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Euler-Cromer Algorithm Applied to the Schroedinger Equation

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0. Introduction and Summary

Euler's well known algorithm is simple and explicit; however, it is notoriously unstable and imprecise. On the other hand, the Crank-Nicolson algorithm[1,2] is, in general, stable and precise. The latter algorithm, however, is implicit and thus slow. Although advances in hardware development enable the use of implicit and slow algorithm, the intuitive relation between the problem and the algorithm is lost in the implicit algorithm. Consequently in computer education, the introduction of the algorithm into simulation studies becomes difficult on the elementary level.

In this paper, we apply a simple and direct algorithm accurate enough to solve the Cauchy problem of the Schroedinger equation. The algorithm is essentially the same one as that introduced by Cromer[3], who used it for solving some simple examples and pointed out its relative stability. However, the detailed step by step examination of stability, in general, and the analysis of unitarity crucial for the Schroedinger equation, in particular, were not performed.

In section 1, we introduce the direct method, as well as the other widely used one. The stability and (almost-) unitarity are discussed in section 2; an example of initial data is shown in section 3. For the sake of comparison, Crank-Nicolson's algorithm is applied to the Schroedinger equation in the Appendix.

1. Algorithm

The partial differential equation to be solved in this paper is that of the Schroedinger equation:

$$i\hbar\frac{\partial\psi}{\partial t}=H\psi\,,\qquad H=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+W(x)\,,\tag{1. 1}$$

Using characteristic dimensional constants, we do the following rescaling:

$$\frac{mc^2}{2\hbar}t\rightarrow t\,,\qquad \frac{mc}{\hbar}x\rightarrow x\ \text{and}\ \frac{2}{mc^2}W(x)\rightarrow W(x)\,.\tag{1. 2}$$

In other words, the length, the time, the momentum and the energy are measured

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in the units, $\frac{h}{mc}$, $\frac{2h}{mc^2}$, mc, and $\frac{mc^2}{2}$, respectively. Then we get the equation written in terms of dimensionless variables:

$$i\frac{\partial\psi}{\partial t}=H\psi, \qquad H=-\frac{\partial^2}{\partial x^2}+W(x). \tag{1.3}$$

It has to be noted that the constant, c, with the dimension of velocity was introduced *by hand* in the above rescaling; it does not necessarily have the meaning of the light velocity unless the potential energy W contains the electromagnetic interaction.

After separating real- and imaginary-parts of the wave function,

$$\psi(t,x)=u(t,x)+iv(t,x), \tag{1.4}$$

we discretize the partial differential equation:

$$u(nk,jh)=u_j^n, \qquad v(nk,jh)=v_j^n \tag{1.5}$$

(n and j are integers).

The simplest algorithm is Euler's forward iteration:

$$u_j^{n+1}=u_j^n-\mu(v_{j+1}^n+v_{j-1}^n-2v_j^n)+kW_jv_j^n, \tag{1.6a}$$

$$v_j^{n+1}=v_j^n+\mu(u_{j+1}^n+u_{j-1}^n-2u_j^n)-kW_ju_j^n, \tag{1.6b}$$

where $\mu=\frac{k}{h^2}$. As is well known, this explicit algorithm is very unstable because it is a non-unitary approximation to the unitary temporal evolution:

$$\psi(t,x)=e^{-iHt}\psi(0,x). \tag{1.7}$$

Goldberg, Schey and Schwartz[3,4] used the Cayley form

$$\psi(t+k,x)=\frac{1-i\frac{k}{2}H}{1+i\frac{k}{2}H}\psi(t,x), \tag{1.8}$$

as a *unitary* approximation to (1.7). Actually, this gives the Crank-Nicolson algorithm[1,5]:

$$u_j^{n+1}+\frac{\mu}{2}(v_{j+1}^{n+1}+v_{j-1}^{n+1}-2v_j^{n+1})-\frac{k}{2}W_jv_j^{n+1}$$
$$=u_j^n-\frac{\mu}{2}(v_{j+1}^n+v_{j-1}^n-2v_j^n)+\frac{k}{2}W_jv_j^n, \tag{1.9a}$$

$$v_j^{n+1}-\frac{\mu}{2}(u_{j+1}^{n+1}+u_{j-1}^{n+1}-2u_j^{n+1})+\frac{k}{2}W_ju_j^{n+1}$$
$$=v_j^n+\frac{\mu}{2}(u_{j+1}^n+u_{j-1}^n-2u_j^n)-\frac{k}{2}W_ju_j^n, \tag{1.9b}$$

which is unitary (see Appendix) but implicit.

