Explicit integration method for the time-dependent Schrodinger equation for collision problems

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To date, only the implicit (Crank–Nicholson) integration method has ben used for numerical integration of the Schrodinger equation for collision processes. The standard explicit methods are known to be unstable and a high price is paid for the implicit method due to the inversion of the large matrices involved. Furthermore, the method is prohibitive in more than two dimensions due to restrictions on memory and large computation times. An explicit method (i.e., a method which doesn't require the solution of simultaneous equations) is presented, and is shown to be stable in n dimensions to the same order of accuracy as the implicit method with the unitarity being secured to two orders higher accuracy than that for the wave function.

I. INTRODUCTION

Currently, the only successful method used in the integration of the time-dependent Schrödinger equation for the complex valued wave function is the implicit Crank–Nicholson method, since this method is known to be stable.[1-3] However, in this method large matrices need to be inverted; although they are banded, the inversion of these matrices gets to be prohibitively expensive as the number of unknowns gets larger. To date, only one and two dimensional problems in space have been solved by means of direct integration.[2,3]

Explicit integration schemes which do not require the repeated solution of a large system of equations are clearly more desirable, provided that they can be shown to be stable. The absence of such a stable explicit scheme in the quantum mechanics literature has led to the present usage of implicit schemes.

In this paper an explicit integration method is presented for the time-dependent Schrödinger equation that is stable, has the same degree of accuracy as the implicit Crank–Nicholson method, is straight forward and simple, and is applicable in n dimensions without extensive memory requirements.

II. THE EXPLICIT CRUDE EULER AND IMPLICIT CRANK-NICHOLSON METHODS

Consider the time-dependent Schrödinger equation in one-space dimension, in the units $m = \hbar = 1$

$$\partial\psi/\partial t = -iH\psi ,\qquad (2.1)$$

where

$$H = -\tfrac{1}{2}(\partial^2/\partial x^2) + V .\qquad (2.2)$$

The time evolution operator

$$U(\Delta t) = e^{-i\Delta t H}\qquad (2.3)$$

has the property

$$\psi^n = U^n(\Delta t)\,\psi^0 ,\qquad (2.4)$$

where $\psi^n \equiv \psi_{t=n\Delta t}$. In particular

$$\psi^{n+1} = e^{-i\Delta t H}\,\psi^n , \qquad \psi^{n-1} = e^{i\Delta t H}\,\psi^n .\qquad (2.5)$$

The simplest method is to expand $e^{-i\Delta t H}$ into a Taylor series and keep the leading terms. Thus,

$$\psi^{n+1} = (1 - i\Delta t H)\,\psi^n .\qquad (2.6)$$

To discretize the differential system above, the notation ψ_j^n is adopted where the superscript indicates the time step and the subscript the values of the function at the location x_j. Thus,

$$\psi_j^n \equiv \psi(x_j, t_n) .\qquad (2.7)$$

An expression correct to $0(\Delta x^2)$ for the second space derivative for an equally spaced mesh is

$$\left.\frac{\partial^2\psi}{\partial x^2}\right|_j^n = \frac{\psi_{j+1}^n + \psi_{j-1}^n - 2\psi_j^n}{\Delta x^2} .\qquad (2.8)$$

Substitution of Eq. (2.8) into Eq. (2.1) yields

$$\psi_j^{n+1} = [1 - i(2\alpha + V_j\Delta t)]\,\psi_j^n + i\alpha(\psi_{j+1}^n + \psi_{j-1}^n) ,\qquad (2.9)$$

where

$$\alpha = \tfrac{1}{2}(\Delta t/\Delta x^2) .\qquad (2.10)$$

Defining the ψ^n as the vector having the ψ_j^n as its components, the system of equations in (2.9) takes the form

$$\psi^{n+1} = \mathbf{A} \cdot \psi^n ,\qquad (2.11)$$

where the matrix $\mathbf{A}$ is easily deduced from Eq. (2.9).

