Solutions of homework # 4

Exercise 1

The uncertainty in position is ruled by the uncertainty principle, that states that $\Delta x \Delta p \geq \frac{\hbar}{2}$. Therefore the minimum uncertainty in position is given by $\Delta x = \frac{\hbar}{2\Delta p}$, with $\Delta p = m\Delta v$. In the two cases we have:

1. Sinner's tennis ball: $\Delta x = \frac{\hbar}{2m\Delta v} = \frac{h}{4\pi m\Delta v} = \frac{6.63\cdot 10^{-34}\,\mathrm{J\cdot s}}{4\pi\cdot(60\cdot 10^{-3}\,\mathrm{kg})\cdot(10^{-3}\,\mathrm{m/s})} = 8.8\cdot 10^{-31}\,\mathrm{m} \approx 0$.
2. An electron: $\Delta x = \frac{\hbar}{2m\Delta v} = \frac{h}{4\pi m\Delta v} = \frac{6.63\cdot 10^{-34}\,\mathrm{J\cdot s}}{4\pi\cdot(9.109\cdot 10^{-31}\,\mathrm{kg})\cdot(10^{-3}\,\mathrm{m/s})} = 5.79\,\mathrm{cm}$.

Clearly, while for a macroscopic object the uncertainty principle does not play a role (we know the exact position of a ball in space), it is fundamental in the microscopic realm; note also that increasing the precision in the velocity measurement would spread further the position measurement.

Exercise 2

1. The trial wave function

$$\Psi(x) = \alpha \sin\left(\frac{2\pi x}{a}\right) + \beta \sin\left(\frac{4\pi x}{a}\right), \tag{1}$$

satisfies the boundary conditions $\Psi(0) = \Psi(a) = 0$ for any values of the parameters α and β. Therefore, these conditions do not put any constraints on these parameters.

The variational principle of quantum mechanics states that

$$E[\Psi] = \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \geq E_0\,, \tag{2}$$

where E_0 is the true ground-state energy of the system. Let us consider first the denominator. The normalization condition for the trial wave functions gives us:

$$\begin{aligned} 1 = \langle\Psi|\Psi\rangle &= \int_0^a \Psi^*(x)\,\Psi(x)\,dx = \int_0^a \left[\alpha \sin\left(\frac{2\pi x}{a}\right) + \beta \sin\left(\frac{4\pi x}{a}\right)\right]^2 dx \\ &= \alpha^2 \int_0^a \sin^2\left(\frac{2\pi x}{a}\right) dx\, + 2\alpha\beta \int_0^a \sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{4\pi x}{a}\right) dx \\ &\quad + \beta^2 \int_0^a \sin^2\left(\frac{4\pi x}{a}\right) dx = \frac{a}{2}\left(\alpha^2 + \beta^2\right). \end{aligned} \tag{3}$$

Therefore, from Eq. (3) we have the condition on the parameters:

$$\alpha^2 + \beta^2 = \frac{2}{a}\,. \tag{4}$$

According to Eq. (2) we need to evaluate the matrix element of the Hamiltonian of the system $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$, namely:

$$\begin{aligned}
\langle\Psi|\hat{H}|\Psi\rangle &= \int_0^a \Psi^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\Psi(x)\,dx \\
&= -\frac{\hbar^2}{2m}\int_0^a \left[\alpha\sin\left(\frac{2\pi x}{a}\right)+\beta\sin\left(\frac{4\pi x}{a}\right)\right]\frac{d^2}{dx^2}\left[\alpha\sin\left(\frac{2\pi x}{a}\right)+\beta\sin\left(\frac{4\pi x}{a}\right)\right]dx \\
&= \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2\int_0^a \left[\alpha\sin\left(\frac{2\pi x}{a}\right)+\beta\sin\left(\frac{4\pi x}{a}\right)\right]\left[\alpha\sin\left(\frac{2\pi x}{a}\right)+4\beta\sin\left(\frac{4\pi x}{a}\right)\right]dx \\
&= \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2\left\{\alpha^2\int_0^a \sin^2\left(\frac{2\pi x}{a}\right)dx + 5\alpha\beta\int_0^a \sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{4\pi x}{a}\right)dx\right. \\
&\qquad \left. + 4\beta^2\int_0^a \sin^2\left(\frac{4\pi x}{a}\right)dx\right\} = \frac{\hbar^2\pi^2}{ma}(\alpha^2+4\beta^2)\,. \qquad (5)
\end{aligned}$$