An explicit, relatively stable, and direct algorithm can be given by the Euler-Cromer algorithm[2]:

$$u_j^{n+1}=u_j^n-\mu(v_{j+1}^n+v_{j-1}^n-2v_j^n)+kW_jv_j^n, \quad (1.10\text{a})$$

$$v_j^{n+1}=v_j^n+\mu(u_{j+1}^{n+1}+u_{j-1}^{n+1}-2u_j^{n+1})-kW_ju_j^{n+1}. \quad (1.10\text{b})$$

The following program fragment written in *C* shows the straightforwardness of the algorithm (we set $W=0$ for the sake of simplicity):

```
for (j = 0; j<N; j++) {
    u[j] = u[j] - mu*(v[(j+1)%N] + v[(N+j-1)%N] - v[j]);
}
for (j = 0; j<N; j++) {
    v[j] = v[j] + mu*(u[(j+1)%N] + u[(N+j-1)%N] - u[j]);
}
```

It is easily seen that the results obtained in the first FOR-LOOP (so-called "left-values") are already assigned to the right hand side of the statement in the second FOR-LOOP so that the coding automatically realizes the Euler-Cromer algorithm.

2. Stability and Almost-Unitarity of the Euler-Cromer Algorithm

In this section, we analyse the stability of the Euler-Cromer algorithm when used for solving the Schrodinger equation. The explicit iteration formula given by eq. (1.10) can be written in a matrix form:

$$\begin{bmatrix} 1 & 0 \\ -\mu\Delta & 1 \end{bmatrix}\begin{bmatrix} u_j^{n+1} \\ v_j^{n+1} \end{bmatrix}=\begin{bmatrix} 1 & -\mu\Delta \\ 0 & 1 \end{bmatrix}\begin{bmatrix} u_j^n \\ v_j^n \end{bmatrix}, \quad (2.1)$$

where Δ is the discrete Laplace operator defined by

$$\Delta\xi_j=\xi_{j+1}+\xi_{j-1}-2\xi_j.$$

$\cos(pjh)$ and $\sin(pjh)$ are the eigenfunctions of the Laplace operator:

$$\Delta\cos(pjh)=-4\sin^2\left(\frac{ph}{2}\right)\cos(pjh), \quad (2.2\text{a})$$

$$\Delta\sin(pjh)=-4\sin^2\left(\frac{ph}{2}\right)\sin(pjh). \quad (2.2\text{b})$$

Using these eigenfuctions, we write the wave function in the Fourier series form:

$$\begin{bmatrix} u_j^n \\ v_j^n \end{bmatrix}=\sum_p\begin{bmatrix} \cos(pjh) & -\sin(pjh) \\ \sin(pjh) & \cos(pjh) \end{bmatrix}\begin{bmatrix} \xi_n(p) \\ \eta_n(p) \end{bmatrix}. \quad (2.3)$$

Then we have

$$\begin{bmatrix} 1 & 0 \\ 4\mu\sin^2\left(\frac{ph}{2}\right) & 1 \end{bmatrix}\begin{bmatrix} \cos(pjh) & -\sin(pjh) \\ \sin(pjh) & \cos(pjh) \end{bmatrix}\begin{bmatrix} \xi_{n+1}(p) \\ \eta_{n+1}(p) \end{bmatrix}$$

$$=\begin{bmatrix} 1 & 4\mu\sin^2\left(\frac{ph}{2}\right) \\ 0 & 1 \end{bmatrix}\begin{bmatrix} \cos(pjh) & -\sin(pjh) \\ \sin(pjh) & \cos(pjh) \end{bmatrix}\begin{bmatrix} \xi_n(p) \\ \eta_n(p) \end{bmatrix}.$$

That is,

$$\begin{bmatrix} \cos(pjh) & -\sin(pjh) \\ \sin(pjh) & \cos(pjh) \end{bmatrix} \begin{bmatrix} \xi_{n-1}(p) \\ \eta_{n+1}(p) \end{bmatrix}$$
$$= \begin{bmatrix} 1 & \kappa \\ -\kappa & 1-\kappa^2 \end{bmatrix} \begin{bmatrix} \cos(pjh) & -\sin(pjh) \\ \sin(pjh) & \cos(pjh) \end{bmatrix} \begin{bmatrix} \xi_n(p) \\ \eta_n(p) \end{bmatrix}, \quad (2.4)$$

where $\kappa = 4\mu \sin^2\left(\frac{ph}{2}\right)$. (2.5)

