Diffusion equation; finite difference : $\frac{1}{D}\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2} + S$

$$\frac{\psi_j^{(n+1)} - \psi_j^{(n)}}{\Delta t} = D\frac{\psi_{j+1}^{(n)} - 2\psi_j^{(n)} + \psi_{j-1}^{(n)}}{\Delta x^2} + s_j^{(n)}. \tag{5.2}$$

We use (n) to denote time index, and put it as a superscript to distinguish it from the space indices j $[k, l]$. Of course this notation is *not* raising to a power. Notice in this equation the *second-order* derivative in space is naturally centered and symmetric. However, the time derivative is not centered in time. It is really the value at $n + 1/2$, not at the time index of everything else: n. This scheme is therefore Forward in Time, but Centered in Space (FTCS); see Fig. 5.2. We immediately know from our previous experience that, because it is not centered in time, this scheme's accuracy is going to be only first order in Δt. Also, this scheme is *explicit* in time. The ψ at $n + 1$ is obtained using only prior (n) values of the other quantities:

$$\psi_j^{(n+1)} = \psi_j^{(n)} + \frac{D\Delta t}{\Delta x^2}(\psi_{j+1}^{(n)} - 2\psi_j^{(n)} + \psi_{j-1}^{(n)}) + \Delta t\, s_j^{(n)}. \tag{5.3}$$

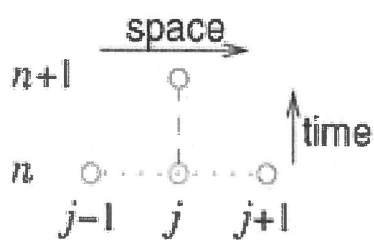

Figure 5.2 Forward time, centered space (FTCS) difference scheme.

A question then arises as to whether this scheme is *stable*. For an ordinary differential equation, we saw that with explicit integration there was a maximum step size that could be allowed before the scheme became unstable. The same is true for hyperbolic and parabolic partial differential equations. For stability analysis, we ignore the source S (because we are really analysing the deviation of the solution [1]). However, even so, it's a bit difficult to see immediately how to evaluate the amplification factor, because for partial differential equations there is variation in the spatial dimension(s) that has to be accounted for. It wasn't present for ordinary differential equations. The way this is generally handled is to turn the partial differential equation into an ordinary differential equation by examining separately all the *Fourier components* of the spatial variation. This sort of analysis is called Von Neumann stability analysis. It gives a precisely correct answer only for uniform grids and coefficients, but it is usually approximately correct, and hence in practice very useful even for non-uniform cases.

A Fourier component varies in space like $\exp(ik_x x)$ where k_x is the wave number in the x-direction (and i is here the square root of minus 1). For such a Fourier component, $\psi_j \propto \exp(ik_x \Delta x j)$, so that $\psi_{j+1} = \exp(ik_x \Delta x)\psi_j$ and $\psi_{j-1} = \exp(-ik_x \Delta x)\psi_j$. Therefore,

$$\psi_{j+1} - 2\psi_j + \psi_{j-1} = (e^{ik_x\Delta x} - 2 + e^{-ik_x\Delta x})\psi_j = -4\sin^2(\frac{k_x\Delta x}{2})\psi_j. \tag{5.4}$$

$$\psi^{(n+1)} = \underbrace{\left[1 - \frac{D\Delta t}{\Delta x^2} 4\sin^2(\frac{k_x \Delta x}{2})\right]}_{\text{Amplification factor}} \psi^{(n)}. \tag{5.5}$$

The amplification factor from each step to the next is the square-bracket term. If it has a magnitude greater than 1, then instability will occur. If D is negative it will in fact be greater than 1. This instability is not a numerical instability, though. It is a *physical* instability. The diffusion coefficient must be positive otherwise the diffusion equation is unstable regardless of numerical methods. So D must be positive; and so are Δt, Δx. Therefore, numerical instability will arise if the magnitude of the second (negative) term in the amplification factor exceeds 2.

If $k_x \Delta x$ is small, then that will make the second term small and unproblematic. We are most concerned about larger k_x values that can make $\sin^2(k_x \Delta x/2)$ approximately unity. In fact, the largest k_x value that can be represented on a finite grid [2] is such that the phase difference ($k_x \Delta x$) between adjacent values is π radians. That corresponds to a solution that oscillates in sign between adjacent nodes. For that Fourier component, therefore, $\sin^2(k_x \Delta x/2) = 1$.

Stability requires *all* Fourier modes to be stable, including the worst mode that has $\sin^2(k_x \Delta x/2) = 1$. Therefore, the condition for stability is

$$\frac{4D\Delta t}{\Delta x^2} < 2. \tag{5.6}$$

There is, for the FTCS scheme, a maximum stable timestep equal to $\Delta x^2/2D$.

Incidentally, the fact that Δt must therefore be no bigger than something proportional to Δx^2 makes the first-order accuracy in time less of a problem. In fact, for a timestep at the stability limit, as we decrease Δx, improving the spatial accuracy proportional to Δx^2 because of the second-order accuracy in space, we also improve the temporal accuracy by the same factor, proportional to Δx^2 because $\Delta t \propto \Delta x^2$.