Problem 9.1

We expect that in the ground state the particle should be localized around the center of the trap, much like in a harmonic oscillator. Therefore we try with with a Gaussian trial wave function

$$\psi(x) = Ae^{-bx^2} \tag{1}$$

with a real and positive variational parameter, b.

In this exercise, we will be needing some Gaussian integral identities. The derivations of the identities will not be shown here.

$$\int_{-\infty}^{\infty} dx\ e^{-\beta x^2} = \sqrt{\frac{\pi}{\beta}}$$
$$\int_{-\infty}^{\infty} dx\ x\ e^{-\beta x^2} = 0$$
$$\int_{-\infty}^{\infty} dx\ x^2 e^{-\beta x^2} = \frac{\partial}{\partial\beta}\int_{-\infty}^{\infty} dx\ e^{-\beta x^2} = \frac{1}{2}\sqrt{\pi}\beta^{-\frac{3}{2}}$$

With that in place, we begin by requiring the wavefunction to be normalized:

$$1 = \int_{-\infty}^{\infty} dx\ \psi^*_{trial}\psi_{trial} = |A|^2 \int_{-\infty}^{\infty} dx\ e^{-2bx^2} = |A|^2\sqrt{\frac{\pi}{2b}}$$
$$\Rightarrow |A|^2 = \sqrt{\frac{2b}{\pi}}$$

We now write down the Hamiltonian:

$$H = T + V = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \alpha\,|x|\,.$$

The variational principle states that

$$E_{gs} \leq \langle\psi|\,H\,|\psi\rangle \equiv \langle H\rangle$$

for any state $|\psi\rangle$, where E_{gs} is the ground state energy. Now, let us calculate $\langle H\rangle$ for our trial wavefunction:

$$\langle H\rangle = \langle T\rangle + \langle V\rangle$$

Beginning with the kinetic term:

$$\begin{aligned}
\langle T\rangle &= |A|^2\int_{-\infty}^{\infty} dx\ e^{-bx^2}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)e^{-bx^2} \\
&= -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}}\left[-2b\int_{-\infty}^{\infty} dx\ e^{-2bx^2} + 4b^2\int_{-\infty}^{\infty} dx\ x^2 e^{-2bx^2}\right] \\
&= -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}}\left[-2b\sqrt{\frac{\pi}{2b}} + \frac{(2b)^2}{2}\sqrt{\pi}(2b)^{-\frac{3}{2}}\right] \\
&= \frac{\hbar^2 b}{2m}
\end{aligned}$$

As for the potential term:

$$\begin{aligned}
\langle V \rangle &= |A|^2 \int_{-\infty}^{\infty} dx\ e^{-bx^2} \alpha\, |x|\, e^{-bx^2} \\
&= \alpha \sqrt{\frac{2b}{\pi}} \int_{-\infty}^{\infty} dx\ \ |x|\, e^{-2bx^2} \\
&= 2\alpha \sqrt{\frac{2b}{\pi}} \int_{0}^{\infty} dx\ xe^{-2bx^2} \\
&\underset{u=x^2}{=} \alpha \sqrt{\frac{2b}{\pi}} \int_{0}^{\infty} du\ e^{-2bu} \\
&= \alpha \sqrt{\frac{2b}{\pi}} \frac{1}{2b} \\
&= \frac{\alpha}{\sqrt{2\pi b}}
\end{aligned}$$

Thus

$$\langle H \rangle = \frac{\hbar^2 b}{2m} + \frac{\alpha}{\sqrt{2\pi b}}.$$

Now, in order to find an upper bound on E_{gs}, we minimize $\langle H \rangle$ with respect to b:

$$\begin{aligned}
\frac{\partial}{\partial b} \langle H \rangle &= \frac{\hbar^2}{2m} - \frac{\alpha}{2\sqrt{2\pi} b^{3/2}} = 0 \\
\Rightarrow b &= \left(\frac{\alpha m}{\sqrt{2\pi}\hbar^2} \right)^{2/3}
\end{aligned}$$

