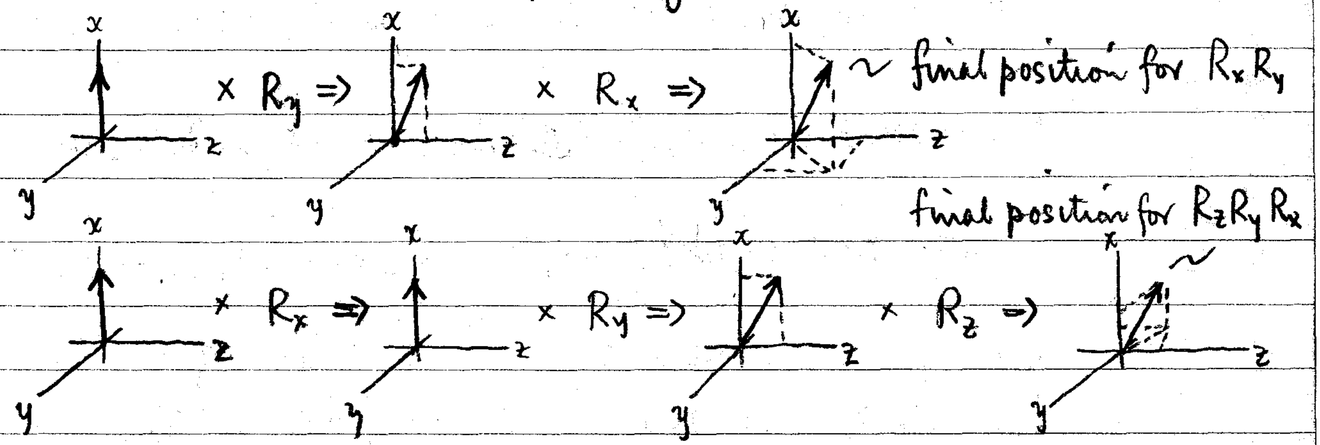
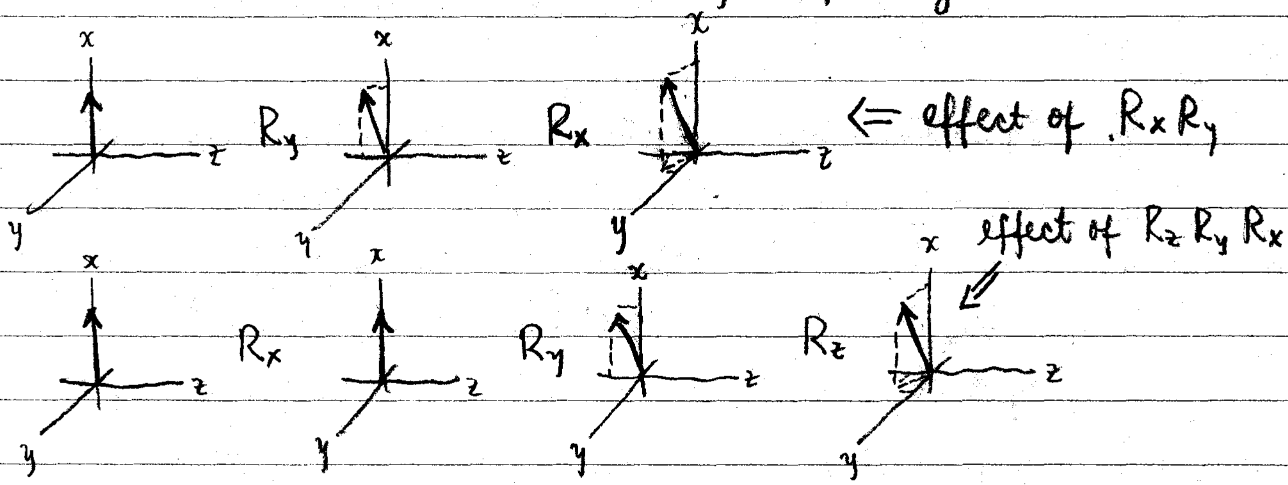
51 We seem to be screwed up but good here. If we leave $\vec{A}$ stationary, and rotate around the cd. axes by the Right-Hand Rule each time, then...

rtn. of cd. sys.



We note the final positions are <u>not</u> the same! On the other hand, if we rotate $\vec{A}$ rather than the cd. system, we get

rtn of vector



In this case, we conclude $R_x R_y = R_z R_y R_x$, which is essential for the proof of $[J_x, J_y] = i J_z$, as we note...

$R_x R_y = R_z R_y R_x$, with $\measuredangle^s$ $\Delta\alpha_x, \Delta\alpha_y, \Delta\alpha_z = \Delta\alpha_x \Delta\alpha_y \Rightarrow$

$$\left(e^{-i\Delta\alpha_x J_x}\right)\left(e^{-i\Delta\alpha_y J_y}\right) = \left(e^{-i\Delta\alpha_x \Delta\alpha_y J_z}\right)\left(e^{-i\Delta\alpha_y J_y}\right)\left(e^{-i\Delta\alpha_x J_x}\right)$$

Expanding these individually to $O(\Delta\alpha^2)$, we get...

$$\left(1 - i\,\Delta\alpha_x J_x - \tfrac{1}{2}\Delta\alpha_x^2 J_x^2\right)\left(1 - i\,\Delta\alpha_y J_y - \tfrac{1}{2}\Delta\alpha_y^2 J_y^2\right) = \qquad (12)$$

$$= \left(1 - i\,\Delta\alpha_x\Delta\alpha_y J_z\right)\left(1 - i\,\Delta\alpha_y J_y - \tfrac{1}{2}\Delta\alpha_y^2 J_y^2\right)\left(1 - i\,\Delta\alpha_x J_x - \tfrac{1}{2}\Delta\alpha_x^2 J_x^2\right)$$

or, $$\cancel{1} - \cancel{i\,\Delta\alpha_y J_y} - \cancel{\tfrac{1}{2}\Delta\alpha_y^2 J_y^2} - \cancel{i\,\Delta\alpha_x J_x} - \Delta\alpha_x\Delta\alpha_y J_x J_y - \cancel{\tfrac{1}{2}\Delta\alpha_x^2 J_x^2} =$$

$$= \cancel{1} - \cancel{i\,\Delta\alpha_x J_x} - \cancel{\tfrac{1}{2}\Delta\alpha_x^2 J_x^2} - \cancel{i\,\Delta\alpha_y J_y} - \Delta\alpha_x\Delta\alpha_y J_y J_x - \cancel{\tfrac{1}{2}\Delta\alpha_y^2 J_y^2} - i\,\Delta\alpha_x\Delta\alpha_y J_z$$

Cancelling the same terms on RHS & LHS gives $[J_x, J_y] = i J_z$. We note that if any one of $\Delta\alpha_x$, $\Delta\alpha_y$ or $\Delta\alpha_z$ were to have its sign changed, this would be equivalent to introducing a $(-)$ sign in front of the component J_x, J_y or J_z to which it belongs. Then the C. Rule would come out backwards, i.e. $[J_y, J_x] = i J_z$.

By rotating the cd. system rather than the vector, we cannot show the essential $R_x R_y = R_z R_y R_x$. Instead, we get $R_x R_y = \bar{R}_z R_y R_x$, where $\bar{R}_z$ denotes rotation by $-\Delta\alpha_z$ rather than $+\Delta\alpha_z$. If this is the case, then we get $[J_y, J_x] = i J_z$, i.e. the wrong C. Rule. By drawing pictures, we can show that for cd. system rotation

$$R_x R_y = \bar{R}_z R_y R_x, \quad R_x \bar{R}_y = R_z \bar{R}_y R_x, \quad \text{or} \quad \bar{R}_x R_y = R_z R_y \bar{R}_x$$

With $R(\vec{\alpha}) = e^{-i\vec{\alpha}\cdot\vec{J}}$, all these relations give $[J_y, J_x] = i J_z$. The proper relation $R_x R_y = R_z R_y R_x$ under C.S. rotation is obtained only if we work in a left-handed cd. system! Shit! Crap! Fuck!

The trouble seems to be that $R(\vec{\alpha}) = e^{-i\vec{\alpha}\cdot\vec{J}}$ does **not** represent rotation of the cd. system w.r.t. a vector $\vec{A}$, but in fact represents rotating the vector itself. This is "confirmed" in Schiff, p. 197.

