ECE 456 - Problem Set 2

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Problem 1

(a) Code:

```
clear all;
%physical constants in MKS units

hbar = 1.054e-34;
q = 1.602e-19;
m = 9.110e-31;

%generate lattice

N  = 100;                    %number of lattice points
n  = [1:N];                  %lattice points
a  = 1e-10;                  %lattice constant
x  = a * n;                  %x-coordinates
t0 = (hbar^2)/(2*m*a^2)/q;   %encapsulating factor
L  = a * (N+1);              %total length of consideration

%set up Hamiltonian matrix

U = 0*x; %0 potential at all x
main_diag  = diag(2*t0*ones(1,N)+U,0); %create main diagonal matrix
lower_diag = diag(-t0*ones(1,N-1),-1); %create lower diagonal matrix
upper_diag = diag(-t0*ones(1,N-1),+1); %create upper diagonal matrix

H = main_diag + lower_diag + upper_diag; %sum to get Hamiltonian matrix

[eigenvectors,E_diag] = eig(H); %"eigenvectors" is a matrix wherein each
                                %column is an eigenvector
                                %"E_diag" is a diagonal matrix where the
                                %corresponding eigenvalues are on the
                                %diagonal.

E_col = diag(E_diag); %folds E_diag into a column vector of eigenvalues

% return eigenvectors for the 1st and 50th eigenvalues

phi_1  = eigenvectors(:,1);
phi_50 = eigenvectors(:,50);

% find the probability densities of position for 1st and 50th eigenvectors

P_1 = phi_1 .* conj(phi_1);
P_50 = phi_50 .* conj(phi_50);

% Find first N analytic eigenvalues
E_col_analytic = (1/q) * (hbar^2 * pi^2 * n.*n) / (2*m*L^2);

% Plot the probability densities for 1st and 50th eigenvectors

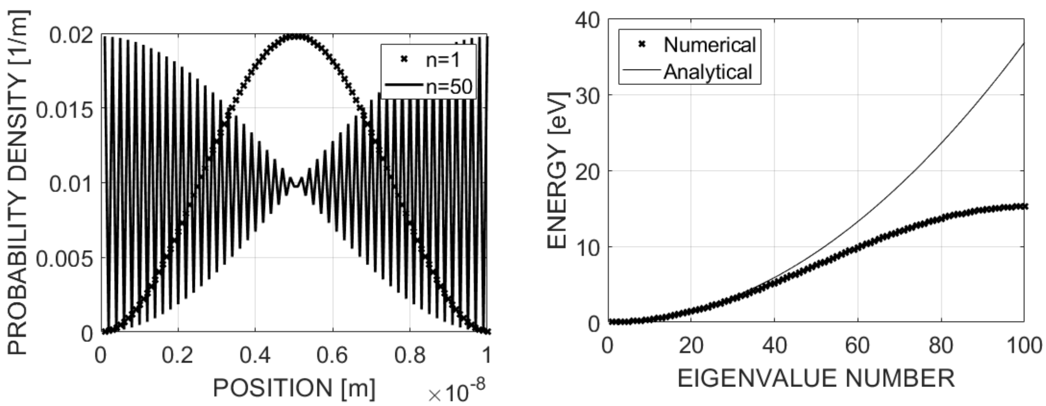
figure(1); clf; h = plot(x,P_1,'kx',x,P_50,'k-');
grid on; set(h,'linewidth',[2.0]); set(gca,'Fontsize',[18]);
xlabel('POSITION [m]'); ylabel('PROBABILITY DENSITY [1/m]');
legend('n=1','n=50');

```

```
% Plot numerical eigenvalues
figure(2); clf; h = plot(n,E_col,'kx'); grid on;
set(h,'linewidth',[2.0]); set(gca,'Fontsize',[18]);
xlabel('EIGENVALUE NUMBER'); ylabel('ENERGY [eV]');
axis([0 100 0 40]);

% Add analytic eigenvalues to above plot

hold on;
plot(n,E_col_analytic,'k-');
legend({'Numerical','Analytical'},'Location','northwest');
```



(a)

(b) Comparison of first 101 numerical and analytic eigenvalues.

Figure 1: (a) Probability densities for $n = 1$ and $n = 50$. (b) Comparison of first 101 numerical and analytic eigenvalues.

