

[I]

$$\begin{aligned} \frac{1}{4\pi} e^{-\alpha r^2 - \beta \mathbf{r} \cdot \mathbf{r}' - \gamma r'^2} &= \frac{1}{4\pi} e^{-(2\alpha r - \beta \mathbf{r}') \cdot \mathbf{r}} \\ &= (-2\alpha + 4\alpha^2 r^2 + \beta^2 r'^2 + 4\alpha\beta \mathbf{r} \cdot \mathbf{r}') e^{-\dots} \end{aligned}$$

$$e^{-\beta \mathbf{r} \cdot \mathbf{r}'} = 4\pi \sum_{LM} i^L j_L(i\beta r r') Y_{LM}^*(\hat{\mathbf{r}}') Y_{LM}(\hat{\mathbf{r}})$$

$$\mathbf{r} \cdot \mathbf{r}' = -\sqrt{3} [\mathbf{r}_p \otimes \mathbf{r}'_q]^{00} = -\sqrt{3} \left( \frac{(1010100)}{-\sqrt{3}} r_0 r'_0 + \frac{(111-1100)}{\sqrt{3}} r_+ r'_- + \frac{(1-111100)}{\sqrt{3}} r_- r'_+ \right)$$

$$= \frac{4\pi}{3} r r' \left( -Y_{10} Y'_{10} + Y_{1+} Y'_{1-} + Y_{1-} Y'_{1+} \right) \left\| \sum_{m_1 m_2} \begin{pmatrix} L_1 S_1 S_2 \\ m_1 m_2 m_3 \end{pmatrix} \begin{pmatrix} L_2 S_2 S_3 \\ m_2 m_3 m_4 \end{pmatrix} \right\| = \frac{1}{\sqrt{3}} \delta_{S_1 S_2} \delta_{m_1 m_2} \delta_{S_2 S_3} \delta_{m_2 m_3}$$

$$= \left[ (4\alpha^2 r^2 + \beta^2 r'^2 - 2\alpha) + 4\alpha\beta \frac{4\pi}{3} r r' (Y_{10} Y'_{10} - Y_{1+} Y'_{1-} - Y_{1-} Y'_{1+}) \right] 4\pi i^L j_L(i\beta r r') Y_{LM}^* Y_{LM}$$

$$e^{-\alpha r^2 - \beta \mathbf{r} \cdot \mathbf{r}'}$$

$$= \sum_{LM} 4\pi i^L j_L(i\beta r r') e^{-\alpha r^2 - \beta \mathbf{r} \cdot \mathbf{r}'} Y_{LM}^* Y_{LM} \cdot \left\{ (4\alpha^2 r^2 + \beta^2 r'^2 - 2\alpha) + (Y'_{10} Y_{10} - Y'_{1+} Y_{1-} - Y'_{1-} Y_{1+}) \frac{16\pi}{3} \alpha\beta r r' \right\}$$

$$\int d\hat{\mathbf{r}}' \int d\mathbf{r}' r'^2 \int d\hat{\mathbf{r}} Y_{LM}^* Y_{LM} = \frac{1}{r'} \sum_{LM} Y_{LM}$$

$$(a) \sum_{LM} Y_{LM}^* Y_{LM} Y_{LM}^* Y_{LM} \rightarrow \delta_{LL} \delta_{MM}$$

$$(b) \sum_{LM} Y_{LM}^* Y_{LM} Y_{LM} Y_{LM} (Y_{10} Y'_{10} - Y_{1+} Y'_{1-} - Y_{1-} Y'_{1+})$$

$$\int d\hat{\mathbf{r}}' Y_{LM}^* Y_{LM} Y_{1q}' = (-1)^M \int d\hat{\mathbf{r}} Y_{L-M}' Y_{LM}' Y_{1q}' = \frac{\hat{L} \hat{L}' \hat{1}}{\sqrt{4\pi}} \begin{pmatrix} L & L' & 1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & L' & 1 \\ -M & M & q \end{pmatrix} (-1)^M$$

$$(-1)^{M'} \int d\hat{\mathbf{r}} Y_{L-M'}^* Y_{LM} Y_{1q}' = \frac{\hat{L}' \hat{L} \hat{1}}{\sqrt{4\pi}} \begin{pmatrix} L' & L & 1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L' & L & 1 \\ -M' & M & q \end{pmatrix} (-1)^{M'}$$

$$= \frac{3(2L+1)\hat{L}\hat{L}'}{4\pi} \sum_{LM} \begin{pmatrix} L & L' & 1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L' & L & 1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & L' & 1 \\ -M & M & q \end{pmatrix} \begin{pmatrix} L' & L & 1 \\ -M' & M' & q \end{pmatrix}$$

$$= \begin{pmatrix} 1 & L & L' \\ q & -M & M \end{pmatrix} \begin{pmatrix} 1 & L & L' \\ p & M & -M' \end{pmatrix} (-1)^{1+L+L'}$$

$$= \begin{pmatrix} 1 & L & L' \\ q & -M & M \end{pmatrix} \begin{pmatrix} 1 & L & L' \\ -q & M & -M' \end{pmatrix} (-1)^{1+L+L'}$$

$$= \begin{pmatrix} 1 & L & L' \\ q & -M & M \end{pmatrix} \begin{pmatrix} 1 & L & L' \\ q & -M & M' \end{pmatrix}$$

$$Y_{LM} Y_{LM}^* Y_{LP} = \begin{pmatrix} L & 1 & L' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & 1 & L' \\ -M & P & M' \end{pmatrix}$$

$$Y_{LM} Y_{LM}^* Y_{LP} = \begin{pmatrix} L & 1 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & 1 & L \\ -M & P & M \end{pmatrix}$$

$$\sum_{L,M} \int d(\Omega_{LM}) Y_{LM}^* Y_{LM} Y_{LP} = \sum_{L,M} \delta_{LM} \delta_{LM} Y_{LP}$$

$$Y_{LM}^* Y_{LM} = \delta_{LM} \delta_{LM}$$

$$\Rightarrow \int d\Omega Y_{LM}^* Y_{LM} = \delta_{LM} \delta_{LM}$$

$$(-1)^M Y_{LM}^* Y_{LM} = \delta_{LM} \delta_{LM}$$

$$= (-1)^M \delta_{LM} \delta_{LM}$$



$$\partial_r^2 e^{-\alpha r^2 - \beta r'^2 - 4\alpha\beta r r'} = (4\alpha^2 r^2 + \beta^2 r'^2 + 4\alpha\beta r r' - 2\alpha) e^{-\alpha r^2 - \beta r'^2 - 4\alpha\beta r r'} = \boxed{N}$$

(§ 34) in UQM:  $e^{-\beta r \cdot r'} = 4\pi \sum_{LM} i^L \underbrace{j_L(i\beta r r')}_{\text{spherical Bessel}} Y_{LM}^* Y'_{LM}$   $j_0 = \frac{\sin x}{x}$ ;  $j_1 = \frac{\cos x}{x^2} - \frac{\sin x}{x}$

$$r \cdot r' = -\sqrt{3} [r_p \otimes r_q]^{00} = -\frac{4\pi}{3} r r' (Y_{1+} Y'_{1-} + Y_{1-} Y'_{1+} - Y_{10} Y'_{10})$$

$$= +\frac{4\pi}{3} r r' \sum_p Y_{1p} Y'_{1-p} (-1)^{+p}$$

$$\Rightarrow \boxed{N} = \sum_{LM} \frac{1}{r'} Y'_{LM} \phi'_{LM} \cdot \int d\hat{r} Y_{LM}^* \int d\hat{r}' r'^2 dr$$

$$= \sum_{LM} \int dr' r'^2 \int d(\hat{r}, \hat{r}') \frac{1}{r'} 4\pi i^L j_L(i\beta r r') Y_{LM}^* Y'_{LM} (4\alpha^2 r^2 + \beta^2 r'^2 - 2\alpha + 4\alpha\beta \frac{4\pi}{3} r r' \sum_p Y_{1p} Y'_{1-p} (-1)^p)$$

$$\cdot Y'_{LM} Y_{LM}^* \phi'_{LM}$$

$$= \sum_{LM} \int dr' r' \int d(\hat{r}, \hat{r}') 4\pi i^L j_L(i\beta r r') \underbrace{Y_{LM}^* Y_{LM}^*}_{= Y_{LM} Y_{LM}^*} Y_{LM}^* Y'_{LM} (-1)^{LM} (4\alpha^2 r^2 + \beta^2 r'^2 - 2\alpha) \phi'_{LM}$$

$$+ \int dr' r' \int d(\hat{r}, \hat{r}') \sum_{LM} \frac{(4\pi)^2}{3} i^L j_L(i\beta r r') 4\alpha\beta r r' (-1)^{M+P} Y_{LM} Y_{LM} Y'_{LM} \underbrace{Y_{LM}^* Y_{LM}^*}_{Y_{LM}^* (-1)^M} Y_{1p} Y'_{1-p} \phi'_{LM}$$

$$= \int dr' r' 4\pi \sum_{LM} \delta_{LM} \delta_{LM} \delta_{LM} \delta_{LM} (-1)^{2M} (4\alpha^2 r^2 + \beta^2 r'^2 - 2\alpha) \phi'_{LM}$$

