1 Question 1

The solution set to the 1-Dimensional infinite potential well is well known and upon projection into position space yields the normalised eigenfunctions and eigenenergies

$$\langle x|\psi_n\rangle = \sqrt{\frac{1}{a}}sin(\frac{n\pi x}{a}) \qquad E_n = \frac{n^2\pi^2\hbar^2}{8ma^2}$$

Giving the lowest three eigenfunctions and eigenenergies as

$$\langle x|\psi_1\rangle = \sqrt{\frac{1}{a}}sin(\frac{\pi x}{a}) \qquad E_1 = \frac{\pi^2\hbar^2}{8ma^2}$$

$$\langle x|\psi_2\rangle = \sqrt{\frac{1}{a}}sin(\frac{2\pi x}{a}) \qquad E_2 = \frac{4\pi^2\hbar^2}{8ma^2}$$

$$\langle x|\psi_3\rangle = \sqrt{\frac{1}{a}}sin(\frac{3\pi x}{a}) \qquad E_3 = \frac{9\pi^2\hbar^2}{8ma^2}$$

a) First order correction to eigenenergy ϵ_n of eigenstate $|n\rangle$ is given by

$$E_n^{(N)} = \langle n| V |n\rangle$$

For the ground state case $n = 1$ of the infinite square well, using the solutions above, this is

$$\begin{aligned} E_1^{(N)} &= \langle 1| V |1\rangle \\ &= b\int_0^{a/2} dx|\psi_1(x)|^2 + (0)\int_{a/2}^{a} dx|\psi_1(x)|^2 \\ &= b\int_0^{a/2} dx|\psi_1(x)|^2 \end{aligned} \tag{1}$$

Given that we know the wave function of the ground state solution to the infinite square well to be symmetric about the point $a/2$, we know the probability density will also be symmetric about this point, being 0.5 on both sides. Thus

$$E_1^{(N)} = \frac{b}{2} \tag{2}$$

The second excited state wave function $\psi_2(x)$ is again symmetric about the point $\frac{a}{2}$ and so the same logic holds thus

$$\begin{aligned} E_1^{(N)} &= b\int_0^{a/2} dx|\psi_2(x)|^2 + (0)\int_{a/2}^{a} dx|\psi_2(x)|^2 \\ &= b\int_0^{a/2} dx|\psi_2(x)|^2 \\ &= \frac{b}{2} \end{aligned} \tag{3}$$

2 Question 2

Upper bound to the ground state energy is given by

$$E_0 \leq \frac{\langle\psi|\, H\, |\psi\rangle}{\langle\psi|\psi\rangle}$$

Where H is the hamiltonian in question. Using the trial function

$$\langle r|\psi\rangle = Ae^{\frac{-r}{a}}$$

it is reasonable to treat the hamiltonian

$$H = \frac{-1}{2m}\nabla^2 + k\frac{r^2}{2}$$

with the laplacian in spherical coordinates, given our wave function is in terms of r. Thus

$$\begin{aligned} \langle\psi|\psi\rangle &= \int_0^{2\pi} d\phi \int_0^{\pi} d\theta sin(\theta) \int_0^{\infty} drr^2A^2e^{\frac{-2r}{a}} \\ &= 4\pi A^2\int_0^{\infty} drr^2e^{\frac{-2r}{a}} \end{aligned} \tag{4}$$

Making use of the relation

$$\int_0^{\infty} dxx^n e^{-bx} = \frac{n!}{a^{n+1}}$$

We have

$$\begin{aligned}
\langle\psi|\psi\rangle &= 4\pi A^2\left(\frac{2!}{(\frac{2}{a})^3}\right) \\
&= 4\pi A^2\left(\frac{2a^3}{8}\right) \\
&= \pi A^2 a^3
\end{aligned} \tag{5}$$

The hamiltonian term is given by

$$\langle\psi| H |\psi\rangle = \frac{-1}{2m}\langle\psi| \nabla^2 |\psi\rangle + \frac{k}{2}\langle\psi| r^2 |\psi\rangle$$

Since

$$\nabla^2 = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) = \frac{2}{r}\frac{d}{dr} + \frac{d^2}{dr^2}$$

So

$$\nabla^2 Ae^{\frac{-r}{a}} = \frac{-2}{ar}Ae^{\frac{-r}{a}} + \frac{1}{a^2}Ae^{\frac{-r}{a}}$$

So

$$\begin{aligned}
\langle\psi| \nabla^2 |\psi\rangle &= 4\pi\int_0^\infty drr^2\left(\frac{-2}{ar}A^2e^{\frac{-2r}{a}} + \frac{1}{a^2}A^2e^{\frac{-2r}{a}}\right) \\
&= 4\pi A^2\left(\frac{-2}{a}\int_0^\infty drre^{\frac{-2r}{a}} + \frac{1}{a^2}\int_0^\infty drr^2e^{\frac{-2r}{a}}\right) \\
&= 4\pi A^2\left(\frac{-2}{a}\frac{a^2}{4} + \frac{1}{a^2}\frac{a^3}{4}\right) \\
&= -piA^2a
\end{aligned} \tag{6}$$

The second term is given by

$$\begin{aligned}
\langle\psi| r^2 |\psi\rangle &= 4\pi\int_0^\infty drr^3A^2e^{\frac{-2r}{a}} \\
&= 4\pi A^2\left(\frac{3!}{\left(\frac{2}{a}\right)^4}\right) \\
&= 4\pi A^2\frac{6a^4}{16} \\
&= \pi A^2\frac{3a^4}{2}
\end{aligned} \tag{7}$$

And so total expression is

$$
\begin{aligned}
\langle\psi| H |\psi\rangle &= \frac{-1}{2m} \langle\psi| \nabla^2 |\psi\rangle + \frac{k}{2} \langle\psi| r^2 |\psi\rangle \\
&= \frac{-1}{2m} 2\pi A^2 a + \frac{k}{2}\pi A^2 \frac{3a^4}{2} \\
&= \frac{-\pi A^2 a}{m} + \frac{\pi A^2 3a^4}{4k} \\
&= \pi A^2 a \left(\frac{3a^3}{4k} - \frac{1}{m} \right)
\end{aligned}
\tag{8}
$$

Now combining numerator and denominator to find upper bound for E_0 we have

$$
\begin{aligned}
\frac{\langle\psi| H |\psi\rangle}{\langle\psi|\psi\rangle} &= \frac{\pi A^2 a \left(\frac{3a^3}{4k} - \frac{1}{m} \right)}{\pi A^2 a^3} \\
&= \frac{1}{a^2} \left(\frac{3a^3}{4k} - \frac{1}{m} \right) \\
&= \left(\frac{3a}{4k} - \frac{1}{ma^2} \right)
\end{aligned}
\tag{9}
$$