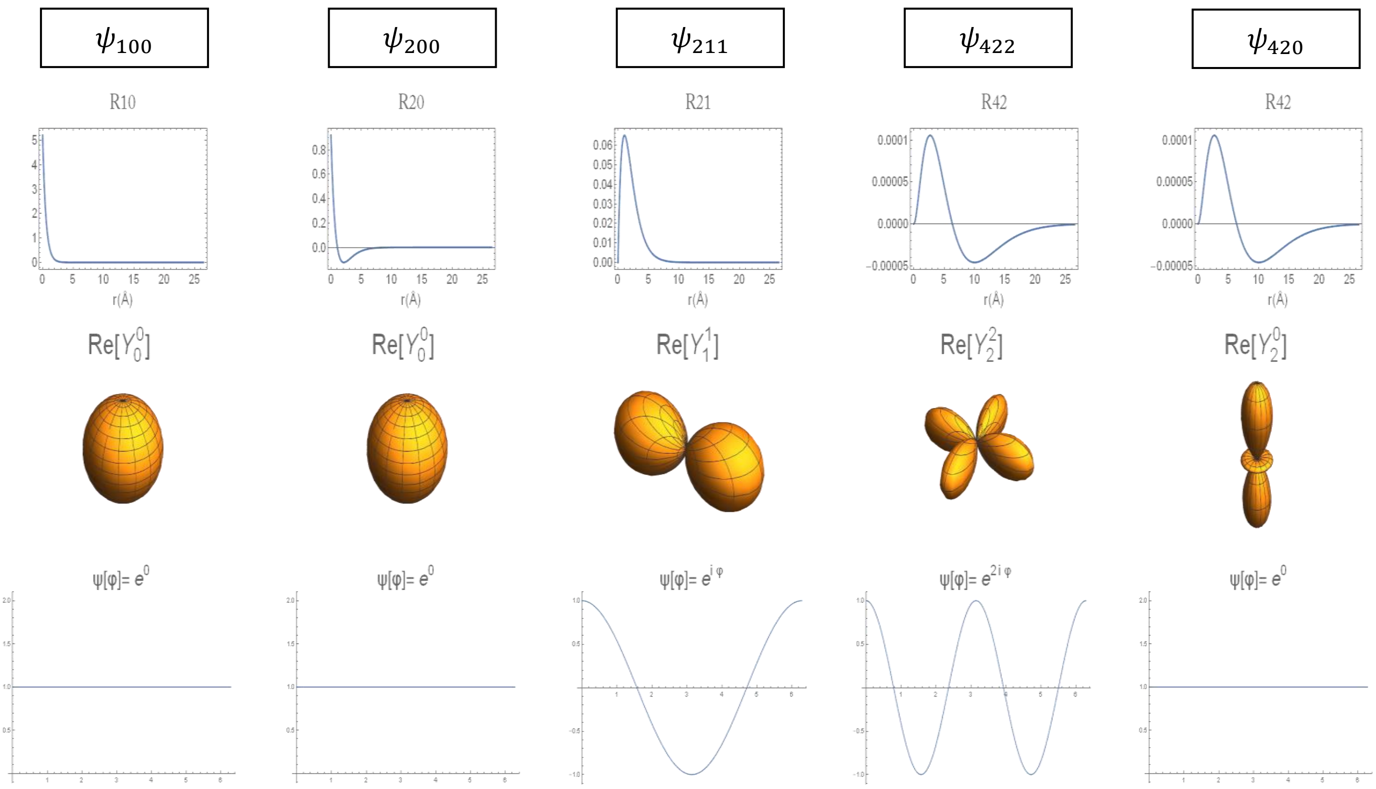
Πανεπιστήμιο Κρήτης,
Τμήμα Φυσικής

Κβαντομηχανική Ι

5ο Σετ Ασκήσεων

Άσκηση 1



Άσκηση 2

Ζητά :

μέση τιμή της πιθανότητας της ακτινικής κατανομής ≡προσδοκώμενη τιμή της ακτινικής κατανομής

⇒ μέση τιμή της πιθανότητας της ακτινικής κατανομής ≡μέση τιμή της απόστασης r

⇒ μέση τιμή της πιθανότητας της ακτινικής κατανομής ≡ $\langle r\rangle = \dfrac{4\pi \int_0^\infty r\, r^2\, |R(r)|^2 dr}{4\pi \int_0^\infty r^2\, |R(r)|^2 dr} = \int_0^\infty r\, r^2\, |R(r)|^2 dr$

