have lower accuracy than the fourth-order Runge–Kutta algorithm when applied to the same problem, and this is different from what the apparent local accuracies imply. For more numerical examples of the Sturm–Liouville problem and the Numerov algorithm in the related problems, see Pryce (1993) and Onodera (1994).

4.9 The one-dimensional Schrödinger equation

The solutions associated with the one-dimensional Schrödinger equation are of importance in understanding quantum mechanics and quantum processes. For example, the energy levels and transport properties of electrons in nanostructures such as quantum wells, dots, and wires are crucial in the development of the next generation of electronic devices. In this section, we will apply the numerical methods that we have introduced so far to solve both the eigenvalue and transport problems defined through the one-dimensional Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + V(x)\phi(x) = \varepsilon\phi(x), \tag{4.91}$$

where m is the mass of the particle, $\hbar$ is the Planck constant, ε is the energy level, $\phi(x)$ is the wavefunction, and $V(x)$ is the external potential. We can rewrite the Schrödinger equation as

$$\phi''(x) + \frac{2m}{\hbar^2}[\varepsilon - V(x)]\phi(x) = 0, \tag{4.92}$$

which is in the same form as the Sturm–Liouville problem with $p(x) = 1, q(x) = 2m[\varepsilon - V(x)]/\hbar^2$, and $s(x) = 0$.

The eigenvalue problem

For the eigenvalue problem, the particle is confined by the potential well $V(x)$, so that $\phi(x) \to 0$ with $|x| \to \infty$. A sketch of a typical $V(x)$ is shown in Fig. 4.7. In order to solve this eigenvalue problem, we can integrate the equation with the Numerov algorithm from left to right or from right to left of the potential region. Because the wavefunction goes to zero as $|x| \to \infty$, the integration from one side to another requires integrating from an exponentially increasing region to an oscillatory region and then into an exponentially decreasing region.

The error accumulated will become significant if we integrate the solution from the oscillatory region into the exponentially decreasing region. This is because an exponentially increasing solution is also a possible solution of the equation and can easily enter the numerical integration to destroy the accuracy of the algorithm. The rule of thumb is to avoid integrating into the exponential regions, that is, to carry out the solutions from both sides and then match them in the well region. Usually the matching is done at one of the turning points, where the energy is equal to the potential energy, such as x_l and x_r in Fig. 4.7. The

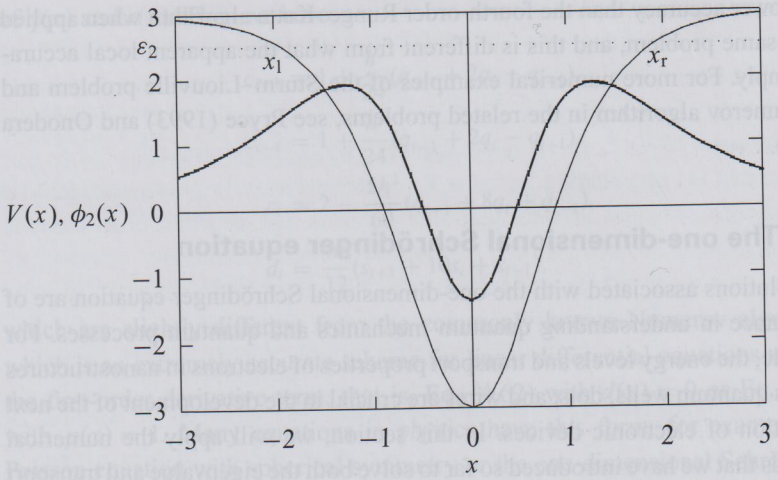

Fig. 4.7 The eigenvalue problem of the one-dimensional Schrödinger equation. Here a potential well $V(x)$ (solid thin line) and the corresponding eigenvalue ε_2 (dotted line) and eigenfunction $\phi_2(x)$ (solid thick line on a relative scale) for the second excited state are illustrated. The turning points x_l and x_r are also indicated.

