University of Bath Department of Physics

Year 3
PH30030 – Quantum Mechanics

Friday, 26th January 2018, 09:30 to 11:30

Answer ALL questions

The only calculators that may be used are those supplied by the University.

Please fill in your name and sign the section on the right of your answer book, peel away adhesive strip and seal.

Take care to enter the correct candidate number as detailed on your desk label.

CANDIDATES MUST NOT TURN OVER THE PAGE AND READ THE EXAMINATION PAPER UNTIL THE CHIEF INVIGILATOR GIVES PERMISSION TO DO SO. 1. The wave function of a particle in a one-dimensional infinite potential well of width a is given by

$$\psi(x,t=0) = \frac{1}{\sqrt{2}}\phi_1(x) + c_2\phi_2(x) + c_3\phi_3(x),$$

where ϕ_1 , ϕ_2 and ϕ_3 are the orthonormal eigenfunctions of the total energy operator, \widehat{H} , corresponding to eigenvalues $E_1 = \frac{\hbar^2 \pi^2}{2ma^2}$, $E_2 = 4 \frac{\hbar^2 \pi^2}{2ma^2}$, $E_3 = 9 \frac{\hbar^2 \pi^2}{2ma^2}$, respectively.

- (a) It has been determined experimentally that the probability of obtaining the energy E_2 is $P(E_2) = \frac{1}{4}$. Determine the coefficients c_2 and c_3 (assume that the phases of these coefficients are zero).
- (b) Calculate the expectation value $\langle \widehat{H} \rangle$. (3)
- (c) What is the form of the wave function $\psi(x,t)$ at a later time t? (2)
- 2. (a) Using the expressions from classical mechanics, derive the operators describing the Cartesian components \hat{L}_x , \hat{L}_y and \hat{L}_z , of the orbital angular momentum. (3)
 - (b) With the help of the relation $[\hat{z}, \hat{p}_z] = i\hbar$, find the commutation relation for \hat{L}_x and \hat{L}_y . (4)
 - (c) Briefly discuss the consequences of this commutation relation for measuring the xand y- components of the orbital angular momentum of a particle. (1)

3. An operator \hat{A} has normalised eigenfunctions ϕ_1 and ϕ_2 with corresponding distinct eigenvalues α_1 and α_2 . A second operator \hat{B} has two normalised eigenfunctions χ_1 and χ_2 with corresponding distinct eigenvalues β_1 and β_2 . The eigenfunctions of the two operators are related by

$$\phi_1 = \sqrt{\frac{1}{10}} (3\chi_1 + \chi_2),$$

$$\phi_2 = \sqrt{\frac{1}{10}} \, (\chi_1 - 3\chi_2).$$

- (a) Given that χ_1 and χ_2 are normalised and orthogonal to each other, show that both ϕ_1 and ϕ_2 are also normalised and orthogonal to each other. (4)
- (b) A particle is prepared in a state

$$\psi = \frac{\sqrt{3}}{2}\phi_1 + \frac{1}{2}\phi_2.$$

Two measurements are then performed: first, of the observable associated with the operator \hat{A} and after that of the observable associated with the operator \hat{B} . What is the probability of obtaining β_1 in the second measurement? (4)

- 4. Consider a particle with spin s = 1.
 - (a) What are the possible outcomes of a measurement of

i. the z-component of spin;
$$(1)$$

ii. the
$$y$$
-component of spin? (1)

(b) The matrix form of the x-component of spin s = 1 operator is

$$\hat{I}_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

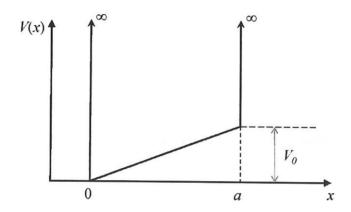
Find the normalised eigenvector corresponding to the eigenvalue $-\hbar$ of the x-component of spin. (2)

(c) The spin-part of the wave function of a particle with spin s=1 is described by the state

$$|\sigma\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\ -i\\ 0 \end{pmatrix}.$$

What is the probability of measuring $-\hbar$ in a measurement of the x-component of spin? (2)

5. A particle of mass m is confined in a one-dimensional infinite square well of width a, where its normalised eigenfunctions are given by $\phi_{0n}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ and the corresponding eigenvalues are given by $E_{0n} = n^2 \frac{\pi^2 \hbar^2}{2ma^2}$. Employ first order perturbation theory to estimate the ground state energy if the infinite square well is perturbed by the potential $V(x) = V_0 \frac{x}{a}$ for 0 < x < a, as shown in the figure. (5)



Note:
$$\int_{0}^{a} dx \, x \sin^{2} \left(\frac{m \, \pi x}{a} \right) = \frac{a^{2}}{4}$$

6. (a) An electron in an unperturbed system described by the Hamiltonian \hat{H}_0 has two orthonormal degenerate states $|\phi_{01}\rangle$ and $|\phi_{02}\rangle$ of energy E_0 . A perturbation \hat{H}' is applied to the system, and solutions to the Schrödinger equation $(\hat{H}_0 + \hat{H}')|\phi\rangle = E|\phi\rangle \text{ in the form } |\phi\rangle = a_1|\phi_{01}\rangle + a_2|\phi_{02}\rangle \text{ are searched for, where } a_1$ and a_2 are constants. Show that the governing equation can be written as

$$\begin{pmatrix} (E_0 + \hat{H}'_{11}) - E & H'_{12} \\ H'_{21} & (E_0 + \hat{H}'_{22}) - E \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = 0$$

where
$$\hat{H}'_{\alpha\beta} = \langle \phi_{0\alpha} | \hat{H}' | \phi_{0\beta} \rangle$$
. (8)

(b) Assume that the degenerate states are given by the eigenstates of the spin operator $\hat{S}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \text{ i.e., } |\phi_{01}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |\phi_{02}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \text{ If a magnetic field } \underline{B} = \begin{pmatrix} 0, 0, B \end{pmatrix}$ is applied to the system, a perturbation of the form

$$\hat{H}' = \frac{e}{mc} \underline{B} \cdot \underline{\hat{S}}$$

is applied where e is the elementary charge, m is electron mass, c is the speed of light, and $\underline{\hat{S}}$ is the spin operator with Cartesian components $\underline{\hat{S}} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$.