Διδάσκων:Πέτρος Ρακιτζής
Βοηθός: Αλέξανδρος Σπηλιώτης

Όπου κανονικοποιούμε, ώστε το αποτέλεσμά μας να είναι μια ακτίνα (το ολοκλήρωμα στον παρονομαστή είναι πάντα ίσο με 1)

a) $\langle r\rangle_{1s} = \int_0^\infty r\, r^2\, |R_{10}|^2 dr$
$$= \int_0^\infty r^3 \left(2a_o^{-\frac{3}{2}}\right)^2 e^{-\frac{2r}{a}}\, dr$$
$$= 4a_o^{-3} \int_0^\infty r^3 e^{-\frac{2r}{a_o}}\, dr$$
$$= 4a_o^{-3} \left[-\frac{1}{8} a_o\, e^{-\frac{2r}{a_o}} (3a_o^3 + 6a_o^2 r + 6a_o r^2 + 4r^3)\right]\Big|_0^\infty$$
$$= 0 - \frac{1}{2} {a_o}^{-3} (-a_o 3a_o^3)$$
$$= \frac{3a_o}{2}$$

b) $\langle r\rangle_{2s} = \int_0^\infty r\, r^2\, |R_{20}|^2 dr$
$$= \int_0^\infty r^3 \left(\frac{1}{\sqrt{2}} {a_o}^{-\frac{3}{2}}\right)^2 \left(1 - \frac{1}{2}\frac{r}{a_o}\right)^2 e^{-\frac{2r}{2a_o}}\, dr$$
$$= \frac{1}{2} {a_o}^{-3} \int_0^\infty r^3 \left(1 - \frac{r}{a_o} + \frac{1}{4}\frac{r^2}{{a_o}^2}\right) e^{-\frac{r}{a_o}}\, dr$$
$$= \frac{1}{2} {a_o}^{-3} \left(\int_0^\infty r^3 e^{-\frac{r}{a_o}}\, dr - \int_0^\infty \frac{r^4}{a} e^{-\frac{r}{a_o}}\, dr + \int_0^\infty \frac{1}{4}\frac{r^5}{{a_o}^2} e^{-\frac{r}{a_o}}\, dr \right)$$
$$= \frac{1}{2} {a_o}^{-3} (6 - 24 + 30) {a_o}^4$$
$$= 6a_o$$

c) $\langle r\rangle_{2p} = \int_0^\infty r\, r^2\, |R_{21}|^2 dr$
$$= \int_0^\infty r^3 \left(\frac{1}{\sqrt{24}} {a_o}^{-\frac{3}{2}}\right)^2 \left(\frac{r}{a}\right)^2 e^{-\frac{2r}{2a_o}}\, dr$$
$$= \frac{1}{24} {a_o}^{-3} \int_0^\infty r^3 \frac{r^2}{a^2} e^{-\frac{r}{a_o}}\, dr$$
$$= \frac{1}{24} {a_o}^{-5} \int_0^\infty r^5 e^{-\frac{r}{a_o}}\, dr$$
$$= \frac{1}{24} {a_o}^{-5} 120 {a_o}^6$$
$$= 5a_o$$

d) $\langle r\rangle_{3s} = \int_0^\infty r\, r^2\, |R_{30}|^2 dr$
$$= \int_0^\infty r^3 \left(\frac{2}{\sqrt{27}} {a_o}^{-\frac{3}{2}}\right)^2 \left(1 - \frac{2}{3}\frac{r}{a_o} + \frac{2}{27}\left(\frac{r}{a_o}\right)^2\right)^2 e^{-\frac{2r}{3a_o}}\, dr$$
$$= \frac{16}{108} {a_o}^{-3} \left(\int_0^\infty r^3 e^{-\frac{2r}{3a_o}}\, dr - \int_0^\infty \frac{4r^4}{3a_o} e^{-\frac{2r}{3a_o}}\, dr + \int_0^\infty \frac{16}{27}\frac{r^5}{{a_o}^2} e^{-\frac{2r}{3a}}\, dr - \int_0^\infty \frac{8}{81}\frac{r^6}{{a_o}^3} e^{-\frac{2r}{3a_o}}\, dr \right.$$
$$\left. + \int_0^\infty \frac{4}{729}\frac{r^7}{{a_o}^4} e^{-\frac{2r}{3a}}\, dr \right)$$

$$= \frac{16}{108} {a_o}^{-3} {a_o}^{4} \left(\frac{243}{8} - 243 + 810 - 1215 + \frac{2835}{4}\right)$$
$$= \frac{16}{108} a_o \frac{729}{8}$$
$$= 13.5 a_o$$

e) $\langle r \rangle_{3d} = \int_0^\infty r\, r^2\, |R_{32}|^2 dr$

$$= \int_0^\infty r^3 \left(\frac{4}{81\sqrt{30}} {a_o}^{-\frac{3}{2}}\right)^2 \left[\left(\frac{r}{a_o}\right)^2\right]^2 \quad e^{-\frac{2r}{3a_o}} dr$$
$$= \frac{16}{30\, 81^2} {a_o}^{-3} \int_0^\infty r^3 \frac{r^4}{{a_o}^4} e^{-\frac{2r}{3a_o}} dr$$
$$= \frac{16}{30\, 81^2} {a_o}^{-7} \int_0^\infty r^7 e^{-\frac{2r}{3a_o}} dr$$
$$= \frac{16}{30\, 81^2} {a_o}^{-7} 129170 {a_o}^8$$
$$= 10.5 a_o$$