The trouble is, you dummy, that in the above rtn of cd. sys., you were not rotating about the old axes each time -- but in fact were rotating about new axes. It actually works if you rotate about old axes -- see p. 184a of notes. N

2/28/71 (52) Write $J_x = \frac{1}{2}(J_+ + J_-)$, $J_y = \frac{1}{2i}(J_+ - J_-)$, where $J_\pm = J_x \pm i J_y$ are step up & step down operators, for which (p. 199)

#⑥
$507
(1992)

$$J_+|jm\rangle = \left[(j-m)(j+m+1)\right]^{\frac{1}{2}}|j\,m+1\rangle$$

$$J_-|jm\rangle = \left[(j+m)(j-m+1)\right]^{\frac{1}{2}}|j\,m-1\rangle$$

$$\therefore \langle j'm'|J_x|jm\rangle = \frac{1}{2}\langle j'm'|J_+|jm\rangle + \frac{1}{2}\langle j'm'|J_-|jm\rangle$$

$$= \frac{1}{2}\left[(j-m)(j+m+1)\right]^{\frac{1}{2}}\delta_{j'j}\delta_{m',m+1} + \frac{1}{2}\left[(j+m)(j-m+1)\right]^{\frac{1}{2}}\delta_{j'j}\delta_{m',m-1}$$

i.e. $\langle j\,m+1|J_x|jm\rangle = \frac{1}{2}\left[(j-m)(j+m+1)\right]^{\frac{1}{2}}$

or $\langle j\,m-1|J_x|jm\rangle = \frac{1}{2}\left[(j+m)(j-m+1)\right]^{\frac{1}{2}}$

all other matrix elements of J_x are $\equiv 0$.

Similarly for J_y ...

$$\langle j'm'|J_y|jm\rangle = \frac{1}{2i}\langle j'm'|J_+|jm\rangle - \frac{1}{2i}\langle j'm'|J_-|jm\rangle$$

$$= \frac{1}{2i}\left[(j-m)(j+m+1)\right]^{\frac{1}{2}}\delta_{j'j}\delta_{m',m+1} - \frac{1}{2i}\left[(j+m)(j-m+1)\right]^{\frac{1}{2}}\delta_{j'j}\delta_{m',m-1}$$

i.e. $\langle j\,m+1|J_y|jm\rangle = \frac{1}{2i}\left[(j-m)(j+m+1)\right]^{\frac{1}{2}}$

or $\langle j\,m-1|J_y|jm\rangle = -\frac{1}{2i}\left[(j+m)(j-m+1)\right]^{\frac{1}{2}}$

all other matrix elements of J_y are $\equiv 0$

Selection rules are $\Delta j = 0$, $\Delta m = \pm 1$.

2/28/71 (53) $\vec{\sigma} \times \vec{\sigma} = 2i\vec{\sigma}$. Choose $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. Note σ_x & σ_y Herm.

$\hookrightarrow$ $\sigma_y\sigma_z - \sigma_z\sigma_y = 2i\sigma_x$

$\sigma_z\sigma_x - \sigma_x\sigma_z = 2i\sigma_y$

Choose: $\sigma_x = \begin{pmatrix} a & b \\ b^* & c \end{pmatrix}$, $\sigma_y = \begin{pmatrix} \alpha & \beta \\ \beta^* & \gamma \end{pmatrix}$

Eqts give...

$$\begin{pmatrix}\alpha & \beta\\ \beta^* & \gamma\end{pmatrix}\begin{pmatrix}1&0\\0&-1\end{pmatrix}-\begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}\alpha & \beta\\ \beta^* & \gamma\end{pmatrix}=\begin{pmatrix}\alpha & -\beta\\ \beta^* & -\gamma\end{pmatrix}-\begin{pmatrix}\alpha & \beta\\ -\beta^* & -\gamma\end{pmatrix}=$$

$$=\begin{pmatrix}0 & -2\beta\\ 2\beta^* & 0\end{pmatrix}=2i\begin{pmatrix}a & b\\ b^* & c\end{pmatrix}\Rightarrow \begin{matrix}a=c=0\\ \beta=-ib\end{matrix}$$

$$\begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}0 & b\\ b^* & 0\end{pmatrix}-\begin{pmatrix}0 & b\\ b^* & 0\end{pmatrix}\begin{pmatrix}1&0\\0&-1\end{pmatrix}=\begin{pmatrix}0 & b\\ -b^* & 0\end{pmatrix}-\begin{pmatrix}0 & -b\\ b^* & 0\end{pmatrix}=$$

$$=\begin{pmatrix}0 & 2b\\ -2b^* & 0\end{pmatrix}=2i\begin{pmatrix}\alpha & \beta\\ \beta^* & \gamma\end{pmatrix}\Rightarrow \begin{matrix}\alpha=\gamma=0\\ b=i\beta\end{matrix}$$

Have: $\beta=-ib$ & $b=i\beta \Rightarrow$ no additional info on b

Now use $\sigma_x\sigma_y-\sigma_y\sigma_x=2i\sigma_z$ to give

$$\begin{pmatrix}0 & b\\ b^* & 0\end{pmatrix}\begin{pmatrix}0 & \beta\\ \beta^* & 0\end{pmatrix}-\begin{pmatrix}0 & \beta\\ \beta^* & 0\end{pmatrix}\begin{pmatrix}0 & b\\ b^* & 0\end{pmatrix}=\begin{pmatrix}b\beta^* & 0\\ 0 & b^*\beta\end{pmatrix}-\begin{pmatrix}b^*\beta & 0\\ 0 & b\beta^*\end{pmatrix}=$$

$$=\begin{pmatrix}b\beta^*-b^*\beta & 0\\ 0 & b^*\beta-b\beta^*\end{pmatrix}=2i\begin{pmatrix}1&0\\0&-1\end{pmatrix}\Rightarrow b\beta^*-b^*\beta=2i$$

But $b=i\beta$ & $b\beta^*-b^*\beta=2i \Rightarrow |\beta|^2=1$. Can choose $\beta=-i$, so that $b=+1$. This gives the std repn

$$\sigma_x=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_y=\begin{pmatrix}0&-i\\+i&0\end{pmatrix},\quad \sigma_z=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

P&C, p. 358
Schiff, p. 206
Merz., p. 270

All that is really necessary is that $|\beta|^2=1$ & $b=i\beta$.

Clearly, all $\sigma_k^2=\underline{1}$, so that $\vec{S}^2=\frac{\hbar^2}{4}\sum_k\sigma_k^2=\frac{3}{4}\hbar^2\,\underline{1}$

$$\left[x\frac{d^2}{dx^2}+(b-x)\frac{d}{dx}-a\right]{}_1F_1(a,b;x)\overset{?}{=}0$$

2/22/71 (54) #1 ϕ507 (1992)

a) By directly differentiating the series, we find

$$\frac{dF}{dx}=\sum_{k=1}^{\infty}\frac{(a)_k}{(b)_k}\frac{x^{k-1}}{(k-1)!}=\sum_{k=0}^{\infty}\frac{(a)_{k+1}}{(b)_{k+1}}\frac{x^k}{k!}$$

But $(a)_{k+1}=a(a+1)_k$, trivally. In fact $(a)_{k+n}=a(a+1)\cdots(a+n-1)(a+n)_k$.

$$\therefore \frac{d}{dx}{}_1F_1(a,b;x)=\frac{a}{b}\sum_{k=0}^{\infty}\frac{\overset{a+1}{(a)_k}}{\underset{b+1}{(b)_k}}\frac{x^k}{k!}=\frac{a}{b}{}_1F_1(a+1,b+1;x)$$ A Fundamental Identity

and//
$$\frac{d^2}{dx^2}{}_1F_1(a,b;x)=\frac{a(a+1)}{b(b+1)}{}_1F_1(a+2,b+2;x)$$

Plugging back into the diff eqtn, we have

$$\frac{a(a+1)}{b(b+1)}x\,{}_1F_1(a+2,b+2;x)+(b-x)\frac{a}{b}{}_1F_1(a+1,b+1;x)-a\,{}_1F_1(a,b;x)\overset{?}{=}0$$

or// $$\sum_{k=0}^{\infty}\frac{x^{k+1}}{k!}\left[\frac{(a)_{k+2}}{(b)_{k+2}}-\frac{(a)_{k+1}}{(b)_{k+1}}\right]+a\sum_{k=0}^{\infty}\frac{x^k}{k!}\left[\frac{(a+1)_k}{(b+1)_k}-\frac{(a)_k}{(b)_k}\right]\overset{?}{=}0$$

Here we have used the above rule for $(a)_{k+n}$. Noting that the $k=0$ term of the 2ND sum LHS is $\equiv 0$, we can rewrite it as

$$\frac{a}{k+1}\sum_{k=0}^{\infty}\frac{x^{k+1}}{k!}\left[\frac{(a+1)_{k+1}}{(b+1)_{k+1}}-\frac{(a)_{k+1}}{(b)_{k+1}}\right]$$

But $(a+1)_{k+1}=(a+1)(a+2)_k$. Combining this with the 1ST sum, get

$$\sum_{k=0}^{\infty}\frac{x^{k+1}}{k!}\left\{\frac{(a)_{k+2}}{(b)_{k+2}}\left[1+\frac{b}{k+1}\right]-\frac{(a)_{k+1}}{(b)_{k+1}}\left[1+\frac{a}{k+1}\right]\right\}\overset{?}{=}0$$

