Differencing the Time-Dependent Schrödinger Equation

Now let's turn to the problem of solving the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\,\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi\,.$$

Its form is basically that of the diffusion equation, except that the coefficients are complex and there is an additional "$V\psi$" term on the right-hand side. The Crank-Nicolson scheme is still the method of choice. What's more, it can be shown that the Crank-Nicolson map from time n to time $n+1$ is *unitary*, so it preserves the normalization of ψ:

$$\int \psi^* \psi \, dx = 1\,.$$

As before, we derive the Crank-Nicolson differencing scheme by averaging together the fully explicit and fully implicit difference forms of the differential equation:

$$\begin{aligned}
i\hbar \frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} &= -\frac{\hbar^2}{2m}\,\frac{\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n}{\Delta x^2} + V_j \psi_j^n \qquad \text{(explicit)}\,, \\
i\hbar \frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} &= -\frac{\hbar^2}{2m}\,\frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}}{\Delta x^2} + V_j \psi_j^{n+1} \quad \text{(implicit)}\,,
\end{aligned}$$

where $V_j = V(x_j)$. Averaging and rearranging, we find

$$\begin{aligned}
\psi_j^{n+1} &= \psi_j^n + \tfrac{1}{2} i\alpha \left\{ \psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n + \psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1} \right\} \\
&\qquad - \tfrac{1}{2} i V_j \Delta t (\psi_j^{n+1} + \psi_j^n)/\hbar\,,
\end{aligned}$$

where $\alpha = \hbar \Delta t/(2m\Delta x^2)$. Moving the unknown "$n+1$" terms to the left-hand side, we have

$$\begin{aligned}
&-\tfrac{1}{2} i\alpha\, \psi_{j-1}^{n+1} + \left[1 + i\alpha + \tfrac{1}{2} i V_j \Delta t/\hbar\right] \psi_j^{n+1} - \tfrac{1}{2} i\alpha\, \psi_{j+1}^{n+1} \\
&\qquad = \tfrac{1}{2} i\alpha\, \psi_{j-1}^n + \left[1 - i\alpha - \tfrac{1}{2} i V_j \Delta t/\hbar\right] \psi_j^n + \tfrac{1}{2} i\alpha\, \psi_{j+1}^n\,.
\end{aligned}$$

This complex matrix equation is then solved in exactly the same way as before.