NOTE:

1. No clarifications or corrections will be provided during the exam.
2. If you think there is an error/inconsistency/omission in the paper, please state your assumptions about it.

Useful Information: $h = 6.626 \times 10^{-34}\,\mathrm{J\,s}$; $c = 3.0 \times 10^{8}\,\mathrm{m\,s^{-1}}$; $m_e = 9.109 \times 10^{-31}\,\mathrm{kg}$

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

1. A particle moving on the x-axis has a probability of $\frac{1}{5}$ for being in the interval $(-d-a, -d+a$ and $\frac{4}{5}$ for being in the interval $(d-a, d+a)$, where $d \gg a$.
   (a) Call the normalized wavefunction for the "left" interval $\phi_-(x)$ and that of the "right" interval $\phi_+(x)$. What is the normalized wavefunction $\phi(x)$ for the particle? [1]
   (b) With $d \gg a$, what is the probaility density $P(x)$ for the particle? What does the integral over all x of $P(x)$ give? [1]

2. A quantum dot relevant to semiconductor devices, may be modeled as an electron in a spherical well:

$$V(r) = \begin{cases} 0 & \text{for } 0 \le r \le a \\ \infty & \text{otherwise} \end{cases}$$

   (a) Write the Schrödinger equation for an electron in such a well. [1]
   (b) If the wavefunctions are written in the form $R_{nl}(r)Y_{lm}(\theta,\phi)$, what is the differential equation satisfied by $R_{nl}(r)$? Use $k = \sqrt{\frac{2mE}{\hbar^2}}$. [2]
   (c) Two solutions of the differential equation satisfied by $R_{nl}(r)$ are

$$R_1 = -\frac{\cos kr}{kr}$$

$$R_2 = \frac{\sin kr}{(kr)^2} - \frac{\cos kr}{kr}$$

   Which of these is an acceptable quantum mechanical wavefunction? Why? [1]
   (d) Is the acceptable wavefunction in part (c) the ground state or an excited state? Does it possess angular momentum? Give justifications. [2]
   (e) The energies of a particle in a sphere are

$$E_{nl} = z_{nl}^2\frac{\hbar^2}{2ma^2},$$

   where z_{nl} are the zeroes of $R_{nl}(r)$. Obtain the radius, a, of the spherical well if the frequency of light emitted when an electron goes from the first excited to the ground state is 10×10^{9} Hz. The z_{nl} of the ground and first excited states are π and 4.493 respectively. The effective mass of the electron is $m = 0.067m_e$. [2]
   (f) At what distance is an electron most likely to be found, if its normalized wavefunction is $\psi = \sqrt{\frac{\pi}{2a^3}}\frac{\sin\left(\frac{\pi r}{a}\right)}{\left(\frac{\pi r}{a}\right)}$? [2]

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Answer: (a)

$$\phi(x) = \frac{1}{\sqrt{5}}\phi_-(x) + \frac{2}{\sqrt{5}}\phi_+(x) \qquad [1]$$

(a) No marks if square root is missing. (b) No marks if ϕ_- and ϕ_+ are switched.

(b)

$$P(x) = \frac{1}{5}\phi_-^2(x) + \frac{4}{5}\phi_+^2(x), \qquad [0.5]$$

where it is assumed that $\int_\infty^\infty \phi_-(x)^* \phi_+(x) dx = 0$.

$$\int_{-\infty}^{\infty} P(x)dx = \frac{1}{5}\int_{-\infty}^{\infty} \phi_-(x)^2 dx + \frac{4}{5}\int_{-\infty}^{\infty} \phi_+(x)^2 dx = \frac{1}{5} + \frac{4}{5} = 1$$

Particle will be found somewhere on the x-axis because $P(x) = 1$. Alternatively, the particle has $frac15$ probability of being found between $(-d-a, -d+a$ and $\frac{4}{5}$ for being in the interval $(d-a, d+a)$ [0.5]

2. A quantum dot relevant to semiconductor devices, may be modeled as an electron in a spherical well:

$$V(r) = \begin{cases} 0 & \text{for } 0 \leq r \leq a \\ \infty & \text{otherwise} \end{cases}$$

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Answer: (a)

$$\hat{\mathcal{H}} = \begin{cases} -\frac{\hbar^2}{2m}\nabla^2 & \text{for } 0 \le r \le a \\ -\frac{\hbar^2}{2m}\nabla^2 + \infty & \text{otherwise} \end{cases}$$

For $0 \le r \le a$

$$\left(-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\right)\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

For $a < r \le \infty$

$$\left(-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] + \infty\right)\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

Only the Schrödinger equation for $0 \le r \le a$ needs to be provided.

(b) Note that the angular wavefunction is identical to that in the hydrogen atom for which we know that $\hat{L}^2 Y_{lm} = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)Y_{lm} = l(l+1)\hbar^2 Y_{lm}$. The differential equation satisfied by $R_{nl}(r)$ may thus be written by analogy.

