Physics 137A: Quantum Mechanics	**Fall 2023**

PSET 1, Due December 04

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Problem 1:

In this question, we consider the 3D Particle in a box potential.

$$V(x,y,z) = \begin{cases} 0, & x,y,z \text{ all between zero and 'a'} \\ \infty, & \text{otherwise} \end{cases}$$

a To find the wavefunctions of the time-independent energy eigenstates we will solve the Time Independent Schroedinger Equations, which presents itself in 3D as

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

Outside the region $\{(x,y,z) : 0 \leq x,y,z \leq a\}$, the potential is infinite i.e. $V(x,y,z) = \infty$. So, the PDE is

$$-\frac{\hbar^2}{2m}\nabla^2\psi + \infty\psi = E\psi$$

But the energy E must be some finite value, so the only valid wavefunction for this region is

$$\boxed{\psi(x,y,z) = 0}$$

Inside of the box, we solve this PDE by **Separation of Variables** in cartesian coordinates.

Let's assume that the solutions to the PDE have the form

$$\psi(x,y,z) = X(x)Y(y)Z(z)$$

Then, the TISE reads as

$$\begin{aligned} &-\frac{\hbar^2}{2m}\left[\partial_x^2 + \partial_y^2 + \partial_z^2\right](XYZ) + V(x,y,z)XYZ = E\cdot XYZ \\ \implies &\frac{-\hbar 2}{2m}\left[\frac{\partial^2 X}{\partial x^2}YZ + \frac{\partial^2 Y}{\partial y^2}XZ + \frac{\partial^2 Z}{\partial z^2}XY\right] + V(x,y,z)(XYZ) = E(XYZ) \end{aligned}$$

Dividing through by $X(x)Y(y)Z(z)$, we have

$$\frac{-\hbar 2}{2m}\left[\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} + \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right] + V(x,y,z) = E$$

And also, recall that inside the box, we have $V(x,y,z) = 0$. This, TISE in this region is equivalent to the equation

$$\frac{-\hbar^2}{2m}\left[\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} + \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right] = E$$

Notice that the LHS consists of three different functions, each dependent SOLELY on one of x, y, or z being summed together to some constant.

The only way for this to holds for all possible (x, y, z) inside the box is for each of the functions to be constant itself. i.e. we have

$$\frac{-\hbar^2}{2m}\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = E_x$$
$$\frac{-\hbar^2}{2m}\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} = E_y$$
$$\frac{-\hbar^2}{2m}\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} = E_z$$

where $E_x + E_y + E_z = E$.

But each of these equations is just the TISE for a free particle in the region $[0, a]$ for each of the directions x, y, z! This is a problem we've already solved, but Let's go through the solution for one of the dimensions and then extrapolate.

Considering the x-direction, we have

$$\frac{-\hbar^2}{2m}\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = E_x$$
$$\Longrightarrow X^{''}(x) = -\frac{2mE_x}{\hbar^2}X(x)$$

Or, setting $k = \sqrt{\frac{2mE_x}{\hbar^2}}$, we have

$$X^{''}(x) = -k^2 X(x)$$

and this differential equation has the general solution

$$\boxed{X(x) = Ae^{ikx} + Be^{-ikx}}$$

Further, the wavefunction $X(x)$ must be continuous. Outside the region $0 \leq x \leq a$, the wavefunction must be zero, so invoking continuity gives us the boundary conditions $X(0) = 0$ and $X(a) = 0$.

The first condition gives us

$$X(0) = A + B = 0$$
$$\Longrightarrow X(x) = A(e^{ikx} - e^{-ikx}) = 2A\sin(kx)$$

And so, now, the second condition tells us that

$$X(a) = 2A\sin(ka) = 0$$
$$\Longrightarrow ka = n\pi, \quad n \in \mathbb{Z}$$
$$\Longrightarrow k = \frac{n\pi}{a}$$

Our k is quantized to only have certain values, which means the energy of the particle in the x-direction is also quantized.