(b) (i) The analytical solution is

$$\phi(x) = Asin\left(\frac{n\pi}{L}x\right) \tag{1}$$

In order to normalise this equation it must conform to the following:

$$\int_0^L |\phi(x)|^2 \, dx = 1. \tag{2}$$

We use the following identity:

$$\int \sin^2(ax) \, dx = \frac{1}{2}x - \frac{1}{4a}\sin(2ax). \tag{3}$$

Given that *sin* of a real value is always real, we can disregard the norm operation, and directly relate (1) to the above identity. Evaluating the integral gives us the following relationship

$$\frac{1}{A^2} = \frac{1}{2}L - \cancel{\frac{L}{4n\pi}sin\left(\frac{2n\pi}{L}L\right)} - \cancel{\frac{1}{2}\cdot 0} + \cancel{\frac{L}{4n\pi}sin(0)}$$

From this, we find:

$$\boxed{A = \sqrt{\frac{2}{L}}}$$

(ii) Starting with the normalization condition for the numerical case:

$$a \sum_{l=1}^{N} |\phi_l|^2 = a \tag{4}$$

$$a \sum_{l=1}^{N} \left| B \sin\left(\frac{n\pi}{L} x_l\right) \right|^2 = a, \tag{5}$$

recalling that $x = al$, and allowing $a \to 0$ while holding L constant implies that $N \to \infty$, since $a = \frac{L}{N}$. An integral is defined as the limit of a Riemann sum as follows:

$$\int_c^d f(x)\, dx \equiv \lim_{n\to\infty} \sum_{i=1}^{n} \Delta x \cdot f(x_i). \tag{6}$$

where $\Delta x = \frac{d-c}{n}$ and $x_i = c + \Delta x \cdot i$. In our case, $n = N$, $i = l$, $c = 0$, $d = L$, and $\Delta x = a$, $x_i = x_l$, $f(x) = \left|B \sin\left(\frac{n\pi}{L} x\right)\right|^2$. Therefore we can write

$$\int_0^L \left| B \sin\left(\frac{n\pi}{L} x\right) \right|^2 dx = \lim_{N\to\infty} \sum_{l=1}^{N} a \cdot \left| B \sin\left(\frac{n\pi}{L} x_l\right) \right|^2 = a.$$

Using (3), we have

$$\int_0^L \left| B \sin\left(\frac{n\pi}{L} x\right) \right|^2 dx = \frac{1}{2} L - \cancel{\frac{L}{4n\pi} \sin\left(\frac{2n\pi}{L} L\right)} - 0 + 0 = \frac{a}{B^2}.$$

This means that B must be

$$\boxed{B = \sqrt{\frac{2a}{L}} = \sqrt{a} \times A.}$$

(c) (i) From the base form of $\phi_\ell = Bsin\left(\frac{n\pi}{L} a\ell\right)$, we can see that $\phi_{\ell+1}$ and $\phi_{\ell-1}$ correspond to the trigonometric identities $sin(a+B) = sin(a)cos(B) + cos(a)sin(B)$ and $sin(a+B) = sin(a)cos(B) + cos(a)sin(B)$, respectively, where $a = \frac{n\pi a\ell}{L}$ and $B = \frac{n\pi a}{L}$.

Plugging these identities into equation (7) from the assignment and simplifying, we get to this equation:

$$-t_0 Bsin\left(\frac{n\pi a\ell}{L}\right) + 2t_0\phi_\ell - t_0 sin\left(\frac{n\pi a\ell}{L}\right)$$

At this point, we notice that $\phi_\ell = Bsin\left(\frac{n\pi}{L} a\ell\right)$, so we can factor it out.

With some minor rearranging, this leaves us with the final expression for E:

$$\boxed{E = 2t_0\left(1 - cos\left(\frac{n\pi a}{L}\right)\right)} \tag{7}$$

(ii) We can see here that the "predicted" numerical response matches nearly exactly the actual calculated numerical solution.