The identity is true iff $\{\ \}=0$. This is true in turn iff

$$(b+1+k)\frac{(a)_{k+2}}{(b)_{k+2}}-(a+1+k)\frac{(a)_{k+1}}{(b)_{k+1}}\overset{?}{=}0$$

But $(b+1+k)/(b)_{k+2}=1/(b)_{k+1}$ & $(a+1+k)(a)_{k+1}=(a)_{k+2}$. So

$$(a)_{k+2}/(b)_{k+1}-(a)_{k+2}/(b)_{k+1}\overset{?}{=}0.$$ Yass! QED

b) The k^{th} term in the series for ${}_1F_1(a,b;x)$ is

$$T_k = \frac{\Gamma(b)}{\Gamma(a)}\frac{\Gamma(k+a)}{\Gamma(k+b)}\frac{x^k}{k!} \qquad \left(\text{i.e. } {}_1F_1(a,b;x) = \sum_{k=0}^{\infty} T_k\right)$$

For $x \to +\infty$, the terms with k "large" will predominate. Noting

$$\Gamma(k+a)/\Gamma(k+b) \simeq k^{a-b} \simeq \Gamma(k)/\Gamma(k-(a-b)) = k!/(k-(a-b))!$$

(from NBS Math Handbook, formula 6.1.46, p.257), we have

$$T_k \simeq \frac{\Gamma(b)}{\Gamma(a)} x^k/(k-(a-b))! \quad , \quad \text{for } k \to \text{large}$$

$$\therefore \; {}_1F_1(a,b;x) \underset{x\to+\infty}{\simeq} \frac{\Gamma(b)}{\Gamma(a)} \sum_k \frac{x^k}{(k-(a-b))!} = \frac{\Gamma(b)}{\Gamma(a)} x^{a-b} \underbrace{\left(\sum_m \frac{x^m}{m!}\right)}_{e^x}$$

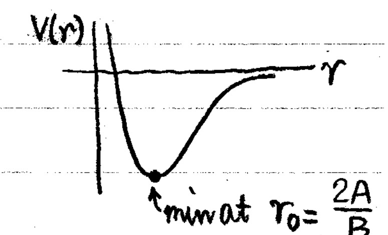
$$\text{i.e. } {}_1F_1(a,b;x) \simeq \frac{\Gamma(b)}{\Gamma(a)} x^{a-b} e^x, \; x \to +\infty \quad \text{QED}$$

For $x \to -\infty$, use Kummer's Transformation to get

$${}_1F_1(a,b;+x) = e^x \, {}_1F_1(b-a,b;-x)$$

$$\text{or } {}_1F_1(a,b;-x) = e^{-x} \, {}_1F_1(b-a,b;+x) \underset{x\to\infty}{\simeq} \frac{\Gamma(b)}{\Gamma(b-a)} x^{-a} \quad \text{QED}$$

2/22/71 **#4** **φ507** **(1992)** (55) This problem is ~ solved in Landau & Lifshitz p.123. Consult PHYS. 506 Lecture (46), 2/22/71. The radial eqtn is



$$\left\{\frac{d^2}{dr^2} + \left[\frac{2mE}{\hbar^2} + \frac{2m}{\hbar^2}\left(\frac{B}{r} - \frac{A}{r^2}\right) - \frac{\ell(\ell+1)}{r^2}\right]\right\} u(r) = 0$$

Define: $\lambda(\lambda+1) = \ell(\ell+1) + \frac{2mA}{\hbar^2} \equiv C$

$$\Rightarrow \lambda = \frac{1}{2}\left[\sqrt{1+4C} - 1\right] = \frac{1}{2}\left[\left((2\ell+1)^2 + \frac{8mA}{\hbar^2}\right)^{\frac{1}{2}} - 1\right]$$

$$\therefore \left\{ \frac{d^2}{dr^2} + \left[\frac{2mE}{\hbar^2} + \frac{2mB}{\hbar^2 r} - \frac{\lambda(\lambda+1)}{r^2} \right] \right\} u(r) = 0$$

This is precisely the same form as H-atom eqtn, except λ replaces l.

Define : $a = \hbar^2/mB$ & $\rho = r/a \Rightarrow r = a\rho = (\hbar^2/mB)\rho$

$$\mathcal{E} = B/a = mB^2/\hbar^2 \; \& \; \epsilon = E/\mathcal{E} \Rightarrow E = \mathcal{E}\epsilon$$

In terms of ρ & ϵ, diff. eqtn becomes...

$$\left\{ \frac{d^2}{d\rho^2} + \left[2\epsilon + \frac{2}{\rho} - \frac{\lambda(\lambda+1)}{\rho^2} \right] \right\} u(\rho) = 0$$

For bound states, let $\kappa^2 = -2\epsilon$. As for H-atom, define

$$u(\rho) = \text{cnst} \times \rho^{\lambda+1} e^{-\kappa\rho} v(\rho)$$

Then, just as for H-atom, diff eqtn for $v(\rho)$ is

$$\rho \frac{d^2 v}{d\rho^2} + \left[2(\lambda+1) - 2\kappa\rho \right] \frac{dv}{d\rho} + \left[2 - 2\kappa(\lambda+1) \right] v = 0$$

Finally : $z = 2\kappa\rho$, $b = 2(\lambda+1)$, $a = \lambda+1 - \frac{1}{\kappa}$ gives

$$z \frac{d^2 v}{dz^2} + (b-z) \frac{dv}{dz} - av = 0 \Rightarrow v(z) = {}_1F_1(a, b; z)$$

Quantization proceeds from truncating the ${}_1F_1$ series, i.e. must have

$$a = \lambda+1 - \frac{1}{\kappa} = -N, \; N = 0, 1, 2, \ldots \Rightarrow \frac{1}{\kappa} = N+\lambda+1$$

or $\kappa^2 = -2\epsilon = 1/(N+\lambda+1)^2 \Rightarrow E = -\frac{1}{2}\mathcal{E}/(N+\lambda+1)^2$ } Quantized Energies

Define principal q. # ; $n = N + l + 1$. Then can write...

$\hookrightarrow N = 0, 1, 2, \ldots \Rightarrow$ at ~~most~~ $l = n-1$

$$E_{n\ell} = -\tfrac{1}{2}\,\mathcal{E}/(n+\Delta_\ell)^2$$

where: $\Delta_\ell = \lambda - \ell = \frac{1}{2}\sqrt{(2\ell+1)^2 + 8mA/\hbar^2} - (\ell+\frac{1}{2})$

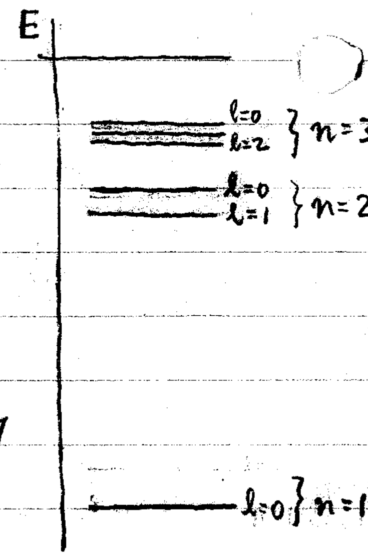
$$= (\ell+\tfrac{1}{2})\left\{\left[1+\frac{2mA/\hbar^2}{(\ell+\frac{1}{2})^2}\right]^{\frac{1}{2}} - 1\right\}, \text{ exact}$$

This result agrees with L&L, p. 124

For $mA/\hbar^2 \ll 1$, $\Delta_\ell \simeq \dfrac{2mA/\hbar^2}{2\ell+1}$ & $(n+\Delta_\ell)^{-2} \simeq \dfrac{1}{n^2}\left[1-\dfrac{4mA/\hbar^2}{n(2\ell+1)}\right]$

$$\therefore\ E_{n\ell} \simeq -\frac{mB^2}{2\hbar^2 n^2}\left[1-\frac{4mA/\hbar^2}{n(2\ell+1)}\right]$$

Note – we recover the H-atom energies, as should be, for $A=0$, or for $\ell\to\infty$. For $A\neq 0$, the ℓ-degeneracy is lifted. Since $E_{n\ell} < E_{n0}$, the states with highest ℓ are most tightly bound (!) -- so the gnd state is $n=1$, $\ell=0$. Spectrum is H-like, but with a cluster of close-lying ℓ states at each given n. See sketch



2/24/71 53 3D Spherical Oscillator. See Davydov, p. 131; Ter Haar, p. 217.

