Quiz #2 Solutions

(1) The radial probability density for the 1s state is

$$P(r) = r^2 |R_{10}(r)|^2 = \frac{4}{a_0^3} r^2 e^{-2r/a_0}$$

(a) The maximum of $P(r)$ occurs when $\frac{\partial P}{\partial r} = 0$

$$\frac{\partial P}{\partial r} = 0 = \left(\frac{4}{a_0^3}\right)\left[2re^{-2r/a_0} - \frac{2r^2}{a_0} e^{-2r/a_0}\right]$$

$$= \left(\frac{4}{a_0^3}\right) 2re^{-2r/a_0}\left[1 - \frac{r}{a_0}\right]$$

$$\Rightarrow \left(1 - \frac{r}{a_0}\right) = 0 \quad \Rightarrow r = a_0 \quad \text{at the maximum}$$

(b) $$P(r) = r^2 |R_{20}|^2 = \frac{1}{(2a_0)^3} r^2 \left(2 - \frac{r}{a_0}\right)^2 e^{-r/a_0}$$

$$\frac{\partial P}{\partial r} = 0 = \frac{1}{(2a_0)^3}\left[2r\left(2-\frac{r}{a_0}\right)^2 e^{-r/a_0} + 2r^2\left(2-\frac{r}{a_0}\right)\left(\frac{-1}{a_0}\right)e^{-r/a_0} - \left(\frac{1}{a_0}\right) r^2 \left(2-\frac{r}{a_0}\right)^2 e^{-r/a_0}\right]$$

$$= \frac{1}{(2a_0)^3} r\left(2 - r/a_0\right) e^{-r/a_0}\left[2\left(2-\frac{r}{a_0}\right) + 2r\left(\frac{-1}{a_0}\right) - \left(\frac{1}{a_0}\right) r \left(2 - r/a_0\right)\right]$$

$$= \frac{1}{(2a_0)^3} r\left(2-\frac{r}{a_0}\right)\left[4 - \frac{2r}{a_0} - \frac{2r}{a_0} - \frac{2r}{a_0} + \frac{r^2}{a_0^2}\right]$$

$$0 = \frac{1}{(2a_0)^3} r\left(2 - r/a_0\right)\left[\frac{r^2}{a_0^2} - \frac{6r}{a_0} + 4\right] = \frac{1}{(2a_0)^3}\frac{1}{a_0^2} r\left(2-r/a_0\right)\left[r^2 - 6a_0 r + 4a_0^2\right]$$

the maximum cannot occur when $r(2-r/a_0) = 0$ since at these points $R_{20} \sim r(2-r/a_0)e^{-r/a_0} = 0$. Thus, the maximum must occur when

($r = 0$, $r = 2a_0$) give minima

$$r^2 - 6a_0 r + 4a_0^2 = 0$$

$$\Rightarrow r = \frac{6a_0 \pm \sqrt{(6a_0)^2 - 4(4a_0^2)}}{2}$$

$$= \frac{3a_0 \pm \sqrt{20\, a_0^2}}{2} = 3a_0 \pm a_0\sqrt{5}$$

$$= (3 \pm \sqrt{5})\, a_0 = (5.236\, a_0 \text{ and } 1.586\, a_0)$$

two maxima

(2) Recall that the expectation value of a function $f(x)$ in one-dimensions is

$$\langle f(x)\rangle = \int_{-\infty}^{\infty} f(x)\,|\Psi(x)|^2\,dx$$

In 3-dimensions, we integrate over all space

$$\langle f(r,\theta,\phi)\rangle = \int_{\text{all space}} f(r,\theta,\phi)\,|\Psi(r,\theta,\phi)|^2\,dV$$

Thus, the expectation value of $\frac{1}{r}$ is (for the 1s state)

(a)
$$\left\langle \frac{1}{r}\right\rangle = \int_{\text{all space}} \left(\frac{1}{r}\right)\left|\frac{1}{\sqrt{\pi a_0^3}}\,e^{-r/a_0}\right|^2 dV$$

$$= \int_{r=0}^{\infty}\left(\frac{1}{r}\right)\left(\frac{1}{\pi a_0^3}\right)e^{-2r/a_0}\,r^2\,dr \int_{\theta=0}^{\pi}\sin\theta\,d\theta \int_{\phi=0}^{2\pi} d\phi$$