This scheme is called the one-step forward or the "Crude Euler" method. It is an explicit scheme as the function at any time step is calculated in terms of the known values of the function at past time(s) without the need to solve a system of equations. In order to study the numerical stability of this system of equations according to the Courant–Levi–Fredrichs criterion,[4] consider the error

$$\epsilon_j^n = \hat{\epsilon}^n \exp(iq x_j)\qquad (2.12)$$

in ψ_j^n and consider the evolution of this error by computing the error ϵ_j^{n+1} in ψ_j^{n+1}. Thus, introducing $\psi_j^n + \epsilon_j^n$ and $\psi_j^{n+1} + \epsilon_j^{n+1}$ into Eq. (2.5) one has

$$\hat{\epsilon}^{n+1} = \{1 - i[2\alpha(1 - \cos q\Delta x) + V_j\Delta t]\}\hat{\epsilon}^n .\qquad (2.13)$$

The ratio $\hat{\epsilon}^{n+1}/\hat{\epsilon}^n$ is called the growth factor g; thus,

$$g = 1 - i[2\alpha(1 - \cos q\Delta x) + V_j\Delta t] .\qquad (2.14)$$

$|g| > 1$ is a sufficient condition for numerical instability. Indeed, in this case

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$$|g|^2 = 1 + [2\alpha(1 - \cos q\Delta x) + V_j ht]^2 > 1 \qquad (2.15)$$

for all wave numbers q of the errors. Consequently the explicit scheme in Eq. (2.9) along with several others[1,2] may not be used in intergrating the Schrodinger equation.

The basic difficulty in the scheme in Eq. (2.9) is that it is not centered; i.e., while the right-hand side is calculated at time step n to accuracy Δt, the left-hand side is a derivative at time step $n + \frac{1}{2}$ to accuracy Δt^2. It is this noncentered aspect that causes the instability of the numerical scheme.

The Crank–Nicholson scheme is based on eliminating ψ^n between the two equations (2.5) to obtain the identity

$$e^{i\Delta t H} \psi^{n+1} = e^{-i\Delta t H} \psi^{n-1} \quad . \qquad (2.16)$$

The discretization in time is obtained by the leading terms of the Taylor series expansion of $e^{\mp i\Delta t H}$

$$(1 + i\Delta t H) \psi^{n+1} = (1 - i\Delta t H) \psi^{n-1} \quad . \qquad (2.17)$$

Further expressing $H\psi_j^{n+1}$ in finite differences according to Eq. (2.8) as

$$H\psi_j^{n+1} = -\tfrac{1}{2}(\psi_{j+1}^{n+1} + \psi_{j-1}^{n+1} - 2\psi_j^{n+1})/\Delta x^2 + V_j \psi_j^{n+1} \quad , \qquad (2.18)$$

yields the Crank–Nicholson scheme

$$[1 + i(2\alpha + V_j \Delta t)] \psi_j^{n+1} - i\alpha(\psi_{j+1}^{n+1} + \psi_{j-1}^{n+1})$$
$$= [1 - i(2\alpha + V_j \Delta t)] \psi_j^{n-1} + i\alpha(\psi_{j+1}^{n-1} + \psi_{j-1}^{n-1}) \quad . \qquad (2.19)$$

Similar to Eq. (2.11), defining the ψ^{n+1} as the vector with components ψ_j^{n+1}, Eq. (2.19) reads

$$\mathbf{A} \cdot \psi^{n+1} = \mathbf{B} \cdot \psi^{n-1} \quad , \qquad (2.20)$$

where $\mathbf{B} = \mathbf{A}^*$ and the elements of A and B are easily deduced from Eq. (2.19). The scheme in Eq. (2.19) is an "implicit" integration scheme as a system of equation is needed to be solved, i.e., the matrix A needs to be inverted in order to calculate ψ^{n+1}. The stability analysis along the previous steps, yields the growth factor to be

$$g = \frac{1 - i[2\alpha(1 - \cos q\Delta x) + 2V_j\Delta t]}{1 + i[2\alpha(1 - \cos q\Delta x) + 2V_j\Delta t]} \quad , \qquad (2.21)$$

and thus

$$|g| = 1 \quad . \qquad (2.22)$$

Consequently, the errors will not grow exponentially.