We see that this is a minimum by evaluating the second derivative:

$$\frac{\partial^2}{\partial b^2} \langle H \rangle = \frac{3\alpha}{4\sqrt{2\pi} b^{5/2}} > 0$$

We thus find

$$\begin{aligned}
\langle H \rangle &= \frac{\hbar^2}{2m} \left(\frac{\alpha m}{\sqrt{2\pi}\hbar^2} \right)^{2/3} + \frac{\alpha}{\sqrt{2\pi}} \left(\frac{\alpha m}{\sqrt{2\pi}\hbar^2} \right)^{-1/3} = \frac{3}{2} \left(\frac{\hbar^2 \alpha^2}{2\pi m} \right)^{1/3} \\
\Rightarrow E_{gs} &\leq \frac{3}{2} \left(\frac{\hbar^2 \alpha^2}{2\pi m} \right)^{1/3} \simeq 1.024 \left(\frac{\hbar^2 \alpha^2}{2m} \right)^{1/3}
\end{aligned}$$

The problem can be solved exaclty, and the eigenfunctions of the system are so-called Airy functions. The actual groundstate of this system has the energy

$$E_0 \simeq 1.019 \left(\frac{\hbar^2 \alpha^2}{2m} \right)^{1/3},$$

meaning that our upper limit was a very good approximation.

Problem 9.2

This problem again involves a lot of calculations with Gaussian integrals, some of them basically identical to those of Problem 9.1. In those places, I will skip some of the obvious intermediate steps. Please note: The compulsory part is a) below. I include the voluntary calculations for two and one dimensions as b) and c), respectively.

a)

We again have a gaussian trial wave function,

$$\psi_L(x, y, z) = Ae^{-(x^2+y^2+z^2)/2L^2}. \tag{2}$$

We start by normalising,

$$|A|^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx\, dy\, dz e^{-(x^2+y^2+z^2)/L^2} = |A|^2(\pi L^2)^{3/2} \equiv 1, \tag{3}$$

which gives $A = (\pi L^2)^{-3/4}$. Now we are to calculate the expectation value of the Hamiltonian, and again start with the kinetic term,

$$\begin{aligned}
\langle T \rangle &= -\frac{\hbar^2}{2m}|A|^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx\, dy\, dz e^{-(x^2+y^2+z^2)/2L^2} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) e^{-(x^2+y^2+z^2)/2L^2} \\
&= -\frac{\hbar^2}{2m}|A|^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx\, dy\, dz e^{-(x^2+y^2+z^2)/L^2} \left(-\frac{3}{L^2} + \frac{x^2+y^2+z^2}{L^4}\right) \\
&= \frac{\hbar^2}{2m}(\pi L^2)^{-3/2}\frac{3}{L^2}(\pi L^2)^{3/2} - \frac{\hbar^2}{2m}(\pi L^2)^{-3/2}\frac{1}{L^4}3(\sqrt{\pi L^2})^2\frac{1}{2}\sqrt{\pi}\left(\frac{1}{L^2}\right)^{-3/2} \\
&= \frac{\hbar^2}{2m}\frac{3}{L^2} - \frac{\hbar^2}{2m}\frac{3}{2L^2} \\
&= \underline{\frac{3\hbar^2}{4mL^2}}.
\end{aligned} \tag{4}$$

Now for $\langle V \rangle$, which is easy:

$$\begin{aligned}
\langle V \rangle &= -\left(\frac{1}{\pi L^2}\right)^{3/2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx\, dy\, dz e^{-(x^2+y^2+z^2)/L^2} \alpha\delta(x)\delta(y)\delta(z) \\
&= -\frac{\alpha}{\pi^{3/2}L^3}.
\end{aligned} \tag{5}$$