Note that: $\int_0^{2\pi} d\phi = \phi\Big]_0^{2\pi} = 2\pi - 0 = 2\pi$

$$\int_0^{\pi}\sin\theta\,d\theta = -\cos\theta\Big]_0^{\pi} = -\left(\cos\pi - \cos(0)\right) = -(-1-1) = 2$$

The integral over angles then gives a factor $(2)(2\pi) = 4\pi$

and

$$\left\langle \frac{1}{r}\right\rangle = \frac{(4\pi)}{\pi a_0^3}\int_0^{\infty} r\,e^{-2r/a_0}\,dr$$

$$= \left(\frac{4}{a_0^3}\right)\left[\frac{1!}{(2/a_0)^2}\right] = \left(\frac{4}{a_0^3}\right)\left(\frac{a_0^2}{4}\right) = \frac{1}{a_0}$$

(b) Since $U = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$

then $\langle U\rangle = \left\langle -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}\right\rangle = -\frac{e^2}{4\pi\epsilon_0}\left\langle\frac{1}{r}\right\rangle = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{a_0}$

since $\left\langle \frac{1}{r}\right\rangle = \frac{1}{a_0}$

(c) Given that $\langle E \rangle = \langle K \rangle + \langle U \rangle$

Then $\langle K \rangle = \langle E \rangle - \langle U \rangle$

For the 1s state: $E = E_1 = -\dfrac{\hbar^2}{2ma_0^2}$

The expectation value of a constant is simply the constant since Ψ_{100} is normalized:

$$\langle E \rangle = \int_{\text{all space}} E_1 |\Psi_{100}|^2 \, dV$$

$$= E_1 \int |\Psi_{100}|^2 \, dV \qquad (\text{since } E_1 = \text{constant})$$

$$= E_1 \qquad (\text{since } \Psi_{100} \text{ is normalized})$$

Then $\langle K \rangle = \dfrac{-\hbar^2}{2ma_0^2} - \left(-\dfrac{1}{4\pi\epsilon_0} \dfrac{e^2}{a_0} \right)$

$$= \frac{-\hbar^2}{2ma_0\left(4\pi\epsilon_0 \frac{\hbar^2}{me^2}\right)} + \frac{1}{4\pi\epsilon_0}\frac{e^2}{a_0} \qquad \left(\text{since } a_0 = 4\pi\epsilon_0 \frac{\hbar^2}{me^2} \right)$$

$$= -\frac{1}{4\pi\epsilon_0}\frac{e^2}{2a_0} + \frac{1}{4\pi\epsilon_0}\frac{e^2}{a_0}$$

$$= \frac{1}{4\pi\epsilon_0}\frac{e^2}{2a_0} = \frac{\hbar^2}{2ma_0^2}$$

3 (a) Schrodinger Equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}Cx^2\psi = E\psi$$

For $\psi(x) = Ae^{-bx^2}$

$$\frac{d\psi}{dx} = -2bx \cdot Ae^{-bx^2}$$

$$\frac{d^2\psi}{dx^2} = -2bAe^{-bx^2} + 4b^2x^2Ae^{-bx^2}$$

Plugging into the Schrodinger Eq. gives

$$-\frac{\hbar^2}{2m}\left[-2b + 4b^2x^2\right]\cancel{Ae^{-bx^2}} + \frac{1}{2}Cx^2\left(\cancel{Ae^{-bx^2}}\right) = E\left(\cancel{Ae^{-bx^2}}\right)$$

$$\underbrace{\left(\frac{1}{2}C - \frac{4b^2\hbar^2}{2m}\right)x^2}_{Bx^2} + \underbrace{\left(\frac{2b\hbar^2}{2m} - E\right)}_{D} = 0$$

