ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Computational Quantum Physics
Exercise 1

FS 09
Prof. P. Werner,
Prof. P. De Forcrand

Problem 1.1 1-D quantum scattering problem

We consider a particle in one dimension, which is scattered at a potential barrier. This problem can be numerically solved using the Numerov algorithm.
Proceed as described in the lecture notes in section 3.1.2. You can use a constant potential ($V = 1$) in the interval $[0, a]$.

1. Observe the tunneling effect for energies $E \in [0, V]$, where the transmission probability $T = 1/|A|^2$ is non-vanishing.

2. Plot T versus the barrier width a and observe the exponential decay.

This dependency $T(a)$ plays a crucial role for the realization of the scanning tunneling microscope (STM). (Review of Modern Physics 59, 615 (1987). Nobel prize 1986).

Problem 1.2 Bound states in 1-D Schrödinger equation and eigenvalue problem

Find the bound states solutions of the 1D Schrödinger equation with $E < 0$ using the Numerov algorithm and a root solver. Note that the solution exists only for discrete energy eigenvalues.
Proceed as described in lecture notes in section 3.1.3.
Take the potential zero outside the interval [0,1] and inside the interval it can be taken as

$$v(x) = c(x^2 - x), 0 \leq x \leq 1, \tag{1}$$

where c is a constant. Please check the dependency of the number of bound states on the values of c.

Start with finding the ground state energy (zero node in your solution) and proceed further with 1, 2, 3... nodes.
Hint: Check the number of zeros (nodes) in the solution. For your guessed energy, if you find more nodes in your solution than the desired number of nodes, decrease the guess-energy and vice versa.

Chapter 3

The quantum one-body problem

3.1 The time-independent 1D Schrödinger equation

We start the numerical solution of quantum problems with the time-indepent one-dimensional Schrödinger equation for a particle with mass m in a Potential $V(x)$. In one dimension the Schrödinger equation is just an ordinary differential equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi(x) = E\psi(x). \tag{3.1}$$

We start with simple finite-difference schemes and discretize space into intervals of length Δx and denote the space points by

$$x_n = n\Delta x \tag{3.2}$$

and the wave function at these points by

$$\psi_n = \psi(x_n). \tag{3.3}$$

3.1.1 The Numerov algorithm

After rewriting the second order differential equation to a coupled system of two first order differential equations, any ODE solver such as the Runge-Kutta method could be applied, but there exist better methods. For the special form

$$\psi''(x) + k(x)\psi(x) = 0, \tag{3.4}$$

of the Schrödinger equation, with $k(x) = 2m(E - V(x))/\hbar^2$ we can derive the Numerov algorithm by starting from the Taylor expansion of ψ_n:

$$\psi_{n\pm1} = \psi_n \pm \Delta x\psi'_n + \frac{\Delta x^2}{2}\psi''_n \pm \frac{\Delta x^3}{6}\psi^{(3)}_n + \frac{\Delta x^4}{24}\psi^{(4)}_n \pm \frac{\Delta x^5}{120}\psi^{(5)}_n + \mathrm{O}(\Delta x^6) \tag{3.5}$$

Adding ψ_{n+1} and ψ_{n-1} we obtain

$$\psi_{n+1} + \psi_{n-1} = 2\psi_n + (\Delta x)^2\psi''_n + \frac{(\Delta x)^4}{12}\psi^{(4)}_n. \tag{3.6}$$

Replacing the fourth derivatives by a finite difference second derivative of the second derivatives

$$\psi_n^{(4)} = \frac{\psi''_{n+1} + \psi''_{n-1} - 2\psi''_n}{\Delta x^2} \tag{3.7}$$

and substituting $-k(x)\psi(x)$ for $\psi''(x)$ we obtain the Numerov algorithm

$$\begin{aligned}\left(1 + \frac{(\Delta x)^2}{12} k_{n+1}\right)\psi_{n+1} = \quad & 2\left(1 - \frac{5(\Delta x)^2}{12} k_n\right)\psi_n \\ & - \left(1 + \frac{(\Delta x)^2}{12} k_{n-1}\right)\psi_{n-1} + \mathrm{O}(\Delta x^6),\end{aligned} \tag{3.8}$$

which is locally of sixth order!

Initial values

To start the Numerov algorithm we need the wave function not just at one but at two initial values and will now present several ways to obtain these.

For potentials $V(x)$ with reflection symmetry $V(x) = V(-x)$ the wave functions need to be either even $\psi(x) = \psi(-x)$ or odd $\psi(x) = -\psi(-x)$ under reflection, which can be used to find initial values:

- For the even solution we use a half-integer mesh with mesh points $x_{n+1/2} = (n + 1/2)\Delta x$ and pick initial values $\psi_(x_{-1/2}) = \psi(x_{1/2}) = 1$.
- For the odd solution we know that $\psi(0) = -\psi(0)$ and hence $\psi(0) = 0$, specifying the first starting value. Using an integer mesh with mesh points $x_n = n\Delta x$ we pick $\psi(x_1) = 1$ as the second starting value.

In general potentials we need to use other approaches. If the potentials vanishes for large distances: $V(x) = 0$ for $|x| \geq a$ we can use the exact solution of the Schrödinger equation at large distances to define starting points, e.g.

$$\psi(-a) = 1 \tag{3.9}$$

$$\psi(-a - \Delta x) = \exp(-\Delta x\sqrt{2mE/\hbar}). \tag{3.10}$$

Finally, if the potential never vanishes we need to begin with a single starting value $\psi(x_0)$ and obtain the second starting value $\psi(x_1)$ by performing an integration over the first time step $\Delta\tau$ with an Euler or Runge-Kutta algorithm.