Collecting everything we've found so far, we know

$$X(x) = 2A\sin\left(\frac{n\pi}{a}x\right)$$

Finally, we use the normalization condition to find A as

$$\begin{aligned}
&\int_0^a |X(x)|^2 dx = 1\\
\implies & 4A^2\int_0^a \sin^2\left(\frac{n\pi x}{a}\right)dx = 1\\
\implies & 4A^2\int_0^a \frac{1-\cos(\frac{2n\pi x}{a})}{2}dx = 1\\
\implies & 4A^2\left[\frac{x}{2} - \frac{a}{2n\pi}\frac{\sin(\frac{2n\pi x}{a})}{2}\right]_0^a = 1\\
\implies & 4A^2\left[\frac{a}{2} - 0\right] = 1\\
\implies & 2aA^2 = 1\\
\implies & A = \frac{1}{\sqrt{2a}}
\end{aligned}$$

Thus, the eigenfunction to the differential equation in the x-direction is

$$\boxed{X(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)}$$

with eigenvalue

$$\boxed{E_x = \frac{\hbar^2k^2}{2m} = \frac{\hbar^2n^2\pi^2}{2ma^2}}$$

where $n = 1, 2, 3...$

Solving the differential equations in the y and z directions, we would get the exact same result. Thus, we can conclude that the energy eigenstates of the 3D particle in a box are

$$\begin{aligned}
\psi(x,y,z) &= X(x)Y(y)Z(z)\\
&= \left(\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)\right)\cdot\left(\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}y\right)\right)\cdot\left(\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}z\right)\right)\\
&= \sqrt{\frac{8}{a^3}}\sin\left(\frac{n\pi}{a}x\right)\sin\left(\frac{n\pi}{a}y\right)\sin\left(\frac{n\pi}{a}z\right)
\end{aligned}$$

with energy eigenvalues

$$\begin{aligned}
E &= E_x + E_y + E_Z\\
&= \frac{\hbar^2n_x^2\pi^2}{2ma^2} + \frac{\hbar^2n_y^2\pi^2}{2ma^2} + \frac{\hbar^2n_z^2\pi^2}{2ma^2}\\
&= \frac{\hbar^2\pi^2}{2ma^2}(n_x^2 + n_y^2 + n_z^2)
\end{aligned}$$

To conclude,

$$\boxed{\psi_E(x,y,z) = \sqrt{\frac{8}{a^3}} \sin\left(\frac{n_x \pi}{a} x\right) \sin\left(\frac{n_y \pi}{a} y\right) \sin\left(\frac{n_z \pi}{a} z\right)}$$

$$\boxed{E = \frac{\hbar^2 \pi^2}{2ma^2}(n_x^2 + n_y^2 + n_z^2)}$$

where $n_x, n_y, n_z = 1, 2, 3...$

b The Distinct Energies $E_1, E_2, E_3, E_4, E_5, E_6$ are found by finding calculating E for different values of n_x, n_y, n_z.

If we denote the number of degeneracies corresponding to each energy level as d, then

$$\begin{aligned}
E_1 &= \frac{\hbar^2 \pi^2}{2ma^2}(3) \quad : \quad d = 1; \\
E_2 &= \frac{\hbar^2 \pi^2}{2ma^2}(6) \quad : \quad d = 3; \\
E_3 &= \frac{\hbar^2 \pi^2}{2ma^2}(9) \quad : \quad d = 3; \\
E_4 &= \frac{\hbar^2 \pi^2}{2ma^2}(11) \quad : \quad d = 3; \\
E_5 &= \frac{\hbar^2 \pi^2}{2ma^2}(12) \quad : \quad d = 1; \\
E_6 &= \frac{\hbar^2 \pi^2}{2ma^2}(14) \quad : \quad d = 6;
\end{aligned}$$

c Supposing we have 5 non-interacting particles doomed to live together in a box, the lowest attainable energy depends on what kind of particles are present.

(a) If the particles are **classical, distinguishable particles** then the ground state energy is zero. This is because, classically, energy is not quantized and can attain any value in a continuous range which includes zero.

(b) If the particles are Spin-1 particles, the Spin-Statistics Theorem tells us that they are **Bosons**, which means they do not need to satisfy the Pauli Exclusion principle.

Thus, all five particles will have the lowest possible energies i.e. each one will have energy $E = \frac{3\hbar^2\pi^2}{2ma^2}$. So, the ground state energy of the 5 particle system will be

$$\boxed{E_{ground} = \frac{15\hbar^2\pi^2}{2ma^2}}$$

(c) If the particles are Spin-1/2, the Spin-Statistics Theorem tells us they are **fermions**. Thus, by the Pauli Exclusion Principle, each energy level can only accomodate two particles (of opposite spin).

Thus, two particles will have energy $E_1 = \frac{\hbar^2\pi^2}{2ma^2}(3)$, two will have energy $E_2 = \frac{\hbar^2\pi^2}{2ma^2}(6)$, and one will have energy $E_3 = \frac{\hbar^2\pi^2}{2ma^2}(9)$.
Thus, the ground state energy of the 5-particle system will be

$$\boxed{E_{ground} = 18\frac{\hbar^2\pi^2}{2ma^2}}$$

d

Problem 2:

Problem 3:
