

Answer each question in the space provided; use back of page if extra space is needed. Answer questions so the grader can READILY understand your work; only work on the exam sheet will be considered. Write answers, where appropriate, with reasonable numbers of significant figures. You may use **only** the "Student Handbook," a calculator, and a straight edge.

1. (10 points) Which of the following functions are eigenfunctions of the operator $\frac{d^2}{dx^2}$?

Prove your statement explicitly.

a) $F = \exp(-ix^2)$:

$$\begin{aligned} \frac{d^2}{dx^2} \exp(-ix^2) &= \frac{d}{dx} \left(\frac{d}{dx} \exp(-ix^2) \right) = \frac{d}{dx} (-2ix \times \exp(-ix^2)) \\ &= -2i \times \exp(-ix^2) - 4x^2 \exp(-ix^2) \neq \text{Const} \times F \end{aligned}$$

F_1 is not the eigenfunction of this operator

b) $F_2 = \exp(-ix)$:

$$\frac{d^2}{dx^2} \exp(-ix) = \frac{d}{dx} \left(\frac{d}{dx} \exp(-ix) \right) = \frac{d}{dx} (-i \exp(-ix)) = -\exp(-ix) = \text{Const} \times F$$

F_2 is an eigenfunction of this operator

c) $F_3 = -i \sin(x)$:

$$\frac{d^2}{dx^2} (-i \sin(x)) = \frac{d}{dx} \left(\frac{d}{dx} (-i \sin(x)) \right) = \frac{d}{dx} (-i \cos(x)) = i \sin(x) = \text{Const} \times F$$

F_4 is an eigenfunction of this operator

**DO NOT WRITE
IN THIS SPACE**

p. 1 _____/10

p. 2 _____/10

p. 3 _____/15

p. 4 _____/10

p. 5 _____/15

p. 6 _____/15

p. 7 _____/10

p. 8 _____/15

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p. 9 _____/5
(Extra credit)

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TOTAL PTS

/100

2. (10 points) For each statement in column A, put the number of the phrase in column B that best fits the expression.

<p>1. If several distinct eigenfunctions of the total energy operator correspond to the same energy, such energy level is called <u>h</u></p> <p>2. De Broglie's relation states <u>c</u></p> <p>3. In the relation below, R is called <u>k</u></p> $\nu = R \left(\frac{1}{n_1^2} - \frac{1}{n^2} \right), \text{ where } n > n_1$ <p>4. In order for us to know the outcome of two quantum mechanical measurements with infinite precision <u>d</u></p> <p>5. According to quantum mechanics, a particle could escape through a barrier even if does not have sufficient energy to go over it. This effect is called <u>i</u></p>	<p>a. excited</p> <p>b. entangled</p> <p>c. $\lambda = \frac{h}{p}$</p> <p>d. the operators corresponding to these two measurements must commute</p> <p>e. absorption constant</p> <p>f. the measurements have to be simultaneous</p> <p>g. $\lambda = \frac{h}{p} + h\nu$</p> <p>h. degenerate</p> <p>i. tunneling</p> <p>j. the operators must be nonlinear</p> <p>k. the Rydberg constant</p> <p>l. the operators corresponding to these two measurements must be Stern-Gerlach</p> <p>m. Rutherford backscattering constant</p>
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3. (15 points)

a) a) (8 points). Find the simplest form of the following commutator $\left[x \frac{d}{dx}, \frac{d^2}{dx^2} \right]$.

The simplest form is found by operation on an arbitrary function, f, of x.

$$\begin{aligned} \left[x \frac{d}{dx}, \frac{d^2}{dx^2} \right] f(x) &= x \frac{d}{dx} \left(\frac{d^2 f(x)}{dx^2} \right) - \frac{d^2}{dx^2} \left(x \frac{df(x)}{dx} \right) = x \frac{d^3 f(x)}{dx^3} - \frac{d}{dx} \left(\frac{dx}{dx} \frac{df(x)}{dx} + x \left(\frac{d^2 f(x)}{dx^2} \right) \right) = \\ &= x \frac{d^3 f(x)}{dx^3} - \frac{d^2 f(x)}{dx^2} - \frac{d^2 f(x)}{dx^2} - x \frac{d^3 f(x)}{dx^3} = -2 \frac{d^2 f(x)}{dx^2} \end{aligned}$$

Therefore, the simplest form of the commutator (an operator) is: $-2 \frac{d^2}{dx^2}$.

Note that the question asked for the form of the operator, not the form of the operator applied to the function.

b) (7 points). Demonstrate whether the following two operators commute or not. Show all work clearly.

$$\hat{p}_x, \hat{p}_x^2$$

The way to show is to find the commutator:

$$\left[\hat{p}_x, \hat{p}_x^2 \right] = \hat{p}_x^3 - \hat{p}_x^3 = 0$$

Since the commutator is equal to zero, the operators commute.

4. (10 points) For a particle in a 1-dimensional box of width a and infinite potential outside this box, determine the probability of a particle being within the middle third of this box for $n=1$. [HINT: $\Psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$]

For $n=1$:

$$P_{1/3} = \int_{a/3}^{2a/3} \frac{2}{a} \sin^2\left(\frac{\pi x}{a}\right) dx = \frac{2}{a} \left(\frac{1}{2} x - \frac{a}{4\pi} \sin\left(\frac{2\pi x}{a}\right) \right) \Bigg|_{a/3}^{2a/3} = \frac{2}{a} \left(\frac{a}{3} - \frac{a}{4\pi} \sin\left(\frac{4\pi a}{3a}\right) - \frac{a}{6} + \frac{a}{4\pi} \sin\left(\frac{2\pi a}{3a}\right) \right) =$$
$$= \frac{1}{3} + 0.13783 + 0.13783 = 0.60899$$

