UNIVESITY OF ESWATINI FACULTY OF SCIENCE AND ENGINEERING DEPARTMENT OF PHYSICS

Main Examination 2019/2020 COURSE NAME: Quantum Mechanics I COURSE CODE: PHY341/PHY342 TIME ALLOWED: 3 hours

ANSWER ANY FIVE QUESTIONS. ALL QUESTIONS CARRY EQUAL (20) MARKS

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(a). Show that if \hat{A} , \hat{B} and \hat{C} are operators, then inj general

$$\left[\hat{\mathbf{A}}\hat{\mathbf{B}},\hat{\mathbf{C}}\right] = \hat{\mathbf{A}}\left[\hat{\mathbf{B}},\hat{\mathbf{C}}\right] - \left[\hat{\mathbf{A}},\hat{\mathbf{C}}\right]\hat{\mathbf{B}}.$$

[3 marks]

(b). Given that $[\hat{x},\hat{p}]=i\hbar$, compute $[\hat{x},\hat{p}^n]$ and $[\hat{p},\hat{x}^n]$.

[6 marks]

(c). If $V(\hat{x})$ is a function with a convergent Taylor expansion, $V(\hat{x}) =$ $\sum_{n=0}^{\infty} c_n \hat{x}^n$, show that

$$[\hat{p}, V(\hat{x})] = i\hbar \frac{dV(\hat{x})}{d\hat{x}}.$$

[4 marks]

- (d). For a simple harmonic oscillator, the ladder operators \hat{a} and \hat{a}^{\dagger} have the property that $[\hat{a}, \hat{a}^{\dagger}] = 1$. Compute
 - (i). $\left[\hat{a}^{\dagger}\hat{a},\hat{a}\right]$.

[2 marks]

(ii). $[\hat{a}^{\dagger}\hat{a}, \hat{a}^{\dagger}]$.

2 marks

(e). The Angular momentum operator \hat{L} has components \hat{L}_x , \hat{L}_y and \hat{L}_z , such that $\left[\hat{\mathbf{L}}_x, \hat{\mathbf{L}}_y\right] = i\hat{\mathbf{L}}_z$, $\left[\hat{\mathbf{L}}_y, \hat{\mathbf{L}}_z\right] = i\hat{\mathbf{L}}_x$, $\left[\hat{\mathbf{L}}_z, \hat{\mathbf{L}}_x\right] = i\hat{\mathbf{L}}_y$ and $\hat{\mathbf{L}}^2 = i\hat{\mathbf{L}}_y$ $\hat{\mathbf{L}}_x^2 + \hat{\mathbf{L}}_y^2 + \hat{\mathbf{L}}_z^2$. Compute

 $\left[\hat{\mathbf{L}}_z,\hat{\mathbf{L}}^2\right]$.

[3 marks]

Explain what was learned about quantization of radiation from the following experiments,

(a). The photo-electric effect.

[5 marks]

(b). Franck-Hertz experiment.

[5 marks]

(c). Compton scattering.

[5 marks]

(d). The black body radiation spectrum.

[5 marks]

Consider a Gaussian wave packet

$$\psi(x) = N \exp\left(i\frac{p_0}{\hbar}x - \frac{x^2}{2\sigma^2}\right)$$

(a). Find the normalization constant N.

[3 marks]

(b). Find the expectation values $\langle \hat{x} \rangle$ and $\langle \hat{x}^2 \rangle$.

[6 marks]

(c). What is the corresponding momentum space wave function $\psi(p)$?

[5 marks]

(d). Find the expectation values $\langle \hat{p} \rangle$ and $\langle \hat{p}^2 \rangle$,

[6 marks]

Question 4

A particle of mass m is confined to a one-dimensional region, $0 \le x \le a$, as shown in figure 1. At t = 0, its normalised wave function is

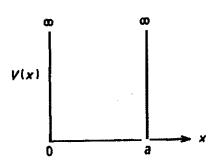


Figure 1:

$$\psi(x,t=0) = \sqrt{\frac{8}{5a}} \left[1 + \cos\left(\frac{\pi x}{a}\right) \right] \sin\left(\frac{\pi x}{a}\right).$$

(a). What is the wave function at a later time $t=t_0$?

[10 marks]

(b). What is the average energy of the system at t = 0 and at $t = t_0$?

[5 marks]

(c). What is the probability that the particle is found in the left half of the box, at $t = t_0$?

[5 marks]

(a). A quantum particle is in the state $|\psi,t\rangle$, which is a solution to the time-dependent Schrödinger equation, $i\hbar\frac{d}{dt}|\psi,t\rangle=\hat{H}|\psi,t\rangle$. Show that the expectation value of the time-independent operator \hat{O} satisfy

$$rac{d}{dt}raket{\psi,t}{\hat{O}}\ket{\psi,t} = rac{1}{i\hbar}raket{\psi,t}{\hat{O},\hat{H}}\ket{\psi,t}$$

[5 marks]

(b). State, with justification, whether each of the following sets of quantum numbers could be used to label a possible wave-function of the hydrogen atom.

[5 marks]

(i).
$$n = 1, \ell = 1, m_{\ell} = 1, m_s = \frac{1}{2}$$

(ii).
$$n = 3, \ell = 1, m_{\ell} = 2, m_s = 0$$

(iii).
$$n=4, \ell=1, m_{\ell}=-1, m_s=\frac{-1}{2}$$

(iv).
$$n=2, \ell=1, m_{\ell}=0, m_s=0$$

(v).
$$n=4, \ell=3, m_{\ell}=-1, m_s=\frac{1}{2}$$

(c). The following wave functions are energy eigenfunctions of the hydrogen atom.

$$\begin{split} \Psi_1(r,\theta,\phi) &= \frac{1}{\sqrt{32\pi a_0^2}} \left(2 - \frac{r}{a_0} \right) e^{\frac{-r}{2a_0}} \\ \Psi_2(r,\theta,\phi) &= \frac{1}{81\sqrt{\pi a_0^3}} \left(\frac{r}{a_0} \right)^2 e^{\frac{-r}{3a_0}} \sin\theta \cos\theta e^{-i\phi} \end{split}$$

(i). Deduce the quantum numbers n, ℓ , and m_{ℓ} for each wave function.

