Physics 721: Homework # 6
Due Wednesday November 25
website: http://www.physics.umd.edu/courses/Phys721

Numerical solutions of the Schrödinger equation

We want to numerically find the bound-state energies and wavefunctions of the one-dimensional or radial Schrödinger equation

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)\right)\psi(r)=E\psi(r)$$

on the interval $r \in [a,b]$ with boundary conditions $\psi(a) = \psi(b) = 0$. We break this Hamiltonian into a kinetic energy operator

$$K=-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\,,$$

and potential $V(r)$. The particle-in-a-box solutions $\phi_n(r)$ form a complete set of real orthonormal functions $\phi_n(r)$ with $K\phi_n(r) = \epsilon_n\phi_n(r)$ with $n = 1, 2, \cdots$. We assume $\epsilon_n < \epsilon_m$ when $n < m$.

The homework exercise will work through the numerical method called the discrete variable representation (DVR).

1. Expand the wavefunction $\psi(r)$ in terms of particle-in-a-box solutions and give expressions for the matrix elements of the kinetic energy and potential operator in this basis. (At this stage you do not need to evaluate V explicitly.)

We are now going to use a quadrature method to evaluate spatial integrals assuming N spatial points r_i and weights w_i so that

$$\int dr\,\Xi(r)\approx\sum_i w_i\,\Xi(r_i)\,.$$

2. Write a discrete form of the orthogonality

$$\int dr\phi_m(r)\phi_n(r)=\delta_{nm}$$

and completeness relation

$$\sum_n \phi_n(r)\phi_n(r')=\delta(r-r')\,.$$

Realize that the delta function $\delta(r-r')$ is a distribution with $\int dr\, f(r)\delta(r-r') = f(r')$ for *all* well-behaved $f(r)$. (Again you do not yet need the explicit form of the particle-in-a-box solutions)

3. Write a discrete form of the potential matrix elements V_{nm}.

We restrict ourselves to the first N particle-in-a-box solutions and we define the $N \times N$ matrices $U_{ij} = \delta_{ij}V(r_i)$ and $O_{ni} = \sqrt{w_i}\phi_n(r_i)$.

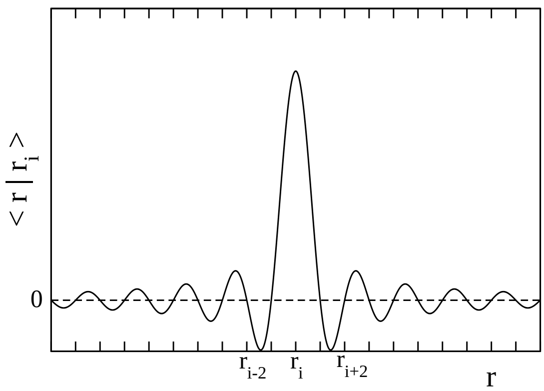
4. Show that $O^TO = 1$.

5. Show that OO^T is equivalent to the completeness relation derived in (2) and thus $O^TO = 1$. What type of matrix is O?

6. Show that $U = O^TVO$.

7. What are the basis functions in the spatial grid basis? Ie. determine the functions $g_i(x)$ in terms of $\phi_n(x)$ such that $\psi(x) = \sum_{n=1}^{N} c_n \phi_n(x) = \sum_{i=1}^{N} b_i g_i(x)$. Show that $g_i(x_j) = \delta_{ij}$? What is the relation between c_n and b_i?.

The functions $g_i(x)$ are localized in space. See figure for an example (you do not need to reproduce this)



Note that we have transformed the potential from a "finite basis representation" to a "discrete variable representation" or grid basis. We can now return to the particle-in-a-box solutions and use its explicit form.

8. Show that with $r_i = a + i(b-a)/(N+1)$ and $w_i = (b-a)/(N+1)$ for $i = 1, \ldots, N$ the matrix O satisfies $O^T O = O O^T = 1$. It helps to separately evaluate the diagonal and off-diagonal matrix elements.

9. Find a closed expression for the kinetic energy operator in the grid basis. I.e. evaluate and simplify $O^T K O$ using the geometric series. It helps to separately evaluate the diagonal and off-diagonal matrix elements.

We now want to find the eigenenergies for an actual physical system. We choose the harmonic oscillator potential $V(r) = \mu\omega^2 r^2/2$ on the region $[-L, L]$. Note that if $L \to \infty$ the eigenenergies are $E_n = (n - 1/2)\hbar\omega$ for $n = 1, 2, 3, \ldots$.

10. Using your favorite numerical tool, program the Hamiltonian

$$O^T K O + U$$

and study the lowest ten eigenenergies as a function of N and L. In particular, plot the difference of the numerical values and the exact values E_n as a function N. Which eigenenergy converges quickest and why is this so? How does the energy depend on L. How large should L be?

You might want to keep the following in mind: a) Choose the most natural units for the problem: you can make the Schrödinger equation dimensionless, b) Is this a good way to debug your code? For example, using SI units does not lead to easily debugged code.