The eigenvalues of the time-transfer matrix,
$T = \begin{bmatrix} 1 & \kappa \\ -\kappa & 1-\kappa^2 \end{bmatrix}$, are given by the solution to the equation:

$$\lambda^2 + (\kappa^2 - 2)\lambda + 1 = 0. \quad (2.6)$$

The solutions are

$$\lambda_\pm = 1 - \frac{\kappa^2}{2} \pm i\frac{\kappa}{2}[4-\kappa^2]^{1/2}, \qquad \text{for } 0 \leqq \kappa \leqq 4\mu \leqq 2. \quad (2.7)$$

$$\text{If } \frac{\kappa}{h^2} \leqq \frac{1}{2}, \ |\lambda| = 1; \quad (2.8)$$

the stability condition in iteration is satisfied accordingly.

Note that the time-transfer matrix is unitray only up to $O(\kappa^2)$. Indeed, the matrix can be diagonalized by using a similarity transformation, but not by using a unitary transformation. Let $X = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{bmatrix}$ be the similarity transformation matrix such that

$$\begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{bmatrix}^{-1} \begin{bmatrix} 1 & \kappa \\ -\kappa & 1-\kappa^2 \end{bmatrix} \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{bmatrix} = \begin{bmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{bmatrix}.$$

Then its matrix elements are given by

$$x_{11} = 1, \qquad x_{12} = -\frac{\kappa}{2} + \frac{i}{2}(4-\kappa^2)^{1/2},$$

$$x_{21} = -\frac{\kappa}{2} + \frac{i}{2}(4-\kappa^2)^{1/2}, \qquad x_{22} = 1. \quad (2.10)$$

Therefore the matrix $X = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{bmatrix}$ itself is not unitary.

We rewrite the time-transfer matrix in terms of $\sin\theta = \frac{\kappa}{2}$.

From $\lambda_\pm = 1 - \frac{\kappa^2}{2} \pm i\frac{\kappa}{2}(4-\kappa^2)^{1/2} = e^{\pm 2i\theta}$ (2.11)

and $x_{12} = x_{21} = -\frac{\kappa}{2} + \frac{i}{2}(4-\kappa^2)^{1/2} = ie^{i\theta}$, (2.12)

we obtain the following relation:

$$T=\begin{bmatrix} 1 & 2\sin\theta \\ -2\sin\theta & 1-4\sin^2\theta \end{bmatrix}$$

$$=\frac{1}{\cos\theta}\begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}\begin{bmatrix} \cos 2\theta & \sin 2\theta \\ -\sin 2\theta & \cos 2\theta \end{bmatrix}\begin{bmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix} \tag{2. 13}$$

where $\sin\theta=\frac{\kappa}{2}$, $\cos\theta=\left[1-\frac{\kappa^2}{4}\right]^{1/2}$.

$$\sin 2\theta=\kappa\left[1-\frac{\kappa^2}{4}\right]^{1/2}, \qquad \cos 2\theta=1-\frac{\kappa^2}{2},$$

$$\sin\frac{\theta}{2}=\frac{1}{2}\left[1+\frac{\kappa}{2}\right]^{1/2}-\frac{1}{2}\left[1-\frac{\kappa}{2}\right]^{1/2},$$

$$\cos\frac{\theta}{2}=\frac{1}{2}\left[1+\frac{\kappa}{2}\right]^{1/2}+\frac{1}{2}\left[1-\frac{\kappa}{2}\right]^{1/2}.$$

Now, it is an easy task to get the exact expression of the time evolution matrix aftre the n-th step temporal iteration. Eq. (2. 13) allows us to write the time-transfer matrix as

$T=YRY^{-1}$, where

$$Y=\begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix} \text{ and } Y^{-1}=\frac{1}{\cos\theta}\begin{bmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix} \tag{2. 14}$$

are the transformation matrix and its inverse, respectively.