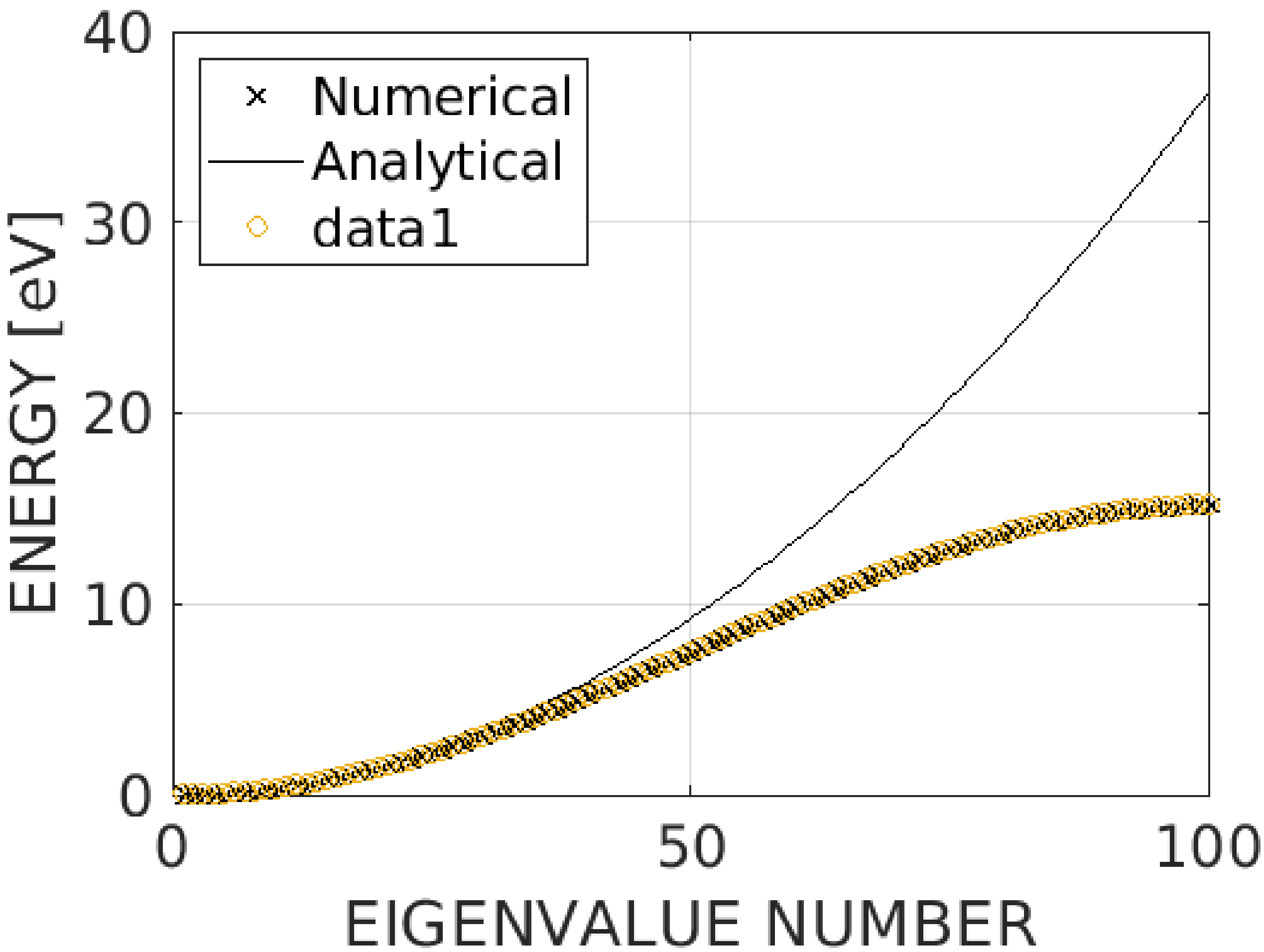


Figure 2: Analytic solution to numeric system, plotted.

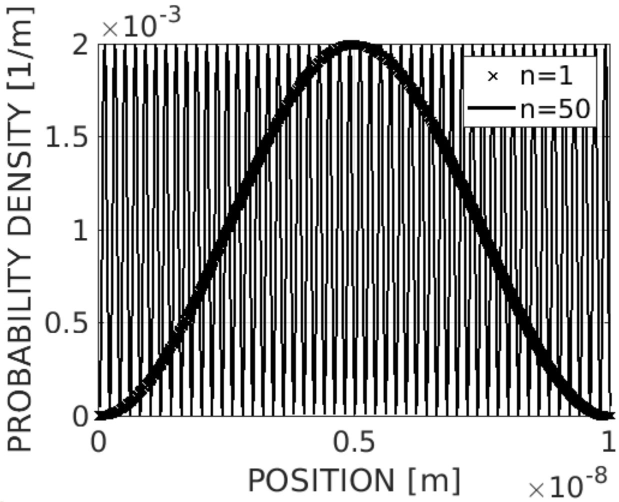
(iii) Applying the approximation $cos(\theta) = 1 - \frac{\theta^2}{2}$ for small θ, on equation (7), we get the following expression