Άσκηση 3

$$x = r\sin(\theta)\cos(\varphi), \qquad y = r\sin(\theta)\sin(\varphi), \qquad z = r\cos(\theta)$$

$$r = \sqrt{x^2 + y^2 + z^2}, \qquad \theta = \arccos\left(\frac{z}{r}\right), \qquad \varphi = \mathrm{arc}tan\left(\frac{y}{x}\right)$$

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$$

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial u}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial u}{\partial \varphi}\frac{\partial \varphi}{\partial x}$$

$$\frac{\partial u}{\partial y} = \frac{\partial u}{\partial r}\frac{\partial r}{\partial y} + \frac{\partial u}{\partial \theta}\frac{\partial \theta}{\partial y} + \frac{\partial u}{\partial \varphi}\frac{\partial \varphi}{\partial y}$$

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial r}\frac{\partial r}{\partial z} + \frac{\partial u}{\partial \theta}\frac{\partial \theta}{\partial z} + \frac{\partial u}{\partial \varphi}\frac{\partial \varphi}{\partial z}$$

$$\frac{\partial r}{\partial x} = sin(\theta)cos(\varphi), \qquad \frac{\partial \theta}{\partial x} = \frac{1}{r}cos(\theta)cos(\varphi), \qquad \frac{\partial \varphi}{\partial x} = -\frac{1}{r}sin(\varphi)\, sin(\theta),$$

$$\frac{\partial r}{\partial y} = sin(\theta)sin(\varphi), \qquad \frac{\partial \theta}{\partial y} = \frac{1}{r}cos(\theta)sin(\varphi), \qquad \frac{\partial \varphi}{\partial y} = \frac{1}{r}cos(\varphi)\, sin(\theta),$$

$$\frac{\partial r}{\partial z} = cos(\theta), \qquad \frac{\partial \theta}{\partial z} = -\frac{1}{r}sin(\theta), \qquad \frac{\partial \varphi}{\partial z} = 0$$

$$\frac{\partial u}{\partial x} = \sin(\theta)\cos(\varphi)\frac{\partial u}{\partial r} + \frac{1}{r}\cos(\theta)\cos(\varphi)\frac{\partial u}{\partial \theta} - \frac{1}{r}\sin(\varphi)\,\sin(\theta)\frac{\partial u}{\partial \varphi}$$

Άρα

$$\frac{\partial^2 u}{\partial x^2} = \sin(\theta)\cos(\varphi)\frac{\partial}{\partial r}\frac{\partial u}{\partial x} + \frac{1}{r}\cos(\theta)\cos(\varphi)\frac{\partial}{\partial \theta}\frac{\partial u}{\partial \theta} - \frac{1}{r}\sin(\varphi)\,\sin(\theta)\frac{\partial}{\partial \varphi}\frac{\partial u}{\partial \varphi}$$

$$\frac{\partial^2 u}{\partial x^2} = (\dots\frac{\partial^2 u}{\partial r^2} + \cdots\frac{\partial u}{\partial \theta} + \cdots + \frac{\partial^2 u}{\partial r \partial \theta} + \cdots + \cdots + \cdots + \cdots\frac{\partial^2 u}{\partial \varphi^2})$$

$$\frac{\partial^2 u}{\partial y^2} = (\dots\frac{\partial^2 u}{\partial r^2} + \cdots\frac{\partial u}{\partial \theta} + \cdots + \frac{\partial^2 u}{\partial r \partial \theta} + \cdots + \cdots + \cdots + \cdots\frac{\partial^2 u}{\partial \varphi^2})$$

$$\frac{\partial^2 u}{\partial z^2} = (\dots\frac{\partial^2 u}{\partial r^2} + \cdots\frac{\partial u}{\partial \theta} + \cdots + \frac{\partial^2 u}{\partial r \partial \theta} + \cdots + \cdots + \cdots + \cdots\frac{\partial^2 u}{\partial \varphi^2})$$

…Και με κάποιες «τετριμμένες» πράξεις, καταλήγουμε στο:

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial u}{\partial r}) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}(\sin\theta\frac{\partial u}{\partial \theta}) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 u}{\partial \varphi}$$

Η αναλυτική λύση βρίσκεται [εδώ]