3.1.2 The one-dimensional scattering problem

The scattering problem is the numerically easiest quantum problem since solutions exist for all energies $E > 0$, if the potential vanishes at large distances ($V(x) \to 0$ for $|x| \to \infty$). The solution becomes particularly simple if the potential is nonzero only on a finite interval $[0, a]$. For a particle approaching the potential barrier from the left ($x < 0$) we can make the following ansatz for the free propagation when $x < 0$:

$$\psi_L(x) = A\exp(-iqx) + B\exp(iqx) \tag{3.11}$$

where A is the amplitude of the incoming wave and B the amplitude of the reflected wave. On the right hand side, once the particle has left the region of finite potential ($x > a$), we can again make a free propagation ansatz,

$$\psi_R(x) = C \exp(-iqx) \tag{3.12}$$

The coefficients A, B and C have to be determined self-consistently by matching to a numerical solution of the Schrödinger equation in the interval $[0, a]$. This is best done in the following way:

- Set $C = 1$ and use the two points a and $a + \Delta x$ as starting points for a Numerov integration.
- Integrate the Schrödinger equation numerically – backwards in space, from a to 0 – using the Numerov algorithm.
- Match the numerical solution of the Schrödinger equation for $x < 0$ to the free propagation ansatz (3.11) to determine A and B.

Once A and B have been determined the reflection and transmission probabilities R and T are given by

$$R = |B|^2/|A|^2 \tag{3.13}$$
$$T = 1/|A|^2 \tag{3.14}$$

3.1.3 Bound states and solution of the eigenvalue problem

While there exist scattering states for all energies $E > 0$, bound states solutions of the Schrödinger equation with $E < 0$ exist only for discrete energy eigenvalues. Integrating the Schrödinger equation from $-\infty$ to $+\infty$ the solution will diverge to $\pm\infty$ as $x \to \infty$ for almost all values. These functions cannot be normalized and thus do not constitute solutions to the Schrödinger equation. Only for some special eigenvalues E, will the solution go to zero as $x \to \infty$.

A simple eigensolver can be implemented using the following shooting method, where we again will assume that the potential is zero outside an interval $[0, a]$:

- Start with an initial guess E
- Integrate the Schrödinger equation for $\psi_E(x)$ from $x = 0$ to $x_f \gg a$ and determine the value $\psi_E(x_f)$
- use a root solver, such as a bisection method (see appendix A.1), to look for an energy E with $\psi_E(x_f) \approx 0$

This algorithm is not ideal since the divergence of the wave function for $x \pm \infty$ will cause roundoff error to proliferate.

A better solution is to integrate the Schrödinger equation from both sides towards the center:

- We search for a point b with $V(b) = E$

- Starting from $x = 0$ we integrate the left hand side solution $\psi_L(x)$ to a chosen point b and obtain $\psi_L(b)$ and a numerical estimate for $\psi'_L(b) = (\psi_L(b) - \psi_L(b - \Delta x))/\Delta x$.
- Starting from $x = a$ we integrate the right hand solution $\psi_R(x)$ down to the same point b and obtain $\psi_R(b)$ and a numerical estimate for $\psi'_R(b) = (\psi_R(b + \Delta x) - \psi_R(b))/\Delta x$.
- At the point b the wave functions and their first two derivatives have to match, since solutions to the Schrödinger equation have to be twice continuously differentiable. Keeping in mind that we can multiply the wave functions by an arbitrary factor we obtain the conditions

$$\begin{aligned} \psi_L(b) &= \alpha\psi_R(b) && (3.15)\\ \psi'_L(b) &= \alpha\psi'_R(b) && (3.16)\\ \psi''_L(b) &= \alpha\psi''_R(b) && (3.17) \end{aligned}$$

  The last condition is automatically fulfilled since by the choice $V(b) = E$ the Schrödinger equation at b reduces to $\psi''(b) = 0$. The first two conditions can be combined to the condition that the logarithmic derivatives vanish:

$$\frac{d\log\psi_L}{dx}|_{x=b} = \frac{\psi'_L(b)}{\psi_L(b)} = \frac{\psi'_R(b)}{\psi_R(b)} = \frac{d\log\psi_R}{dx}|_{x=b} \qquad (3.18)$$

- This last equation has to be solved for in a shooting method, e.g. using a bisection algorithm

Finally, at the end of the calculation, normalize the wave function.

3.2 The time-independent Schrödinger equation in higher dimensions

The time independent Schrödinger equation in more than one dimension is a partial differential equation and cannot, in general, be solved by a simple ODE solver such as the Numerov algorithm. Before employing a PDE solver we should thus always first try to reduce the problem to a one-dimensional problem. This can be done if the problem factorizes.

3.2.1 Factorization along coordinate axis

A first example is a three-dimensional Schrödinger equation in a cubic box with potential $V(\vec{r}) = V(x)V(y)V(z)$ with $\vec{r} = (x, y, z)$. Using the product ansatz

$$\psi(\vec{r}) = \psi_x(x)\psi_y(y)\psi_z(z) \qquad (3.19)$$

the PDE factorizes into three ODEs which can be solved as above.