- (i) Write an expression for the perturbation in terms of a suitable 2×2 matrix.
 - (1)
- (ii) Hence, evaluate the matrix elements \hat{H}'_{11} , \hat{H}'_{12} , \hat{H}'_{21} and \hat{H}'_{22} . (3)
- (iii) Use the governing equation to find the energy levels of each of the perturbed states. Comment on the effect of the magnetic field. (4)

7. During the performance of a spectroscopic experiment, a hydrogen atom is perturbed by the application of a time dependent electric field. Transitions between initial states i and final states f are observed with a probability $W \propto \left|H'_{fi}\right|^2$ where the quantum numbers $m_i = m_f = 0$ such that $H'_{fi} \propto \int\limits_0^\pi d\theta \sin\theta \cos\theta \ Y_{\ell_f 0}^{**}(\theta) Y_{\ell_i 0}(\theta)$. Three of the spherical

harmonics for m=0 are given by $Y_{00}=\sqrt{\frac{1}{4\pi}}$, $Y_{10}=\sqrt{\frac{3}{4\pi}}\cos\theta$ and

$$Y_{20} = \sqrt{\frac{5}{16\pi}} \left(3\cos^2 \theta - 1 \right).$$

- (a) Find the transition probability for the cases when:
 - (i) $\ell_i = 0$, $\ell_f = 0$
 - (ii) $\ell_i = 1$, $\ell_f = 0$
 - (iii) $\ell_i = 1$, $\ell_f = 1$
 - (iv) $\ell_i = 1$, $\ell_f = 2$

(5)

(3)

- (b) On the basis of these results, deduce the selection rule. (1)
- (c) How will these transitions manifest themselves in a spectroscopic experiment?

Note: $\int dx \sin(ax) \cos^m(ax) = -\frac{1}{(m+1)a} \cos^{m+1}(ax)$

(MMK/PSS)

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FUNDAMENTAL CONSTANTS

Note: Numerical values have been rounded to four significant figures.

Quantity	Symbol	<u>Value</u>	<u>Unit</u>	Dimensions
Atomic mass unit	u	1.661×10^{-27}	kg	M
Avogadro constant	N_A	6.022×10^{23}	mol ⁻¹	
Bohr magneton (e \hbar /2m _e)	μ_{B}	9.274 × 10 ⁻²⁴	$ m JT^{-1}$	I L ²
Bohr radius $(4\pi \hbar^2/\mu_o c^2 e^2 m_e)$	a_{o}	5.292 × 10 ⁻¹¹	m	L
Boltzmann constant	k	1.381×10^{-23}	J K ⁻¹	$ML^2T^{-2}\theta^{-1}$
Charge of electron (magnitude)	e	1.602×10^{-19}	C	ΙΤ
Charge (magnitude)/rest mass ratio (electron)	e/m _e	1.759×10^{11}	C kg ⁻¹	I M ⁻¹ T
Fine–structure constant ($\mu_0 ce^2/2h$)	α	7.292×10^{-3}		
	$1/\alpha$	137.0		
Gravitational constant	G	6.672×10^{-11}	Nm ² kg ⁻²	M ⁻¹ L ³ T ⁻²
Mass ratio, m_p/m_e	m_p/m_e	1836		
Molar gas constant	R	8.314	J mol ⁻¹ K ⁻¹	$ML^2T^{-2}\theta^{-1}$
Molar volume (ideal gas, STP)	$V_{\rm m}$	2.241×10^{-2}	m^3	L^3
Permeability of vacuum	μ_{o}	$4\pi \times 10^{-7}$	Hm ⁻¹	I ⁻² MLT ⁻²
Permittivity of vacuum $(1/\mu_o c^2)$	$\epsilon_{ ext{o}}$	8.854×10^{-12}	Fm ⁻¹	$I^2M^{-1}L^{-3}T^4$
	$4\pi\epsilon_o$	1.113×10^{-10}	Fm ⁻¹	$I^2M^{-1}L^{-3}T^4$
Planck constant	h ħ	6.626×10^{-34} 1.055×10^{-34}	Js Js	$\mathrm{ML}^{2}\mathrm{T}^{-1}$ $\mathrm{ML}^{2}\mathrm{T}^{-1}$
Rest mass of electron	m_e	9.110×10^{-31}	kg	M
Rest mass of proton	m_p	1.673×10^{-27}	kg	M
Speed of light in vacuum	c	2.998×10^{8}	ms ⁻¹	LT ⁻¹
Stefan-Boltzmann constant $(2\pi^5k^4/15h^3c^2)$	σ	5.670×10^{-8}	Wm ⁻² K ⁻⁴	$MT^{-3}\theta^{-4}$