x_0 \) and \( x_H \) are independent variables, let us call \( x_0 = x \) and \( x_H = y \). Equations (3) and (4) become
\[ \frac{\partial D'_H}{\partial y} = f[x, y, D'_0(x, y), D''_0(x, y)] \]  
\[ \frac{\partial D'_0}{\partial x} = g[x, y, D'_0(x, y), D''_0(x, y)]. \]  
(A4.1)

Let us integrate \( D''_H \) along the direction \( y \): we need derivations which use the function \( g \) (formula A4.1). The analogue of \( k_1 \) (Appendix 3) is
\[ pg[1, D'_0(1), D''_0(1)] \]
(Fig. 2). The analogue of \( k_2 \) (Appendix 3) is
\[ pg(4, D'_0(2) + \frac{p}{2} f[2, D'_0(2), D''_0(2), D''_0(1)]) \]
\[ + \frac{p}{2} g[1, D'_0(1), D''_0(1)]. \]  
(A4.4)

The analogue of \( k_3 \) (Appendix 3) is
\[ pg(7, D'_0(3) - pg[3, D'_0(3), D''_0(3)]) \]
\[ + 2pf \left\{ 5, D'_0(3) + \frac{p}{2} f[3, D'_0(3), D''_0(3)], D''_0(2) + \frac{p}{2} g[2, D'_0(2), D''_0(2)] \right\}. \]
THE INTEGRATION OF THE TAKAGI-TAUPIN EQUATIONS

\[ D_h'(1) - pg[1, D_0(1), D_h'(1)] \]
\[ + 2pg \left\{ 4, D_0(2) + \frac{p}{2} f[2, D_0(2), D_h'(2)] \right\} \]
\[ D_h'(1) + \frac{p}{2} g[1, D_0(1), D_h'(1)] \). \] (A4.5)

We finally get
\[ D_h'(7) = D_h'(1) + \frac{p}{6} (k_1 + 4k_2 + k_3). \] (A4.6)

APPENDIX 5

We have described Taupin's extension of the one-dimensional Runge-Kutta third-order method in Appendix 4.

For the sake of simplicity, the Takagi-Taupin equations (3) and (4) can be written as
\[
\begin{align*}
\frac{\partial u}{\partial x} &= f(x, y, u, v) \tag{A5.1} \\
\frac{\partial v}{\partial y} &= g(x, y, u, v), \tag{A5.2}
\end{align*}
\]
where \( D_0 = u, D_h = v, x_0 = x, x_h = y \); Taupin's method consists of writing (Fig. 2 and Appendix 4)
\[
\begin{align*}
v(x_0, y_0) &= v(x_0, y_0 - p) \\
+ p \left( g(x_0, y_0 - p, u_{x_0 - p}, v_{x_0 - p}) \right) \\
+ 4g \left( x_0, y_0 - \frac{p}{2} u_{x_0 - p/2, y_0 - p/2} \right) \\
+ \frac{p}{2} f_{x_0 - p/2, y_0 - p/2} v_{x_0 - p/2} \\
+ \frac{p}{2} g_{x_0 - p} \\
+ g \left( x_0, y_0 - p, u_{x_0 - p}, v_{x_0 - p} \right) \\
+ p \left[ 2f \left( x_0 - \frac{p}{2}, y_0, u_{x_0 - p}, y_0 \right) \right] \\
+ \frac{p}{2} f_{x_0 - p, y_0} v_{x_0 - p/2, y_0 - p/2} \\
+ p \left[ \frac{g_{x_0 - p/2}}{2} \left( x_0 - p, y_0, u_{x_0 - p}, v_{x_0 - p, y_0} \right) \right]. \tag{A5.3}
\end{align*}
\]

By expanding this expression up to third order in \( p \), one obtains
\[
\begin{align*}
t(x_0, y_0) - t(x_0, y_0 - p) &= pg(x_0, y_0 - p) \\
+ \frac{p^2}{2} \left( g_{y} + g_{y} u_y + g_{y} v_y \right) \\
+ \frac{p^3}{6} \left( g_{y}^2 + g_{y} u_y^2 + g_{y} v_y^2 \right) \\
+ 2g_{y} u_y g + 2g_{y} v_y g + 2g_{y} u_y^2 + 2g_{y} v_y^2 + g_{y}^2 g + O(p^4).
\end{align*}
\]

This expression is exactly, up to third order, Taylor's expansion of the function \( t(x, y) \) relative to \( y \) near the point \((x_0, y_0 - p)\). So, when we use Taupin's method to integrate the Takagi-Taupin equations, we neglect terms proportional to \( p^4 \).

References


