5.1

a)

**Sol:**

Starting with the following information:

\[
\mathbf{R} = \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{m_1 + m_2}, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \quad (1)
\]

\[
\mu = \frac{m_1 \cdot m_2}{m_1 + m_2} \quad (2)
\]

we want to derive:

\[
\mathbf{r}_1 = \mathbf{R} + \mu \frac{m_1}{m_1 + m_2} \mathbf{r}, \quad \mathbf{r}_2 = \mathbf{R} - \mu \frac{m_2}{m_1 + m_2} \mathbf{r} \quad (3)
\]

\[
\nabla_1 = \mu \frac{m_2}{m_1 + m_2} \mathbf{R} + \nabla_\mathbf{r}, \quad \nabla_2 = \mu \frac{m_1}{m_1 + m_2} \mathbf{R} - \nabla_\mathbf{r}. \quad (4)
\]

Finding $\mathbf{R}$ as a function of $\mathbf{r}_1$:

\[
\mathbf{R} = \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{m_1 + m_2}
\]

\[
\mathbf{R} = \frac{m_1 \mathbf{r}_1 + m_2 (\mathbf{r}_1 - \mathbf{r})}{m_1 + m_2}
\]

\[
\mathbf{R}(m_1 + m_2) = (m_1 + m_2) \mathbf{r}_1 - m_2 \mathbf{r}
\]

\[
\frac{\mathbf{R}(m_1 + m_2) + m_2 \mathbf{r}}{m_1 + m_2} = \mathbf{r}_1
\]

\[
\mathbf{R} + \frac{m_2}{m_1 + m_2} \mathbf{r} = \mathbf{r}_1
\]

\[
\mathbf{R} + \frac{\mu}{m_1} \mathbf{r} = \mathbf{r}_1.
\]

Finding $\mathbf{R}$ as a function of $\mathbf{r}_2$:

As an exercise, redo the steps but now make the exchange $\mathbf{r}_1 = \mathbf{r} + \mathbf{r}_2$ to obtain:

\[
\mathbf{R} - \frac{\mu}{m_2} \mathbf{r} = \mathbf{r}_2.
\]
Now we focus on showing that \( \nabla_1 = \frac{\mu}{m_2} \nabla_r + \nabla_r \quad \nabla_2 = \frac{\mu}{m_1} \nabla_R - \nabla_r \).

To do this we first note the following:

\[ \nabla = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right). \]

Let us define:

\[ R = (X, Y, Z) \quad \text{and} \quad r = (x, y, z) \]

\[ r_1 = (x_1, y_1, z_1) \quad \text{and} \quad r_2 = (x_2, y_2, z_2). \]

**Let’s proceed by finding \( \nabla_1 \):**

Note that since \( r_1 \) and \( r_2 \) are symmetric in their coordinates we can just consider one component of \( \nabla_1 \), say the \( x \)-component. We will therefore focus on \( \left( \frac{\partial}{\partial x} \right)_1 \).

Also note that \( r_1 \) depends on both \( r, R \), i.e \( r_1(r, R) \). It then follows that we must make use of the chain rule:

\[ \frac{\partial}{\partial x_1} = \frac{\partial X}{\partial x_1} \frac{\partial}{\partial X} + \frac{\partial x}{\partial x_1} \frac{\partial}{\partial x}. \]

By combining eq.(1) and eq.(2) we can write \( R \) on the form \( (X, Y, Z) \):

\[ R = \frac{\mu}{m_2} r_1 + \frac{\mu}{m_1} r_2 = \left( \frac{\mu}{m_2} x_1 + \frac{\mu}{m_1} x_2, \frac{\mu}{m_2} y_1 + \frac{\mu}{m_1} y_2, \frac{\mu}{m_2} z_1 + \frac{\mu}{m_1} z_2 \right) \]

which gives:

\[ \frac{\partial X}{\partial x_1} = \frac{\partial}{\partial x_1} \left[ \frac{\mu}{m_2} x_1 + \frac{\mu}{m_1} x_2 \right] = \frac{\mu}{m_2} \]

In the same manner we now use eq.(1) and eq.(2) to write \( r \) on the form \( (x, y, z) \):

\[ r = r_1 - r_2 = (x_1 - x_2, y_1 - y_2, z_1 - z_2) = (x, y, z) \]

\[ \Rightarrow \frac{\partial x}{\partial x_1} = \frac{\partial}{\partial x_1} [x_1 - x_2] = 1. \]