[5 marks]

(ii). Verify if $\Psi_1(r, \theta, \phi)$ is normalised and calculate the expectation value of the electron-nuclear separation in the hydrogen atom for this wave function.

[5 marks]

(a). A infinite cubical well ("or particle in a box") has a potential, defined in Cartesian 3D coordinates as

 $V(x,y,z) = egin{cases} 0, & ext{if } x,y,z ext{ are all between 0 and a} \\ \infty, & ext{otherwise} \end{cases}$

(i). What is the time-dependant Schrödinger equation for the particle inside the box

[3 marks]

(ii). Use the separation of variables ansatz $(\Psi(x, y, z) = X(x)Y(y)Z(z))$ to derive **three** separate ordinary differential equations for X, Y and Z in terms of K_x, K_y and K_z , where $E = \frac{\hbar^2}{2m}(K_x^2 + K_y^2 + K_z^2)$.

[3 marks]

(iii). Find solutions to the equations above. Apply the boundary conditions to show that

$$K_x a = n_x \pi$$

$$K_y a = n_y \pi$$

$$K_z a = n_z \pi$$

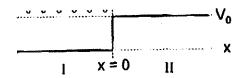
where $n_x, n_y, n_z = 1, 2, 3, ...$

[3 marks]

(b). Consider a step potential;

$$V(x) = \begin{cases} 0, & \text{if } x < 0 \\ V_0, & \text{if } x \ge 0 \end{cases}.$$

Consider the initial condition where a single particle of energy $E > V_0$ is incident from the left and no particle is incident from the right. Use



 $k=\frac{\sqrt{2mE}}{\hbar}$ and $l=\frac{\sqrt{2m(E-V_0)}}{\hbar}$ to show that the time-independent Schrödinger equation for region I and II are

$$\frac{\partial^2 \Psi_I(x)}{\partial x^2} + k^2 \Psi_I(x) = 0$$
$$\frac{\partial^2 \Psi_{II}(x)}{\partial x^2} + l^2 \Psi_{II}(x) = 0.$$

[3 marks]

Appendix

3

$$\int x^2 \sin(ax) dx = \frac{2x}{a^2} \sin(ax) + \left(\frac{2}{a^3} - \frac{x^2}{a}\right) \cos(ax)$$

$$\int x^2 \cos(ax) dx = \frac{2x}{a^2} \cos(ax) + \left(\frac{2}{a^3} - \frac{x^2}{a}\right) \sin(ax)$$

$$\int x^2 \cos^2(bx) dx = \frac{4b^3x + 3(2b^2x^2 - 1)\sin(2bx) + 6bx\cos(2bx)}{24b^3}$$

$$\int_0^\infty e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}$$

- 5 $\int_0^\infty x^n e^{\frac{-x}{a}} dx = n! a^{n+1}$ for any non-negative integer, n.
- 6 Planck's constant $h = 6.663 \times 10^{-34} J \cdot s$
- 7 Dirac's constant $\hbar = 1.05 \times 10^{-31} J \cdot s$
- 8 Permittivity of vaccum $\epsilon_0 = 8.854 \times 10^{-12} C^2 N^{-1} m^{-2}$
- 9 Ground state hydrogen energy $-E_1 = 13.6057eV$
- 10 Bohr energies $E_n = \frac{E_1}{n^2}$
- 11 Hydrogen ground state wavefunction $\Psi_0 = \frac{1}{\sqrt{\pi a^3}} e^{\frac{-r}{a}}$

Y_0^0	$\left(\frac{1}{4\pi}\right)^{\frac{1}{2}}$
Y_1^0	$\left(\frac{3}{4\pi}\right)^{\frac{1}{2}}\cos\theta$
$Y_1^{\pm 1}$	$\mp \left(\frac{3}{8\pi}\right)^{\frac{1}{2}} \sin\theta e^{\pm i\phi}$
Y_2^0	$\left(\frac{5}{16\pi}\right)^{\frac{1}{2}}(3\cos^2\theta - 1)$
$Y_2^{\pm 1}$	$\mp \left(\frac{15}{8\pi}\right)^{\frac{1}{2}} \sin\theta \cos\theta e^{\pm i\phi}$

Table 1: The first few spherical harmonics, $Y_l^m(\theta, \phi)$

R_{10}	$2a^{\frac{-3}{2}}e^{\frac{-r}{a}}$
R_{20}	$\frac{1}{\sqrt{2}}a^{\frac{-3}{2}}\left(1-\frac{r}{2a}\right)e^{\frac{-r}{2a}}$
R_{21}	$\frac{1}{\sqrt{24}}a^{\frac{-3}{2}}\left(\frac{r}{a}\right)e^{\frac{-r}{2a}}$
R_{30}	$\frac{2}{\sqrt{27}}a^{\frac{-3}{2}}\left(1-\frac{2r}{3a}+\frac{2}{27}\left(\frac{r}{a}\right)^{2}\right)e^{\frac{-r}{3a}}$
R_{32}	$\frac{4}{81\sqrt{30}}a^{\frac{-3}{2}}\left(\frac{r}{a}\right)^{2}e^{\frac{-r}{3a}}$

Table 2: The first few hydrogen radial wavefunctions, $R_{nl}(r)$