

210 Quantum Mechanics Test

In the following *show all your working*

1. Determine if the following functions are eigenfunctions of the p_x operator. If yes, identify the eigenvalue, if no, explain why not. **Show your working.**

(b) x^3

(c) e^{ikx}

5 marks

$\Omega f = \omega f$ Ω = operator ω = eigenvalue f = eigenfunction $\Omega = p_x = \frac{-i}{h} \frac{d}{dx}$	$f = x^3$ evaluate: $\frac{h}{i} \frac{d}{dx} x^3 = \omega x^3$ $\frac{d}{dx} x^3 = 3x^2$ $\frac{h}{i} \frac{d}{dx} x^3 = \frac{h}{i} 3x^2$ $\frac{3h}{i} x^2 \neq \omega x^3$	$f = e^{ikx}$ evaluate: $\frac{h}{i} \frac{d}{dx} e^{ikx} = \omega e^{ikx}$ $\frac{d}{dx} e^{ikx} = ike^{ikx}$ $\frac{h}{i} \frac{d}{dx} e^{ikx} = \frac{h}{i} ike^{ikx}$ $hke^{ikx} = \omega e^{ikx}$ where $\omega = hk$
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definition (1 mark)

maths (1 mark each)

x^3 is not an eigenfunction because the eigenvalue equation does not hold, the *function* is different on the LHS and RHS of the equation (1 mark)

e^{ikx} is an eigenvector because the equation does hold with an eigenvalue of hk . (1 mark)

This question is of a familiar format presented in lectures and problems.

2. **Discuss** the function below, **define** each of the variables, **identify** the named functions and quantum numbers, **describe** the functional components and **explain** their origins/relevance.

$$Y_2^{-2}(\theta, \phi) = \frac{1}{4} \sqrt{\frac{15}{2\pi}} \sin^2\theta e^{-i2\phi}$$

10 marks

Associated Legendre function gives 3p orbital forms and l (1 mark)

particle on a ring solution gives m_l (1 mark)

normalisation factor (1 mark)

spherical harmonic (1 mark)

polar coords

here $l=2$ and $m_l=-2$

m_l = magnetic QN (1 mark)

l = angular QN

1 mark for components given until 10 marks is reached

θ and ϕ are the spherical polar variables/coordinates (1 mark)

$Y_l^{m_l}(\theta, \phi)$ is a spherical harmonic (1 mark)

and gives rise to the angular nature of AOs (1 mark)

1 angular quantum number and $l=2$ (1 mark)

the $l=2$ is for a dAO (1 mark)

m_l magnetic quantum number and $m_l=-2$ (1 mark)

the coefficients in the front are the *normalisation* (1 mark)

normalisation provides the "magnitude", and ensures only 2e occupy each orbital, and that orbitals are comparable (1 marks)

$\sin^2\theta$ is an associated Legendre function (gives 1 QN) (1 mark)

θ gives the 3D angular shape of the orbitals (1 mark)

$e^{-i2\phi}$ is the solution for a particle on a ring ϕ (gives the m_l QN) (1 mark)

ϕ gives the imaginary part of the wavefunction, and or is the decay feature (1 mark)

The form of this question was a direct "copy" of a problem given in the L7 problems, but not this particular wavefunction.

3. For "particle in a box" wavefunction given below

$$\psi(x) = N \sin\left(\frac{nx\pi}{L}\right) \text{ with } n = 1, 2, \dots$$

(a) **derive** an expression for the $n=3$ normalisation coefficient, **show your working**.

(b) **evaluate** N for the $n=3$ level for a box of length $L=2\text{nm}$, **show your working**

(c) **sketch** the $n=3$ level probability curve on a diagram of the box.

10 marks

normalisation requires $\int_{limits} \psi^* \psi d\tau = 1$ particle in a box $n=3$ level $\psi = N \sin\left(\frac{3\pi x}{L}\right)$ $\tau \rightarrow x$ $\psi = \text{real so } \psi^* \psi = \psi^2$ limits are between 0 and L $\int_{limits} \psi^* \psi d\tau \rightarrow \int_0^L N^2 \sin^2\left(\frac{3\pi x}{L}\right) dx$ evaluate $\int_0^L N^2 \sin^2\left(\frac{3\pi x}{L}\right) dx$ we know $\int \sin^2(2ax) dx = \frac{1}{2}x - \frac{1}{4a} \sin(2ax)$ where $2a = \frac{3\pi}{L}$ $\int_0^L N^2 \sin^2\left(\frac{3\pi x}{L}\right) dx = N^2 \left[\frac{1}{2}x - \frac{L}{6\pi} \sin\left(\frac{3\pi x}{L}\right) \right]_0^L$ $\left[\frac{1}{2}x - \frac{L}{6\pi} \sin\left(\frac{3\pi x}{L}\right) \right]_0^L = \left[\frac{1}{2}L - \frac{L}{6\pi} \sin\left(\frac{3\pi L}{L}\right) \right] - \left[\frac{1}{2}0 - \frac{L}{6\pi} \sin\left(\frac{3\pi 0}{L}\right) \right]$ $= \left[\frac{1}{2}L - \frac{L}{6\pi} \sin(3\pi) \right] - \left[0 - \frac{L}{6\pi} \sin(0) \right]$ but $\sin(3\pi) = \sin(0) = 0$ $= \left[\frac{1}{2}L - 0 \right] - [0 - 0]$ $= \frac{1}{2}L$ evaluate $\int_0^L N^2 \sin^2\left(\frac{3\pi x}{L}\right) dx = 1$ $N^2 \frac{1}{2}L = 1$ $N = \sqrt{\frac{2}{L}}$	general expression (1 mark) express the integral (1 mark) evaluate A (1 mark) evaluate B (1 mark) evaluate C (1 mark) final expression (1 mark) 6 marks total
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evaluating for $L=2\text{nm}$

(2 marks)

$$\begin{aligned} N &= \sqrt{\frac{2}{L}} \\ \text{for } L &= 2\text{nm} \\ &= \sqrt{\frac{2}{20 \times 10^{-10}}} \\ &= \left(\frac{2}{2 \times 10^{-10}} \right)^{\frac{1}{2}} \\ &= \left(\frac{2}{2} \right)^{\frac{1}{2}} \left(\frac{1}{10^{-10}} \right)^{\frac{1}{2}} \\ \text{where } \left(\frac{1}{10^{-10}} \right)^{\frac{1}{2}} &= (10^{10})^{\frac{1}{2}} = 10^{\frac{10}{2}} = 10^5 \\ &= \sqrt{1} \times 10^5 \end{aligned}$$

express the probability on a infinite square well, three humps, all values positive

(2 marks)

The students have been given the evaluation of the general N as a class problem. Here we have asked for a particular n . This is a very small stretch from the notes. Evaluating the N for a specific length is new, drawing the energy diagram was part of the assignment.