Now insert the results from eq.(12) and eq.(10) into eq.(8) to obtain:

\[ \frac{\partial}{\partial x_1} = \frac{\mu}{m_2} \frac{\partial}{\partial X} + \frac{\partial}{\partial x} \]

\[^1\text{If you don’t see it now, just be patient, you will see it at the end.}\]
Because \( \mathbf{R} \) and \( \mathbf{r} \) are completely symmetric with respect to the three components, it immediately follows that:

\[
\frac{\partial}{\partial y_1} = \frac{\mu}{m_2} \frac{\partial}{\partial Y} + \frac{\partial}{\partial y}
\]

\[
\frac{\partial}{\partial z_1} = \frac{\mu}{m_2} \frac{\partial}{\partial Z} + \frac{\partial}{\partial z}
\]

(14)

and finally inserting these into eq.(5) gives our result:

\[
\nabla_1 = \frac{\mu}{m_2} (\nabla_X, \nabla_Y, \nabla_Z) + (\nabla_x, \nabla_y, \nabla_z) = \frac{\mu}{m_2} \nabla_R + \nabla_r
\]

(15)

If you want to test the steps by yourself you can now redo them for \( \nabla_2 \):

\[
\nabla_2 = \frac{\mu}{m_1} \nabla_R - \nabla_r
\]

(16)

be wary of the minus sign that appears from eq.(12).

b)

Sol:

The Hamiltonian is given by the sum of each particle's kinetic energy and the total potential \( V(\mathbf{r}) \):

\[
\hat{H} = \left( -\frac{\hbar^2}{2m_1} \nabla_1^2 + -\frac{\hbar^2}{2m_2} \nabla_2^2 \right) + V(\mathbf{r})
\]

The time independent Schrödinger equation, \( \hat{H} \psi = E \psi \), then becomes:

\[
- \left( \frac{\hbar^2}{2m_1} \nabla_1^2 + \frac{\hbar^2}{2m_2} \nabla_2^2 \right) \psi + V(\mathbf{r}) \psi = E \psi.
\]

(17)

The goal is now to show that eq.(17) is equivalent with:

\[
- \frac{\hbar^2}{m_1 + m_2} \nabla_R^2 \psi - \frac{\hbar^2}{2\mu} \nabla_r^2 \psi + V(\mathbf{r}) \psi = E \psi
\]

and we will show this by first evaluating \( \nabla_1^2 (\psi) \):

\[
\nabla_1^2 (\psi) = \nabla_1 (\nabla_1 (\psi)) = \left( \frac{\mu}{m_2} \nabla_R + \nabla_r \right) \left( \frac{\mu}{m_2} \nabla_R + \nabla_r \right) \psi.
\]

\[
= \left( \frac{\mu}{m_2} \nabla_R + \nabla_r \right) \left( \frac{\mu}{m_2} \nabla_R (\psi) + \nabla_r (\psi) \right)
\]

\[
= \left( \frac{\mu}{m_2} \right)^2 \nabla_R^2 \psi + \frac{\mu}{m_2} \nabla_R \nabla_r \psi + \frac{\mu}{m_2} \nabla_r \nabla_R \psi + \nabla_r^2 \psi
\]

and since we always consider functions with commuting partial derivatives we get:

\[
\nabla_1^2 (\psi) = \left( \frac{\mu}{m_2} \right)^2 \nabla_R^2 \psi + 2 \frac{\mu}{m_2} \nabla_R \cdot \nabla_r (\psi) + \nabla_r^2 (\psi).
\]

(18)
Similarly one gets (do this as an exercise!):

\[
\nabla^2_2 (\psi) = \left( \frac{\mu}{m_1} \right)^2 \nabla^2_R (\psi) - 2 \frac{\mu}{m_1} \nabla_R \cdot \nabla_r (\psi) + \nabla^2_r (\psi).
\]

(19)

Multiplying these two with the respective factor \( \frac{\hbar^2}{2m_i} \):

\[
\begin{align*}
- \frac{\hbar^2}{2m_1} \nabla^2_1 \psi &= - \frac{\hbar^2}{2m_1} \left[ \left( \frac{\mu}{m_2} \right)^2 \nabla^2_R (\psi) + 2 \frac{\mu}{m_2} \nabla_R \cdot \nabla_r (\psi) + \nabla^2_r (\psi) \right] \\
- \frac{\hbar^2}{2m_2} \nabla^2_2 \psi &= - \frac{\hbar^2}{2m_2} \left[ \left( \frac{\mu}{m_1} \right)^2 \nabla^2_R (\psi) - 2 \frac{\mu}{m_1} \nabla_R \cdot \nabla_r (\psi) + \nabla^2_r (\psi) \right]
\end{align*}
\]

we see that the middle terms will cancel if we add the two lines. Doing this we obtain:

\[
\begin{align*}
- \frac{\hbar^2}{2m_1} \nabla^2_1 \psi - \frac{\hbar^2}{2m_2} \nabla^2_2 \psi &= - \frac{\hbar^2}{2} \left[ \left( \frac{\mu^2}{m_1 m_2} + \frac{\mu^2}{m_2 m_1} \right) \nabla^2_R (\psi) + \left( \frac{1}{m_1} + \frac{1}{m_2} \right) \nabla^2_r (\psi) \right] \\
- \frac{\hbar^2}{2m_1} \nabla^2_1 \psi - \frac{\hbar^2}{2m_2} \nabla^2_2 \psi &= - \frac{\hbar^2}{2} \left[ \frac{\mu^2 m_2 + m_1}{m_1 m_2} \nabla^2_R (\psi) + \left( \frac{m_2 + m_1}{m_1 m_2} \right) \nabla^2_r (\psi) \right] \\
- \frac{\hbar^2}{2m_1} \nabla^2_1 \psi - \frac{\hbar^2}{2m_2} \nabla^2_2 \psi &= - \frac{\hbar^2}{2} \left[ \frac{1}{m_2 + m_1} \nabla^2_R (\psi) + \left( \frac{1}{\mu} \right) \nabla^2_r (\psi) \right]
\end{align*}
\]

Inserting this into eq.(17) now gives:

\[
- \frac{\hbar^2}{2(m_2 + m_1)} \nabla^2_R (\psi) = \frac{\hbar^2}{2\mu} \nabla^2_r (\psi) + V(\mathbf{r}) \psi = E \psi.
\]

(20)

c)

Sol:

Assuming now that the wave function can be written as a product of two wave functions: \( \psi(\mathbf{R}, \mathbf{r}) = \psi_R \psi_r \). We get:

\[
\begin{align*}
- \frac{\hbar^2}{2(m_2 + m_1)} \nabla^2_R (\psi_R \psi_r) &= \frac{\hbar^2}{2\mu} \nabla^2_r (\psi_R \psi_r) + V(\mathbf{r}) \psi_R \psi_r = E \psi_R \psi_r, \\
- \frac{\hbar^2}{2(m_2 + m_1)} \psi_r \nabla^2_R (\psi_R) &= \frac{\hbar^2}{2\mu} \psi_R \nabla^2_r (\psi_r) + V(\mathbf{r}) \psi_R \psi_r = E \psi_R \psi_r
\end{align*}
\]

division by \( \psi_R \psi_r \) gives:

\[
\begin{align*}
- \frac{\hbar^2}{2(m_2 + m_1)} \psi_R \nabla^2_R (\psi_R) &= \frac{\hbar^2}{2\mu} \psi_R \nabla^2_r (\psi_r) + V(\mathbf{r}) = E.
\end{align*}
\]

(21)
Since the right hand side is a constant and the two terms on the left hand side are solely functions of separate variables, assumed to be non-dependent of each other, each term must be constant. Thus:

\[-\frac{\hbar^2}{2(m_2 + m_1)} \frac{1}{\psi_R} \nabla^2_R (\psi_R) = E_R \]

(22)

\[-\frac{\hbar^2}{2\mu} \frac{1}{\psi_r} \nabla^2_r (\psi_r) + V(r) = E_r \]

(23)

with \(E_R + E_r = E\).

Note that eq.(22) is the Schrödinger equation for a free particle (no potential) while eq.(23) is the Schrödinger equation for a particle of mass \(\mu\) moving in a potential \(V(r)\).

5.4

Q. If \(\psi_a\) and \(\psi_b\) are orthogonal and both normalized, what is the constant \(A\) in:

\[\psi_\pm(r_1, r_2) = A [\psi_a(r_1)\psi_b(r_2) \pm \psi_b(r_2)\psi_a(r_1)] \]

(24)

\[
\begin{align*}
1 &= |A|^2 \iint \left| \psi_a(r_1)\psi_b(r_2) \pm \psi_b(r_2)\psi_a(r_1) \right|^2 dr_1 dr_2 \\
1 &= \frac{1}{|A|^2} \iint \left| \psi_a(r_1)\psi_b(r_2) \pm \psi_b(r_2)\psi_a(r_1) \right|^2 dr_1 dr_2 \\
&= \frac{1}{|A|^2} \iint \left[ \left| \psi_a(r_1)\right|^2 \left| \psi_b(r_2)\right|^2 + \left| \psi_b(r_2)\right|^2 \left| \psi_a(r_1)\right|^2 + \right. \\
&\quad \left. \mp \int \psi_a^*(r_1)\psi_b^*(r_2)\psi_a(r_2)\psi_b(r_1) dr_1 dr_2 + \right. \\
&\quad \left. \int \psi_b^*(r_2)\psi_a^*(r_1)\psi_b(r_1)\psi_a(r_2) dr_1 dr_2 \right] \\
&= 2 \frac{1}{|A|^2} \iint \left[ \psi_a^*(r_2)\psi_b^*(r_1)\psi_a(r_1)\psi_b(r_2) \right. dr_1 dr_2 + \left. \psi_b^*(r_1)\psi_a^*(r_2)\psi_b(r_2)\psi_a(r_1) \right] dr_1 dr_2
\]

We will now show that each double integral in the square bracket is 0 by focusing on the left one:
\[ \int\int \psi^*_a(r_2)\psi^*_b(r_1)\psi_a(r_1)\psi_b(r_2)\, dr_1 dr_2 = \int\psi^*_a(r_1)\psi_a(r_1)\, dr_1 \int \psi^*_b(r_2)\psi_b(r_2)\, dr_2 \]

because \( \psi_a(r_1) \) and \( \psi_b(r_1) \) are orthogonal. Do the same for the other double integral as an exercise.