$V(r) = \frac{1}{2}m\omega^2 r^2$. Bound states are (+)ve E. Radial eqtn is

$$\left\{\frac{d^2}{dr^2} + \left[\frac{2mE}{\hbar^2} - \frac{2m}{\hbar^2}\times\frac{1}{2}m\omega^2 r^2 - \frac{\ell(\ell+1)}{r^2}\right]\right\}u(r) = 0$$

Let $a = \sqrt{\hbar/m\omega}$ & $\rho = r/a$, $\mathcal{E} = \hbar\omega$ & $\epsilon = E/\mathcal{E}$. Then

$$\frac{d^2u}{d\rho^2} + \left[2\epsilon - \rho^2 - \frac{\ell(\ell+1)}{\rho^2}\right]u = 0 \leftarrow \text{Same as Davydov eq. (37.5), p.132}$$

Asymptotic behaviour: $u(\rho) \sim \rho^{\ell+1}$ as $\rho \to 0$. For $\rho \to \infty$, have

$$\frac{d^2u}{d\rho^2} - \rho^2 u \simeq 0 \Rightarrow u(\rho) \sim e^{-\frac{1}{2}\rho^2}$$

$$\hookrightarrow \frac{d^2u}{d\rho^2} = (\rho^2 - 1)u \simeq \rho^2 u \text{ for large } \rho$$

$\therefore$ let: $u(\rho) = \text{const} \times \rho^{\ell+1} e^{-\frac{1}{2}\rho^2} v(\rho)$. After some algebra, get

$$\frac{d^2v}{d\rho^2} + 2\left(\frac{\ell+1}{\rho} - \rho\right)\frac{dv}{d\rho} - \left[2(\ell+\tfrac{3}{2}) - 2\epsilon\right]v = 0$$

$$\hookrightarrow \text{or}// \quad \frac{d^2v}{dr^2} + 2\left(\frac{\ell+1}{r} - \lambda r\right)\frac{dv}{dr} - \left[2\lambda(\ell+\tfrac{3}{2}) - \frac{2mE}{\hbar^2}\right]v = 0 \quad \left\{ \begin{array}{l} \lambda = 1/a^2. \text{ This} \\ \text{is Ter Haar eq. (3)} \\ \text{p. 217} \end{array} \right.$$

Define new variable: $z = \rho^2$. Then

$$\frac{d}{d\rho} = 2\sqrt{z}\,\frac{d}{dz} \quad \text{and} \quad \frac{d^2}{d\rho^2} = 4z\frac{d^2}{dz^2} + 2\frac{d}{dz}$$

Diff eqtn becomes...

$$z\frac{d^2v}{dz^2} + \left((\ell+\tfrac{3}{2}) - z\right)\frac{dv}{dz} - \left[\tfrac{1}{2}(\ell+\tfrac{3}{2}) - \tfrac{1}{2}\epsilon\right]v = 0$$

$$\Rightarrow v(z) = {}_1F_1(a,b;z) \quad \left\{ \begin{array}{l} a = \frac{1}{2}(\ell+\frac{3}{2}) - \frac{1}{2}\epsilon \\ b = \ell + \frac{3}{2} \end{array} \right. \quad \text{and } z = \rho^2$$

Quantization: $a = \frac{1}{2}(\ell+\frac{3}{2}) - \frac{1}{2}\epsilon = -N$, $N = 0, +1, +2, \ldots$

$$\therefore E_\Lambda = (2N + \ell + \tfrac{3}{2})\mathcal{E} = (\Lambda + \tfrac{3}{2})\hbar\omega$$

where $\Lambda = 2N + \ell \left\{ \begin{array}{l} N = 0,1,2,\ldots \\ \ell = 0,1,2,\ldots \end{array} \right\} \Lambda = 0, 1, 2, 3, \ldots$

The radial eigenfcns are

$$u_{\Lambda \ell}(\rho) = \text{cnst} \times \rho^{\ell+1} e^{-\frac{1}{2}\rho^2} {}_1F_1\left(-\tfrac{1}{2}(\Lambda-\ell),\ \ell+\tfrac{3}{2};\ \rho^2\right)$$

Note $-\frac{1}{2}(\Lambda-\ell) = -N \Rightarrow \Lambda - \ell = 2N = 0, 2, 4, \ldots$ $\quad \underset{\sim\sim}{\ell \leq \Lambda}$

E_Λ does not depend on ℓ, only on the combination $\Lambda = 2N + \ell$.

$\Lambda = 0 \Rightarrow (N, \ell) = (0,0)$ only. This state is denoted $1s$

$\Lambda = 1 \Rightarrow (N, \ell) = (0,1)$ only. " " " " $1p$

$\Lambda = 2 \Rightarrow (N, \ell) = (1,0)$ & $(0,2)$. These states are $2s$ & $1d$.

$\Lambda = 3 \Rightarrow (N, \ell) = (1,1)$ & $(0,3)$ " " " $2p$ & $1f$

Parity of the state is $(-1)^\ell$ ... from the associated $Y_{\ell m}$. We note that only even values of ℓ appear for $\Lambda =$ even, while only odd values of ℓ appear for $\Lambda =$ odd. (this is apparent from $\ell = \Lambda - 2N$). So parity is $= (-1)^\Lambda$. Noting that the degeneracy of each ℓ state is $2\ell + 1$, we find the total # states for level E_Λ as

$\Lambda = 0$ $(1s) \rightarrow$ # states $= 1$

$\Lambda = 1$ $(1p) \rightarrow$ # states $= 3$

$\Lambda = 2$ $(2s$ & $1d) \rightarrow$ # states $= 1 + 5 = 6$

$\Lambda = 3$ $(2p$ & $1f) \rightarrow$ # states $= 3 + 7 = 10$

$\Lambda = 4$ $(3s, 2d, 1g) \rightarrow$ # states $= 1 + 5 + 9 = 15$

$\Lambda = 5$ $(3p, 2f, 1h) \rightarrow$ # states $= 3 + 7 + 11 = 21$

The general formula is $\frac{1}{2}(\Lambda+1)(\Lambda+2)$.

2/25/71 (57) We look up the results in Pauling "The Nature of the Chemical Bond" (Cornell Univ. Press, 1960, 3RD ed.), Appendix III, p. 576. In Pauling's notation, the spherical harmonics are

$$Y_{lm}(\vartheta,\varphi) = \Theta_{lm}(\vartheta)\,\Phi_m(\varphi)$$

We shall use exponential form for the Φ_m's, i.e. $\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$, which are normalized so that $\int_0^{2\pi} \Phi_m^*(\varphi)\,\Phi_m(\varphi)\,d\varphi = 1$. Then we get...

$$Y_{00}(\vartheta,\varphi) = 1/\sqrt{4\pi}$$

$$Y_{10}(\vartheta,\varphi) = \sqrt{3/4\pi}\,\cos\vartheta$$

$$Y_{1,\pm1}(\vartheta,\varphi) = \sqrt{3/8\pi}\,\sin\vartheta\, e^{\pm i\varphi}$$

$$Y_{20}(\vartheta,\varphi) = \sqrt{5/16\pi}\,(3\cos^2\vartheta - 1)$$

$$Y_{2,\pm1}(\vartheta,\varphi) = \sqrt{15/8\pi}\,\sin\vartheta\cos\vartheta\, e^{\pm i\varphi}$$

$$Y_{2,\pm2}(\vartheta,\varphi) = \sqrt{15/32\pi}\,\sin^2\vartheta\, e^{\pm 2i\varphi}$$

Except for $\mp$ signs in the $m=\pm1$ cases, these agree with the listing in Schiff, p. 80, and Merzbacher, p. 186. As for the $R_{nl}(r)$, Pauling gives, with $\boxed{x = (2Z/na_0)r}$..

$$R_{10}(r) = (Z/a_0)^{3/2} \times 2e^{-x/2}$$

$$R_{20}(r) = \frac{(Z/a_0)^{3/2}}{2\sqrt{2}}(2-x)e^{-x/2} = \left(\frac{Z}{2a_0}\right)^{\frac{3}{2}}(2-x)e^{-x/2}$$

$$R_{21}(r) = \frac{(Z/a_0)^{3/2}}{2\sqrt{6}}\,x\,e^{-x/2} = \left(\frac{Z}{2a_0}\right)^{\frac{3}{2}}\frac{x}{\sqrt{3}}e^{-x/2}$$

These agree with Schiff, p. 94. Merzbacher has none. In addition

$$|1,0,0\rangle = (1/\pi a_0'^3)^{\frac{1}{2}} e^{-r/a_0'} , \quad a_0' = a_0/Z$$

$$|2,1,0\rangle = (1/32\pi a_0'^3)^{\frac{1}{2}} \left(\frac{z}{a_0'}\right) e^{-r/2a_0'} , \quad z = r\cos\vartheta$$

52

$$R_{30}(r) = \frac{(Z/a_0)^{3/2}}{9\sqrt{3}} (6 - 6x + x^2) e^{-x/2}$$

$$R_{31}(r) = \frac{(Z/a_0)^{3/2}}{9\sqrt{6}} (4 - x)\, x\, e^{-x/2}$$

$$R_{32}(r) = \frac{(Z/a_0)^{3/2}}{9\sqrt{30}} x^2 e^{-x/2}$$

From the above, we find, explicitly...