The above scheme is implicit in the sense that unknown values of the function at various points in the mesh are coupled with each other. Consequently the system of algebraic Eqs. (2.20) needs to be solved.

For the accuracy, the Taylor series expansions of (2.19) yields

$$(\dot\psi + iH\psi) + \frac{\Delta t^2}{2}(\tfrac{1}{3}\dddot\psi + iH\ddot\psi) - i\frac{\Delta x^2}{6}\frac{\partial^4\psi}{\partial x^4} + \cdots = 0 \qquad (2.23)$$

Consequently, the accuracy of the system of difference Eqs. (2.9) with $\alpha = \Delta t/2\Delta x^2 = O(1)$, is $O(\Delta x^4)$.

In order to study the unitarity of the scheme, rewrite Eq. (2.17) as

$$\psi^{n+1} = L \psi^{n-1} \quad , \qquad (2.24)$$

where

$$L = (1 + i\Delta t H)^{-1} (1 - i\Delta t H) \quad . \qquad (2.25)$$

Consider now the adjoint L^+ of L

$$L^+ = (1 + i\Delta t H)(1 - i\Delta t H)^{-1} \quad , \qquad (2.26)$$

where use is made of the self adjointness of H, i.e., of $H^+ = H$. The unitarity of L is determined by the study of

$$L L^+ = (1 + i\Delta t H)^{-1}(1 - i\Delta t H)(1 + i\Delta t H)(1 - i\Delta t H)^{-1} \quad . \qquad (2.27)$$

Since $(1 - i\Delta t H)$ and $(1 + i\Delta t H)$ commute,

$$L L^+ = (1 + i\Delta t H)^{-1}(1 + i\Delta t H)(1 - i\Delta t H)(1 - i\Delta t H)^{-1} = I \quad . \qquad (2.28)$$

This latter result is obtained by noting that $(1 + i\Delta t H)^{-1} \times (1 + i\Delta t H) = I$ and $(1 - i\Delta t H)(1 - i\Delta t H)^{-1} = I$, where I is the identity operator. Consequently,

$$(\psi^{n+1}, \psi^{n+1}) = (L\psi^{n-1}, L\psi^{n-1}) = (L^+ L\psi^{n-1}, \psi^{n-1}) = (\psi^{n-1}, \psi^{n-1}) \quad . \qquad (2.29)$$

III. A STABLE EXPLICIT SCHEME

Within the above framework, unlike in the Crank–Nicholson method, keeping ψ^n in the pair of Eqs. (2.5) and subtracting one equation from the other yields the identity

$$\psi^{n+1} - \psi^{n-1} = (e^{-i\Delta t H} - e^{i\Delta t H}) \psi^n \quad . \qquad (3.1)$$

Similarly, the expansion of $e^{\mp i\Delta t H}$ into a Taylor series to the same number of terms as in obtaining Eq. (2.6) yields

$$\psi^{n+1} = -2 i\Delta t H \psi^n + \psi^{n-1} \quad . \qquad (3.2)$$

The proposed numerical method is achieved by a finite difference expression of $H\psi$ as in Eq. (2.8) to get

$$\psi_j^{n+1} = -2i[(2\alpha + V_j\Delta t) \psi_j^n - \alpha(\psi_{j+1}^n + \psi_{j-1}^n)] + \psi_j^{n-1} \quad . \qquad (3.3)$$

By the definition of the vector ψ^n with components ψ_j^n, (3.3) reads

$$\psi^{n+1} = \mathbf{A} \cdot \psi^n + \psi^{n-1} \quad . \qquad (3.4)$$

This scheme is an explicit one as the state of the system at time step $(n + 1)$ is directly calculated in terms of the states at past times without the need to invert an equation. Equation (3.4) should be contrasted with the implicit Crank–Nicholson scheme (2.20).

