THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS

FINAL EXAMINATION: JUNE 2012

PHYS3011 & PHYS3210
Quantum Mechanics

P1

Time allowed – 2 hours
Total number of questions – 4
Answer ALL 4 questions
All questions are of equal value

Candidates must supply their own,
university-approved calculator.

Answers must be written in ink.
Except where they are expressly required,
pencils may only be used for drawing,
sketching, or graphical work.
Please do not use red ink.

Candidates may keep this question paper.

QUANTUM MECHANICS – Formula Sheet

You can use any of the information given in these pages, without proof, in the exam.

Fundamental constants:

Planck's constant, $h \; = \; 6.63 \times 10^{-34}$ Js

Reduced Planck constant, $\hbar \; = \; h/2\pi \; = \; 1.05 \times 10^{-34}$ Js

Speed of light, $c = 3 \times 10^8$ ms^{-1}

Elementary charge, $e \; = 1.60 \text{ x } 10^{-19}$ C 1eV $= 1.60 \text{ x } 10^{-19}$ J

Electron mass $m_e \; = \; 0.511$ MeV/$c^2 = 9.11 \text{ x } 10^{-31}$ kg

$$a_0 \; = \; \frac{(4\pi\epsilon_0)\,\hbar^2}{m_e e^2} \; = 0.529 \text{ Å} \; = \; 0.529{\times}10^{-10}\text{ m} \quad \text{(Radius of 1st Bohr orbit)}$$

$$\alpha \; = \; \frac{e^2}{(4\pi\epsilon_0)\,\hbar c} \; = \; \frac{1}{137.04} \qquad \text{(Fine structure constant – dimensionless)}$$

$$E_B \; = \; -\frac{1}{2}\,\frac{e^2}{(4\pi\epsilon_0)\,a_0} \; = \; -\tfrac{1}{2} m_e c^2 \alpha^2 \; = \; -\frac{1}{2}\,\frac{m_e e^4}{(4\pi\epsilon_0)^2\,\hbar^2} \; = \; -13.6\,e\text{V}$$

(Binding energy of H atom)

$$\mu_B \; = \; \frac{e\hbar}{2m_e} \; = \; 9.27{\times}10^{-24}\text{ Amp-m}^2 \; = \; 9.27{\times}10^{-24}\text{ J T}^{-1} \qquad \text{(Bohr magneton)}$$

Reduced mass of system of two particles with masses m_1, m_2 : $\mu \; = \; \dfrac{m_1 m_2}{m_1 + m_2}$

∇^2 in spherical polar coordinates:

$$\nabla^2 \; = \; \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) \; + \; \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) \; + \; \frac{1}{r^2\sin^2\theta}\,\frac{\partial^2}{\partial\phi^2}$$

3-dimensional volume element $= r^2 \sin\theta \; dr \; d\theta \; d\phi$

Schroedinger Wave Equation:

To obtain the time-dependent equation from the classical expression for energy:

substitute $\quad \mathbf{p} \rightarrow -i\hbar\nabla \qquad E \rightarrow i\hbar\frac{\partial}{\partial t}$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V(x,t)\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

Time independent equation in 1 dimension: $\dfrac{-\hbar^2}{2m}\dfrac{d^2\psi}{dx^2} + V\psi = E\psi$

In 3 dimensions: $\dfrac{-\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$

Normalised wave functions:

For Hydrogen-like atom:

$$\psi_{100} = \left(\frac{Z^3}{\pi a_0^3}\right)^{\frac{1}{2}} \exp\left(-\frac{Zr}{a_0}\right)$$

$$\psi_{200} = \left(\frac{Z^3}{32\pi a_0^3}\right)^{\frac{1}{2}} \left(2-\frac{Zr}{a_0}\right) \exp\left(-\frac{Zr}{2a_0}\right)$$

$$\psi_{210} = \left(\frac{Z^3}{32\pi a_0^3}\right)^{\frac{1}{2}} \frac{Zr}{a_0} \exp\left(-\frac{Zr}{2a_0}\right) \cos\theta$$

$$\psi_{21\pm1} = \left(\frac{Z^3}{64\pi a_0^3}\right)^{\frac{1}{2}} \frac{Zr}{2a_0} \exp\left(-\frac{Zr}{2a_0}\right) \sin\theta \exp(\pm i\phi)$$

