

Thus 10 May 07
week 6

QM6b - Finish Ch 12.6 *12.6.1, 12.6.2

Ch 13 ^{2,3,4}¹H Atom *13.1.1, 13.1.3, 13.3.3

- 4.1 Exercise 12.6.1.* A particle is described by the wave function

$$\psi_E(r, \theta, \phi) = Ae^{-r/a_0} \quad (a_0 = \text{const})$$

- (i) What is the angular momentum content of the state?
- (ii) Assuming ψ_E is an eigenstate in a potential that vanishes as $r \rightarrow \infty$, find E . (Match leading terms in Schrödinger's equation.) $E = -\hbar^2/2\mu a_0^2$
- (iii) Having found E , consider finite r and find $V(r)$.

$$V = \frac{e^2}{\mu a_0 r}$$

(a) This wave function does not depend on θ or ϕ . The only Y_l^m that doesn't is $Y_0^0 = \sqrt{\frac{1}{4\pi}}$, so $l=0$ and $m=0$.
 $L^2|\Psi_E\rangle = l(l+1)|\Psi_E\rangle = 0 \quad |\Psi_E\rangle ; \quad l=0$

(b) This radial wave function must satisfy the radial Sch. eqn for some spherically symmetric potential $V(r)$:

$$(12.6.3) \quad \left\{ -\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} \right] + V(r) \right\} R_{E,l} = E R_{E,l}$$

$$\text{We know } l=0: \quad \left\{ -\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \right] + V(r) \right\} \Psi_E = E \Psi_E$$

$$\text{Do the } \frac{\partial}{\partial r} \text{ parts: } \frac{\partial}{\partial r} \Psi_E = \frac{\partial}{\partial r} A e^{-r/a_0} = -\frac{A}{a_0} e^{-r/a_0}$$

$$\frac{\partial}{\partial r} \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \Psi_E \right] = -\frac{A}{a_0} \frac{\partial}{\partial r} \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 e^{-r/a_0} \right] = -\frac{A}{a_0} e^{-r/a_0} \left[-\frac{\hbar^2}{a_0^2} + 2r \right]$$

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

(12.6.1...) So Sch. Egu. becomes (sub m & simplify)

$$\frac{-t^2}{2\mu} \frac{Ae^{-\frac{r}{a_0}}}{a_0} \left[\frac{2}{r} - \frac{1}{a_0} \right] + V(r) Ae^{-\frac{r}{a_0}} = EAe^{-\frac{r}{a_0}}$$

$$\frac{-t^2}{2\mu} \frac{1}{a_0} \left(\frac{2}{r} - \frac{1}{a_0} \right) = E - V /$$

Let's look at the limits for infinite and finite r:

$$\lim_{r \rightarrow \infty} : \frac{-t^2}{2\mu} \frac{1}{a_0} \left(\frac{1}{a_0} \right) = E - V(r \rightarrow \infty) = E \xrightarrow[t^2]{a_0^2}$$

Looks like an oscillator?

Sch. equ. also has to work for finite r, and that will tell us $V(r)$. Use the E we just found:

$$V = E + \frac{-t^2}{2\mu} \frac{1}{a_0} \left(\frac{2}{r} - \frac{1}{a_0} \right)$$

$$= \frac{-t^2}{2\mu a_0^2} \left(\frac{-t^2}{2\mu a_0} + \frac{t^2}{\mu a_0 r} \right)$$

$$V(r) = \frac{-t^2}{\mu a_0 r} /$$

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Shankar

#12.6.2 - Derive (12.6.5) from (12.6.3)

$$(12.6.3) \quad \frac{1}{2\mu} \left\{ -\frac{\hbar^2}{r^2} \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} \right] + V(r) \right\} R_{el} = ER_{el}$$

Substitute for the radial wavefunction $R_{el} = \frac{U_{el}}{r}$, or $R = \frac{U}{r}$

$$\frac{\partial R}{\partial r} = \frac{2}{\partial r} \left(\frac{U}{r} \right) = \frac{1}{r} \frac{\partial U}{\partial r} - \frac{U}{r^2}$$

$$r^2 \frac{\partial R}{\partial r} = \frac{r^2}{r} \frac{\partial U}{\partial r} - \frac{r^2}{r^2} U = r \frac{\partial U}{\partial r} - U$$

$$\frac{2}{\partial r} r^2 \frac{\partial R}{\partial r} = \frac{2}{\partial r} \left(r \frac{\partial U}{\partial r} - U \right) = \frac{\partial U}{\partial r} + r \frac{\partial^2 U}{\partial r^2} - \frac{\partial U}{\partial r} = r \frac{\partial^2 U}{\partial r^2}$$

$$ER = E \frac{U}{r} = \left\{ -\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} \right] + V(r) \right\} \frac{U}{r}$$

$$E \frac{U}{r} = \left\{ -\frac{\hbar^2}{2\mu} \frac{1}{r} \frac{\partial^2 U}{\partial r^2} + \frac{\hbar^2}{2\mu} \frac{l(l+1)U}{r^2} + V(r) \frac{U}{r} \right\}$$

Multiply both sides by $-2\mu/\hbar^2$ to get

$$-\frac{-2\mu r}{\hbar^2} E \frac{U}{r} = -\frac{2\mu}{\hbar^2} EU = \frac{\partial^2 U}{\partial r^2} - \frac{l(l+1)}{r^2} U - \frac{2\mu}{\hbar^2} V(r) U$$

$$0 = \frac{\partial^2 U_{el}}{\partial r^2} + \frac{2\mu}{\hbar^2} \left[E - V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2} \right] U_{el}$$

$$\left\{ \frac{\partial^2}{\partial r^2} + \frac{2\mu}{\hbar^2} \left[E - V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2} \right] \right\} U_{el} = 0 / (12.6.5)$$