$\frac{1}{\sqrt{8}}\left(\frac{1}{2}\right)^{\frac{3}{2}} = \frac{1}{8}$

$$|2,1,\pm 1\rangle = \frac{1}{\sqrt{8\pi}} \left(\frac{Z}{2a_0}\right)^{\frac{3}{2}} \left[\left(\frac{Zr}{a_0}\right) e^{-\frac{1}{2}(Zr/a_0)}\right] e^{\pm i\varphi} \sin\vartheta$$

$$|3,0,0\rangle = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{3a_0}\right)^{\frac{3}{2}} \left[1 - \frac{2}{3}\left(\frac{Zr}{a_0}\right) + \frac{2}{27}\left(\frac{Zr}{a_0}\right)^2\right] e^{-\frac{1}{3}(Zr/a_0)}$$

2/25/71 53 This is Merzbacher's prob 14, p. 213. ∃ a "Solution" (right -- but for wrong reasons) in Powell & Crasemann, pp. 398-400.

Note - for energy levels in a Yukawa potential, see Rawls & Schultz AJP 33, 444 ('65)

$$V(r) = -V_0 \left(\frac{e^{-r/a}}{r/a}\right) \quad \text{in } \ell = 0 \text{ state}$$

Choose $R(r) = e^{-\beta(r/a)} = \frac{1}{r} u(r)$ as trial fcn, β = adjustable

Note K.E. op. in Sph. Cds. is -- for $\ell = 0$ state (p. 182 of PHYS 506 lectures)

$$T = -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right)$$

$$\therefore \langle T \rangle = -\frac{\hbar^2}{2m} \int_0^\infty R^*(r) \left[\frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right)\right] R(r) \times r^2 dr$$

$$\text{N.B.} \quad T R(r) = -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) \frac{u(r)}{r} = -\frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial^2 u}{\partial r^2}$$

$$\therefore \langle T \rangle = \int_0^\infty \left[\frac{u^*(r)}{r} (T) \frac{u(r)}{r}\right] r^2 dr = -\frac{\hbar^2}{2m} \int_0^\infty u \frac{\partial^2 u}{\partial r^2} dr$$

But $u(r)$ vanishes at $r=0$ & $r=\infty$, so we can partial integrate...

$$\langle T\rangle = -\frac{\hbar^2}{2m}\left[\underbrace{\left(u\frac{\partial u}{\partial r}\right)\Big|_{r=0}^{r=\infty}}_{\to 0} - \int_0^\infty\left(\frac{\partial u}{\partial r}\right)^2 dr\right] = +\frac{\hbar^2}{2m}\int_0^\infty\left(\frac{\partial u}{\partial r}\right)^2 dr$$

With $u(r)=rR(r)$, $\frac{\partial u}{\partial r} = r\frac{\partial R}{\partial r}+R$, and $\left(\frac{\partial u}{\partial r}\right)^2 \neq r^2\left(\frac{\partial R}{\partial r}\right)^2$. So the Powell & Crasemann eqtn (11-86), p. 399 is <u>wrong</u>! For the assumed trial fcn, have...

$$u(r) = re^{-\beta(r/a)} \Rightarrow \frac{\partial u}{\partial r} = \left(1-\beta\frac{r}{a}\right)e^{-\beta(r/a)}$$

$$\therefore \langle T\rangle = \frac{\hbar^2}{2m}a\int_0^\infty(1-\beta x)^2 e^{-2\beta x}dx, \quad x = r/a$$

Use $\int_0^\infty x^n e^{-kx}dx = \Gamma(n+1)/k^{n+1}$. Then

$$\langle T\rangle = \frac{\hbar^2 a}{2m}\left\{\frac{1}{2\beta} - 2\beta\left(\frac{1}{(2\beta)^2}\right) + \beta^2\left(\frac{2}{(2\beta)^3}\right)\right\} = \frac{\hbar^2 a}{2m}\times\frac{1}{4\beta}$$

Amazingly enough, P&C have "right" answer in (11-86), by accident. Now calculate exp. value of $V(r)$...

$$\langle V\rangle = -V_0\int_0^\infty R^*(r)\left(\frac{e^{-r/a}}{r/a}\right)R(r)r^2dr = -V_0a^3\int_0^\infty x e^{-(2\beta+1)x}dx$$

$$= -V_0a^3/(2\beta+1)^2 \leftarrow \text{agrees with P\&C (11-87), p. 399.}$$

$$\therefore \langle T\rangle + \langle V\rangle = \frac{\hbar^2 a}{2m}\left[\frac{1}{4\beta} - \frac{2mV_0a^2/\hbar^2}{(2\beta+1)^2}\right]$$

To get $\langle E\rangle$, we must divide by a norm factor...

$$N = \int_0^\infty R^*(r)R(r)r^2dr = a^3\int_0^\infty x^2e^{-2\beta x}dx = \boxed{a^3/4\beta^3} \leftarrow \text{P\&C (11-85)}$$

$$\therefore \langle E\rangle = \frac{1}{N}\left[\langle T\rangle+\langle V\rangle\right] = \frac{\hbar^2}{2ma^2}\beta^2\left[1-\frac{4\gamma^2\beta}{(2\beta+1)^2}\right], \quad \gamma^2 = \frac{2mV_0a^2}{\hbar^2}$$

$$\langle E\rangle = \frac{\hbar^2\beta^2}{2ma^2}\left[1 - \frac{4V_0\beta^3}{(2\beta+1)^2}\right]$$

Want to minimize this w.r.t. β. Get

eq ① $\frac{\partial}{\partial\beta}\langle E\rangle = 0 \Rightarrow \gamma^2 = (2\beta+1)^3/2\beta(2\beta+3)$ ∫ for a given V_0 & a, this gives β such that $\langle E\rangle = $ min.

This min condition $\Rightarrow \frac{4\gamma^2\beta}{(2\beta+1)^2} = 2(2\beta+1)/(2\beta+3)$

eq. ② $\therefore \langle E\rangle_{min} = -\frac{\hbar^2}{2ma^2}\beta^2\left(\frac{2\beta-1}{2\beta+3}\right)$ ← agrees with P&C (11-90)

Apply this to deuteron binding? For given V_0 & a, γ^2 is determined by

$$V_0 a^2 = \left(\frac{\hbar^2}{2m}\right)\gamma^2 = 41.50\,\gamma^2 \text{ MeV-}\mathring{f}^2 \quad \begin{cases} V_0 \text{ in MeV, } a \text{ in } \mathring{f} = 10^{-13}\text{ cm} \\ m = \frac{1}{2}M,\ M = p\text{-mass} = 1.6726\times10^{-24}\text{ gm} \end{cases}$$

(This ~ agrees with P&C (11-92)). Now with γ^2 known, eq ① gives β. Plugging this β (and the assumed a) into eq. ② gives the desired $\langle E\rangle_{min}$

Assume $a = 1.40\,\mathring{f} \Rightarrow \hbar^2/2ma^2 = 41.50/a^2 = 21.17$ MeV. Then

$$\langle E\rangle_{min} = -21.17\,\beta^2\left(\frac{2\beta-1}{2\beta+3}\right)$$

"Know" $\langle E\rangle_{min} = -2.226$ MeV. Then ...

$$f(\beta) = \beta^2\left(\frac{2\beta-1}{2\beta+3}\right) = \frac{-\langle E\rangle_{min}}{21.17} = 0.10515 \Rightarrow \beta = 0.8452$$

$$\therefore \gamma^2 = (2\beta+1)^3/2\beta(2\beta+3) = 2.456, \text{ and } V_0 = \frac{41.50}{a^2}\gamma^2 = 51.99 \text{ MeV}$$

$V_0 a^2 = 101.924$ (MeV-$\mathring{f}^2$)

For these parameters, deuteron has an enormous size!

$$\langle r\rangle = \frac{1}{N}\int_0^\infty r\,|R(r)|^2 r^2\,dr = \frac{3}{2}a/\beta = 2.48\,\mathring{f}$$

$$\langle r^2\rangle^{\frac{1}{2}} = \sqrt{3}\,a/\beta = 2.87\,\mathring{f}$$

For $a \to \infty$, but $V_0 a \to \text{cnst} = Ze^2 \Rightarrow V(r) \to \frac{Ze^2}{r}$, Coulomb potential we have...

