Physics 492
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Lecture 5: Radial Equation

$$\langle \vec{r} | E, \ell, m \rangle = R_{E,\ell}(r) Y_{\ell m}(\theta, \phi)$$

$$R = U(r)/r$$

$$\left[\frac{-\hbar^2}{2\mu} \frac{d^2}{dr^2} + \underbrace{\boxed{\frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + V(r)}}_{V_{eff}(r)} \right] U_{E,\ell} = E_\ell U_{E,\ell}$$

where $0 < r < \infty$

$$\langle E \ell m | E \ell m \rangle = 1 = \int_0^\infty r^2 dr\, R^* R = \int_0^\infty U^* U \, dr$$

Wave function at $r=0$

For potential like Coulomb

$$V(r) \underset{r \to 0}{\sim} \frac{1}{r} \qquad \left(\alpha = e^2/\hbar c \right)$$

$$V_{eff}(r) \underset{r \to 0}{\sim} \frac{1}{r^2}$$

then "near" $r = 0$, $\quad r \ll \frac{\hbar c}{\alpha (2\mu c^2)}$ for Coulomb

$$\approx 0.27 \text{ Å}$$

$$\frac{-\hbar^2}{2\mu} \frac{d^2}{dr^2} U + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} U = E U$$

from which we find:

$$\boxed{u(r) \underset{r\to 0}{\sim} r^{l+1}}$$

$$R(r) \underset{r\to 0}{\sim} r^{l}$$

Only $l=0$ states have non-zero $\psi(0)$.

Example:

positronium is a hydrogen like bound state of e^+, e^-. When e^+ meets e^-,

$$e^+ e^- \to \gamma\gamma$$

Positronium must cascade down (emitting photons) to $l=0$ state to annihilate.

Annihilation rate of positronium Γ,

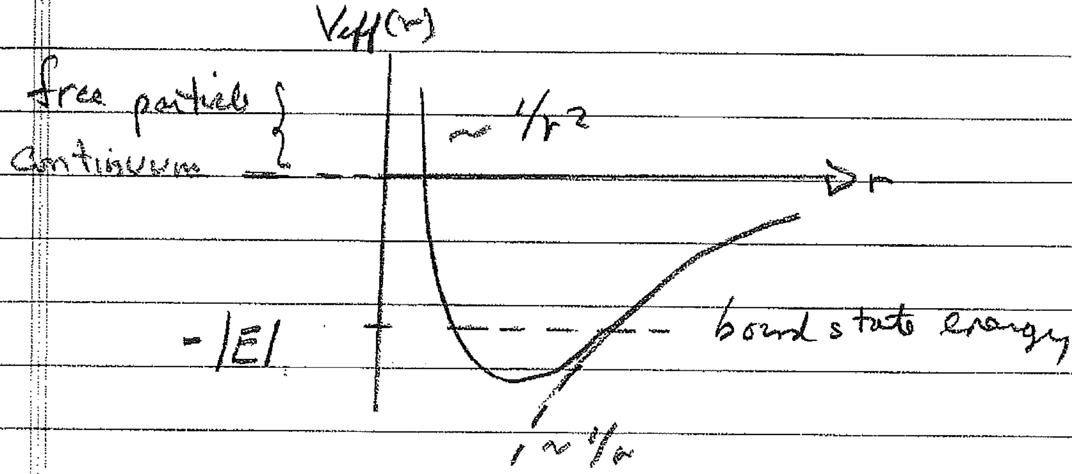
$$\Gamma \propto |\psi(0)|^2$$

Coulomb Potential

$$V(r) = \frac{-e^2}{r} = -\frac{\hbar c \alpha}{r}$$

$\alpha^{-1} = 137.036$ fine structure constant

$\mu c^2 \approx m_e c^2 = 0.511$ MeV electron mass



define dimensionless variable

$$\rho \equiv \sqrt{\frac{8\mu|E|}{\hbar^2}}\, r$$

dimensionless coupling

$$\lambda = \frac{e^2}{\hbar c}\sqrt{\frac{\mu c^2}{2|E|}} = \alpha\sqrt{\frac{\mu c^2}{2|E|}}$$

and let $\frac{du}{d\rho} \equiv u'$

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}u + \frac{l(l+1)\hbar^2}{2\mu r^2}u - \frac{e^2}{r}u = Eu$$

becomes

$$u'' - \frac{l(l+1)}{\rho^2}u + \left(\frac{\lambda}{\rho} - \frac{1}{4}\right)u = 0$$

Asymptotic behavior as $\rho \to \infty$.