So for the trial wavefunction of Eq. (1), Eq. (2) can be rewriteen as:

$$E[\Psi] = \langle\Psi|\hat{H}|\Psi\rangle = \frac{\hbar^2\pi^2}{ma}(\alpha^2+4\beta^2) \qquad (6)$$

Therefore, using Eqs. (4) and (6), Eq. (2) can be rewritten in terms of one parameter only, using either α or β:

$$E(\alpha) = \frac{\hbar^2\pi^2}{ma}\left(\frac{8}{a}-3\alpha^2\right)\,. \qquad (7)$$

$$E(\beta) = \frac{\hbar^2\pi^2}{ma}\left(\frac{2}{a}+3\beta^2\right) \qquad (8)$$

Minima of the energy are found when the first derivative of the function vanishes and when its **second derivative is positive**. The first derivative in the two cases reads:

$$\frac{dE(\alpha)}{d\alpha} = -\frac{6\hbar^2\pi^2}{ma}\alpha = 0 \quad\Longrightarrow\quad \alpha = 0 \qquad (9)$$

$$\frac{dE(\beta)}{d\beta} = \frac{6\hbar^2\pi^2}{ma}\beta = 0 \quad\Longrightarrow\quad \beta = 0. \qquad (10)$$

However, the second derivative of the function is positive only for Eq. (8):

$$\frac{d^2E(\alpha)}{d\alpha^2} = -\frac{6\hbar^2\pi^2}{ma} < 0 \qquad (11)$$

$$\frac{d^2E(\beta)}{d\beta^2} = \frac{6\hbar^2\pi^2}{ma} > 0 \qquad (12)$$

So the minimum of the function is obtained for $\beta = 0$, while α is fixed from the normalization condition of Eq. (4):

$$\alpha^2 = \frac{2}{a} \quad\Longrightarrow\quad \alpha = \pm\sqrt{\frac{2}{a}}\,. \qquad (13)$$

The case with $\alpha = 0$ and $\beta = \pm\sqrt{2/a}$ corresponds instead to a maximum of the energy. Therefore, the trial wave function minimizing the energy takes the form

$$\Psi_{\text{min}}(x) = \pm\sqrt{\frac{2}{a}}\sin\left(\frac{2\pi x}{a}\right). \tag{14}$$

2. The wave function, Eq. (14), corresponds to the energy of the particle ($\beta = 0$, $\alpha = \pm\sqrt{\frac{2}{a}}$):

   $$E[\Psi_{\text{min}}] = \frac{2\hbar^2\pi^2}{ma^2} > \frac{\hbar^2\pi^2}{2ma^2} = E_0\,. \tag{15}$$

   Therefore, the obtained energy $E[\Psi_{\text{min}}]$ is four times greater than the true ground-state energy. This means that the variational principle is satisfied.

   We can recognize that our trial wave function, Eq. (1), is actually a linear combination of the two eigenfunctions of the particle in the box (with $n = 2$ and $n = 4$) and that it does not contain the wave function with $n = 1$. So, after the minimization procedure we did above, there is no way to end up with the true ground-state wave function $\psi_1(x) = \pm\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)$: indeed, eigenstates corresponding to different eigenvalues are orthonormal. Since the true ground state has $n = 1$ and the minimum-energy trial wave function is nothing but the first excited state, $n = 2$, the two are orthogonal.

Exercise 3

First of all, we need to calculate the 3 components of $\hat{L}$ solving the vector product. They are:

$$\begin{aligned}
\hat{L}_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y,\\
\hat{L}_y &= \hat{z}\hat{p}_x - \hat{x}\hat{p}_z,\\
\hat{L}_z &= \hat{x}\hat{p}_y - \hat{y}\hat{p}_x.
\end{aligned}$$

Let's start with the commutator $[\hat{x}, \hat{L}_x]$:

$$\begin{aligned}
[\hat{x}, \hat{L}_x]\psi &= \Big([\hat{x}, \hat{y}\hat{p}_z - \hat{z}\hat{p}_y]\Big)\psi\\
&= \Big([\hat{x}, \hat{y}\hat{p}_z] - [\hat{x}, \hat{z}\hat{p}_y]\Big)\psi\\
&= \Big(\cancel{[\hat{x}, \hat{y}]}\hat{p}_z + \hat{y}\cancel{[\hat{x}, \hat{p}_z]} - \cancel{[\hat{x}, \hat{z}]}\hat{p}_y - \hat{z}\cancel{[\hat{x}, \hat{p}_y]}\Big)\psi\\
&= 0\,,
\end{aligned}$$

where all terms cancel because of the commutator rules calculated in 2.b and 2.c.