$$\text{And } R=\begin{bmatrix} \cos 2\theta & -\sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{bmatrix} \tag{2. 15}$$

is unitarily equivalent to the diagonalized (complex) form of the T matrix. In this form, the result of n steps iteration is given by

$$T^n=YR^nY^{-1}, \tag{2. 16}$$

$$\text{where } R^n=\begin{bmatrix} \cos(2n\theta) & -\sin(2n\theta) \\ \sin(2n\theta) & \cos(2n\theta) \end{bmatrix}. \tag{2. 17}$$

Note that the discrepancy of X from a unitary matrix does not accumulate in the course of iteration ; the simple algorithm given above is not only stable but also a good approximation to the unitary iteration.

$$T^n=\frac{1}{\cos\theta}\begin{bmatrix} \cos[(2n-1)\theta] & \sin(2n\theta) \\ -\sin(2n\theta) & \cos[(2n+1)\theta] \end{bmatrix}. \tag{2. 18}$$

The exact dispersion relation is given by

$$\omega(p)=\frac{2}{k}\theta=\frac{2}{k}\sin^{-1}\left[2\mu\sin^2\left(\frac{ph}{2}\right)\right]. \tag{2. 19}$$

In the continuum limit ($h \to 0$), we get $\omega(p)=p^2$.

3. Gaussian Wave Packet

In this section we give a specific example of the Cauchy data, Gaussian wave packet:

$$\psi(0, x)=\frac{2\pi}{L}\sum_{l=-N}^{N} e^{-(l-l_0)^2\left(\frac{2\pi\sigma}{L}\right)^2+i\frac{2\pi l j}{N}}, \tag{3. 1}$$

where the correspondence, $p=\frac{2\pi l}{L}$, $x=j\frac{L}{N}$, is used.
In eq. (3. 1) the range of index j is from 0 to $N-1$, and the average momentum is given by

$$\bar{p}=\frac{2\pi l_0}{L}, \qquad (l_0=\text{an integer}). \tag{3. 2}$$

Note that initial data (3. 1) satisfies the boundary condition:

$$\psi(0, x+L)=\psi(0, x).$$

The above choice corresponds to the following value in eq. (2. 5)

$$\kappa=4\mu\sin^2\left(\frac{ph}{2}\right)=\frac{8\pi k N^2}{L^2}\sin^2\left(\frac{2\pi l}{N}\right),$$

that is, $p=\frac{2\pi l}{L}$, $Nh=L$.

In the continuum limit $h \to 0$, we get the following Fourier transform of the Gaussian distribution:

$$\psi(0, x)=\int_{-\infty}^{+\infty} e^{-(p-\bar{p})^2\sigma^2+ipx}dp=\frac{\sqrt{\pi}}{\sigma}\exp\left[-\frac{x^2}{4\sigma^2}+i\bar{p}x\right], \tag{3. 3}$$

where $\bar{p}$ is the average momentum.
The time evolution operator e^{-itH} acts on $\psi(0, x)$ as follows:

$$\begin{aligned}\psi(t, x)=e^{-itH}\psi(0, x)&=\int_{-\infty}^{+\infty} e^{-(p-\bar{p})^2\sigma^2}e^{-ip^2t+ipx}dp\\&=\left[\frac{\pi}{\sigma^2+it}\right]^{1/2}\exp\left[-\frac{(x-vt)^2}{4(\sigma^2+it)}-i\bar{p}^2t+i\bar{p}x\right],\end{aligned} \tag{3. 4}$$

where the last line of the above equation is obtained by using an analytic continuation of the Fourier transform, and $v=2\bar{p}$ is the group velocity of the wave packet.

$\left(\text{In our scaling, } \omega(\bar{p})=\bar{p}^2,\ v=\frac{\partial\omega}{\partial\bar{p}}\right)$

The probability density at time t is given by

$$|\psi(x, t)|^2=\left[\frac{\pi^2}{\sigma^4+t^2}\right]^{1/2}\exp\left[-\frac{(x-vt)^2\sigma^2}{2(\sigma^4+t^2)}\right], \tag{3. 6}$$

which describes the spreading of the distribution.

Appendix: Crank-Nicolson Method.

