

Physics 4350 Computational Physics

1. (Variational method in QM. Perturbed particle in a box.). Using Octave/Matlab, calculate the energy levels of a perturbed "particle in a box" using the variational method as described in class. The perturbation (as defined in the code below) is a step in the last 1/4 of the box. Calculate the energy levels for a perturbation (step height in the box) of $\lambda H_1 = 0.2$ using the lowest 8 base states from the unperturbed Hamiltonian. Use atomic units ($\hbar = m = L = 1$). You may use the code snippets below in your Octave/Matlab program.

```
# First, we define the basis set
function y = u(n,x)
    global hbar m L;
    y = sqrt(2/L)*sin(n*pi*x/L);
endfunction

function y = upp(n,x) % the second derivative of u
    global hbar m L;
    y = -(n^2*pi^2/L^2)*sqrt(2/L)*sin(n*pi*x/L);
endfunction

# Define some functions for integration
function y = umult(n1,n2,x)
    global hbar m L;
    y = u(n1,x)*u(n2,x);
endfunction

# Define the perturbed potential
function y = vpert(x)
    global perturbation;
    if ( x <= 0.75 ) y = 0; endif
    if ( x > 0.75 ) y = perturbation; endif
endfunction

function y = uH0u(n1,n2,x)
    global hbar m L;
    y = -( hbar^2 / (2*m) ) * u(n1,x)*upp(n2,x);
endfunction

function y = uVu(n1,n2,x)
    global hbar m L;
    y = u(n1,x)*vpert(x)*u(n2,x);
endfunction

# calculate the integrals
function y = H0(i,j)
    global hbar m L;
    [v,error,nval] = quad( @(x) uH0u(i,j,x),0,L);
    y = v;
endfunction

function y = V(i,j)
    global hbar m L;
    [v,error,nval] = quad( @(x) uVu(i,j,x),0,L);
    y = v;
endfunction
```