$$\neq 0 \Leftrightarrow M-p=-m \text{ and } -M+p=m \Rightarrow M+m'=p$$

$$+ \sqrt{\frac{2\hat{L}\hat{L}'}{4\pi}} \sqrt{\frac{2\hat{L}\hat{L}'}{4\pi}} \int dr' r' \sum_{LM} \frac{(4\pi)^2}{3} i^L j_L(i\beta r r') (-1)^{M+M'} \begin{pmatrix} L & 1 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & 1 & L' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & 1 & L \\ M-p & m & \end{pmatrix} \begin{pmatrix} L & 1 & L' \\ -M & p & -m' \end{pmatrix} \phi'_{LM}$$

$$= (-1)^{L+L'+1} \begin{pmatrix} L & 1 & L' \\ M-p & m & \end{pmatrix}$$

$$= \int dr' 4\pi r' \phi'_{LM} (4\alpha^2 r^2 + \beta^2 r'^2 - 2\alpha) j_L(i\beta r r')$$

$$+ \int dr' r' 4\pi i^L \sum_{LM} \hat{L} \hat{L}' j_L(i\beta r r') (-1)^{L+L'+1} \begin{pmatrix} L & 1 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & 1 & L' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & 1 & L \\ M-p & m & \end{pmatrix} \begin{pmatrix} L & 1 & L' \\ -M & p & -m' \end{pmatrix} \phi'_{LM}$$

note:  $\sum_p f(-p) = \sum_p f(p)$

because  $\sum_p$  is over a symmetric interval  $-1, 0, 1$  &



III

$$= \int dr' 4\pi r' i^{\ell'} s_{\ell'} (4\alpha^2 r'^2 + \beta^2 r'^2 - 2\alpha) \phi'_{\ell'm'}$$

$$+ \int dr' 4\pi r' \sum_{\ell_m} i^{\ell} s_{\ell} \hat{L} \hat{\ell} \hat{L} 4\alpha \beta r r' (-)^{\ell+\ell'+1} \begin{pmatrix} L & 1 & \ell' \\ 0 & 0 & 0 \end{pmatrix} \frac{1}{\ell'} \delta_{\ell\ell'} \delta_{mm'} \delta(L1\ell') \phi'_{\ell'm'}$$

$$= \int dr' 4\pi r' \left[ i^{\ell'} s_{\ell'} (4\alpha^2 r'^2 + \beta^2 r'^2 - 2\alpha) \phi'_{\ell'm'} \right.$$

$$\left. + \sum_{\ell} i^{\ell} s_{\ell} \hat{L} \hat{\ell} \hat{L} 4\alpha \beta r r' (-)^{\ell+\ell'+1} \begin{pmatrix} L & 1 & \ell' \\ 0 & 0 & 0 \end{pmatrix}^2 \delta(L1\ell') \phi'_{\ell'm'} \right]$$

$\neq 0 \Leftrightarrow L+1+\ell' = \text{even}$

$$= \int dr' 4\pi r' \left[ i^{\ell'} s_{\ell'} (4\alpha^2 r'^2 + \beta^2 r'^2 - 2\alpha) + \sum_{\ell} i^{\ell} s_{\ell} \hat{L} \hat{\ell} \hat{L} 4\alpha \beta r r' \begin{pmatrix} L & 1 & \ell' \\ 0 & 0 & 0 \end{pmatrix}^2 \delta(L1\ell') \right] \phi'_{\ell'm'}$$

$\uparrow \text{a.t.}$

$L+1+\ell' = \text{even}$

$\ell' = 1L-1, \dots, L+1$

S wave ( $\ell'=0$ )

$$\begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = -\frac{1}{\sqrt{3}}$$

$$\int dr' 4\pi r' \left[ s_0(i\beta r r') (4\alpha^2 r'^2 + \beta^2 r'^2 - 2\alpha) + i s_1(i\beta r r') (\sqrt{3})^4 4\alpha \beta r r' \right] \phi'_{00}$$

$L=0, 2, 4$

P wave ( $\ell'=1$ )

$1 = L=0 \checkmark$

$L=2 \checkmark$

$$\int dr' 4\pi r' \left[ i s_1(i\beta r r') (4\alpha^2 r'^2 + \beta^2 r'^2 - 2\alpha) + \left( s_0(i\beta r r') \sqrt{3}^{-1} - s_2(i\beta r r') 2\sqrt{3}^{-1}\sqrt{5}^{-1} \right) 4\alpha \beta r r' \right] \phi'_{1m}$$