$$\begin{aligned}
[\hat{x}, \hat{L}_y]\psi &= \Big([\hat{x}, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z] \Big)\psi \\
&= \Big([\hat{x}, \hat{z}\hat{p}_x] - [\hat{x}, \hat{x}\hat{p}_z] \Big)\psi \\
&= \Big(\cancel{[\hat{x}, \hat{z}]}\hat{p}_x + \hat{z}[\hat{x}, \hat{p}_x] - \cancel{[\hat{x}, \hat{x}]}\hat{p}_y - \hat{x}\cancel{[\hat{x}, \hat{p}_y]} \Big)\psi \\
&= i\hbar\hat{z}\psi \,.
\end{aligned}$$

We can generalize for all the operators x, y, z and L_x, L_y, L_z saying that:

$$[\hat{r}_i, \hat{L}_j] = i\hbar\,\varepsilon_{ijk}\hat{r}_k \,.$$

The commutator is 0 if $i = j$, as the first case $[\hat{x}, \hat{L}_x]$, while it is different from 0 in the other cases, and the sign ±1 is given by the Levi-Civita symbol. For quantum momentum:

$$\begin{aligned}
[\hat{p}_x, \hat{L}_x]\psi &= \Big([\hat{p}_x, \hat{y}\hat{p}_z - \hat{z}\hat{p}_y] \Big)\psi \\
&= \Big([\hat{p}_x, \hat{y}\hat{p}_z] - [\hat{p}_x, \hat{z}\hat{p}_y] \Big)\psi \\
&= \Big(\cancel{[\hat{p}_x, \hat{y}]}\hat{p}_z + \hat{y}\cancel{[\hat{p}_x, \hat{p}_z]} - \cancel{[\hat{p}_x, \hat{z}]}\hat{p}_y - \hat{z}\cancel{[\hat{p}_x, \hat{p}_y]} \Big)\psi \\
&= 0
\end{aligned}$$

as before, if $i = j$, in this case $i = j = x$, the commutator is 0, while:

$$\begin{aligned}
[\hat{p}_x, \hat{L}_y]\psi &= \Big([\hat{p}_x, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z] \Big)\psi \\
&= \Big([\hat{p}_x, \hat{z}\hat{p}_x] - [\hat{p}_x, \hat{x}\hat{p}_z] \Big)\psi \\
&= \Big(\cancel{[\hat{p}_x, \hat{z}]}\hat{p}_x + \hat{z}\cancel{[\hat{p}_x, \hat{p}_x]} - [\hat{p}_x, \hat{x}]\hat{p}_z - \hat{x}\cancel{[\hat{p}_x, \hat{p}_z]} \Big)\psi \\
&= \Big(-(-i\hbar)\hat{p}_z\psi = i\hbar\hat{p}_z \Big)\psi
\end{aligned}$$

also here, the general case reads:

$$[\hat{p}_i, \hat{L}_j] = i\hbar\,\varepsilon_{ijk}\hat{p}_k \,.$$

Using the results just obtained, one can also verify the following important relation for the angular momentum operators:

$$[\hat{L}_i, \hat{L}_j] = i\hbar\,\varepsilon_{ijk}\hat{L}_k \,.$$

Using, e.g., L_x and L_y we have:

$$\begin{aligned}
[\hat{L}_x, \hat{L}_y]\psi &= \Big([\hat{L}_x, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z] \Big)\,\psi \\
&= \Big([\hat{L}_x, \hat{z}\hat{p}_x] - [\hat{L}_x, \hat{x}\hat{p}_z] \Big)\,\psi \\
&= \Big([\hat{L}_x, \hat{z}]\hat{p}_x + \hat{z}\cancel{[\hat{L}_x, \hat{p}_x]} - \cancel{[\hat{L}_x, \hat{x}]}\hat{p}_z - \hat{x}[\hat{L}_x, \hat{p}_z] \Big)\,\psi \\
&= i\hbar\left(\hat{y}\hat{p}_x - \hat{x}\hat{p}_y\right)\psi = i\hbar\hat{L}_z\psi
\end{aligned}$$