The particle spends over 60% of its time in the middle third of the box

5. (15 points) **Prove** that the most probable distance between the electron of a hydrogen atom in a 1s orbital and the nucleus is the Bohr radius. Show all your work clearly.

$$\psi_n = R_{nl}(r)Y_{lm}(\Theta, \varphi)$$

$$R_{nl}\left(\frac{r}{a_0}\right) = A_{nl}\left(\frac{Zr}{a_0}\right)^l L_{nl}\left(\frac{r}{a_0}\right) \exp\left(-\frac{Zr}{na_0}\right); R_{10}\left(\frac{r}{a_0}\right) = A_{10}\left(\frac{r}{a_0}\right)^0 \exp\left(-\frac{r}{a_0}\right)$$

The radial distribution function is $P(r) = R_{nl}^2 r^2$, whose derivative with respect to r should equal zero at a maximum:

$$\frac{dP}{dr} = \frac{d\left(A_{10}^2 r^2 \exp\left(-\frac{2r}{a_0}\right)\right)}{dr} = 0 = A_{10}^2 \times 2r \times \exp\left(-\frac{2r}{a_0}\right) - \frac{2}{r} A_{10}^2 \times r^2 \exp\left(-\frac{2r}{a_0}\right)$$

Thus,

$$A_{10}^2 \times 2r \times \exp\left(-\frac{2r}{a_0}\right) = \frac{2}{a_0} A_{10}^2 \times r^2 \exp\left(-\frac{2r}{a_0}\right)$$

or:

$$2r = \frac{2}{a_0} r^2, \text{ which means that } r = a_0$$

6. (15 points) For each practical problem in the left column, indicate the model in the right column that **best** represents the quantum mechanics of the practical problem.

Problem	Model
1. <u> C </u> An organic molecule moving across the surface of a metal catalyst	a. Free particle
2. <u> G </u> A helium ion	b. Particle in a 1-D box
3. <u> B </u> A xenon atom adsorbed in a carbon nanotube	c. Particle in a 2-D box
4. <u> D </u> An oxygen atom in a high vacuum chamber	d. Particle in a 3-D box
5. <u> A </u> A piece of dust in deep interstellar space	e. 1-D harmonic oscillator
	f. Rigid rotor
	g. Central-force problem

7. (10 points) For a particle of mass m in a three-dimensional cubic box of side a , write down the energies of the lowest five energy levels, in order from lowest to highest, in units of $\frac{h^2}{8ma^2}$. For each, indicate the degeneracy of the level.

Energy (in units of $\frac{h^2}{8ma^2}$)	Degeneracy
3	1
6	3
9	3
11	3
12	1

8. (15 points) For the helium atom in the $1s^2$ state, a proposed approximate spatial wave function is

$\psi = A e^{-\zeta r_1/a_0} e^{-\zeta r_2/a_0}$, the product of a hydrogen-like wave functions for the electrons. Carrying out a calculation of the expectation value total energy, including electron-electron repulsion, for the system using this wave function gives the following approximate energy for this system

$$E_{app} = \left(\zeta^2 - 4\zeta + \frac{5}{8}\zeta \right) E_h$$

where E_h is the Hartree energy, and ζ is the apparent charge on the nucleus. (a) For the helium atom, what value of ζ gives the best approximate energy? (b) What is the predicted energy, in electron volts, of this state of the helium atom relative to the vacuum level?

(a) This is a use of the variation principle:

$$\frac{\partial E_{app}}{\partial \zeta} = 0 = \frac{\partial}{\partial \zeta} \left(-\zeta^2 - 4\zeta + \frac{5}{8}\zeta \right) E_h = \left(2\zeta - 4 + \frac{5}{8} \right) E_h$$

Solution of this equation gives a value $\zeta = \frac{27}{16}$

Note that this is less than the actual charge on the helium nucleus, and indication of shielding of the nuclear charge by the second electron.

(b)

$$\begin{aligned} E_{app} &= \left(\zeta^2 - 4\zeta + \frac{5}{8}\zeta \right) E_h = \left(\left(\frac{27}{16} \right)^2 - 4 \left(\frac{27}{16} \right) + \frac{5}{8} \left(\frac{27}{16} \right) \right) (27.2144 \text{ eV}) \\ &= -77.49 \text{ eV} \end{aligned}$$

9. (5 points, extra credit) For 3-D free particle of mass m , $\psi(x, y, z) = A e^{-i(k_x x + k_y y + k_z z)}$, where A is some normalization constant and (k_x, k_y, k_z) are the quantum numbers for motion in the three orthogonal directions. In terms of the quantum numbers and any other fundamental constants, give an equation for the **speed** of this particle.

This is straightforward, if you realize that the speed and the linear momentum are related. Operation with the square of the linear momentum gives:

$$\hat{p}^2 \psi = (\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2) \psi = p^2 \psi$$

Substitution of the wave function and the form for the operators in this equation gives

$$(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2) \psi = -\hbar^2 \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) e^{-i(k_x x + k_y y + k_z z)} = \hbar^2 (k_x^2 + k_y^2 + k_z^2) e^{-i(k_x x + k_y y + k_z z)}$$

By comparison, one sees that the eigenvalue for p^2 is $\hbar^2 (k_x^2 + k_y^2 + k_z^2)$.

But by physics, $m^2 v^2 = p^2$, so by rearrangement

$$v^2 = \frac{p^2}{m^2} = \frac{\hbar^2}{m^2} (k_x^2 + k_y^2 + k_z^2)$$

The speed is the square root of this, so one finally reaches the answer for the speed of the particle:

$$v = \sqrt{v^2} = \sqrt{\frac{p^2}{m^2}} = \frac{\hbar}{m} \sqrt{k_x^2 + k_y^2 + k_z^2}$$