Chem. 550
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BASICS – COMPUTER ASSIGNMENT 2

In this assignment you will write a computer code to calculate the time evolution of a wavefunction in a one-dimensional potential $V(x)$ by expanding the time-dependent wavefunction $\Psi(x;t)$ in a basis set $\{\Phi_n\}$ with time-dependent coefficients $c_n(t)$. For this assignment you will use the lowest *N* particle-in-a-box basis functions, which are very easy to code. Proceed by following the steps given below.

(a) Define the box size *L* as a parameter (to be adjusted later) and code the particle-in-a-box wavefunctions.

(b) Calculate the matrix elements H_{mn} of the Hamiltonian with respect to these basis functions by using the trapezoid rule or Simpson's rule. These are very easy to code, but you may also obtain library subroutines if you prefer.

(c) Evaluate the overlap integrals of a chosen initial wavefunction $\Psi(x;0)$ with the basis functions in order to calculate the expansion coefficients $c_n(0)$ of this wavefunction.

(d) Look up a subroutine that solves coupled 1st order differential equations. Make sure you understand how to use it and perform a few tests on systems where you know the answer. Using the computed expansion coefficients $c_n(0)$ as initial values, solve the coupled differential equations to obtain the expansion coefficients $c_n(t)$ as a function of time.

Implement your code to explore the time evolution of a wavefunction which initially has a Gaussian form,

$$\Psi(x;0) = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}(x-a)^2}$$

with $\hbar, m, \omega$ set equal to 1 and $a = 0.1$ under the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 + b\hat{x}^4$$

with $b = 0.1$. Reconstruct the evolving wavefunction $\Psi(x;t)$ from the expansion and calculate the expectation value of the position operator by evaluating the integral numerically.

Note that the box size *L* and the number *n* of basis functions are convergence parameters. To converge, start by plotting the initial wavefunction and choose a box length that is just large enough to "fit" this function. Choose a value for the number *n* of basis functions. Then, keeping the chosen value of *L* fixed, run your code and focus on a particular result, e.g. the expectation value of position after some time, increasing n until this value converges. Next, try a slightly larger value of L and converge again with respect to the number of basis functions, until you have converged with respect to the box size as well.

With the final values of L and n, plot snapshots of the probability density at a few select values of time. Also plot the survival probability as a function of time for 2-3 periods of motion.