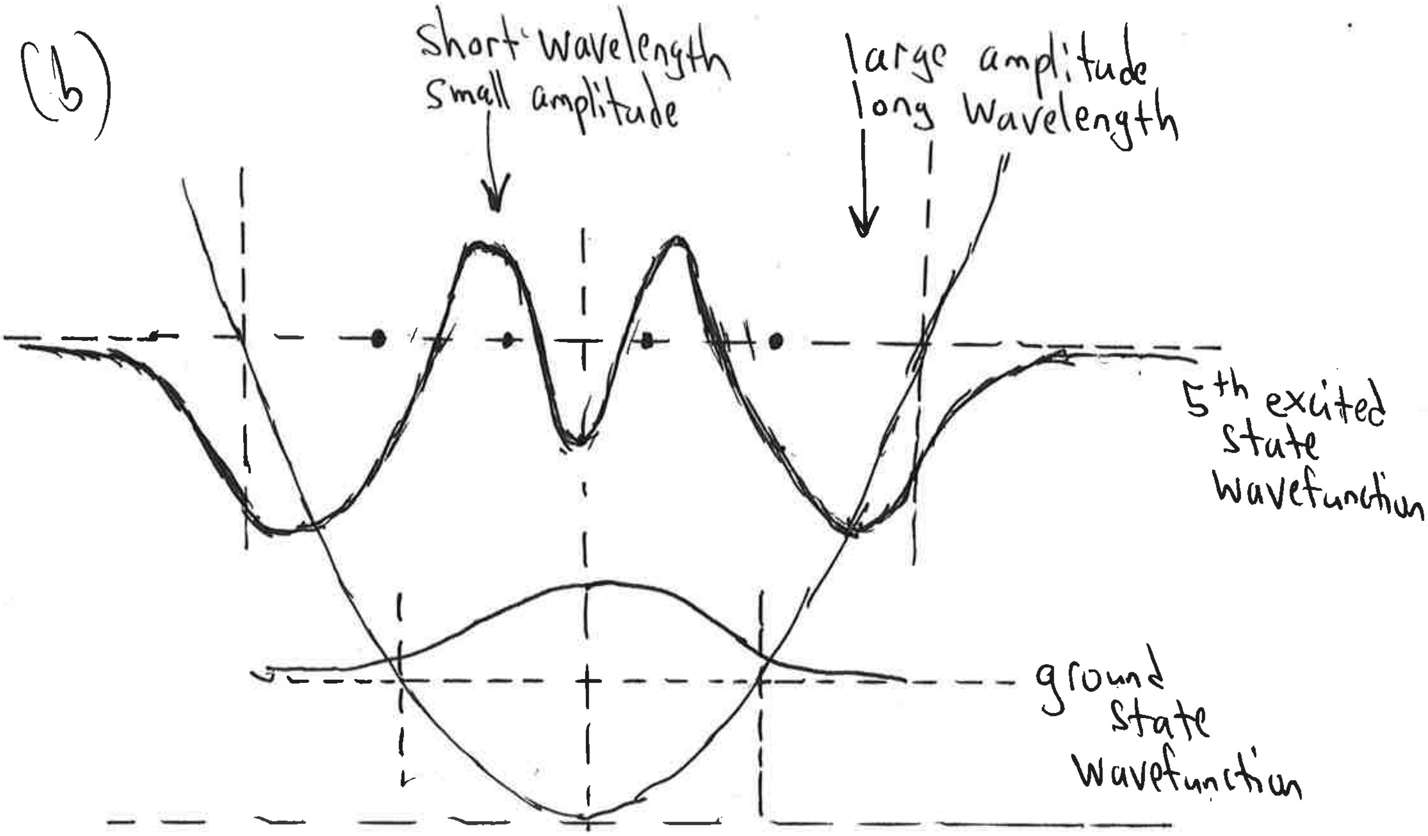
For $D = 0$: $\frac{2b\hbar^2}{2m} - E = 0 \Rightarrow E = \frac{b}{m}\hbar^2$

For $B = 0$: $\frac{1}{2}C - \frac{4b^2\hbar^2}{2m} = 0 \Rightarrow \boxed{b = \frac{\sqrt{Cm}}{2\hbar}}$

Then; $\boxed{E = \frac{\hbar^2}{m}\left(\frac{\sqrt{Cm}}{2\hbar}\right) = \frac{1}{2}\hbar\sqrt{\frac{C}{m}}} = \frac{1}{2}\hbar\omega_0$

where ω_0 = resonance frequency

(b)


Short wavelength
Small amplitude
large amplitude
long wavelength
5th excited state wavefunction
ground state wavefunction