The formal solution to the Schroedinger equation and its unitary approximation are given by

$$\psi(t+k, x) = e^{-ikH}\psi(t, x) \tag{A. 1}$$

and $$\psi(t+k, x) = \frac{1-i\frac{k}{2}H}{1+i\frac{k}{2}H}\psi(t, x), \tag{A. 3}$$

respectively. The action of the Hamiltonian operator upon ψ is:

$$(H\psi)(t, x)$$
$$= -\frac{1}{h^2}\left\{\psi(t, x+h)+\psi(t, x-h)-2\psi(t, x)\right\}+W(x)\cdot\psi(t, x).$$

Therefore, from (A. 3) we get

$$\psi(t+k, x)-\frac{ik}{2h^2}\left\{\psi(t+k, x+h)+\psi(t+k, x-h)-2\psi(t+k, x)\right\}$$
$$+i\frac{k}{2}W\cdot\psi(t, x)$$
$$=\psi(t, x)+\frac{ik}{2h^2}\left\{\psi(t, x+h)+\psi(t, x-h)-2\psi(t, x)\right\}-i\frac{k}{2}W\cdot\psi(t, x) \tag{A. 4}$$

To check the stability and the unitarity, let us solve the above difference equation in the free case ($W=0$). Making use of the ansatz, $\psi(t, x)\sim z^n e^{ipjh}$, we get

$$z=\frac{1-i\frac{2k}{h^2}\sin^2\left(\frac{ph}{2}\right)}{1+i\frac{2k}{h^2}\sin^2\left(\frac{ph}{2}\right)}. \tag{A. 5}$$

Therefore $|z|=1$ holds exactly, and we get (as $h\to0$)

$$z\sim\frac{1-i\frac{kp^2}{2}}{1+i\frac{kp^2}{2}}\sim e^{-ikp^2}. \tag{A. 6}$$

$\psi(t, x)=z^n e^{ipjh}=e^{-ip^2t}\cdot e^{ipx}$, as it should be.
On the other hand, an exact dispersion relation for finite k and h is obtained by setting $z=e^{-i\theta}$.
Since, $z^n=e^{-i\omega(p)t}$ and $t=nk$, we get the exact dispersion relation:

$$\omega(p)=\frac{2}{k}\tan^{-1}\left(\frac{\kappa}{2}\right), \tag{A. 7}$$

where $\kappa=\frac{4k}{h^2}\sin^2\left(\frac{ph}{2}\right)$. (This definition is different from that in the main text by the factor of 2.)

Setting $r=\frac{k}{2h^2}$ and $\psi(nk, jh)=u_j^n+iv_j^n$, we get an implicit equation :

$$u_j^{n+1}+r(v_{j+1}^{n+1}+v_{j-1}^{n+1}-2v_j^{n+1})-\frac{k}{2}W_j v_j^{n+1}$$
$$=u_j^n-r(v_{j+1}^n+v_{j-1}^n-2v_j^n)+\frac{k}{2}W_j v_j^n\,, \tag{A. 8}$$

$$v_j^{n+1}-r(u_{j+1}^{n+1}+u_{j-1}^{n+1}-2u_j^{n+1})+\frac{k}{2}W_j u_j^{n+1}$$
$$=v_j^n+r(u_{j+1}^n+u_{j-1}^n-2u_j^n)-\frac{k}{2}W_j u_j^n\,. \tag{A. 9}$$

The time-transfer matrix obtained from (A. 8) and (A. 9),

$$T=\frac{1}{1+(\kappa/2)^2}\begin{bmatrix}1-(\kappa/2)^2 & \kappa\\ -\kappa & 1-(\kappa/2)^2\end{bmatrix}, \tag{A. 10}$$

is unitary ; indeed it is diagonalized as

$$\begin{bmatrix}\frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}}\\ \frac{-i}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix}\begin{bmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{bmatrix}\begin{bmatrix}\frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}}\\ \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix}=\begin{bmatrix}e^{i\theta} & 0\\ 0 & e^{-i\theta}\end{bmatrix}, \tag{A. 11}$$

were $\cos\theta=\frac{1-(\kappa/2)^2}{1+(\kappa/2)^2}$, $\sin\theta=\frac{\kappa}{1+(\kappa/2)^2}$.

That is, $\theta=2\tan^{-1}\left(\frac{\kappa}{2}\right)$.

