Schrödinger equation:

$$i\hbar\frac{d}{dt}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x,t)$$

Finite differences:

$$\frac{d}{dt}f(t) \approx \frac{f(t+\Delta t)-f(t)}{\Delta t} = f_t$$

$$\frac{d^2}{dt^2}f(x) \approx \frac{f(x-\Delta x)-2f(t)+f(x+\Delta x)}{\Delta x^2} = f_{xx}$$

Use the finite difference approximation of the Schrödinger equation:

$$i\hbar\Psi_t = -\frac{\hbar^2}{2m}\Psi_{xx}$$

Explicit:

$$i\hbar\frac{\Psi(x,t+\Delta t)-\Psi(x,t)}{\Delta t} = -\frac{\hbar^2}{2m}\frac{\Psi(x-\Delta x,t)-2\Psi(x,t)+\Psi(x+\Delta x,t)}{\Delta x^2}$$

Implicit:

$$i\hbar\frac{\Psi(x,t+\Delta t)-\Psi(x,t)}{\Delta t} = -\frac{\hbar^2}{2m}\frac{\Psi(x-\Delta x,t+\Delta t)-2\Psi(x,t+\Delta t)+\Psi(x+\Delta x,t+\Delta t)}{\Delta x^2}$$

$$i\hbar\left[\Psi(x,t+\Delta t)-\Psi(x,t)\right] = -\frac{\hbar^2}{2m}\frac{\Delta t}{\Delta x^2}\left[\Psi(x-\Delta x,t+\Delta t)-2\Psi(x,t+\Delta t)+\Psi(x+\Delta x,t+\Delta t)\right]$$

$$-i\hbar\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\Delta t}{\Delta x^2}\left[\Psi(x-\Delta x,t+\Delta t)-2\Psi(x,t+\Delta t)+\Psi(x+\Delta x,t+\Delta t)\right] - i\hbar\Psi(x,t+\Delta t)$$

$$\hbar\Psi(x,t) = -i\frac{\hbar^2}{2m}\frac{\Delta t}{\Delta x^2}\left[\Psi(x-\Delta x,t+\Delta t)-2\Psi(x,t+\Delta t)+\Psi(x+\Delta x,t+\Delta t)\right] + \hbar\Psi(x,t+\Delta t)$$

$$\Psi(x,t) = -i\frac{\hbar}{2m}\frac{\Delta t}{\Delta x^2}\left[\Psi(x-\Delta x,t+\Delta t)-2\Psi(x,t+\Delta t)+\Psi(x+\Delta x,t+\Delta t)\right] + \Psi(x,t+\Delta t)$$

$$r = -i\frac{\hbar}{2m}\frac{\Delta t}{\Delta x^2}$$

$$\Psi(x,t) = r\left[\Psi(x-\Delta x,t+\Delta t)-2\Psi(x,t+\Delta t)+\Psi(x+\Delta x,t+\Delta t)\right] + \Psi(x,t+\Delta t)$$

$$\Psi(x,t) = r\Psi(x-\Delta x,t+\Delta t) + (1-2r)\Psi(x,t+\Delta t) + r\Psi(x+\Delta x,t+\Delta t)$$

Stencil:

$$\Psi(t) = \begin{bmatrix} r & (1-2r) & r \end{bmatrix}\Psi(t+\Delta t)$$

Jacobi method:

$$Ax = b$$

$$A\Psi(t + \Delta t) = \Psi(t)$$

$$x_i^{k+1} = \frac{1}{A_{ii}} \left(b_i - \sum_{i \neq j} A_{ij} x_j^k \right)$$

Intuition for why it works:

$$A_{ii} x_i^{k+1} = b_i - \sum_{i \neq j} A_{ij} x_j^k$$

$$A_{ii} x_i^{k+1} + \sum_{i \neq j} A_{ij} x_j^k = b_i$$

$$Ax = b$$

Application to our FDM:

$$\Psi(x, t + \Delta t)^{k+1} = \frac{1}{1 - 2r} \left[\Psi(x, t) - r\Psi(x - \Delta x, t + \Delta_t)^k - r\Psi(x + \Delta x, t + \Delta_t)^k \right]$$

Iterated over k for some number of steps N, and (arbitrary) initial $\Psi(x, t + \Delta_t)^{k=0}$, usually $= \Psi(x, t)^{k=N}$.