The stability analysis of this scheme along the same steps as above yields the following equation for the growth factor g

$$g^2 + 2i[2\alpha(1 - \cos q\Delta x) + V_j\Delta t]g - 1 = 0 \quad . \qquad (3.5)$$

Two growth factors g_1 and g_2 are obtained from the quadratic equation above as

$$g_{1,2} = -i[2\alpha(1 - \cos q\Delta x) + V_j\Delta t]$$
$$\pm \{1 - [2\alpha(1 - \cos q\Delta x) + V_j\Delta t]^2\}^{1/2} \quad . \qquad (3.6)$$

Consequently, just as for the implicit Crank–Nicholson method, one has for both g_1 and g_2

$$|g_1|^2 = |g_2|^2 = 1 \quad . \qquad (3.7)$$

The stability of the proposed explicit scheme is seen to be governed by the same criterion as the Crank–Nicholson method. As for the accuracy, Taylor series

expansion (3.3) near t_n yields

$$(\dot{\psi} + iH\psi) + \frac{\Delta t^2}{6}\dddot{\psi} + i\frac{\Delta x^2}{24}\frac{\partial^4\psi}{\partial x^4} + \cdots = 0 \ . \tag{3.8}$$

Consequently, the accuracy of this scheme is of the same order of magnitude as for the Crank–Nicholson scheme, i.e., $O(\Delta x^4)$ and this explicit method is shown to be stable.

In order to study the unitarity of the scheme, in Eq. (3.3) eliminate ψ^n by substituting it with the exact equivalent $e^{i\Delta tH}\psi^{n-1}$. Thus, Eq. (3.3) yields

$$\psi^{n+1} = (1 - 2i\Delta t\, e^{-i\Delta tH})\psi^{n-1} \ . \tag{3.9}$$

With the definition

$$L = 1 - 2i\Delta t\, e^{-i\Delta tH} \ , \tag{3.10}$$

the adjoint operator is

$$L^* = 1 + 2i\Delta t\, e^{i\Delta tH} \ ,$$

where use is made of the self adjointness of H, i.e., of $H^* = H$. With L and L^* as above

$$L^*L = 1 - 4\Delta tH\sin\Delta tH + 4\Delta t^2 H^2 \ . \tag{3.11}$$

Expanding the $\sin\Delta tH$ into a Taylor series, Eq. (3.11) yields

$$L^*L = 1 + (4/3!)\Delta t^4 H^4 \ . \tag{3.12}$$

Consequently,

$$\begin{aligned}(\psi^{n+1},\ \psi^{n+1}) &= (L\psi^{n-1},\ L\psi^{n-1}) = (\psi L\psi^{n-1},\ \psi^{n-1})\\ &= (\psi^{n-1},\ \psi^{n-1}) + \tfrac{2}{3}\Delta t^4(H^2\psi^{n-1},\ H^2\psi^{n-1}) \ .\end{aligned} \tag{3.13}$$

Therefore, the scheme here is not strictly unitary. However, the unitarity is secured to order Δt^4, i.e., to $O(\Delta x^8)$ with $\alpha = \Delta t/2\Delta x^2 = O(1)$. Thus, such an error in the norm is acceptable as it is four orders of magnitude less than that of the scheme. Furthermore, the error will not cumulate since the scheme is stable. Consequently, it appears that the sacrifice in the strict unitarity is well compensated by the implicit aspect of the method.

It is worth noting that the scheme here is known to be unstable for the heat diffusion (i.e., parabolic) equation[4] which bears a resemblance to the Schrödinger equation, with the first order time derivative and second order spatial derivative. However, the imaginary number $i \equiv \sqrt{-1}$ in the Schrödinger equation changes the character of the differential equation and results in the corresponding numerical scheme being stable.

IV. MULTIDIMENSIONAL CASE

For the scheme in p dimensions, let

$$\psi[\mathbf{x}(j),\ t_n] \equiv \psi_j^n \tag{4.1}$$

The finite difference analog of the Laplace operator correct to $(\Delta x)^2$ is

$$\nabla^2\psi\big|_j^n = \sum_{l=1}^{p}(\psi_{j_1},\ldots{}_{j_l+1},\ldots{}_{j_p} + \psi_{j_1}^n,\ldots{}_{j_l-1},\ldots{}_{j_p}$$
$$- 2\psi_{j_1}^n,\ldots{}_{j_l},\ldots{}_{j_p})\Delta x_l^2 \ . \tag{4.2}$$

