

## 7.2: Discretizing Partial Differential Equations

With discretized derivatives, differential equations can be formulated as discrete systems of equations. We will discuss this using a specific example: the discretization of the time-independent Schrödinger wave equation in 1D.

### 7.2.1 Deriving a Finite-Difference Equation

The 1D time-independent Schrödinger wave equation is the second-order ordinary differential equation

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x), \quad (7.2.1)$$

where  $\hbar$  is Planck's constant divided by  $2\pi$ ,  $m$  is the mass of the particle,  $V(x)$  is the potential,  $\psi(x)$  is the quantum wavefunction of an energy eigenstate of the particle, and  $E$  is the corresponding energy. The differential equation is usually treated as an eigenproblem, in the sense that we are given  $V(x)$  and seek to find the possible values of the eigenfunction  $\psi(x)$  and the energy eigenvalue  $E$ . For convenience, we will adopt units where  $\hbar = m = 1$ :

$$-\frac{1}{2} \frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x). \quad (7.2.2)$$

To discretize this differential equation, we simply evaluate it at  $x = x_n$ :

$$-\frac{1}{2} \psi''(x_n) + V_n \psi_n = E \psi_n, \quad (7.2.3)$$

where, for conciseness, we denote

$$V_n \equiv V(x_n). \quad (7.2.4)$$

We then replace the second derivative  $\psi''(x_n)$  with a discrete approximation, specifically the three-point rule:

$$-\frac{1}{2h^2} [\psi_{n+1} - 2\psi_n + \psi_{n-1}] + V_n \psi_n = E \psi_n. \quad (7.2.5)$$

This result is called a **finite-difference equation**, and it would be valid for all  $n$  if the number of discretization points is infinite. However, if there is a finite number of discretization points,  $\{x_0, x_1, \dots, x_{N-1}\}$ , then the finite-difference formula fails at the boundary points,  $n = 0$  and  $n = N - 1$ , where it involves the value of the function at the "non-existent" points  $x_{-1}$  and  $x_N$ . We'll see how to handle this problem in the next section.

Boundaries aside, the finite-difference equation describes a matrix equation:

$$\left\{ -\frac{1}{2h^2} \begin{bmatrix} \ddots & \ddots & & & \\ \ddots & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & 1 & -2 & \ddots \\ & & & \ddots & \ddots \end{bmatrix} + \begin{bmatrix} & & & & \\ & \ddots & & & \\ & & V_{n-1} & & \\ & & & V_n & \\ & & & & V_{n+1} \\ & & & & & \ddots \end{bmatrix} \right\} \begin{bmatrix} \vdots \\ \psi_{n-1} \\ \psi_n \\ \psi_{n+1} \\ \vdots \end{bmatrix} = E \begin{bmatrix} \vdots \\ \psi_{n-1} \\ \psi_n \\ \psi_{n+1} \\ \vdots \end{bmatrix}. \quad (7.2.6)$$

The second-derivative operator is represented by a tridiagonal matrix with  $-2$  in each diagonal element, and  $1$  in the elements directly above and below the diagonal. The potential operator is represented by a diagonal matrix, where the elements along the diagonal are the values of the potential at each discretization point. In this way, the Schrödinger wave equation is reduced to a discrete eigenvalue problem.

### 7.2.2 Boundary Conditions

We now have to figure out how to handle the boundaries. Let us suppose  $\psi(x)$  is defined over a finite interval,  $a \leq x \leq b$ . As we recall from the theory of differential equations, the solution to a differential equation is not wholly determined by the differential equation itself, but also by the boundary conditions that are imposed. Thus, we have to specify how  $\psi(x)$  behaves at the end-points of the interval. We will show how this is done for a couple of the most common boundary conditions; other choices of boundary conditions can be handled using the same kind of reasoning.

## Dirichlet Boundary Conditions

Under **Dirichlet boundary conditions**, the wavefunction vanishes at the boundaries:

$$\psi(a) = \psi(b) = 0. \quad (7.2.7)$$

Physically, these boundary conditions apply if we let the potential blow up in the external regions,  $x > b$  and  $x < a$ , thus forcing the wavefunction to be strictly confined to the interval  $a \leq x \leq b$ .

We have not yet stated how the discretization points  $\{x_0, \dots, x_{N-1}\}$  are distributed within the interval; we will make this decision in tandem with the implementation of the boundary conditions. Consider the first discretization point,  $x_0$ , wherever it is. The finite-difference equation at this point is

$$-\frac{1}{2h^2} [\psi_{-1} - 2\psi_0 + \psi_1] + V_0\psi_0 = E\psi_0. \quad (7.2.8)$$

This involves the wavefunction at  $x_{-1}$ , which lies just outside our set of discretization points. But if we choose the discretization points so that  $x_{-1} = a$ , then  $\psi_{-1} = 0$  under Dirichlet boundary conditions, so the above finite-difference formula reduces to

$$-\frac{1}{2h^2} [-2\psi_0 + \psi_1] + V_0\psi_0 = E\psi_0. \quad (7.2.9)$$

As for the other boundary, the finite-difference equation at  $x_{N-1}$  involves  $\psi_N$ . If we choose the discretization points so that  $x_N = b$ , then the finite-difference formula becomes

$$-\frac{1}{2h^2} [\psi_{N-2} - 2\psi_{N-1}] + V_{N-1}\psi_{N-1} = E\psi_{N-1}. \quad (7.2.10)$$

