Physics 115/242

Numerov method for integrating the one-dimensional Schrödinger equation.

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The one-dimensional time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x), \tag{1}$$

where $\psi(x)$ is the wavefunction, $V(x)$ is the potential energy, m is the mass, and $\hbar$ is Planck's constant divided by 2π. This is an eigenvalue problem since one can only find a solution which vanishes at $\pm\infty$ (the boundary conditions) for certain discrete values of E.

In order to find the energy eigenvalues, we need to be able to integrate the equation with respect to x, for a given value of E, starting at $x = x_0$, say, with some specified values for $x = x_0$ and $x = x_1 = x_0 + h$, where h is the step interval. Using the notation $x_n = x_0 + nh$ and $\psi_n \equiv \psi(x_n)$, we have to solve for $\psi_2, \psi_3, \cdots$, given ψ_0 and ψ_1. Having solved the equation for a given value of E we need to vary E until we find a solution which satisfies the boundary conditions, which requires re-solving the equation for each value of E. We will discuss this aspect of the problem, using what is called the "shooting method", in more detail in class.

Here we focus on the problem of integrating the equation for a *given* value of E. One method would be to use 4-th order Runge-Kutta (RK4), since it is is quite accurate. RK4 involves writing Schrödinger's equation, which is second order, as two first order equations:

$$\begin{aligned}\frac{d\psi}{dx} &= \phi(x) \\ \frac{d\phi}{dx} &= -k^2(x)\psi(x),\end{aligned} \tag{2}$$

where

$$k^2(x) = \frac{2m}{\hbar^2}\left(E - V(x)\right). \tag{3}$$

You will recall that this a fourth order method, i.e. the error is proportional to h^4.

An alternative, is to leave the Schrödinger equation as one second order equation,

$$\boxed{\frac{d^2\psi}{dx^2} + k^2(x)\psi(x) = 0,} \tag{4}$$

and take advantage of its particular structure (it is linear in ψ and there is no term involving the first derivative.) A suitable algorithm for this type of problem is the *Numerov* algorithm, which is simpler than RK4 and is one one higher order (fifth).

We now describe the Numerov method (see also Landau and Páez). A Taylor series for $\psi(x+h)$ gives

$$\psi(x+h)=\psi(x)+h\psi'(x)+\frac{h^2}{2}\psi^{(2)}(x)+\frac{h^3}{6}\psi^{(3)}(x)+\frac{h^4}{24}\psi^{(4)}(x)+\cdots\,. \tag{5}$$

Adding this to the series for $\psi(x-h)$ all the odd powers of h vanish:

$$\psi(x+h)+\psi(x-h)=2\psi(x)+h^2\psi^{(2)}(x)+\frac{h^4}{12}\psi^{(4)}(x)+O(h^6)\,. \tag{6}$$

We can therefore write the second derivative which occurs in the Schrödinger equation, Eq. (4), as

$$\psi^{(2)}(x)=\frac{\psi(x+h)+\psi(x-h)-2\psi(x)}{h^2}-\frac{h^2}{12}\psi^{(4)}(x)+O(h^4). \tag{7}$$

We would like to evaluate the term involving the 4th derivative. To do so, we act on Eq. (4) with $1+(h^2/12)d^2/dx^2$, which gives

$$\psi^{(2)}(x)+\frac{h^2}{12}\psi^{(4)}(x)+k^2(x)\psi(x)+\frac{h^2}{12}\frac{d^2}{dx^2}\left[k^2(x)\psi(x)\right]=0. \tag{8}$$

Substituting for $\psi^{(2)}(x)+\frac{h^2}{12}\psi^{(4)}(x)$ from Eq. (8) into Eq. (7) gives

$$\psi(x+h)+\psi(x-h)-2\psi(x)+h^2k^2(x)\psi(x)+\frac{h^4}{12}\frac{d^2}{dx^2}\left[k^2(x)\psi(x)\right]+O(h^6)=0. \tag{9}$$

We evaluate $\frac{d^2}{dx^2}\left[k^2(x)\psi(x)\right]$ by using an elementary difference formula (this has an error $O(h^2)$ but preserves the overall $O(h^6)$ accuracy since it is multiplied by h^4 in Eq. (9)):

$$\frac{d^2}{dx^2}\left[k^2(x)\psi(x)\right]\simeq\frac{k^2(x+h)\psi(x+h)+k^2(x-h)\psi(x-h)-2k^2(x)\psi(x)}{h^2}. \tag{10}$$

Substituting Eq. (10) into Eq. (9) and rearranging we get the Numerov algorithm for one time step:

$$\psi(x+h)=\frac{2\left(1-\frac{5}{12}h^2k^2(x)\right)\psi(x)-\left(1+\frac{1}{12}h^2k^2(x-h)\right)\psi(x-h)}{1+\frac{1}{12}h^2k^2(x+h)}+O(h^6). \tag{11}$$

Setting $x=x_n\equiv x_0+nh$, and defining $k_n\equiv k(x_n)$, this can be written more tidily as

$$\boxed{\psi_{n+1}=\frac{2\left(1-\frac{5}{12}h^2k_n^2\right)\psi_n-\left(1+\frac{1}{12}h^2k_{n-1}^2\right)\psi_{n-1}}{1+\frac{1}{12}h^2k_{n+1}^2},} \tag{12}$$

with an error of order h^6. The Numerov method, Eq. (12), can be used to determine ψ_n for $n=2,3,4,\cdots$, given *two* initial values, ψ_0 and ψ_1. (We need two initial values because Eq. (4) is a second order differential equation.)

The error in one time step is $O(h^6)$, see Eq. (9). However, as we have also discussed in other contexts, the number of steps needed to integrate over a *fixed* range of x, from x_0 to x_f say, is

$(x_f - x_0)/h \propto 1/h$. One might expect that the errors at each step would be roughly comparable so so the total error in the Numerov method would be $O(h^6 h^{-1})$, i.e. $O(h^5)$, a $\boxed{\text{5-th order method,}}$ one higher than RK4. Indeed one ofter sees this statement in the books, e.g. Landau and Paez. However, this is *not* correct, the error grows with succesive steps, and the final error is $O(h^4)$, the *same* as RK4. This will be discussed in the solution to an (optional) homework question.

Note too that there can be problems with roundoff errors in using Eq. (12) so make sure you use double precision arithmetic.