$$\gamma^2 = \frac{2m}{\hbar^2}(V_0 a)a = \frac{2m}{\hbar^2} Ze^2 a \to \text{large} \Rightarrow \beta \text{ also is large. Then}$$

$$\gamma^2 \simeq 2\beta \text{ for } \beta \text{ large} \Rightarrow \beta \simeq \tfrac{1}{2}\gamma^2 = \tfrac{1}{2} \times \frac{2m}{\hbar^2} Ze^2 a = Za/a_0$$

where $a_0 = \hbar^2/me^2$ is Bohr radius

$$\therefore \langle E \rangle \simeq -\frac{\hbar^2}{2ma^2}\beta^2 \simeq -\frac{\hbar^2}{2ma^2}\left(\frac{Za}{a_0}\right)^2 = -\tfrac{1}{2}Z^2 e^2/a_0 \quad \Big\{ \text{H-atom gnd state energy}$$

3/4/71 (9) Consult p. 203 of Phys. 506 Notes. For $E \geq 0$, $\kappa^2 = -2\epsilon = -2E/\mathcal{E} = -2E/\frac{me^4}{\hbar^2}$ is negative, so we should replace κ by $i\kappa$, the new $\kappa^2 = 2E/\frac{me^4}{\hbar^2}$. Then the results on p. 203 et seq. can be taken over more or less intact. The diff eqtn in $u(\rho)$ is the same form as before, namely

$$\frac{d^2u}{d\rho^2} + \left[\kappa^2 + \frac{2Z}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right]u = 0$$

only with κ^2 replacing $-\kappa^2$, $\rho \to 0$ behaviour is $u(\rho) \sim \rho^{\ell+1}$ as before, but now for $\rho \to \infty$, we get $u(\rho) \sim e^{\mp i\kappa\rho}$. There is now no reason to eliminate the +ve exp, since it is oscillatory. Replacing κ by $i\kappa$, we thus have...

$$u_\pm(\rho) = \text{cnst} \times \rho^{\ell+1} e^{\pm i\kappa\rho} {}_1F_1\left(\ell+1 \pm \frac{Z}{i\kappa}, 2\ell+2; \mp 2i\kappa\rho\right)$$

This agrees with Davydov, p. 139, eq (39.5). Now see Landau & Lifshitz, p. 120. They apparently use only $u_-(\rho)$. Define

$$R(\rho) = \frac{1}{\rho}u_-(\rho) = \text{cnst} \times \rho^\ell e^{-i\kappa\rho} {}_1F_1\left(\ell+1+\frac{iZ}{\kappa}, 2\ell+2; 2i\kappa\rho\right)$$

At this point, we shall drop the cnst, remembering that it can be chosen arbitrarily. The asymptotic form for ${}_1F_1$ is (see p. 206 of lecture notes)

$$ {}_1F_1(a,b;z) = \frac{\Gamma(b)}{\Gamma(a)} e^{z} z^{a-b} + \frac{\Gamma(b)}{\Gamma(b-a)} (-z)^{-a} $$

With $a = l+1+\frac{iZ}{\kappa}$, $b = 2l+2$, $z = 2i\kappa\rho$, have

$$ {}_1F_1 = \frac{(2l+1)!}{\Gamma(l+1+\frac{iZ}{\kappa})} e^{2i\kappa\rho} (2i\kappa\rho)^{\frac{iZ}{\kappa}-(l+1)} + \frac{(2l+1)!}{\Gamma(l+1-\frac{iZ}{\kappa})} (-2i\kappa\rho)^{-\frac{iZ}{\kappa}-(l+1)} $$

$$ = (2l+1)!\, e^{i\kappa\rho} \left[\frac{e^{+i\kappa\rho}}{\Gamma(l+1+\frac{iZ}{\kappa})} (+2i\kappa\rho)^{\frac{iZ}{\kappa}-(l+1)} + \frac{e^{-i\kappa\rho}}{\Gamma(l+1-\frac{iZ}{\kappa})} (-2i\kappa\rho)^{-\frac{iZ}{\kappa}-(l+1)} \right] $$

Now $\pm i = e^{\pm i\frac{\pi}{2}}$. Then $(+i)^{\frac{iZ}{\kappa}-(l+1)} = e^{-\frac{Z\pi}{2\kappa}} e^{-i(l+1)\frac{\pi}{2}}$. So

and $(-i)^{-\frac{iZ}{\kappa}-(l+1)} = e^{-\frac{Z\pi}{2\kappa}} e^{+i(l+1)\frac{\pi}{2}}$

$$ {}_1F_1 = \left\{ \frac{(2l+1)!\, e^{+i\kappa\rho}}{(2\kappa\rho)^{l+1}} \right\} e^{-\frac{Z\pi}{2\kappa}} \left[\frac{e^{+i(\kappa\rho-(l+1)\frac{\pi}{2})}}{\Gamma(l+1+\frac{iZ}{\kappa})} (2\kappa\rho)^{\frac{iZ}{\kappa}} + \frac{e^{-i(\kappa\rho-(l+1)\frac{\pi}{2})}}{\Gamma(l+1-\frac{iZ}{\kappa})} (2\kappa\rho)^{-\frac{iZ}{\kappa}} \right] $$

Use $e^{c\ln x} = x^c \Rightarrow (2\kappa\rho)^{\pm\frac{iZ}{\kappa}} = e^{\pm\frac{iZ}{\kappa}\ln 2\kappa\rho}$. Thus have

$$ {}_1F_1 = \{\ \text{"}\ \} e^{-\frac{Z\pi}{2\kappa}} \left[\frac{e^{+i(\kappa\rho-(l+1)\frac{\pi}{2}+\frac{Z}{\kappa}\ln 2\kappa\rho)}}{\Gamma(l+1+\frac{iZ}{\kappa})} + \frac{e^{-i(\kappa\rho-(l+1)\frac{\pi}{2}+\frac{Z}{\kappa}\ln 2\kappa\rho)}}{\Gamma(l+1-\frac{iZ}{\kappa})} \right] $$

Now if we choose a cnst for $R(\rho)$ (as do L & L, eq.(36.17), p. 120)

$$ R(\rho) = \underbrace{\frac{C_\kappa}{(2l+1)!}(2\kappa}_{=\text{cnst}}\rho)^{l} e^{-i\kappa\rho}\, {}_1F_1(l+1+\tfrac{iZ}{\kappa}, 2l+2; 2i\kappa\rho) $$

and note that the two terms in [ ] in ${}_1F_1$ above are complex conjugates, then the desired asymptotic behaviour as $\rho\to\infty$ is

$$ R(\rho) \underset{\rho\to\infty}{\simeq} C_\kappa \frac{e^{-Z\pi/2\kappa}}{\kappa\rho} \operatorname{Re}\left[\frac{e^{-i(\kappa\rho-(l+1)\frac{\pi}{2}+\frac{Z}{\kappa}\ln 2\kappa\rho)}}{\Gamma(l+1-\frac{iZ}{\kappa})} \right] $$

Note: $\kappa\rho = \sqrt{\frac{2E}{me^4/\hbar^2}}\ \frac{r}{a_0} = kr$, $k = \sqrt{\frac{2mE}{\hbar^2}}$ = wave#, also: $\kappa = ka_0$

$a_0 = \hbar^2/me^2$

$K = ka_0 \qquad kr = ka_0\left(\frac{r}{a_0}\right) = K\rho$

Let : $\Gamma(\ell+1-\frac{iZ}{K}) = |\Gamma(\ell+1-\frac{iZ}{ka_0})|\, e^{i\delta_\ell(k)}$, $\boxed{\delta_\ell(k) = \arg\Gamma(\ell+1-\frac{iZ}{ka_0})}$

$$\therefore R_{k\ell}(r) \underset{r\to\infty}{\simeq} \frac{C_k e^{-Z\pi/ka_0}}{|\Gamma(\ell+1-\frac{iZ}{ka_0})|}\frac{1}{kr}\,\mathrm{Re}\left\{e^{-i[kr-(\ell+1)\frac{\pi}{2}+\frac{Z}{ka_0}\ln 2kr+\delta_\ell(k)]}\right\}$$

$\hookrightarrow = \cos(\sim+\frac{\pi}{2}) = -\sin$

or,

$$R_{k\ell}(r) \underset{r\to\infty}{\simeq} \left\{\frac{C_k e^{-Z\pi/ka_0}}{|\Gamma(\ell+1-\frac{iZ}{ka_0})|}\right\}\frac{1}{kr}\sin\left[(kr-\ell\tfrac{\pi}{2})+\frac{Z}{ka_0}\ln 2kr+\delta_\ell(k)\right]$$

where $\delta_\ell(k)$ is as defined above. This essentially agrees with L & L eq. (36.23) p. 121. We "know" the normalizing const { } should be $\sqrt{2/\pi}\,k$ if we are to have $\int_0^\infty R^*_{k'\ell} R_{k\ell}\, r^2\, dr = \delta(k'-k)$, as we can see from

$$\int_0^\infty \sin k'r \sin kr\, dr = -\frac{1}{4}\int_0^\infty (e^{+ik'r}-e^{-ik'r})(e^{+ikr}-e^{-ikr})\,dr$$

$$= +\frac{1}{4}\int_0^\infty \left[e^{+i(k'-k)r}+e^{-i(k'-k)r}-e^{+i(k'+k)r}-e^{-i(k'+k)r}\right]dr$$

$\hookrightarrow$ both k & $k' >$ $\Rightarrow$ these terms oscillate themselves to death.

$$= \frac{1}{4}\int_{-\infty}^{+\infty} e^{+i(k'-k)r}\,dr = \frac{\pi}{2}\delta(k'-k)$$

$\therefore R_{k\ell}(r) = \left\{\sqrt{\frac{2}{\pi}}\,k\right\}\frac{1}{kr}\sin kr$ is normalized to $\int_0^\infty R_{k'\ell}R_{k\ell}\, r^2\, dr = \delta(k-k')$.