We set

$$s_1(j)=u_j^n-r(v_{j+1}^n+v_{j-1}^n-2v_j^n)+\frac{k}{2}W_j v_j^n\,,$$
$$s_2(j)=v_j^n+r(u_{j+1}^n+u_{j-1}^n-2u_j^n)-\frac{k}{2}W_j u_j^n\,. \tag{A. 12}$$

Then, we have to solve the following coupled equations :

$$u_0^{n+1}+r(v_1^{n+1}-2v_0^{n+1})-\frac{k}{2}W_0 v_0^{n+1}=s_1(0)\,,$$
$$v_0^{n+1}-r(u_1^{n+1}-2u_0^{n+1})+\frac{k}{2}W_0 u_0^{n+1}=s_2(0)\,. \tag{A. 13}$$

$$u_n^{j+1}+r(v_{j+1}^{n+1}+v_{j-1}^{n+1}-2v_j^{n+1})-\frac{k}{2}W_j v_j^{n+1}=s_1(j)\,,$$
$$v_j^{n+1}-r(u_{j+1}^{n+1}+u_{j-1}^{n+1}-2u_j^{n+1})+\frac{k}{2}W_j u_j^{n+1}=s_2(j)\,. \tag{A. 14}$$

$$u_N^{n+1}+r(v_{N-1}^{n+1}-2v_N^{n+1})-\frac{k}{2}W_N v_N^{n+1}=s_1(Nh)\,,$$
$$v_N^{n+1}-r(u_{N-1}^{n+1}-2u_N^{n+1})+\frac{k}{2}W_N u_N^{n+1}=s_2(Nh)\,. \tag{A. 15}$$

Or in a matrix form,

$$B(0)\,\phi(0)+A\phi(1)=S(0)\,,$$
$$A\phi(j-1)+B(j)\,\phi(j)+A\phi(j+1)=S(j)\,,\qquad (j=1,2,\cdots,N-1)\,,$$
$$A\phi(N-1)+B(N)\,\phi(N)=S(N)\,. \tag{A. 16}$$

where

$$A=\begin{bmatrix} 0 & r \\ -r & 0 \end{bmatrix},\quad B(j)=\begin{bmatrix} 1 & -2r-(k/2)\,W(jh) \\ 2r+(k/2)\,W(jh) & 1 \end{bmatrix}, \tag{A. 17}$$

$$S(j)=\begin{bmatrix} s_1(j) \\ s_2(j) \end{bmatrix} \text{ and } \phi(j)=\begin{bmatrix} u_j^{n+1} \\ v_j^{n+1} \end{bmatrix}. \tag{A. 18}$$

Next we solve equation (A. 16). From $B(0)\,\phi(0)+A\phi(1)=S(0)$ and $A\phi(0)+B(1)\,\phi(1)+A\phi(2)=S(1)$, we get

$$C(1)\,\phi(1)+\phi(2)=T(1)\,, \tag{A. 19}$$

where $C(1)=A^{-1}B(1)-B^{-1}(0)\,A\,,$ (A. 20)

and $T(1)=A^{-1}S(1)-B^{-1}(0)\,S(0)\,.$ (A. 21)

In other words, setting $C(0)=A^{-1}B(0)$ and $T(0)=A^{-1}S(0)$, we can write

$$C(1)=A^{-1}B(1)-C^{-1}(0)\,, \tag{A. 22}$$

$$T(1)=A^{-1}S(1)-C^{-1}(0)\,T(0)\,, \tag{A. 23}$$

In general, from the ansatz

$$C(j-1)\,\phi(j-1)+\phi(j)=T(j-1) \tag{A. 24}$$

and $A\phi(j-1)+B(j)\,\phi(j)+A\phi(j+1)=S(j)\,,$ (A. 25)

we get

$$A^{-1}B(j)\,\phi(j)-C^{-1}(j-1)\,\phi(j)+\phi(j+1)=A^{-1}S(j)-C^{-1}(j-1)\,T(j-1)\,,$$

therefore, $C(j)=A^{-1}(j-1)\,\phi(j)-C^{-1}(j-1)$ (A. 26)

and $\quad T(j)=A^{-1}S(j)-C^{-1}(j-1)\,T(j-1)\,,$ (A. 27)

recursively. Lastly, from

$$C(N-1)\,\phi(N-1)+\phi(N)=T(N-1) \tag{A. 28}$$

and $A\phi(N-1)+B(N)\,\phi(N)=S(N)\,,$ (A. 29)

we get

$$\{A^{-1}B(N)-C^{-1}(N-1)\}\,\phi(N)=A^{-1}S(N)-C^{-1}(N-1)\,T(N-1)\,. \tag{A. 30}$$

The remaining task to get a procedure for obtaining $\phi(j)$ is standard; we just refer to Smith's classical textbook[5].

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