The expectation value of the Hamiltonian is thus

$$\langle H \rangle = \frac{3\hbar^2}{4mL^2} - \frac{\alpha}{\pi^{3/2}L^3}. \tag{6}$$

The next step would be to minimise this function with respect to L, were the minimum would give an upper bound on the ground state energy. However, this function has no finite minimum. The extremal point where the derivative is zero, is in fact a *maximum* as can be seen by checking the second derivative. Rather, $\langle H \rangle$ diverges to $-\infty$ as $L \to 0$, so no finite ground state energy can be found.

b)

What then, if we look at the problem in two dimensions instead? The calculations are very similar, but obviously some coefficients and powers of L will change when we do two-dimensional integrals instead. The latter will make an important physical difference. So, now assume a trial wave function

$$\psi_L(x,y) = Ae^{-(x^2+y^2)/2L^2}. \tag{7}$$

The normalisation factor is then $A = 1/(\sqrt{\pi}L)$. For the kinetic term we get

$$\begin{aligned}
\langle T\rangle &= -\frac{\hbar^2}{2m}|A|^2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx\,dy e^{-(x^2+y^2)/2L^2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)e^{-(x^2+y^2)/2L^2}\\
&= -\frac{\hbar^2}{2m}\frac{1}{\pi L^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx\,dy e^{-(x^2+y^2)/L^2}\left(-\frac{2}{L^2}+\frac{x^2+y^2}{L^4}\right)\\
&= \frac{\hbar^2}{2mL^2}.
\end{aligned} \tag{8}$$

The potential term:

$$\begin{aligned}
\langle V\rangle &= -\left(\frac{\alpha}{\pi L^2}\right)\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx\,dy\,e^{-(x^2+y^2)/L^2}\alpha\delta(x)\delta(y)\\
&= -\frac{\alpha}{\pi L^2}.
\end{aligned} \tag{9}$$

So we see that while the kinetic energy scales as $1/L^2$ like in three dimensions, the potential term now scales like $1/L^2$ as well,

$$\langle H\rangle = \frac{\hbar^2}{2mL^2} - \frac{\alpha}{\sqrt{\pi}L^2}. \tag{10}$$

Again, this expectation value has no finite minimum as a function of L. It diverges to ∞ or $-\infty$ as $L \to 0$ depending on the relative magnitude of the two terms.

c)

Finally, let us examine what happens in a one-dimensional problem, where the math is even simpler,

$$\psi_L(x) = Ae^{-x^2/2L^2}. \tag{11}$$

Now $A = (\pi L^2)^{-1/4}$. In full analogy to problem 9.1 we find

$$\langle T\rangle = \frac{\hbar^2}{4mL^2} \tag{12}$$

while

$$\langle V\rangle = \frac{-\alpha}{\sqrt{\pi}L}\int_{-\infty}^{\infty}\delta(x)e^{-x^2/2L^2}dx = \frac{-\alpha}{\sqrt{\pi}L}. \tag{13}$$

This time the potential part scales like $1/L$, and by differentiation as before it is straightforward to find that $\langle H\rangle$ now has a finite minimum,

$$\langle H\rangle_{min} = \frac{-m\alpha^2}{\pi\hbar^2}. \tag{14}$$

This is larger than the true ground state, $E_0 = \frac{-m\alpha^2}{2\hbar^2}$ as it should be (and not too far off).

Problem 9.3

It is a good idea to start with a two-dimensional contour plot of E_{tr} as a function of Z_1 and Z_2 (which are positive numbers) to get an idea where to find the minimum, if any. Then use your favorite tool to minimize E_{tr} with respect to the two variables, e.g. the function `FindMinimum` in Mathematica. The solution is $E_{tr} = -1.02661|E_1|$ for $Z_1 = 0.283221, Z_2 = 1.03923$. Since E_{tr} is smaller than E_1, the ground state energy of the hydrogen atom (i.e. with one electron bound), we see that a bound state of a single proton and two electrons is favored.