Our condition is now:

\[ \frac{1}{|A|^2} = 2 \pm 0 \]

\[ |A| = \frac{1}{\sqrt{2}} \]  \hspace{1cm} (25)

b)

Q. What is \( A \) if \( \psi_a = \psi_b \) and \( \psi(r_1, r_2) \) is normalized?

Sol:

In this case we have:

\[ \psi(r_1, r_2) = A [\psi_a(r_1)\psi_a(r_2) + \psi_a(r_2)\psi_a(r_1)] = 2A\psi_a(r_1)\psi_a(r_2) \]  \hspace{1cm} (26)

which gives:

\[ \frac{1}{4|A|^2} = \int\int |\psi_a(r_1)\psi_a(r_2)|^2\, dr_1 dr_2 = \int |\psi_a(r_1)|^2\, dr_1 \int |\psi_a(r_2)|^2\, dr_2 = 1 \cdot 1 \]

\[ |A| = \frac{1}{2} \]  \hspace{1cm} (27)
5.5

a)

Q. Write down the Hamiltonian for two noninteracting identical particles in the infinite square well. Verify that the fermion ground state:

\[ \psi_{12}(x_1, x_2) = \frac{\sqrt{2}}{a} \left[ \sin(\pi x_1/a) \sin(2\pi x_2/a) - \sin(2\pi x_1/a) \sin(\pi x_2/a) \right] \] (28)

is an eigenfunction of \( H \) with the appropriate eigenvalue. (why is \( \psi_{11} \) not the ground state?)

Sol:
The reason why \( \psi_{11} \) cannot be the ground state\(^2\) for fermions is that the two particles would then occupy the same state. (We see that eq.(28) would be 0 in that case.)

Now, from the Hamiltonian for a general two particle system moving in an unknown potential:

\[ H = -\frac{\hbar^2}{2m_1} \nabla_1^2 - \frac{\hbar^2}{2m_2} \nabla_2^2 + V(r_1, r_2, t) \]

we see that for the case of identical particles we must have the same mass:

\[ H = -\frac{\hbar^2}{2m} \left[ \nabla_1^2 + \nabla_2^2 \right] + V(r_1, r_2, t). \] (29)

Furthermore, in our case we know the potential. The infinite square well potential is 0 inside the well and since the particles are non-interacting the total potential is also 0. Therefore:

\[ H = -\frac{\hbar^2}{2m} \left[ \nabla_1^2 + \nabla_2^2 \right] = -\frac{\hbar^2}{2m} \left[ \frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2} \right] \] (30)

where the last step comes from the fact that we are only considering the 1D infinite square well.

Now we check if eq. (28) is an eigenfunction of our Hamiltonian operator:

\[ H \psi_{12} = -\frac{\hbar^2}{2m} \left[ \frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2} \right] \psi_{12} = E \psi_{12} \] (?)

by letting the Hamiltonian in eq.(30) work on the wave function eq.(28):

\(^2\)If we neglect spin.
\[ H_{\psi_{12}} = -\frac{\hbar^2}{2m} \left( \frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2} \right) \sqrt{2} \left[ \sin \left( \frac{\pi x_1}{a} \right) \sin \left( \frac{2\pi x_2}{a} \right) - \sin \left( \frac{2\pi x_1}{a} \right) \sin \left( \frac{\pi x_2}{a} \right) \right] \]

\[ H_{\psi_{12}} = -\frac{\hbar^2 \sqrt{2}}{2ma} \left[ \sin \left( \frac{\pi x_1}{a} \right) \sin \left( \frac{2\pi x_2}{a} \right) - \frac{d^2}{dx_1^2} \sin \left( \frac{2\pi x_1}{a} \right) \sin \left( \frac{\pi x_2}{a} \right) \right] + \sin \left( \frac{\pi x_1}{a} \right) \frac{d^2}{dx_1^2} \sin \left( \frac{2\pi x_2}{a} \right) - \sin \left( \frac{2\pi x_1}{a} \right) \frac{d^2}{dx_1^2} \sin \left( \frac{\pi x_2}{a} \right) \]

