Problem 1. (6 points) Consider a particle of mass m moving along axis x. Which of the functions listed below are eigenfunctions of the kinetic energy operator of the particle? If they are, what at are the corresponding eigenvalues? (here a and b are constants)

(A) $3e^{i7x}$; **(B)** $3e^{iax}+4ie^{-iax}$; **(C)** $\sin(bx)-a\cos(bx)$.

All three function are eigenfunctions of the kinetic energy operator. The eigenvalues are:

(A) $\dfrac{49\hbar^2}{2m}$; **(B)** $\dfrac{a^2\hbar^2}{2m}$; **(C)** $\dfrac{b^2\hbar^2}{2m}$.

Problem 2 (4 points). A quantum mechanical particle of mass m is in a state described by the wave function (not normalized): $\Psi=\left(5e^{ix}-3e^{i2x}+ie^{-i4x}\right)/\sqrt{2L}$. Assume it's a free particle defined in the interval $(-L,L)$ where $L\to\infty$. Using the postulates of QM, answer the following questions:

(**A**) List all values of the linear momentum, p, that can be obtained in a single measurement and their probabilities.

Function Ψ is not an eigenfunction of the momentum operator. Since the eigenfunctions of the momentum operator have the form of e^{ikx} (with the corresponding eigenvalue = $\hbar k$), we can treat Ψ as a linear combination of the eigenfunctions of the momentum operator. Note that each term $e^{ikx}/\sqrt{2L}$ is already normalized, therefore when calculating the probabilities of the individual measured values we can focus on the projection coefficients.

According to the 3rd postulate, when measuring the momentum only the following individual eigenvalues of the momentum operator can be obtained:

$p=\hbar$, probability = $5^2/(5^2+3^2+|i|^2)$ = 25/35 = 0.7143
$p=2\hbar$, probability = $3^2/35$ = 9/35 = 0.2571
$p=-4\hbar$, probability = 1/35 = 0.0286

(**B**) Calculate the average value of p that you expect to obtain as a result of a very large number of measurements.

Using statistical considerations:

$$\langle p\rangle=\sum_i p_i\times\text{Probability}(p_i)=\hbar\frac{25}{35}+2\hbar\frac{9}{35}-4\hbar\frac{1}{35}=\hbar\frac{25+18-4}{35}=\hbar\frac{39}{35}=1.56\hbar$$

Alternatively, you can use the expectation value equation (4th postulate, remember?) and calculate the corresponding integrals in both numerator and denominator (you need to calculate the denominator because Ψ as defined in this problem is not normalized). I include this calculation below so that those of you who did the problem using statistical considerations can follow it

$$\langle p\rangle=\frac{\int\Psi^*\hat{p}\Psi dx}{\int\Psi^*\Psi dx}=\frac{-\dfrac{i\hbar}{2L}\int\limits_{-L}^{L}\left(5e^{-ix}-3e^{-i2x}-ie^{i4x}\right)\dfrac{d}{dx}\left(5e^{ix}-3e^{i2x}+ie^{-i4x}\right)dx}{\dfrac{1}{2L}\int\limits_{-L}^{L}\left(5e^{-ix}-3e^{-i2x}-ie^{i4x}\right)\left(5e^{ix}-3e^{i2x}+ie^{-i4x}\right)dx}=$$

$$=-i\hbar\frac{\dfrac{1}{2L}\int\limits_{-L}^{L}\left(5e^{-ix}-3e^{-i2x}-ie^{i4x}\right)\left(5ie^{ix}-6ie^{i2x}+4e^{-i4x}\right)dx}{\dfrac{1}{2L}\int\limits_{-L}^{L}\left(5e^{-ix}-3e^{-i2x}-ie^{i4x}\right)\left(5e^{ix}-3e^{i2x}+ie^{-i4x}\right)dx}=-i\hbar\frac{\dfrac{1}{2L}\int\limits_{-L}^{L}\left((25+18-4)i+\textit{terms containing } e^{iax}\right)dx}{\dfrac{1}{2L}\int\limits_{-L}^{L}\left((25+9+1)+\textit{terms containing } e^{iax}\right)dx}$$

(remember that $e^{-ia} \times e^{ia} = 1$, so after opening the brackets in the integrand you will have terms that are just numbers and terms that contain exponential functions e^{-ia}). Recall that for a free particle, in order to get Ψ normalized we assumed that the particle is moving in the interval from $-L$ to L, where L is large and eventually set to infinity ($L \rightarrow \infty$). Therefore the integrals of the e^{-iax} – containing terms (where $a \neq 0$) become negligible when $L \rightarrow \infty$:

