Hints for Solution of the Time-Dependent Schrödinger Equation

Consider the one-dimensional, time-dependent Schrödinger equation, on the domain $0 \le x \le 1$, $t \ge 0$, where we have chosen units such that $\hbar = 2m = 1$:

$$i \frac{\partial \psi(x,t)}{\partial t} = -\frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\,\psi(x,t) \qquad (1)$$

Use the following finite difference approximation (*Crank Nicholson* approximation) which is (a) second order in both space and time, and (b) *implicit*, meaning a *system* of linear equations must be solved at each time step:

$$i \frac{\psi_j^{n+1} - \psi_j^n}{\triangle t} = -\frac{1}{2}\left(\frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}}{\triangle x^2} + \frac{\psi_{j+1}^{n} - 2\psi_j^{n} + \psi_{j-1}^{n}}{\triangle x^2} \right) + V_j\,\frac{1}{2}\left(\psi_j^{n+1} + \psi_j^n\right) \qquad (2)$$

where $\psi_j^n \equiv \psi(j\triangle x, n\triangle t)$, $V_j \equiv V(j\triangle x)$, etc. Rewrite the above equations in the form

$$c_j^+\,\psi_{j+1}^{n+1} + c_j^0\,\psi_j^{n+1} + c_j^-\,\psi_{j-1}^{n+1} = S_j \qquad j = 2, 3, ..., \mathtt{nx} - 1 \qquad (3)$$

which, along with the boundary conditions (representing an infinite potential barrier at $x = 0$ and $x = 1$)

$$\psi_1^{n+1} = \psi_{\mathtt{nx}}^{n+1} = 0 \qquad (4)$$

constitute a *complex, tridiagonal, linear* system for the advanced values ψ_j^{n+1}. You will need to determine precise formulae for the c_j^+, c_j^0, c_j^- and S_j yourself, and note that these quantities will generally be complex.

Use `complex*16` (not `complex`) arithmetic, and the `LAPACK` solver `zgtsv` to solve the tridiagonal system. See the source code at

`http://laplace.physics.ubc.ca/People/matt/410/Doc/linsys/src_lapack/zgtsv.f`

for usage details, but note that the routine is available via

```
$(F77_LOAD) ... -llapack $(LIBBLAS) -o ...
```

as with the rest of the `LAPACK` routines.

Use

$$\triangle t = \lambda \triangle x \qquad (5)$$

where $\lambda \sim 1$—you can experiment with various values, but something like $\lambda = 0.5$ should work well.

Note that an excellent way of checking your implementation follows from the fact that there is a conservation law for $\psi(x,t)$ (conservation of total probability):

$$I \equiv \int_0^1 \psi(x,t)\,\psi^*(x,t)\,dx = \text{constant}. \qquad (6)$$

You can approximate the integral using the following second order approximation:

$$I \approx \sum_{j=1}^{\mathtt{nx}-1} \psi_{j+1/2}^n\,{\psi^*}_{j+1/2}^n\,\triangle x = \sum_{j=1}^{\mathtt{nx}-1} \frac{1}{2}\left(\psi_j^n + \psi_{j+1}^n\right)\frac{1}{2}\left({\psi^*}_j^n + {\psi^*}_{j+1}^n\right)\triangle x \qquad (7)$$