From this, we conclude that the discretization points ought to be equally spaced, with  $x_0$  at a distance  $h$  to the right of the left boundary  $a$  and  $x_{N-1}$  a distance  $h$  to the left of the right boundary  $b$ . This is shown in the following figure:

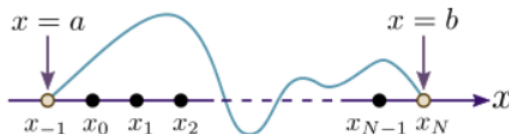


Figure 7.2.1: Position of discretization points for Dirichlet boundary conditions at  $x = a$  and  $x = b$ .

Since there are  $N$  discretization points, the interval should contain  $(N + 1)$  multiples of  $h$ . Hence,

$$h = \frac{b - a}{N + 1} \Rightarrow x_n = a + h(n + 1) = \frac{a(N - n) + b(n + 1)}{N + 1}. \quad (7.2.11)$$

Having made the above choices, the matrix equation becomes

$$\left\{ -\frac{1}{2h^2} \begin{bmatrix} -2 & 1 & & \\ 1 & -2 & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2 \end{bmatrix} + \begin{bmatrix} V_0 & & & \\ & V_1 & & \\ & & \ddots & \\ & & & V_{N-1} \end{bmatrix} \right\} \begin{bmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{N-1} \end{bmatrix} = E \begin{bmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{N-1} \end{bmatrix}. \quad (7.2.12)$$

You can check for yourself that the first and last rows of this equation are the correct finite-difference equations at the boundary points, corresponding to Dirichlet boundary conditions.

## Neuman boundary conditions

**Neumann boundary conditions** are another common choice of boundary conditions. They state that the first derivatives vanish at the boundaries:

$$\psi'(a) = \psi'(b) = 0. \quad (7.2.13)$$

An example of such a boundary condition is encountered in electrostatics, where the first derivative of the electric potential goes to zero at the surface of a charged metallic surface.

We follow the same strategy as before, figuring out the discretization points in tandem with the boundary conditions. Consider again the finite-difference equation at the first discretization point:

$$-\frac{1}{2h^2} [\psi_{-1} - 2\psi_0 + \psi_1] + V_0\psi_0 = E\psi_0. \quad (7.2.14)$$

To implement the condition that first derivative vanishes at the boundary, we invoke the mid-point rule. Suppose the boundary point  $x = a$  falls in between the points  $x_{-1}$  and  $x_0$ . Then, according to the mid-point rule,

$$\frac{\psi_0 - \psi_{-1}}{h} \approx \psi'(a) = 0. \quad (7.2.15)$$

With this choice, therefore, we can make the replacement  $\psi_{-1} = \psi_0$  in the finite-difference equation, which then becomes

$$-\frac{1}{2h^2} [-\psi_0 + \psi_1] + V_0\psi_0 = E\psi_0. \quad (7.2.16)$$

Similarly, to apply the Neumann boundary condition at  $x = b$ , we let the boundary fall between  $x_{N-1}$  and  $x_N$ , so that the finite-difference equation becomes

$$-\frac{1}{2h^2} [\psi_{N-2} - \psi_{N-1}] + V_{N-1}\psi_{N-1} = E\psi_{N-1}. \quad (7.2.17)$$

The resulting distribution of discretization points is shown in the following figure:

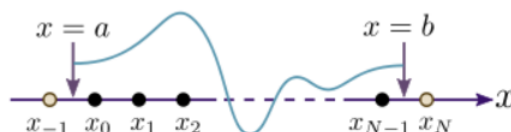


Figure 7.2.2: Position of discretization points for Neumann boundary conditions at  $x = a$  and  $x = b$ .

Unlike the Dirichlet case, the interval contains  $N$  multiples of  $h$ . Hence, we get a different formula for the positions of the discretization points

$$h = \frac{b-a}{N} \Rightarrow x_n = a + h \left( n + \frac{1}{2} \right) = \frac{a(N - n - \frac{1}{2}) + b(n + \frac{1}{2})}{N}. \quad (7.2.18)$$

The matrix equation is:

$$\left\{ -\frac{1}{2h^2} \begin{bmatrix} -1 & 1 & & & \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & -2 & 1 \\ & & & 1 & -1 \end{bmatrix} + \begin{bmatrix} V_0 & & & \\ & V_1 & & \\ & & \ddots & \\ & & & V_{N-1} \end{bmatrix} \right\} \begin{bmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{N-1} \end{bmatrix} = E \begin{bmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{N-1} \end{bmatrix}. \quad (7.2.19)$$

Due to the Neumann boundary conditions and the mid-point rule, the tridiagonal matrix has  $-1$  instead of  $-2$  on its corner entries. Again, you can verify that the first and last rows of this matrix equation correspond to the correct finite-difference equations for the boundary points.

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