$$E = 2t_0 \left(\frac{n^2\pi^2a^2}{2L^2} \right)$$

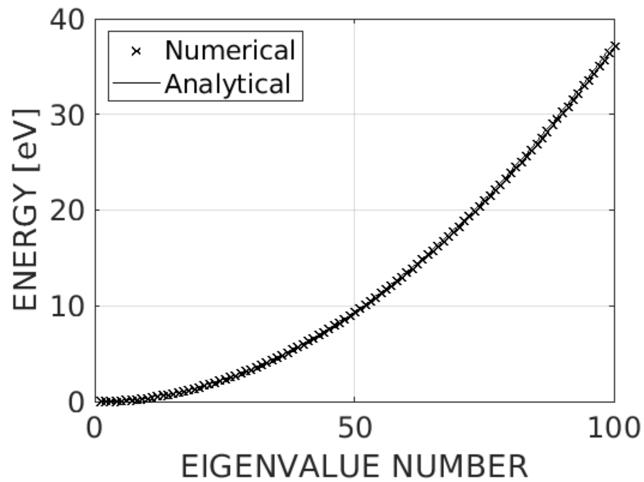
Fully substituting the known value of t_0, and we can get our final analytical expression for E:

$$\boxed{E = \frac{\hbar^2 n^2 \pi^2}{2mL^2}}$$

(iv) With the decreased lattice spacing, and increased number of points, we can see the numerical solution of eigenvalues matches the analytical solution much closer. As well, we can see that the probability density function appears to be "squeezed" in the centre, for the $n = 50$ case. The $n = 50$ case is now a constant-amplitude wave, which corresponds to the expected analytic result - in contrast to the plot in section (a), which has a low-frequency envelope around it.



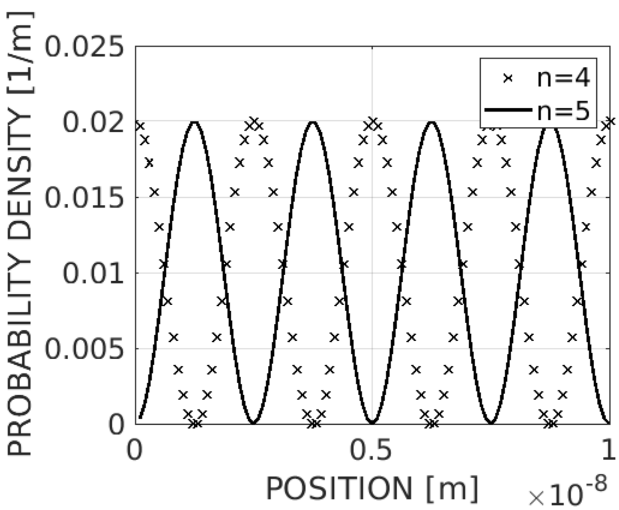
(a) Probability densities for $n = 1$ and $n = 50$.



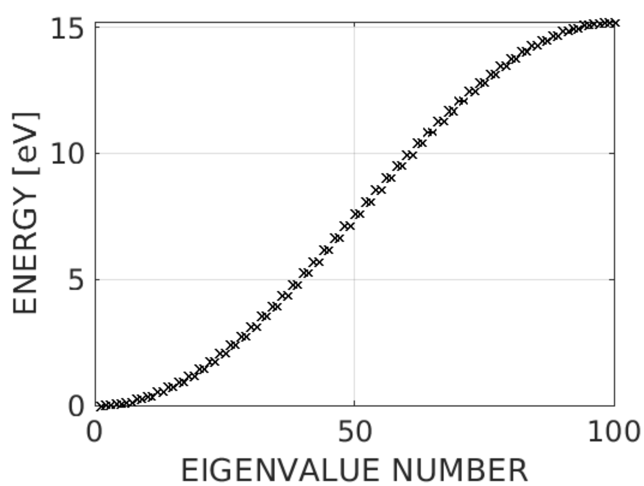
(b) Comparison of first 101 numerical and analytic eigenvalues.

(d) (i) In order to modify the computations to those for a particle in a "ring" we simply had to add $-t_0$ elements as the "corner" elements of the hamiltonian operator array:

```
% Modify hamiltonian for circular boundary conditions
H(1, N) = -t0;
H(N, 1) = -t0;
```



(a) Probability densities for $n = 4$ and $n = 5$.