$\frac{1}{2L}\int_{-L}^{L} e^{iax}dx = \frac{1}{2L}\frac{e^{iaL}-e^{-iaL}}{ia} = \frac{\sin(aL)}{aL} \rightarrow 0 \;\; when \;\; L \rightarrow \infty$, because $\sin(kL)$ is bounded ($|\sin(aL)| \le 1$), and the only non-zero terms come from $\frac{1}{2L}\int_{-L}^{L} dx = \frac{2L}{2L} = 1$. This gives $\langle p \rangle = -i\hbar\frac{39i}{35} = \frac{39}{35}\hbar$, the same result as using statistics-based approach.

Problem 3 **(6 points).** A particle in the 1D box ($0 \le x \le a$) is in the state with n=5. Answer the following questions:

(**A**) Write the expression for the wave function describing this particle. Make sure the wave function is normalized and *explicitly* includes the time dependence.

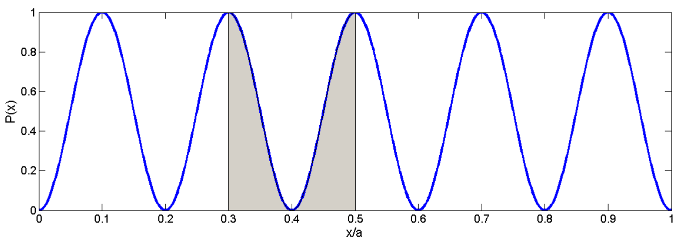
$$\Psi(x,t) = \Psi_{n=5}(x) \times e^{-i\frac{E_{n=5}}{\hbar}t} = \sqrt{\frac{2}{a}}\sin\left(\frac{5\pi}{a}x\right) \times e^{-i\frac{25\pi h}{4ma^2}t}$$

(B) In which points inside the box you are unlikely to find the particle? List their coordinates.

These are points where $\sin(5\pi x/a)=0$: $x = a/5$, $2a/5$, $3a/5$, $4a/5$. The particle also cannot be found at the edges of the box: $x = 0$ and $x = a$.

(**C**) What is the probability to find this particle in the interval between $0.3a$ and $0.5a$?

If you plot P(x) (see below) you will find out that, based on the symmetry of P(x), this is 1/5 of the total area covered by P(x), hence the probability is 0.2.



Direct integration of the probability density over this interval gives the same result:

$$P\left(\frac{3a}{10} \le x \le \frac{5a}{10}\right) = \int_{3a/10}^{5a/10}\left[\Psi_5(x)\right]^2 dx = \frac{2}{a}\int_{3a/10}^{5a/10}\sin^2\left(\frac{5\pi}{a}x\right)dx = \frac{1}{a}\int_{3a/10}^{5a/10}\left[1-\cos\left(\frac{10\pi}{a}x\right)\right]dx =$$

$$= \frac{1}{5} - \frac{1}{a}\frac{a}{10\pi}\left[\sin(5\pi) - \sin(3\pi)\right] = \frac{1}{5}$$

Problem 4 (4 points). As a simplified model of the hydrogen atom, consider an electron in a cube with the size of 1 Å (=10^{-10} m) (approximately the diameter of the lowest orbit in Bohr's model).

(**A**) Calculate the energy difference, ΔE, between the ground state and the first excited state of the electron.

The ground state of a particle (in this case electron) in a 3D box corresponds to all three quantum numbers (n_x, n_y, and n_z) equal 1. The first excited state corresponds to only one of the quantum numbers =2 while the other being =1, and because it's a cube, it doesn't matter which quantum number it is.

$\Delta E = E_{n=2} - E_{n=1} = \frac{h^2}{8ma^2}\left(2^2 - 1\right) = \frac{3h^2}{8ma^2}$. Substituting $m=m_e=9.1 \times 10^{-31}$ kg; $a=10^{-10}$ m, we get $\Delta E_{electron}=1.8\ 10^{-17}$ J.

(**B**) Compare your result in A with the average kinetic energy (½ k_BT per degree of freedom) at room temperature (assume 300 K) to answer the question whether classical or quantum mechanics should be used to describe the electron in this model.

$\langle E_{thermal}\rangle = 3\times ½\ k_BT = 6.21 \times 10^{-21}$ J at T=300 K (it's a 3-D motion, hence three degrees of freedom). Because $\Delta E_{electron} \approx 3000 \times (3\times ½\ k_BT) >> \langle E_{thermal}\rangle$, QM must be used in this case.