\[ H_{\psi_{12}} = -\frac{\hbar^2 \sqrt{2}}{2ma} \left[ -\frac{\pi^2}{a^2} \sin \left( \frac{\pi x_1}{a} \right) \sin \left( \frac{2\pi x_2}{a} \right) - \frac{4\pi^2}{a^2} \sin \left( \frac{2\pi x_1}{a} \right) \sin \left( \frac{\pi x_2}{a} \right) \right] + \sin \left( \frac{\pi x_1}{a} \right) \left[ -\frac{4\pi^2}{a^2} \sin \left( \frac{2\pi x_2}{a} \right) - \frac{\pi^2}{a^2} \sin \left( \frac{\pi x_2}{a} \right) \right] \]

\[ H_{\psi_{12}} = \frac{\hbar^2}{2ma^2} \frac{5\pi^2}{a} \left[ \sin \left( \frac{\pi x_1}{a} \right) \sin \left( \frac{2\pi x_2}{a} \right) - \sin \left( \frac{\pi x_1}{a} \right) \sin \left( \frac{2\pi x_2}{a} \right) \right] \]

\[ = \frac{5\hbar^2 \pi^2}{2ma^2} \psi_{12} \]

which indeed shows that \( \psi_{12} \) is an eigenfunction of \( H \). The factor in front, the eigenvalue, is also what we expect since we expect it to be of the form:

\[ \left( n_1^2 + \frac{n_2^2}{4} \right) \frac{\hbar^2 \pi^2}{2a^2m} = \frac{5\hbar^2 \pi^2}{2a^2m} \]  \hspace{1cm} (31)

b)

Q. Give the wavefunctions and energies of the two next excited states for each of these three cases: distinguishable particles, identical bosons and identical fermions.

Sol:

To tidy up the notation we define:

\[ K = \frac{\hbar^2 \pi^2}{2a^2m}. \]  \hspace{1cm} (32)

The two next excited states would then correspond to states with eigenvalues above \( 5K \).
**Distinguishable particles:**

In this case the wavefunction is just the product of two single particle wavefunctions: $\psi(x_1, x_2) = \psi(x_1)\psi(x_2)$ of the 1D infinite square well: $\psi_n(x) = \sqrt{\frac{2}{a}} \sin(n \pi x / a)$.  

The first excited state above $\psi_{12}$ is $\psi_{22}$:

$$\psi_{22} = \psi_2(x_1)\psi_2(x_2) = \frac{2}{a} \sin(2\pi x_1 / a) \sin(2\pi x_2 / a) \quad \text{with} \quad E = (2^2 + 2^2)K = 8K$$

The second excited state above $\psi_{12}$ can be either of these two states:

$$\psi_{13} = \psi_1(x_1)\psi_3(x_2) = \frac{2}{a} \sin(\pi x_1 / a) \sin(3\pi x_2 / a) \quad \text{(34)}$$

$$\psi_{31} = \psi_3(x_1)\psi_1(x_2) = \frac{2}{a} \sin(3\pi x_1 / a) \sin(\pi x_2 / a) \quad \text{(35)}$$

both with the corresponding eigenvalue $E = 10K$ (this state is thus doubly degenerate).

**Identical bosons:**

Recall that for bosons the wave function has the general appearance:

$$\psi(x_1, x_2) = A [\psi_a(x_1)\psi_b(x_2) + \psi_b(x_1)\psi_a(x_2)]$$

where $A = \frac{1}{\sqrt{2}}$ if $a \neq b$ and $A = \frac{1}{2}$ if $a = b$.

Since bosons can occupy the same state, the first excited state with energy above $E = 5K$ is that for which $a = b = 2$:

$$\psi_{22} = \frac{2}{a} \sin(2\pi x_1 / a) \sin(2\pi x_2 / a) \quad \text{with} \quad E = 8K$$

The second excited state with energy $E > 5K$ is given when either $a$ or $b$ is 1 and the other 3:

$$\psi_{13} = \frac{1}{\sqrt{2}} \frac{2}{a} [\sin(\pi x_1 / a) \sin(3\pi x_2 / a) + \sin(3\pi x_1 / a) \sin(\pi x_2 / a)].$$

*Note that for identical particles, $\psi_{ab}$ and $\psi_{ba}$ are not distinct eigenstates. For bosons they are even mathematically identical. Thus the state $\psi_{13}$ is not degenerate with $\psi_{31}$ - they are the same state.*

The energy of this state is $E = 10K$. 


Identical fermions:
Identical fermions cannot occupy the same state so in this case $a \neq b$.

The first level is given by:
\[
\psi_{13} = \frac{1}{\sqrt{2}} a \sin \left( \frac{n\pi x_1}{a} \right) \sin \left( \frac{3\pi x_2}{a} \right) - \sin \left( \frac{3\pi x_1}{a} \right) \sin \left( \frac{n\pi x_2}{a} \right)
\]
and the second level is given by:
\[
\psi_{23} = \frac{1}{\sqrt{2}} a \sin \left( \frac{2\pi x_1}{a} \right) \sin \left( \frac{3\pi x_2}{a} \right) - \sin \left( \frac{3\pi x_1}{a} \right) \sin \left( \frac{2\pi x_2}{a} \right)
\]
where the negative signs come from the fact that we are dealing with fermions. The energies of the two states are $E_{13} = 10K$ and $E_{23} = 13K$.

Note here, as in the discussion concluding the "Identical bosons", that $\psi_{31}$ depends on $\psi_{13}$. Unlike for bosons where $\psi_{13} = \psi_{31}$, fermionic wavefunctions are antisymmetric with respect to the interchanging of two states: $\psi_{13} = -\psi_{31}$.

This however does not mean that $E_{13}$ and $E_{23}$ are degenerate eigenvalues. Degeneracy only occurs when two linearly dependent eigenstates have the same eigenvalue.

5.6

Q. Imagine two noninteracting particles, each of mass $m$, in the infinite square well (where the potential is 0 for $0 \leq x \leq a$ and infinite elsewhere). If one is in the state:
\[
\psi_n = \sqrt{\frac{2}{a}} \sin \left( \frac{n\pi}{a} x \right)
\]
and the other in the state $\psi_l$ ($l \neq n$), calculate $\langle (x_1 - x_2)^2 \rangle$ assuming that:
a) They are distinguishable particles.
b) They are identical bosons.
c) They are identical fermions.

a)

Sol:
In this case the total wave function is:
\[
\psi(x_1, x_2) = \psi_n(x_1)\psi_l(x_2) = \frac{2}{a} \sin \left( \frac{n\pi}{a} x_1 \right) \sin \left( \frac{l\pi}{a} x_2 \right)
\]
with $n \neq l$. Note now that:
\[
\langle (x_1 - x_2)^2 \rangle = \langle x_1^2 + x_2^2 - x_1 x_2 - x_2 x_1 \rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2\langle x_1 x_2 \rangle
\]
so we study each of the three terms on the RHS separately. Starting with the
two first terms we obtain:

\[
\langle x^2_1 \rangle = \int \int \psi^*(x_1, x_2) \psi(x_1, x_2) dx_1 dx_2 = \int_{x_1} x^2_1 \psi^*_n(x_1) \psi_n(x_1) dx_1 \int_{x_2} \psi^*_l(x_2) \psi_l(x_2) dx_2.
\]

More compactly this is:

\[
\langle x^2_1 \rangle = \int x^2_1 \psi^*_n(x_1) \psi_n(x_1) dx_1 = \langle x^2 \rangle_n. \tag{40}
\]

\[
\langle x^2_2 \rangle = \int \int \psi^*(x_1, x_2) \psi(x_1, x_2) dx_1 dx_2 = \int_{x_1} \psi^*_n(x_1) \psi_n(x_1) dx_1 \int_{x_2} x^2_2 \psi^*_l(x_2) \psi_l(x_2) dx_2.
\]

\[
\langle x^2_2 \rangle = \int x^2_2 \psi^*_l(x_2) \psi_l(x_2) dx_2 = \langle x^2 \rangle_l. \tag{41}
\]

Note that we dropped the indices \(i = 1, 2\) on \(x_i\). Even if they are separate co-
ordinates they both span the same space (the distance within the square well).

Therefore, when you integrate over the whole space the index is not important.

Now we insert our \(\psi_n\) into eq.(40):

\[
\langle x^2 \rangle_n = \int x^2 \psi^*_n(x) \psi_n(x) dx = \frac{2}{a} \int_0^a x^2 \sin^2 \left( \frac{n\pi}{a} x \right) dx \tag{42}
\]

and note to our horror that there does not seem to be a ready made expression
in either Physics Handbook nor Mathematics Handbook for \(x^2 \sin^2(Ax)\).

However\(^3\), the primitive function of \(x^2 \cos(Ax)\) is listed and we can rewrite
\(\sin^2(Ax) = \frac{1}{2} (1 - \cos(2Ax))\). Therefore:

\[
\langle x^2 \rangle_n = \frac{2}{a} \int_0^a x^2 \sin^2 \left( \frac{n\pi}{a} x \right) dx = \frac{1}{2} \int_0^a x^2 - x^2 \cos \left( \frac{2n\pi}{a} x \right) dx
\]

\[
= \frac{1}{a} \left[ \frac{x^3}{3} \right]_0^a - \frac{1}{a} \left[ \frac{2x}{(2n\pi/a)^2} \cos \left( \frac{2n\pi}{a} x \right) + \left( \frac{x^2}{2n\pi/a} - \frac{2}{(2n\pi/a)^2} \right) \sin \left( \frac{2n\pi}{a} x \right) \right]_0^a
\]

\[
= \frac{1}{a} \left[ \frac{a^3}{3} \right] - \frac{1}{a} \left[ \frac{a^3}{2n^2\pi^2} \right] = a^2 \left( \frac{1}{3} - \frac{1}{2n^2\pi^2} \right)
\]

We conclude:

\[
\langle x^2 \rangle_n = a^2 \left( \frac{1}{3} - \frac{1}{2n^2\pi^2} \right). \tag{43}
\]

\(^3\)Thanks to Daniel Blixt for pointing this out!
It obviously follows that:

\[
\langle x^2 \rangle_i = a^2 \left( \frac{1}{3} - \frac{1}{2l^2 \pi^2} \right). \tag{44}
\]

Now we evaluate the mixed term \(\langle x_1 x_2 \rangle\):

\[
\langle x_1 x_2 \rangle = \int \int \psi^*(x_1, x_2) \psi(x_1, x_2) dx_1 dx_2 = \int x_1 \psi_n^*(x_1) \psi_n(x_1) dx_1 \int x_2 \psi_l^*(x_2) \psi_l(x_2) dx_2 = \langle x \rangle_n \langle x \rangle_l.
\]

Following the same structure as above, we now calculate \(\langle x \rangle_n\):

1) Use \(\sin^2(Ax) = \frac{1}{2}(1 - \cos(2Ax))\):

\[
\langle x \rangle_n = 2 a \int_0^a x \sin^2 \left( \frac{n \pi}{a} x \right) dx = \frac{2}{a} \left[ x - \frac{x}{2} \right]_0^a - \frac{1}{2} \left[ \frac{\cos \left( \frac{2n \pi}{a} x \right)} {\left( \frac{2n \pi}{a} \right)^2} + \frac{x \sin \left( \frac{2n \pi}{a} x \right)} {\left( \frac{2n \pi}{a} \right)^2} \right]_0^a = \frac{a}{2}
\]

\[
\langle x \rangle_n = a - \frac{a}{2} + 0 = \frac{a}{2} \tag{45}
\]

This gives us:

\[
\langle (x_1 - x_2)^2 \rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2 \langle x_1 x_2 \rangle
\]

\[
\langle (x_1 - x_2)^2 \rangle = a^2 \left( \frac{1}{3} - \frac{1}{2l^2 \pi^2} \right) + a^2 \left( \frac{1}{3} - \frac{1}{2l^2 \pi^2} \right) - 2 \cdot \frac{a}{2} \cdot \frac{a}{2} = \frac{a^2}{6} - \left( \frac{1}{2n^2 \pi^2} + \frac{1}{2l^2 \pi^2} \right) \tag{46}
\]
b)

**Sol:**
To save some time we refer the reader to the derivation in the text book (section 5.1.2) of:

\[
\langle (x_1 - x_2)^2 \rangle = \langle x_2^2 \rangle_n + \langle x_2^2 \rangle_l - 2\langle x \rangle_n \langle x \rangle_l - 2|\langle x \rangle_{nl}| \tag{47}
\]

where:

\[
\langle x \rangle_{nl} = \int x \psi_n^*(x) \psi_l(x) dx. \tag{48}
\]

Comparing eq.(47) and the one at the top of this page we see that the only difference is the last term. Let us therefore focus on this one:

\[
\langle x \rangle_{nl} = \int_0^a x \psi_n^*(x) \psi_l(x) dx = \frac{2}{a} \int_0^a x \sin \left( \frac{n\pi}{a} x \right) \sin \left( \frac{l\pi}{a} x \right) dx. \tag{49}
\]

Now we make use of the following trigonometric identity:

\[
\sin \left( \frac{n\pi}{a} x \right) \sin \left( \frac{l\pi}{a} x \right) = \frac{1}{2} \left[ \cos \left( \frac{\pi(n - l)}{a} x \right) - \cos \left( \frac{\pi(n + l)}{a} x \right) \right] \tag{50}
\]

and from Physics handbook we find:

\[
g(x) = x \cos(bx) \implies G(x) = \frac{\cos(bx)}{b^2} + x \frac{\sin(bx)}{b} \tag{51}
\]

which gives:

\[
\frac{2}{a} \int_0^a x \psi_n^*(x) \psi_l(x) dx = \frac{1}{a} \left[ \cos \left( \frac{\pi(n - l)}{a} x \right) + x \sin \left( \frac{\pi(n - l)}{a} x \right) - \cos \left( \frac{\pi(n + l)}{a} x \right) - x \sin \left( \frac{\pi(n + l)}{a} x \right) \right]_0^a \]

The second and fourth terms are 0 while the rest evaluates to:

\[
\frac{1}{a} \left[ \cos \left( \frac{\pi(n - l)}{a} x \right) - \cos \left( \frac{\pi(n + l)}{a} x \right) \right]_0^a = \frac{1}{a} \left[ \frac{-1^{n+l} - 1}{\pi^2} + \frac{-1^{n+l} - 1}{\pi^2} \right] = \begin{cases} 0 & \text{if } l + n \text{ is even} \\ \frac{-8a^2l^2}{\pi^4(n^2 - l^2)} & \text{else.} \end{cases} \]

since \(\cos(\pi(n \pm l)) = -1^{n+l}\).