$$u_\infty'' - \frac{1}{4}u_\infty = 0$$

$$u \underset{\rho\to\infty}{\sim} e^{-\rho/2}$$

Thus,

$$u(\rho) = \rho^{l+1} e^{-\rho/2} F(\rho)$$

Find equation for F which is solved by a power series solution.

$$F'' + \left(\frac{2l+2}{\rho} - 1\right)F' + \left(\frac{\lambda}{\rho} - \frac{l+1}{\rho}\right)F = 0$$

$$F(\rho) = \sum_{k=0}^{\infty} c_k \rho^k$$

Solution requires series to terminate giving

$$\lambda = 1 + l + n_r, \quad n_r = 0, 1, 2$$

quantized energies

Since n_r, l are integers define principal quantum number n by

$$n \equiv l + 1 + n_r \quad , n = 1, 2, 3, \ldots$$

see page 6a

$$E_n = -\frac{1}{n^2} \frac{\mu c^2 (Z\alpha)^2}{2} = \frac{-13.6\,eV}{n^2}$$

nucleus with charge Ze

Radial wave functions

Bohr radius $a_0 = \dfrac{\hbar}{\mu c \alpha} = 0.529\,\text{Å} = 0.0529\,\text{nm}$

$$R_{1,0} = 2 \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$$

$$R_{2,0} = 2 \left(\frac{Z}{2a_0}\right)^{3/2} \left(1 - \frac{Zr}{2a_0}\right) e^{-Zr/2a_0}$$

$$R_{2,1} = \frac{1}{\sqrt{3}} \left(\frac{Z}{2a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0}$$

Note: can be written in terms of

"associated Laguerre polynomials"

if you want to write all of them down.

Degeneracy

Energy has no l dependence.

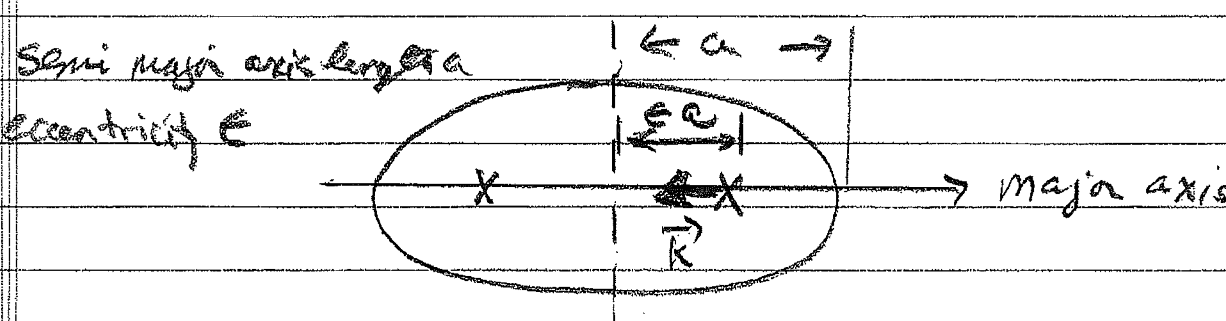
$$\text{degeneracy} \quad d = \sum_{l=0}^{n-1} (2l+1) = n^2$$

where all we expect from spherical symmetry is $2l+1$ degeneracy of states with different m.

n^2 states are basis for chemical "shell" description.

This degeneracy is not accidental, but the result of a dynamical symmetry of the potential.

Classically, $V \propto -\frac{1}{r}$, $V \propto r^2$ are only potentials that have closed orbits.
(GR gives higher order effective r^{-3} term)



Runge - Lenz vector $\vec{K}$.

$$\lambda = \frac{Z\hbar c\alpha}{\hbar}\sqrt{\frac{\mu}{2|E|}} = 1 + n_r + \ell \equiv n$$

$$n^2 = \frac{Z^2\alpha^2\mu c^2}{2|E|}$$

$$\boxed{|E| = \frac{1}{n^2}\left(\frac{1}{2}\right)\left(Z^2\alpha^2\mu c^2\right)}$$

n	ℓ	n_r
1	0	0
2	1	0
	0	1
3	2	0
	1	1
	0	2

etc.

degeneracy and
$\ell < n$

$$\vec{K} = \frac{\vec{r}}{r} + \frac{1}{\mu e^2} \vec{L} \times \vec{p}$$

$$|\vec{K}| = \varepsilon$$

Q.m. $\hat{\vec{K}} = \frac{\hat{\vec{r}}}{r} + \frac{1}{2\mu e^2}\left(\vec{L} \times \vec{p} - \vec{p} \times \vec{L}\right)$

Can be shown that $[\hat{H}, \hat{\vec{K}}] = 0$

Rydberg Formula & Discovery of Deuteron

$$h\nu = \Delta E = \frac{1}{2}\mu c^2 \alpha^2 \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