(b) Comparison of first 101 numerical and analytic eigenvalues.

(ii) The energy levels for eigenvalues number 4 and 5 are both $\boxed{0.06\,\text{eV}}$. These eigenstates are degenerate because they both have the same eigenvalue/energy.

(iii)

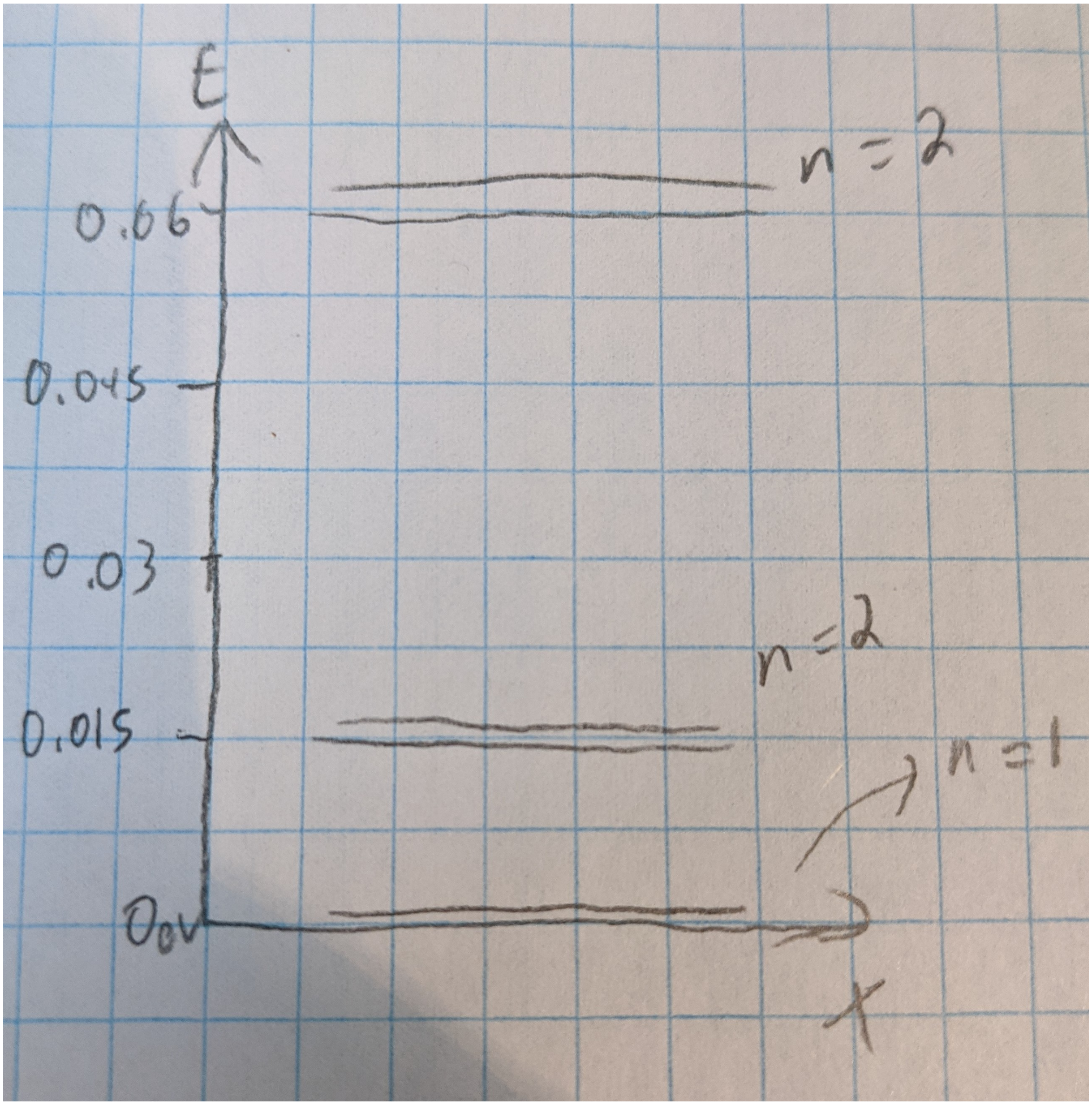


Figure 5: Sketch of degenerate energy levels.