This means that the additional term now is:

\[
-2|\langle x \rangle_{nl}|^2 = -\frac{128a^2n^2l^2}{\pi^4(n^2 - l^2)^4}
\]

Thus we get:

\[
\langle (x_1 - x_2)^2 \rangle = a^2 \left( \frac{1}{6} - \frac{1}{2n^2\pi^2} + \frac{1}{2l^2\pi^2} - \frac{128n^2l^2}{\pi^4(n^2 - l^2)^4} \right). \tag{52}
\]
if \( n + l \) is even. Otherwise we get the same answer as in the previous problem.

c)

Sol:
The only difference for fermions lies in the last sign:

\[
\langle (x_1 - x_2)^2 \rangle = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2\langle x \rangle_a \langle x \rangle_b + 2|\langle x \rangle_{ab}|^2
\]

so we immediately get the answer:

\[
\langle (x_1 - x_2)^2 \rangle = a^2 \left( \frac{1}{6} - \frac{1}{2n^2\pi^2} + \frac{1}{2l^2\pi^2} + \frac{128n^2l^2}{\pi^4(n^2 - l^2)^4} \right).
\]

if \( n + l \) is even. Otherwise we get the same answer as in problem a). Note that:

1) The average distance between two particles being in fixed states might differ depending on if they are distinguishable or not.

2) If they are indistinguishable they are either closer (bosons) or farther (fermions) apart from distinguishable particles in the same state.

5.7

Q. Construct the total wavefunction for three particles in the orthonormal states \( \psi_a, \psi_b, \psi_c \) for the cases of a) distinguishable, b) bosonic and c) fermionic particles.

a)

For distinguishable particles the total wavefunction is just the simple product:

\[
\psi(x_1, x_2, x_3) = \psi_a(x_1)\psi_b(x_2)\psi_c(x_3)
\]

and since \( \psi_a, \psi_b, \psi_c \) are all normalized the product has norm 1. compare this result to eq.(5.15) in the text book.
b) For identical bosons we have to form a completely symmetric combination with respect to the interchange of any two of the three particles. The number of terms will be the same as the number of permutations, so for \( n \) states this will give \( n! \) number of terms. In our case we have three particles so the total wavefunction is a product of six terms:

\[
\psi(x_1, x_2, x_3) = A \left[ \psi_a(x_1)\psi_b(x_2)\psi_c(x_3) + \psi_a(x_1)\psi_c(x_2)\psi_b(x_3) + \psi_b(x_1)\psi_a(x_2)\psi_c(x_3) \\
+ \psi_b(x_1)\psi_c(x_2)\psi_a(x_3) + \psi_c(x_1)\psi_a(x_2)\psi_b(x_3) + \psi_c(x_1)\psi_b(x_2)\psi_a(x_3) \right]
\]

The remaining thing now is to find the normalization constant \( A \). This is easy since each term has norm 1 (compare with the answer in a)) so \( A^2 = 6 \). Our normalization constant is then \( A = \frac{1}{\sqrt{6}} \).

c) For fermions we also need \( n! \) terms but the total wave function should be antisymmetric. This means that it has to change sign for each interchange of two fermions. You could do this either by using the result from problem b) and just change sign on three terms to make the total wave function antisymmetric, or use a faster way; the Slater determinant

\[
\psi(x_1, x_2, x_3) = \frac{1}{\sqrt{3!}} \begin{vmatrix} \psi_a(x_1) & \psi_b(x_1) & \psi_c(x_1) \\
\psi_a(x_2) & \psi_b(x_2) & \psi_c(x_2) \\
\psi_a(x_3) & \psi_b(x_3) & \psi_c(x_3) \end{vmatrix}
\]

\[
\psi(x_1, x_2, x_3) = \frac{1}{\sqrt{6}} \left[ \psi_a(x_1)\psi_b(x_2)\psi_c(x_3) + \psi_b(x_1)\psi_c(x_2)\psi_a(x_3) + \psi_c(x_1)\psi_a(x_2)\psi_b(x_3) \\
- \psi_c(x_1)\psi_b(x_2)\psi_a(x_3) - \psi_b(x_1)\psi_a(x_2)\psi_c(x_3) - \psi_a(x_1)\psi_c(x_2)\psi_b(x_3) \right]
\]

which works for any number of elements (note that the normalization then becomes \( \frac{1}{\sqrt{N!}} \)).