Using Eq. (4.2) in $H\psi = -\tfrac{1}{2}\nabla^2\psi + V\psi$ leads to the explicit scheme in p dimensions

$$\psi_j^{n+1} = \psi_j^{n-1} - i2\left[\left(2\sum_{l=1}^{p}\alpha_l + V_j\Delta t\right)\psi_j^n\right.$$
$$\left. - \sum_{l=1}^{p}\alpha_l(\psi_{j_1}^n,\ldots{}_{j_l+1},\ldots{}_{j_p} + \psi_{j_1}^n,\ldots{}_{j_l-1},\ldots{}_{j_p})\right] \ , \tag{4.3}$$

where

$$\alpha_l = \tfrac{1}{2}(\Delta t/\Delta x_l^2) \ . \tag{4.4}$$

For errors of the form

$$\epsilon_j^n = \hat{\epsilon}^n\exp\left(i\sum_{l=1}^{p}q_l x_l(j)\right) \ , \tag{4.5}$$

the equation for the growth factor, as a generalization of Eq. (3.5), is

$$g^2 + 2i\left(2\sum_{l=1}^{p}\alpha_l(1 - \cos q_l\Delta x_l) + V_j\Delta t\right)g - 1 = 0 \ . \tag{4.6}$$

Consequently, as in Eq. (3.6), the scheme is stable since $|g|_1 = |g|_2 = 1$.

In particular, in two space dimensions, Eq. (4.3) reduces to

$$\begin{aligned}\psi_{j,k}^{n+1} = \psi_{j,k}^{n-1} &- 2i\{[2(\alpha_x + \alpha_y) + V_{j,k}\Delta t]\psi_{j,k}^n\\ &- \alpha_x(\psi_{j+1,k}^n + \psi_{j-1,k}^n) - \alpha_y(\psi_{j,k+1}^n + \psi_{j,k-1}^n)\} \ , \tag{4.7}\end{aligned}$$

and in three space dimensions, to

$$\begin{aligned}\psi_{j,k,l}^{n+1} = \psi_{j,k,l}^{n-1} &+ 2i\{[2(\alpha_x + \alpha_y + \alpha_z) + V_{j,k,l}]\psi_{j,k,l}^n\\ &- \alpha_x(\psi_{j+1,k,l}^n + \psi_{j-1,k,l}^n) - \alpha_y(\psi_{j,k+1,l}^n + \psi_{j,k-1,l}^n)\\ &- \alpha_z(\psi_{j,k,l+1}^n + \psi_{j,k,l-1}^n)\} \ . \tag{4.8}\end{aligned}$$

To be able to use the proposed scheme, at $t = 0$ a projection is made for $t = \Delta t$ by any scheme (implicit or explicit) correct to $O(\Delta t^2)$. From this point on the scheme (4.3) is used to calculate the evolution of the function ψ in time.

V. APPLICATION

In the use of the scheme in (3.3) complex algebra may be used directly. However, in many computations real algebra may be preferred. In this case let

$$\psi(x, t) \equiv u(x, t) + iv(x, t) \ , \tag{5.1}$$

where u and v are real functions. Separating the real and imaginary parts of Eq. (3.3), one has

$$\begin{aligned}u_j^{n+1} &= u_j^{n-1} - 2[\alpha(v_{j+1}^n + v_{j-1}^n) - 2(\alpha + V_j\Delta t)v_j^n]\\ v_j^{n+1} &= v_j^{n-1} + 2[\alpha(u_{j+1}^n + u_{j-1}^n) - 2(\alpha + V_j\Delta t)u_j^n] \ .\end{aligned} \tag{5.2}$$

The p dimensional generalization of Eq. (5.2) after Eq. (4.12) being straightforward, is not given.

The proposed scheme is tried out by repeating the calculations of Weiner and Askar[3] for the evolution of a Gaussian wave packet in two dimensions subject to a potential barrier with a saddle point. As in Ref. 3, the problem is defined by the potential $V(x, y) = 16 - x^2 + y^2$ and the initial condition on the wave packet as

TABLE I. Values of the norm of the wave function $\iint |\psi(x, y, t)|^2 dx\,dy$.