For Harmonic Oscillator: (in 1 Dimension)

Ground state wf: $\psi_0 = \left(\dfrac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(\dfrac{-m\omega x^2}{2\hbar}\right)$

Energy levels: $E_n = \left(n+\frac{1}{2}\right)\hbar\omega$

For 1-D infinite square well: (sides at $x = \pm a/2$)

$$\psi = \sqrt{\frac{2}{a}}\cos\frac{n\pi x}{a}, \quad n = 1,3,5,\ldots$$

$$\text{or } \psi = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}, \quad n = 2,4,6,\ldots$$

Energy levels: $E_n = \dfrac{\hbar^2\pi^2 n^2}{2ma^2}$

Operators for angular momentum:

$$
\begin{aligned}
\hat{L}_x &= y\hat{\mathrm{p}}_x - z\hat{\mathrm{p}}_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\\
\hat{L}_y &= z\hat{\mathrm{p}}_x - x\hat{\mathrm{p}}_z = -i\hbar\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\\
\hat{L}_z &= x\hat{\mathrm{p}}_y - y\hat{\mathrm{p}}_x = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\\
\hat{L}^2 &= -\hbar^2\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\}
\end{aligned}
$$

Some useful integrals: (taken from the Bedside Book of Integrals)

$$\int_0^\infty e^{-\alpha x}\,dx = \frac{1}{\alpha} \qquad \int_0^\infty xe^{-\alpha x}\,dx = \frac{1}{\alpha^2} \qquad \int_0^\infty x^2e^{-\alpha x}\,dx = \frac{2}{\alpha^3}$$

$$\int_{-\infty}^\infty e^{-\lambda x^2}\,dx = \sqrt{\frac{\pi}{\lambda}} \qquad \int_{-\infty}^\infty x^2e^{-\lambda x^2}\,dx = \frac{1}{2\lambda}\sqrt{\frac{\pi}{\lambda}}$$

$$\int_{-\infty}^\infty x^4e^{-\lambda x^2}\,dx = \frac{3}{4\lambda^2}\sqrt{\frac{\pi}{\lambda}}$$

$$\int x^n\sin kx\,dx = -x^n\frac{\cos kx}{k} + n\int x^{(n-1)}\frac{\cos kx}{k}\,dx$$

$$\int x^n\cos kx\,dx = x^n\frac{\sin kx}{k} - n\int x^{(n-1)}\frac{\sin kx}{k}\,dx$$

$$\int_0^\infty x^ne^{-x}\,dx = n!$$

Question 1

(a) Show that $\psi(r,\theta,\phi) = f(r)(3\cos^2\theta - 1)$ is an eigenstate of $\hat{L}^2$ and find its eigenvalue.

(b) Evaluate the commutators $\left[\hat{p}_x, \hat{L}_y\right]$ and $\left[\hat{x}, \hat{L}_y\right]$.

Question 2

A particle in a p-state is represented by the wavefunction $\psi = 4\,Y_1^1 \;+\; 3\,Y_1^{-1}$

where Y_ℓ^m are the (normalised) spherical harmonics for quantum numbers ℓ and m.

(a) Normalise ψ.

(b) What is the probability that a measurement of L_z will give the value $+\hbar$?

(c) What is the expectation value of L_z ?

(d) What is the expectation value of L_z^2 ?

(e) What is the expectation value of L^2 ?

(f) What are the possible values of a measurement of L_x ?

Question 3

The Hamiltonian of a one-dimensional simple harmonic oscillator is modified by the addition of terms in x^3 and x^4, so that the Schroedinger equation becomes:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \tfrac{1}{2}m\omega^2 x^2\psi + \alpha x^3\psi + \beta x^4\psi = E\psi \quad \text{where } \alpha \text{ and } \beta \text{ are small}$$

Find the first-order change in the energy of the ground state of this oscillator:
(a) due to the term in x^3
(b) due to the term in x^4.

Question 4

The electron in a hydrogen-like atom is in the 2s state. It is subjected to a small perturbation $\delta V(r) = \lambda r\cos^2\theta$, where λ is a constant. Find the first-order change in energy of this state.