(iv) Plugging the valid levels for n into equation (10) from the assignment (and dividing by the requisite q), we get the energy levels of $0eV, 0.0147eV, and 0.0589eV$, for the eigenvalue numbers $n = 0, 1, and 2$, respectively. These match very closely, to within acceptable margin of the numerical results from part (ii).

Problem 2

(a) Since $t_0 = \frac{\hbar^2}{2ma^2}$, and $U_l = -\frac{q^2}{4\pi\varepsilon_0 r_l} + \frac{l_o(l_o+1)\hbar^2}{2mr_l^2}$, the middle diagonal elements will have values

$$\boxed{\hat{H}_{ll} = \frac{\hbar^2}{ma^2} - \frac{q^2}{4\pi\epsilon_0 r_l} + \frac{l_o(l_o+1)\hbar^2}{2mr_l^2},}$$

and the upper and lower diagonals elements will have values

$$\boxed{\hat{H}_{l(l\pm1)} = -\frac{\hbar^2}{2ma^2}.}$$

(b) Homogenous boundary conditions imply that the corner entries of $\hat{H}$ will be $\boxed{0}$.

(c) Code:

```
clear all;
%physical constants in MKS units

hbar = 1.054e-34;
q = 1.602e-19;
m = 9.110e-31;
epsilon_0 = 8.854e-12;

%generate lattice

N  = 100;                     %number of lattice points
n  = [1:N];                   %lattice points
a  = 0.1e-10;                   %lattice constant
r  = a * n;                   %x-coordinates
t0 = (hbar^2)/(2*m*a^2)/q;    %encapsulating factor
L  = a * (N+1);               %total length of consideration

%set up Hamiltonian matrix

U = -q^2./(4*pi*epsilon_0.*r) * (1/q); %potential at r in [eV]
main_diag  = diag(2*t0*ones(1,N)+U,0); %create main diagonal matrix
lower_diag = diag(-t0*ones(1,N-1),-1); %create lower diagonal matrix
upper_diag = diag(-t0*ones(1,N-1),+1); %create upper diagonal matrix

H = main_diag + lower_diag + upper_diag; %sum to get Hamiltonian matrix

[eigenvectors,E_diag] = eig(H); %"eigenvectors" is a matrix wherein each column is an eigenvector
                                %"E_diag" is a diagonal matrix where the
                                %corresponding eigenvalues are on the
