KTH PHYSICS May 13, 2022
SH1017 Physics for Engineering Mathematics

Computer Lab 4: Schrödinger equation

In this lab the simplest version of solution to the Schrödinger equation is studied numerically: eigenstates to the one-dimensional time-independent Schrödinger equation for a particle bound by a potential. The problem is: given $V(x)$, compute eigenvalues E_n and eigenstates $\psi_n(x)$. Here a couple of simple potentials are used to explore the possibilities, but you should appreciate that any potential with bound states can be solved by this method. The provided code implements the Verlet method. The focus is not on how the algorithm works or to produce effective code. The purpose is rather to explore and identify some key points in the numerical solution of physics problems. In the code all physics constants have been set to 1 for simplicity so $\hbar = m = 1$ etc. This is often done in simulations. To get realistic answers the solution has to be rescaled to correct physical units but this will not be considered here. The code implements the shooting method. An input value for the energy eigenvalue E is provided as an initial guess. Initial values for ψ, ψ' are also provided at a starting point, then the SE is integrated towards a end point. If the prescribed continuity conditions are fulfilled at the end point then E is an eigenvalue and an eigenstate has been found. Otherwise the program is executed again with an adjusted guess for E. This process is iterated with a sequence of systematically refined values until the eigenvalue is found with desired accuracy. The code produces unnormalized eigenstates. It is easily to normalize numerically but we will not do that here.

1. The provided python code considers a particle in a one-dimensional infinite box potential of width $L = 1$. The solution to this problem was given in the lecture. Why study a problem with a know solution? This is a very useful test in order to (1) verify that the code is correct and (2) check what discretization is needed to get desired accuracy. The exact energy eigenvalues are $E_n = \hbar^2\pi^2n^2/2mL^2$ which gives $E_n = \pi^2n^2/2$ in the units used. First set $E = 0.5\pi^2$ which is the exact ground state energy. The provided code uses $N = 10$ mesh points and produces poor accuracy. The error is conveniently measured as $\Delta = |\psi(1)|$, which is $= 0$ in the exact solution. The first task is to compute $\Delta(N)$ for $N = 10, 100, 1000, 10000$. Plot Δ vs N in a loglog plot in order to verify that the expected $\Delta = constant/N^2$ is fulfilled. This can be done by setting the constant to a suitable value to get data points and the exact line to coincide. For the rest of the lab $N = 10000$ or more can be used.

2. To locate the ground state energy without assuming its value, make an initial guess, say $E = 0.4\pi^2$ and run the code. This does not find the correct endpoint since $\psi \neq 0$ there. Repeat with a new value $E = 0.6\pi^2$, and so on with a sequence of systematically refined values until ψ satisfies the correct continuity condition at the end point and the eigenvalue is located with desired accuracy. This iteration can be done by hand or by writing a binary search loop (intervallhalvering) which is suggested. In this way determine the 4 lowest eigenvalues and provide a plot of their eigenstates $\psi_n, n = 1, 2, 3, 4$.

3. Change model to the harmonic oscillator given by $V(x) = x^2/2$ in units where all constants are set to =1. The known energy eigenvalues then become $E_n = n+1/2$. The code has to be modified in a few ways to solve this problem. (1) The new potential has to be coded. It is already in the code, a comment sign has to be removed. (2) The start condition is $\psi(0) = 1, \psi'(0) = 0$ for even eigenstates and $\psi(0) = 0, \psi'(0) = 1$ for odd. (3) The right endpoint for the integration might need to be adjusted upwards in order to get the solution to match the continuity requirement $\psi(x) = \psi'(x) = 0$ at the upper integration point: change $dx = 1/N$ to $5/N$. Determine the 4 lowest energy eigenvalues and plot the eigenstates. The odd solutions are hard to converge and might need an increased number of mesh points.

4. Next change to an anharmonic potential: $V(x) = x^2/2 + x^4/2$. This problem does not have an analytic solution in terms of well-known special functions and thus demonstrates the power of numerics. Find the lowest 4 energy eigenvalues and the corresponding eigenstates and plot them. In the lecture an approximation method to estimate the solution will be studied and compared with the results found here. With a similar approach virtually any bound state problem can be studied numerically.

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