Applying this to the above, we get...

$$R_{k\ell}(r) \underset{r\to\infty}{\simeq} \sqrt{\frac{2}{\pi}}\,\frac{1}{r}\sin\left[(kr-\ell\tfrac{\pi}{2})+\frac{Z}{ka_0}\ln 2kr+\delta_\ell(k)\right] \qquad \underline{\text{QED}}$$

and : $C_k = \sqrt{\frac{2}{\pi}}\,k\,e^{\frac{Z\pi}{ka_0}}\,|\Gamma(\ell+1-\frac{iZ}{ka_0})|$ $\leftarrow$ agrees with L&L (36.22)

3/16/71 (c) The const $2^\nu\Gamma(\nu+1)$ is chosen by convention for the "proper" behaviour of $J_\nu(x)$ as $x\to\infty$. It is of no consequence in the diff. eqtn., so drop it, and look at

$f_\nu(x) = x^\nu e^{-ix}\,{}_1F_1(\nu+\tfrac{1}{2}, 2\nu+1; 2ix)$. Denote ${}_1F_1$ by F.

$$\frac{d}{dx} f_\nu = \left(\frac{\nu}{x} - i\right) f_\nu + x^\nu e^{-ix} \frac{dF}{dx}$$

$$\frac{d^2}{dx^2} f_\nu = \left(\frac{\nu^2-\nu}{x^2} - 2i\frac{\nu}{x} - 1\right) f_\nu + 2\left(\frac{\nu}{x} - i\right) x^\nu e^{-ix} \frac{dF}{dx} + x^\nu e^{-ix} \frac{d^2F}{dx^2}$$

Let $g = x^\nu e^{-ix}$. Note $\frac{1}{g} f_\nu = F$. Then

$$\frac{1}{g}\, x \frac{d}{dx} f_\nu = (\nu - ix) F + x \frac{dF}{dx}$$

$$\frac{1}{g}\, x^2 \frac{d^2}{dx^2} f_\nu = (\nu^2 - \nu - 2i\nu x - x^2) F + 2(\nu x - ix^2) \frac{dF}{dx} + x^2 \frac{d^2F}{dx^2}$$

Forming Bessel's eqtn (which is satisfied by f_ν), have

$$\frac{1}{g}\left[x^2 \frac{d^2}{dx^2} + x\frac{d}{dx} + (x^2 - \nu^2)\right] f_\nu(x) = 0 \quad \Rightarrow$$

$$\left[-(2\nu+1)ix\right] F + \left[(2\nu+1)x - 2ix^2\right] \frac{dF}{dx} + x^2 \frac{d^2F}{dx^2}$$

Divide thru by x. Let $\rho = 2ix$. Then get

$$\rho \frac{d^2F}{d\rho^2} + \left[(2\nu+1) - \rho\right] \frac{dF}{d\rho} - (\nu + \tfrac{1}{2}) F = 0$$

$\hookrightarrow$ C.H. Eq., with solution $F = {}_1F_1(\nu+\tfrac{1}{2}, 2\nu+1; \underbrace{\rho}_{=2ix})$ **QED.**

As $x \to 0$, $e^{-ix}\,{}_1F_1 \to 1$, so we have

$$J_\nu(x) \simeq \left(\frac{x}{2}\right)^\nu / \Gamma(\nu+1) \quad \text{for } x \to 0.$$ ← agrees with NBS eq. (9.1.7), p. 360

Next - using the formula for large x (p. 206 of notes), we find

$$ {}_1F_1(\nu+\tfrac{1}{2}, 2\nu+1; 2ix) \underset{x\to\infty}{\simeq} \frac{\Gamma(2\nu+1)}{\Gamma(\nu+\frac{1}{2})} \left\{ e^{+2ix}(2ix)^{-(\nu+\frac{1}{2})} + e^{+i\pi(\nu+\frac{1}{2})}(2ix)^{-(\nu+\frac{1}{2})} \right\} $$

$$ = \frac{\Gamma(2\nu+1)}{\Gamma(\nu+\frac{1}{2})} \frac{2e^{+ix}}{(2x)^{\nu+\frac{1}{2}}} \cos\left[x-(\nu+\tfrac{1}{2})\tfrac{\pi}{2}\right] $$

Use $\Gamma(2z)/\Gamma(z) = \dfrac{2^{2z-1}}{\sqrt{\pi}}\Gamma(z+\frac{1}{2})$ ← NBS eq. (6.1.18), p. 256

to get $\dfrac{\Gamma(2\nu+1)}{\Gamma(\nu+\frac{1}{2})} = \dfrac{2^{2\nu}}{\sqrt{\pi}}\Gamma(\nu+1)$. Then we have

$$ J_\nu(x) = \left(\frac{x}{2}\right)^\nu \frac{e^{-ix}}{\Gamma(\nu+1)} {}_1F_1(\nu+\tfrac{1}{2}, 2\nu+1; 2ix) $$

$$ \underset{x\to\infty}{\simeq} \sqrt{\frac{2}{\pi x}} \cos\left[x-(\nu+\tfrac{1}{2})\tfrac{\pi}{2}\right] $$ ← agrees with NBS (9.2.1) p. 364

QED for part a).

13

$$ R_{k\ell}(r) = A_k j_\ell(kr) \rightarrow \frac{A_k}{kr}\sin(kr-\ell\tfrac{\pi}{2}) \quad \text{as } r\to\infty $$

Use this approx. form in orthogonality integral...

$$ \int_0^\infty R^*_{k'\ell}(r) R_{k\ell}(r) r^2 dr \simeq \frac{A^*_{k'} A_k}{k'k} \int_0^\infty \sin(k'r-\ell\tfrac{\pi}{2})\sin(kr-\ell\tfrac{\pi}{2}) dr $$

For large r, neglect the terms in $\ell\frac{\pi}{2}$. Then, as in problem 59, the integral is

$$ \int_0^\infty \sin k'r \sin kr \, dr = \frac{\pi}{2}\delta(k'-k) $$

So we have $\int_0^\infty R^*_{k'\ell}(r) R_{k\ell}(r) r^2 dr = \delta(k'-k)$, if we choose

$$\frac{|A_k|^2}{k^2}\frac{\pi}{2} = 1 \Rightarrow A_k = \sqrt{\frac{2}{\pi}}\, k \quad \underline{\underline{QED}}.$$

Now $E = \frac{\hbar^2}{2m}k^2$ for a free particle. Thus we have

$$\delta(E'-E) = \delta(k'-k) \Big/ \left|\frac{d}{dk}\left(\frac{\hbar^2}{2m}k^2\right)\right| = \frac{m}{\hbar^2 k}\delta(k'-k)$$

or $\delta(k'-k) = \frac{\hbar^2 k}{m}\delta(E'-E) = \hbar\sqrt{\frac{2E}{m}}\,\delta(k'-k)$

$$\therefore \int_0^\infty R^*_{E'\ell}(r) R_{E\ell}(r) r^2 dr = \left(\frac{|A_E|^2}{k^2}\frac{\pi}{2} \times \frac{\hbar^2 k}{m}\right)\delta(E'-E)$$

$$(\quad) = 1 \Rightarrow A_E = \frac{1}{\hbar}\sqrt{\frac{2mk}{\pi}} = \left(\frac{1}{\hbar}\sqrt{\frac{m}{k}}\right)A_k = \frac{1}{\hbar}\sqrt{\frac{2mk}{\pi}}$$

This agrees with Landau & Lifshitz, eq. (33.5), p. 105. $\underline{\underline{QED}}$.

3/16/71 (61) a) $\underset{\sim}{H}\vec{u}_k = E_k \vec{u}_k$ let $u_{k\ell}$ be ℓ^{th} comp. of $\vec{u}_k$. Take ℓ^{th} comp. of each side. Then

$$\sum_m H_{\ell m} u_{km} = E_k u_{k\ell} = \sum_m E_k \delta_{\ell m} u_{km}$$

or $\sum_m (H_{\ell m} - E_k\delta_{\ell m}) u_{km} = 0$

Soln only if: $\det(H_{\ell m} - E_k \delta_{\ell m}) = 0$.