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial R_{nl}(r)}{\partial r}\right] + \frac{l(l+1)\hbar^2}{2mr^2}R_{nl}(r) = ER_{nl}(r) \qquad [1]$$

or

$$-\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial R_{nl}(r)}{\partial r} + \frac{l(l+1)}{r^2}R_{nl}(r) - \frac{2mE}{\hbar^2}R_{nl}(r) = 0$$

or

$$\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial R_{nl}(r)}{\partial r} - \frac{l(l+1)}{r^2}R_{nl}(r) + \frac{2mE}{\hbar^2}R_{nl}(r) = 0$$

or

$$-\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial R_{nl}(r)}{\partial r} + \frac{l(l+1)}{r^2}R_{nl}(r) - k^2R_{nl}(r) = 0$$

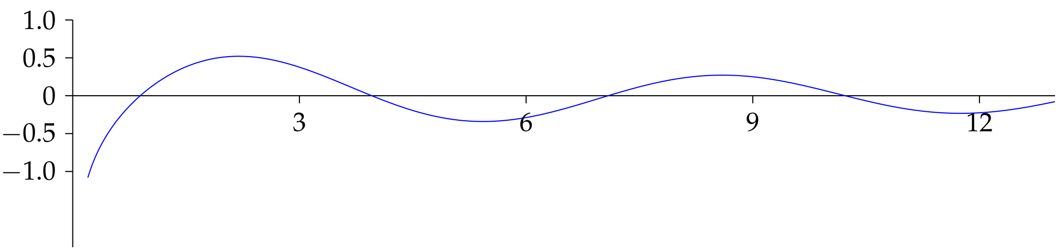
or

$$\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial R_{nl}(r)}{\partial r} - \frac{l(l+1)}{r^2}R_{nl}(r) + k^2R_{nl}(r) = 0$$

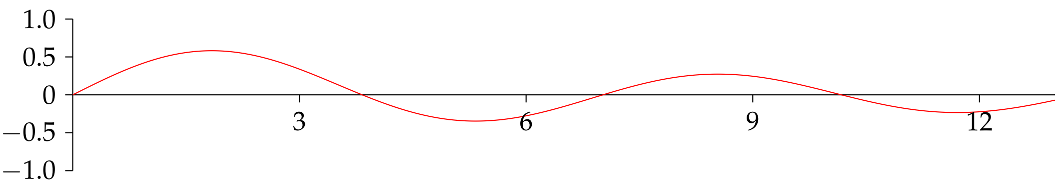
or

$$\frac{d^2R_{nl}(r)}{dr^2} + \frac{2}{r}\frac{dR_{nl}(r)}{dr} + \left(k^2 - \frac{l(l+1)}{r^2}\right)R_{nl}(r) = 0$$

(c) Quantum mechanically acceptable solution is R_2 - the function and its first derivative are finite, single-valued, and continuous. On the other hand, R_1 diverges at $r = 0$. Alternatively, they could arrive at the same conclusion from a sketch of R_1 and R_2. The function R_1 looks like:



The function R_2 has the following appearance:



(d) EXCITED STATE - function has nodes (ground state has no nodes) [1]
NON-ZERO ANGULAR MOMENTUM - function is zero at $r = 0$, which is true for states with $l \neq 0$ [1].

(e)

$$\Delta E = h\nu = \frac{\hbar^2}{2ma^2}\left((4.493)^2 - (3.1415)^2\right) \qquad [0.5]$$

$$\nu = \frac{h \times 10.3180}{8 \times \pi^2 \times 0.067 \times m_e \times a^2} \qquad [0.5]$$

$$a = \sqrt{\frac{10.3180 \times 6.626 \times 10^{-34}\,\mathrm{J\,s}}{8 \times (3.1415)^2 \times 0.067 \times 9.109 \times 10^{-31}\,\mathrm{kg} \times 1.0 \times 10^{10}\,\mathrm{Hz}}} = 376\,\mathrm{nm} \qquad [1]$$

(f) The r at which the radial probability distribution, r^2R^2, is maximum, i. e. the r at which $\frac{d}{dr}r^2R^2 = 0$. [0.5]
For the given ψ, $r^2R^2 = c\sin^2\left(\frac{\pi r}{a}\right)$, where c is a constant. This function reaches its maximum when the argument of sin, $\pi r/a$, is $\pi/2$. In other words, the electron is most likely to be found at $r = a/2$. [1.5]
Alternatively,

$$\frac{d}{dr}c\sin^2\left(\frac{\pi r}{a}\right) = c\frac{\pi}{a}2\sin\left(\frac{\pi r}{a}\right)\cos\left(\frac{\pi r}{a}\right) = 0$$

$$\implies \sin\left(\frac{2\pi r}{a}\right) = 0$$

$$\implies \frac{2\pi r}{a} = \pi \qquad \text{or} \qquad r = \frac{a}{2}$$