$D = pn = {}^2_1H$ discovered spectroscopically.

$$\mu = \frac{m_e m_n}{m_e + m_n} = m_e\left(1 + \frac{m_e}{m_N}\right)^{-1} \cong m_e\left(1 - \frac{m_e}{m_n}\right)$$

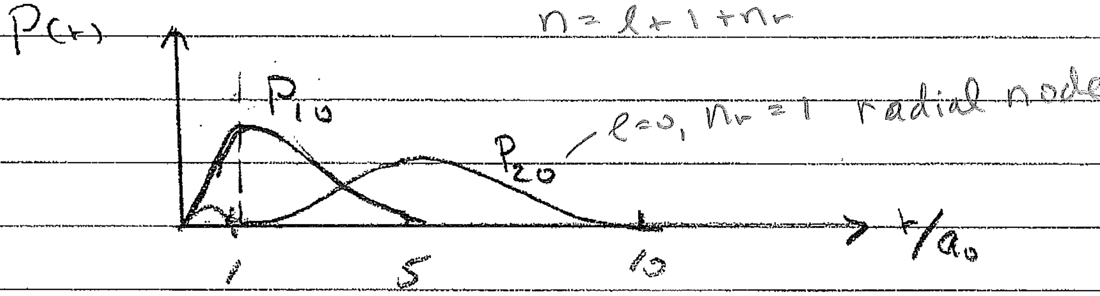
$$m_e/m_n \cong \epsilon = (1800)^{-1}$$

$$\frac{\mu_D}{\mu_H} = \frac{1-\varepsilon}{1-\frac{1}{2}\varepsilon} \approx 1 - \frac{1}{2}\epsilon$$

$$\frac{|\nu_D - \nu_H|}{\nu_H} = \frac{1}{2}\epsilon = 3 \times 10^{-4}$$

Radial Probability Density

$$P_{n\ell}(r) = r^2 |R_{n\ell}|^2$$



P_{10} peaks at $r = a_0$

Higher n values peak at larger r
shell structure

Kramer Relation for $s > -(2\ell+1)$ integer
Griffiths #6.29 (page 253)

$$\boxed{\frac{s+1}{n^2}\langle r^s\rangle - (2s+1)a_0\langle r^{s-1}\rangle + \frac{s}{4}\left((2\ell+1)^2 - s^2\right)a_0^2\langle r^{s-2}\rangle = 0}$$

$s=0$, $\quad \dfrac{\langle r^0\rangle}{n^2} - a_0\left\langle \dfrac{1}{r}\right\rangle = 0$

$$\left\langle \frac{1}{r}\right\rangle = \frac{1}{n^2 a_0}$$

so that $\langle V(r)\rangle = -\alpha\hbar c\left\langle \dfrac{1}{r}\right\rangle = -\dfrac{\alpha\hbar c}{n^2 a_0}$

$$\langle \hat{V} \rangle = -\frac{\alpha^2 \mu c^2}{n^2} = 2\langle \hat{H} \rangle$$

$$\langle K.E. \rangle = \langle \hat{H} \rangle - \langle \hat{V} \rangle = -\frac{1}{2}\langle \hat{V} \rangle$$

This is the an example of the Virial theorem:

$$\left\langle \frac{\vec{p}^2}{2\mu} \right\rangle = \frac{1}{2}\langle \vec{r} \cdot \vec{\nabla} V \rangle$$

or $\langle KE \rangle = -\frac{1}{2}\langle \vec{r} \cdot \vec{F} \rangle$

then for $V(r) = -e^2/r$

$$\vec{r} \cdot \vec{\nabla} V = r \frac{\partial}{\partial r}\left(-\frac{e^2}{r}\right) = r(-e^2)\frac{-1}{r^2} = \frac{e^2}{r} = -V$$

$$\langle KE \rangle = -\frac{1}{2}\langle \hat{V} \rangle \quad \text{as before}$$

$\underline{s=1}$ $$\frac{2}{n^2}\langle r \rangle - 3a_0\langle r^0 \rangle + \frac{1}{4}\left[(2\ell+1)^2 - 1\right]a_0^2 \underbrace{\langle r^{-1} \rangle}_{\frac{1}{n^2}\frac{1}{a_0}} = 0$$

$$\boxed{\langle r \rangle = n^2 a_0 \left[\frac{3}{2} - \frac{\ell(\ell+1)}{2n^2}\right]}$$

$$\langle r \rangle_{10} = \frac{3}{2}a_0$$

$$\langle r \rangle_{n0} = n^2 \langle r \rangle_{10}$$