This is the secular eqtn, with N (assumed distinct) solns for E_k

To show E_k are real & $\vec{u}_k$ are orthogonal, write

$$\underset{\sim}{H}\vec{u}_j = E_j \vec{u}_j, \text{ or } \vec{u}_j^{\dagger}\underset{\sim}{H}^{\dagger} = E_j^* u_j^{\dagger}$$

Use $\underset{\sim}{H}^\dagger = \underset{\sim}{H}$ ($\underset{\sim}{H}$ Hermitian) and operate through this eqtn by $\cdot \vec{u}_k$

$$\vec{u}_j^\dagger \underset{\sim}{H} \cdot \vec{u}_k = \vec{u}_j^\dagger \cdot (\underset{\sim}{H} \vec{u}_k) = E_j^* \vec{u}_j^\dagger \cdot \vec{u}_k$$

But $\underset{\sim}{H} \vec{u}_k = E_k \vec{u}_k$. So we have

$$E_k (\vec{u}_j^\dagger \cdot \vec{u}_k) = E_j^* \vec{u}_j^\dagger \cdot \vec{u}_k, \text{ or } \boxed{(E_j^* - E_k)\, \vec{u}_j^\dagger \cdot \vec{u}_k = 0}$$

For $j = k$, this gives $(E_k^* - E_k)|\vec{u}_k|^2 = 0$. Since $|\vec{u}_k|^2 \neq 0$, then have $E_k^* = E_k$, i.e. all E_k are real. Now for $j \neq k$

$$(E_j - E_k)\, \vec{u}_j^\dagger \cdot \vec{u}_k = 0, \quad j \neq k$$

If all E_k distinct, $E_j - E_k \neq 0$, so $\vec{u}_j^\dagger \cdot \vec{u}_k \equiv 0$ for $j \neq k$. Thus the $\vec{u}_k$ are orthogonal.

b) Normalize the $\vec{u}_k$ to unit vectors $\hat{u}_k$. They are orthonormal

$$\hat{u}_j^\dagger \cdot \hat{u}_k = \sum_l u_{jl}^* u_{kl} = \delta_{jk}$$

This is possible since the $\hat{u}_k$ satisfy a set of homogeneous eqtns, and so are determined only up to a multiplicative const -- which we use here for norm. Now if $\underset{\sim}{U} = (u_{kl}^*)$, then $\underset{\sim}{U}^\dagger = (u_{lk})$, and

$$(\underset{\sim}{U}\underset{\sim}{U}^\dagger)_{km} = \sum_l u_{kl}^* u_{ml} = \delta_{km}, \quad \text{i.e. } \underset{\sim}{U}\underset{\sim}{U}^\dagger = \underset{\sim}{1}$$

also

$$(\underset{\sim}{U}^\dagger \underset{\sim}{U})_{km} = \sum_l u_{lk} u_{lm}^* = \delta_{km}, \quad \text{i.e. } \underset{\sim}{U}^\dagger \underset{\sim}{U} = \underset{\sim}{1}$$

So $\underset{\sim}{U}$ is unitary -- this follows from the orthonormality of the eigenvectors $\hat{u}_k$.

Now show $\underset{\sim}{U}\underset{\sim}{H}\underset{\sim}{U}^\dagger$ is diagonal ...

$$(\underset{\sim}{U}\underset{\sim}{H}\underset{\sim}{U}^\dagger)_{kn} = \sum_{l,m} U_{kl} H_{lm} U^\dagger_{mn} = \sum_{l,m} u^*_{kl} H_{lm} u_{nm}$$

$$= \sum_l u^*_{kl} \underbrace{(\underset{\sim}{H}\hat{u}_n)_l}_{= E_n \hat{u}_n} = E_n \hat{u}^\dagger_k \cdot \hat{u}_n = E_n \delta_{kn}$$

So $\underset{\sim}{U}\underset{\sim}{H}\underset{\sim}{U}^\dagger = \begin{pmatrix} E_1 & & 0 \\ & E_2 & \\ 0 & & \ddots \end{pmatrix} = \underset{\sim}{H}'$ is indeed diagonal -- it is the canonical form for $\underset{\sim}{H}$, with the eigenvalues down the diagonal.

If S.T. were $\underset{\sim}{V}^\dagger \underset{\sim}{H}\underset{\sim}{V} = \underset{\sim}{H}'$, then $\underset{\sim}{V} = \underset{\sim}{U}^\dagger$. So, while $\underset{\sim}{U}$ is the matrix of the $\hat{u}_k^\dagger$ as rows, $\underset{\sim}{V}$ would be the matrix of the $\hat{u}_k$ as columns.

c) $\underset{\sim}{U}\underset{\sim}{H}\underset{\sim}{U}^\dagger = \underset{\sim}{H}' \Rightarrow \underset{\sim}{H} = \underset{\sim}{U}^\dagger \underset{\sim}{H}' \underset{\sim}{U}$ and $\underset{\sim}{H}^{-1} = \underset{\sim}{U}^\dagger \underset{\sim}{H}' \underset{\sim}{U}$

Here we have used $\underset{\sim}{U}^{-1} = \underset{\sim}{U}^\dagger$. Now we have

$H^{-1}_{kl} = \sum_{m,n} U^\dagger_{km} H'^{-1}_{mn} U_{nl}$. But $H'^{-1}_{mn} = \frac{1}{E_m}\delta_{mn}$, trivially

$$\therefore H^{-1}_{kl} = \sum_{m,n} \frac{1}{E_m} u_{mk} \delta_{mn} u^*_{nl} = \sum_m \frac{1}{E_m} u_{mk} u^*_{ml} \qquad \text{QED}$$

If some $E_m = 0$, the matrix $\underset{\sim}{H}$ is singular, i.e. $\det \underset{\sim}{H} = 0$, and no inverse exists (see Powell & Crasemann, p 290, where they show that

$\underset{\sim}{H}^{-1}$ exists if and only if $\underset{\sim}{H}\vec{u} = \vec{0}$ implies $\vec{u} \equiv 0$). Now we have

$$\underset{\sim}{H}\vec{A} = \vec{B} \Rightarrow \vec{A} = \underset{\sim}{H}^{-1} B$$

or// $$A_k = \sum_l H^{-1}_{kl} B_l = \sum_{l,m} \frac{1}{E_m} u_{mk} u^*_{ml} B_l$$

d) ~~Applying a similarity transform by $\underset{\sim}{U}$ to $\underset{\sim}{H}\vec{A} = \vec{B}$, we find~~

$$(\underset{\sim}{U}\,\underset{\sim}{H}\,\underset{\sim}{U}^{\dagger})\underset{\sim}{U}\vec{A} = \underset{\sim}{U}\vec{B}, \text{ or } \underset{\sim}{H}'\vec{A}' = \vec{B}' \left\{ \begin{array}{l} \underset{\sim}{H}' = \underset{\sim}{U}\,\underset{\sim}{H}\,\underset{\sim}{U}^{\dagger} \\ \vec{A}' = \underset{\sim}{U}\vec{A} \ \& \ \vec{B}' = \underset{\sim}{U}\vec{B} \end{array} \right.$$

But $\underset{\sim}{H}'$ is diagonal : $H'_{kl} = E_k \delta_{kl}$, so we have

$$\therefore B'_k = \sum_l H'_{kl} A'_l = E_k A'_k, \text{ or : } A'_k = B'_k / E_k$$

The effect of a similarity transform by $\underset{\sim}{U}$ on the eigenvalue eqtn is

$$\underset{\sim}{H}'\hat{u}'_k = E_k \hat{u}'_k, \quad \hat{u}'_k = \underset{\sim}{U}\hat{u}_k$$

or// $$u'_{ki} = \sum_j U_{ij} u_{kj} = \sum_j u^*_{ij} u_{kj} = \hat{u}_i \cdot \hat{u}_k = \delta_{ik}$$

So $\underset{\sim}{U}$ rotates the unit vectors $\hat{u}_k$ to single component unit vectors $\hat{u}'_k = (0, 0, \ldots, 0, 1, 0, \ldots, 0)$. The eigenvalue eqtn becomes...
k^{th} entry.

$$(E_k \hat{u}'_k)_i = (\underset{\sim}{H}'\hat{u}'_k)_i \text{ or// } E_k u'_{ki} = \sum_j H'_{ij} u'_{kj} = E_i u'_{ki}$$

$$\text{i.e.// } E_k \delta_{ik} = E_i \delta_{ik}$$

$\underset{\sim}{U}$ rotates the vectors CW & cd system CCW ← active transf^{n}
$\underset{\sim}{V} = \underset{\sim}{U}^{\dagger}$ rotates the cd system CW & vectors CCW ← passive transf^{n}