                                %diagonal.

E_col = diag(E_diag); %folds E_diag into a column vector of eigenvalues

% return eigenvectors for the 1st and 50th eigenvalues

phi_1  = eigenvectors(:,1);
phi_2 = eigenvectors(:,2);

% find the probability densities of position for 1st and 50th eigenvectors
```

```

P_1 = phi_1 .* conj(phi_1);
P_2 = phi_2 .* conj(phi_2);

% Plot the probability densities for 1st and 2nd eigenvectors

figure(1); clf; h = plot(r,P_1,'k-');
grid on; set(h,'linewidth',[2.0]); set(gca,'Fontsize',[18]);
xlabel('RADIAL POSITION [m]'); ylabel('PROBABILITY DENSITY [1/m]');
yticks([0.02 0.04 0.06 0.08 0.10 0.12]);
legend('n=1');
axis([0 1e-9 0 0.12]);

figure(2); clf; h = plot(r,P_2,'k-');
grid on; set(h,'linewidth',[2.0]); set(gca,'Fontsize',[18]);
xlabel('RADIAL POSITION [m]'); ylabel('PROBABILITY DENSITY [1/m]');
yticks([0.005 0.01 0.015 0.02 0.025 0.03 0.035 0.04]);
legend('n=2');
axis([0 1e-9 0 0.04]);
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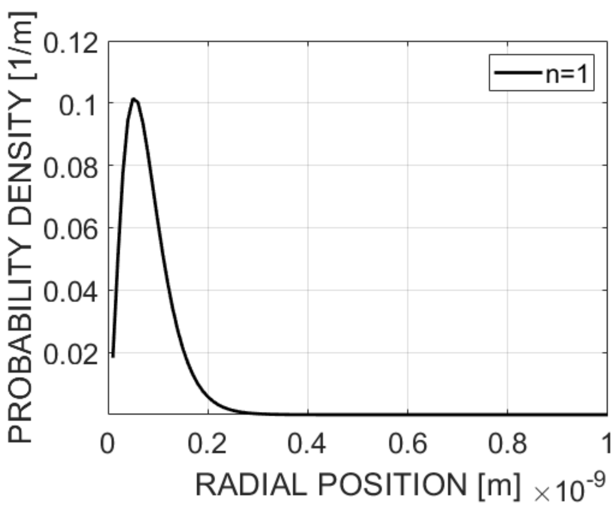
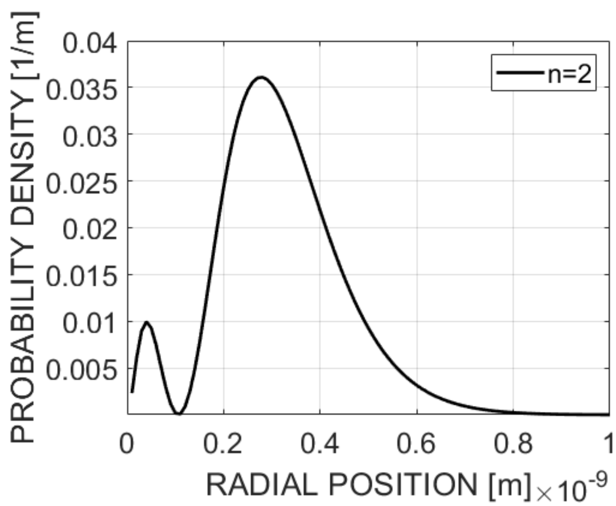


(a) 1s probability density.



(b) 2s probability density.

(d) For the 1s level, $\boxed{E = -13.4978\,\text{eV}}$.

(e) Beginning with equation (11) from the assignment, with $l_o = 0$:

$$\begin{aligned}
\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - \frac{q^2}{4\pi\epsilon_0 r}\right] f(r) &= Ef(r) \\
-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\left(\frac{2r}{a_0^{3/2}}e^{-r/a_0}\right) - \frac{q^2}{4\pi\epsilon_0 r}f(r) &= Ef(r) \\
-\frac{\hbar^2}{2m}\frac{2}{a_0^{3/2}}\frac{d}{dr}\left(e^{-r/a_0} - \frac{r}{a_0}e^{-r/a_0}\right) - \frac{q^2}{4\pi\epsilon_0 r}f(r) &= Ef(r) \\
-\frac{\hbar^2}{2m}\frac{2}{a_0^{3/2}}\left(-\frac{1}{a_0}e^{-r/a_0} - \frac{1}{a_0}e^{-r/a_0} + \frac{r}{a_0^2}e^{-r/a_0}\right) - \frac{q^2}{4\pi\epsilon_0 r}f(r) &= Ef(r) \\