so-called matching here is to adjust the trial eigenvalue until the solution integrated from the right, $\phi_r(x)$, and the solution integrated from the left, $\phi_l(x)$, satisfy the continuity conditions at one of the turning points. If we choose the right turning point as the matching point, the continuity conditions are

$$\phi_l(x_r) = \phi_r(x_r), \tag{4.93}$$

$$\phi_l'(x_r) = \phi_r'(x_r). \tag{4.94}$$

If we combine these two conditions, we have

$$\frac{\phi_l'(x_r)}{\phi_l(x_r)} = \frac{\phi_r'(x_r)}{\phi_r(x_r)}. \tag{4.95}$$

If we use the three-point formula for the first-order derivatives in the above equation, we have

$$f(\varepsilon) = \frac{[\phi_l(x_r + h) - \phi_l(x_r - h)] - [\phi_r(x_r + h) - \phi_r(x_r - h)]}{2h\phi(x_r)} = 0, \tag{4.96}$$

which can be ensured by a root search scheme. Note that $f(\varepsilon)$ is a function of only ε because $\phi_l(x_r) = \phi_r(x_r) = \phi(x_r)$ can be used to rescale the wavefunctions.

We now outline the numerical procedure for solving the eigenvalue problem of the one-dimensional Schrödinger equation:

(1) Choose the region of the numerical solution. This region should be large enough compared with the effective region of the potential to have a negligible effect on the solution.

(2) Provide a reasonable guess for the lowest eigenvalue ε_0. This can be found approximately from the analytical result of the case with an infinite well and the same range of well width.

(3) Integrate the equation for $\phi_l(x)$ from the left to the point $x_r + h$ and the one for $\phi_r(x)$ from the right to $x_r - h$. We can choose zero to be the value of the first points of $\phi_l(x)$ and $\phi_r(x)$, and a small quantity to be the value of the second points of $\phi_l(x)$ and $\phi_r(x)$, to start the integration, for example, with the Numerov algorithm. Before matching the solutions, rescale one of them to ensure that $\phi_l(x_r) = \phi_r(x_r)$. For example, we can multiply $\phi_l(x)$ by $\phi_r(x_r)/\phi_l(x_r)$ up to $x = x_r + h$. This rescaling also ensures that the solutions have the correct nodal structure, that is, changing the sign of $\phi_l(x)$ if it is incorrect.

(4) Evaluate $f(\varepsilon_0) = [\phi_r(x_r - h) - \phi_r(x_r + h) - \phi_l(x_r - h) + \phi_l(x_r + h)]/2h\phi_r(x_r)$.

(5) Apply a root search method to obtain ε_0 from $f(\varepsilon_0) = 0$ within a given tolerance.

(6) Carry out the above steps for the next eigenvalue. We can start the search with a slightly higher value than the last eigenvalue. We need to make sure that no eigenstate is missed. This can easily be done by counting the nodes in the solution; the nth state has a total number of n nonboundary nodes, with $n = 0$ for the ground state. A node is where $\phi(x) = 0$. This also provides a way of pinpointing a specific eigenstate.

Now let us look at an actual example with a particle bound in a potential well

$$V(x) = \frac{\hbar^2}{2m}\alpha^2\lambda(\lambda - 1)\left[\frac{1}{2} - \frac{1}{\cosh^2(\alpha x)}\right], \tag{4.97}$$

where both α and λ are given parameters. The Schrödinger equation with this potential can be solved exactly with the eigenvalues

$$\varepsilon_n = \frac{\hbar^2}{2m}\alpha^2\left[\frac{\lambda(\lambda - 1)}{2} - (\lambda - 1 - n)^2\right], \tag{4.98}$$

for $n = 0, 1, 2, \ldots$. We have solved this problem numerically in the region $[-10, 10]$ with 501 points uniformly spaced. The potential well, eigenvalue, and eigenfunction shown in Fig. 4.7 are from this problem with $\alpha = 1$, $\lambda = 4$, and $n = 2$. We have also used $\hbar = m = 1$ in the numerical solution for convenience. The program below implements this scheme.

```
// An example of solving the eigenvalue problem of the
// one-dimensional Schroedinger equation via the secant
// and Numerov methods.

import java.lang.*;
import java.io.*;
public class Schroedinger {
  static final int nx = 500, m = 10, ni = 10;
  static final double x1 = -10, x2 = 10, h = (x2-x1)/nx;
  static int nr, nl;
  static double ul[] = new double[nx+1];
  static double ur[] = new double[nx+1];
  static double ql[] = new double[nx+1];
  static double qr[] = new double[nx+1];
```