Time (a.u.)	$\Delta x = \Delta y = 0.4$ $\Delta t = 0.01$	$\Delta x = \Delta y = 0.2$ $\Delta t = 0.0025$	$\Delta x = \Delta y = 0.1$ $\Delta t = 0.002$
0	0.999997	0.999989	0.999957
0.1	0.971144	0.998881	1.00077
0.2	1.02808	1.00279	1.00169
0.3	1.00987	1.00094	1.00058
0.4	1.01076	1.00108	1.00064
0.5	1.01081	1.00105	1.00062
0.6	1.01035	1.00104	1.00057
0.7	1.00826	1.00103	1.00048
0.8	1.01306	1.00099	1.00029
0.9	1.03572	1.00099	1.00003
1.0	1.00377	1.00135	1.00068
1.1	0.962018	1.00318	1.00567
1.2	1.04890	1.00929	1.00576
1.3	1.01598	1.01830	1.00097
1.4	0.983113	1.02103	1.01819
1.5	1.03650	1.03082	1.01454
1.6	0.985156	1.05666	1.01514
CPU time	0.81 s	10.8 s	61.7 s
CPU time/step	0.005	0.017	0.077
Number of mesh points	$31 \times 16 = 496$	$61 \times 31 = 1891$	$121 \times 61 = 7381$
CPU time/step– mesh points	10^{-5}	10^{-5}	10^{-5}

$\psi(x, 0)$

$$= \exp\{-\tfrac{1}{4}[\chi_{11}(x - x_0)^2 + 2\chi_{12}(x - x_0)(y - y_0) + \chi_{22}(y - y_0)^2]\}$$
$$\times \exp\{-i[p_0(x - x_0) + q_0(y - y_0)]\}/(2\chi^{1/2})^{-1/2} , \qquad (5.3)$$

with

$$\chi_{11} = 3/16, \quad \chi_{12} = 3/16, \quad \chi_{22} = -3/16,$$
$$\chi = |\chi_{11}\chi_{22} - \chi_{12}^2| = \sqrt{2}\,(3/16)$$
$$x_0 = -4, \quad y_0 = 0, \quad p_0 = \sqrt{6}, \quad q_0 = 0 .$$

This problem corresponds to the scattering of a Gaussian wave packet centered at (-4.0) and oriented at $45°$ and having a translational energy of 75% of the barrier energy. In the calculations in atomic units with $m = \hbar = 1$, a rectangular space $\{-8 \le x \le 4, \; 3 \le y \le 3\}$ is used with a mesh spacing of 0.4, 0.2, and 0.1 with time steps of 0.010, 0.0025, and 0.0020, respectively, for three sets of calculations. The scheme is observed to be stable and the norm is conserved to an accuracy $\le 10^{-2}$ as seen in Table I. The evolution of the collision is illustrated in Figs. 4 and 5 of Ref. 3 and it is seen that $t = 1.6$ is practically the end of the collision. The computer time requirements are, respectively, 0.005, 0.017, and 0.077 s for each time step and 0.81, 10.8, and 61.7 s for the complete calculations on Princeton University's IBM 360/91. For comparison, consider the excellent calculations of McCullough and Wyatt[2] utilizing the implicit Crank–Nicholson method. In these, 10^4 mesh points are involved and the computation time is reported to be 11 s on CDC 6600 for each time step. For the set of calculations reported here 31×16, 61

$\times 31$, and 121×61 mesh points are used. Since no matrix inversions are required the computational effort increases linearly with the number of points as is also seen in the results presented in Table I. Consequently, for the same number of 10^4 mesh points the computation time may be reasonably estimated to be 0.1 s. Considering that the speed CDC 6600 is comparable to that of the IBM 360/91, this scheme is seen to be significantly (i.e., at least two orders of magnitude) faster than the implicit method. Calculations similar to those of McCullough and Wyatt[2] were reported recently by Zuhrt, Kamal, and Zulicke[5] and by Kellerhals, Sathyamurty, and Raff,[6] each using 10^4 mesh points. The computation time for Ref. 5 is not reported, while that of Ref. 6 was 1.7 min for each time step on IBM 360/65. With proper computer speed adjustments, the times involved in this latter work are estimated to be equal to those in Ref. 2.