-\frac{\hbar^2}{2m}\left(-\frac{2}{a_0 r} + \frac{1}{a_0^2}\right) f(r) - \frac{q^2}{4\pi\epsilon_0 r}f(r) &= Ef(r) \\
-\frac{\hbar^2}{2m}\left(-\frac{2}{a_0 r} + \frac{1}{a_0^2}\right) - \frac{q^2}{4\pi\epsilon_0 r} &= E.
\end{aligned}$$

Recalling that $a_0 = 4\pi\epsilon_0\hbar^2/mq^2$, we can eliminate r:

$$\begin{aligned}
\frac{\cancel{\hbar^2}}{\cancel{2}m}\frac{\cancel{2m}q^2}{4\pi\epsilon_0\cancel{\hbar^2}}\frac{1}{r} - \frac{\hbar^2}{2m}\frac{1}{a_0^2} - \frac{q^2}{4\pi\epsilon_0}\frac{1}{r} &= E \\
\cancel{\frac{q^2}{4\pi\epsilon_0}\frac{1}{r}} - \frac{\hbar^2}{2m}\frac{1}{a_0^2} - \cancel{\frac{q^2}{4\pi\epsilon_0}\frac{1}{r}} &= E.
\end{aligned}$$

We can then solve for E:

$$E\,[\mathrm{eV}] = -\frac{1}{q}\cdot\frac{\hbar^2}{2ma_0^2} = -\frac{1}{q}\cdot\frac{(1.054\times10^{-34}\,\mathrm{J\cdot s})^2}{2(9.110\times10^{-31}\,\mathrm{kg})(0.0529\,\mathrm{nm})^2} = \boxed{-13.6\ \mathrm{eV.}}$$

This is very similar to the result in (d).

(f) In the figure below we can see that the numerical and analytical results agree up to scaling by a. The scale difference is expected, as discussed in Problem 1. From (d), we also expect agreement in the curve shapes because the numerical and analytical energies for the 1s level are very similiar. We can see that the peak value of the analytic result is very slightly higher than that of the numerical result, which corresponds to the analytical result for the energy being slightly greater in magnitude (−13.6 eV versus −13.4978 eV).

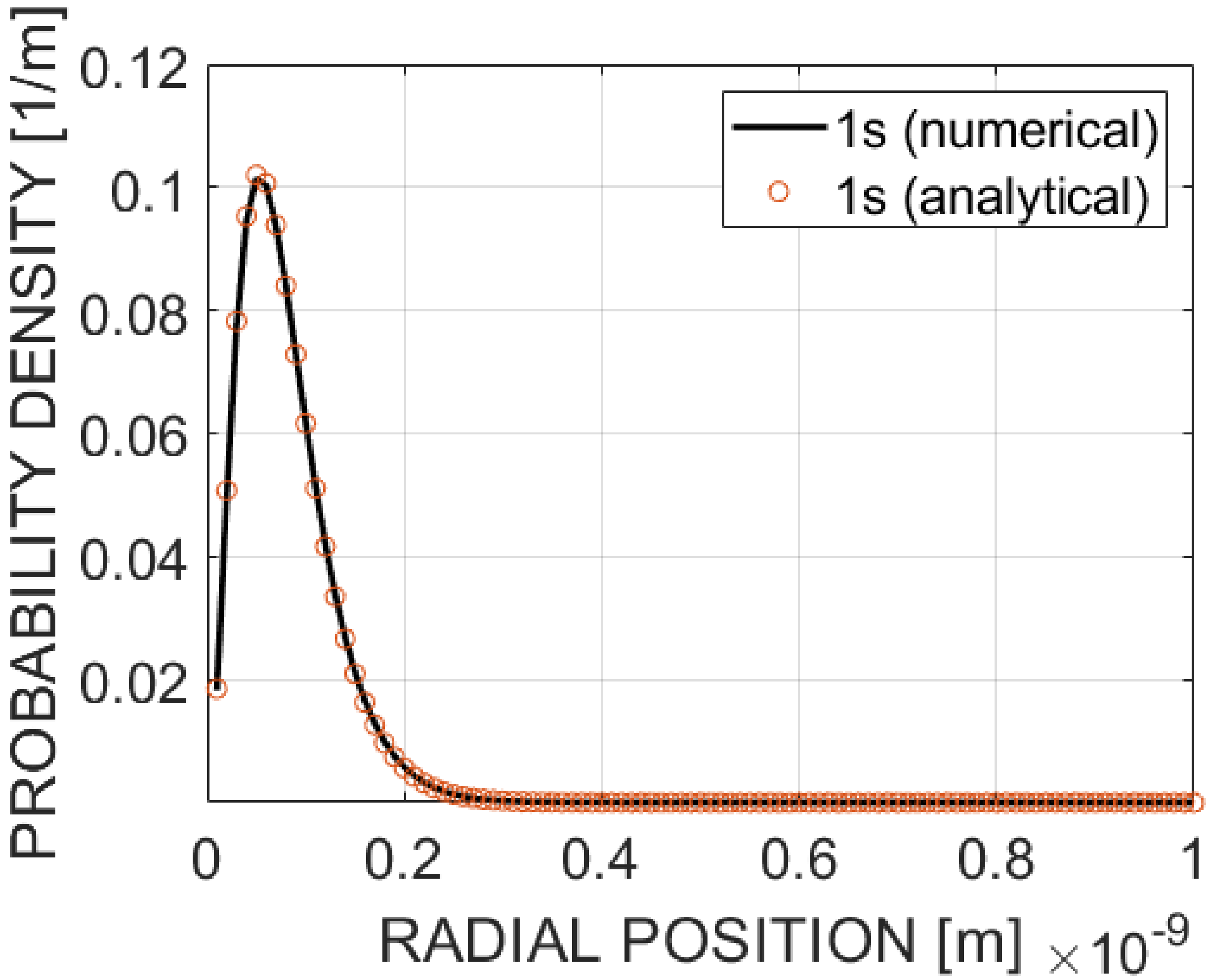


Figure 7: Numerical result (black line) and analytical solution scaled by a (orange circles).

Problem 3

(a)

$$\theta(x') = \sqrt{\frac{2}{L}} sin\left(\frac{\pi(x' + L/2)}{L}\right) = \sqrt{\frac{2}{L}} cos\left(\frac{\pi x'}{L}\right) \tag{8}$$

(b)

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Problem 4

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