VI. DISCUSSION

The importance of the explicit scheme presented here lies primarily in its applicability in two and higher dimensions. In the implicit schemes the matrices involved are almost unmanageable and difficult to visualize in more than two dimensions. In fact, on one- two- and three-space dimensions, the Crank–Nicholson scheme (2.20) reads

$$A_{jk}\psi_k^{n+1} = B_{jk}\psi_k^{n-1} ,$$
$$A_{mnjk}\psi_{jk}^{n+1} = B_{mnjk}\psi_{jk}^{n-1} , \qquad (6.1)$$
$$A_{mnpjkl}\psi_{jkl}^{n+1} = B_{mnpjkl}\psi_{jkl}^{n-1} .$$

Clearly, the one dimensional problem presents no difficulty, A_{jk}, B_{jk} are banded matrices of width 3, and the elements A_{jk} and B_{jk} are easily identifiable. For the two dimensional problem, the algebraic equations with the four dimensional matrices A_{mnjk} and B_{mnjk} nonmanageable in their present forms. Nevertheless, a contraction is made on the indices to reduce the second Eq. (6.1) into[2]

$$A_{KL}\psi_L^{n+1} = B_{KL}\psi_L^{n-1} . \qquad (6.2)$$

Although the contracted matrices are very large, and are not thin banded, this set of equations can nevertheless be solved. For the three dimensional problem, however, even if a contraction is made on the triple indices, the resulting matrices are too large to be inverted with a reasonable computational effort and the elements of the contracted matrices are quite difficult to visualize. However, the equations analogous to Eq. (6.1) corresponding to the method proposed in this paper are of the form

$$\psi_j^{n+1} = \psi_j^{n-1} + A_{jk}\psi_k^n ,$$
$$\psi_{jk}^{n+1} = \psi_{jk}^{n-1} + A_{jkmn}\psi_{mn}^n , \qquad (6.3)$$
$$\psi_{jkl}^{n+1} = \psi_{jkl}^{n-1} + A_{jklpqr}\psi_{pqr}^n .$$

The advantages of Eq. (6.3) in comparison to Eq. (6.1) are obvious: No matrices need be inverted, only one matrix is stored in memory, and no contraction is necessary. Furthermore, the matrices A_{jp}, A_{jkpq}, and A_{jklpqr} are banded in the sense that only the elements

$A_{j,j} A_{j+1,j}$

$A_{jkjk} A_{j\pm1,k,jk} A_{j,k\pm1,j,k} A_{j\pm1,k\pm1,j,k}$

$A_{jkljk} A_{j\pm1,k,l,j,k} A_{j,k\pm1,l,j,k,l} A_{j,k,l\pm1,j,k,l}$

$A_{j\pm1,k\pm1,l,j,k,l} A_{j\pm1,k,l\pm1,j,k,l} A_{j,k\pm1,l\pm1,j,k,l} A_{j\pm1,k\pm1,l\pm1,j,k,l}$

(6.4)

are nonzero. For a mesh with n points in each dimension, the nonzero elements of the banded matrices (6.1) number, respectively, $3n$, $9n^2$, and $30n^3$, rather than n^2, n^4, and n^6 for the full matrices. Although the same is true for the matrices **A** and **B** in Eq. (6.2), when the matrices on the left-hand side are inverted, however, the banded character disappears. This is important for both the computer time requirement and memory space allocation.

The real power of this explicit scheme is due to the elimination of the matrices whose inversion proves prohibitive in the implicit methods. The advantages of the explicit method are even more significant in higher di-

mensions and for denser meshes. The reason is that the computational effort in implicit methods increases as the cube of the number of elements of the matrices involved, while the increase is only linear with the number of unknowns for the explicit method presented here. This linearity is displayed on Table I as the CPU time per step, per mesh point is the same for all three calculations using a different number of points.

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