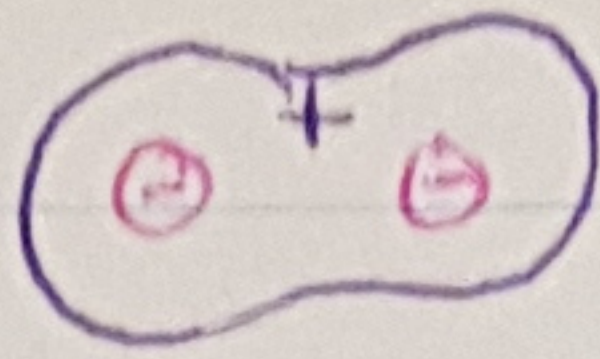
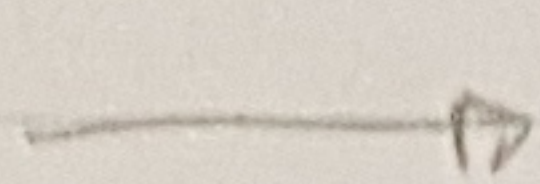
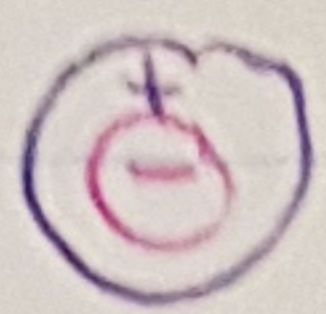
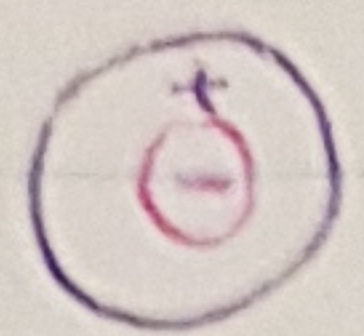


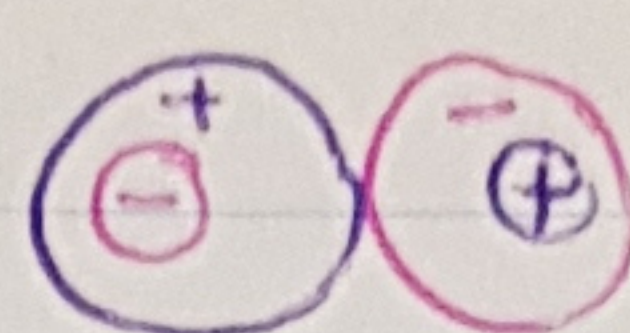
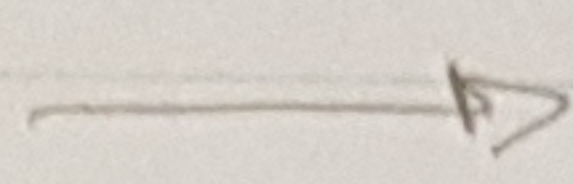
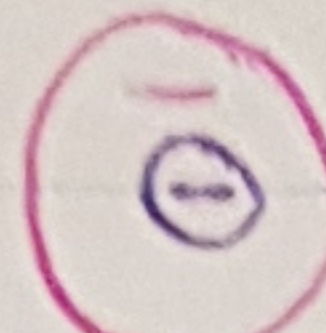
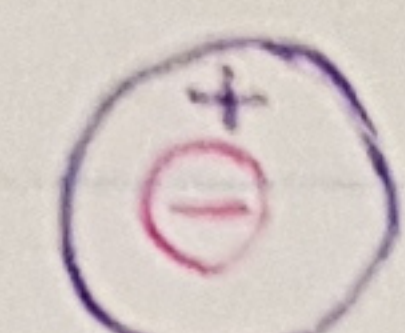
# Assignment (19)

1) a)  $\psi_{2s}^{(l)}(\vec{r}) + \psi_{2s}^{(r)}(\vec{r})$



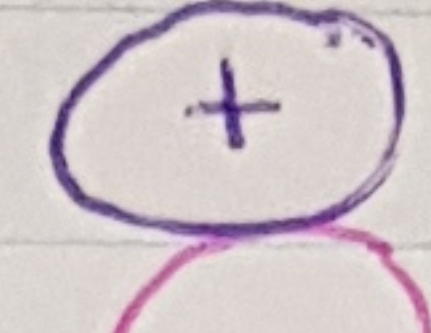
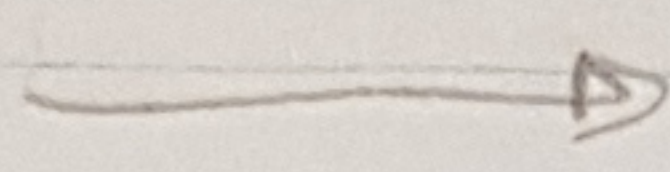
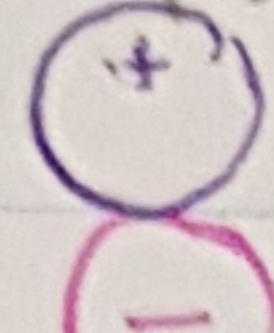
$\sigma_g^+$

b)  $\psi_{2s}^{(l)}(\vec{r}) - \psi_{2s}^{(r)}(\vec{r})$



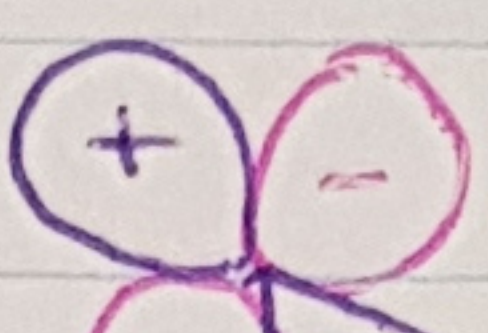
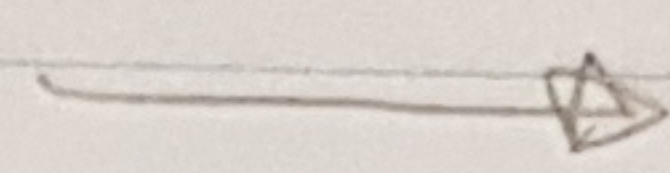
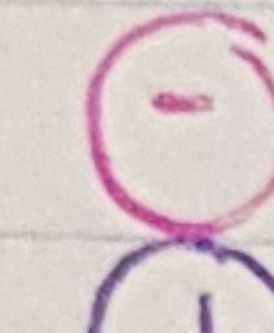
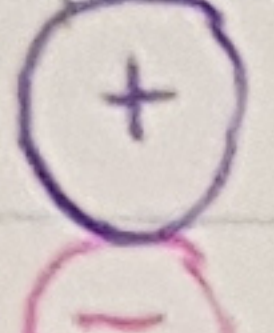
$\sigma_u^+$

c)  $\psi_{2p_z}^{(l)}(\vec{r}) + \psi_{2p_z}^{(r)}(\vec{r})$



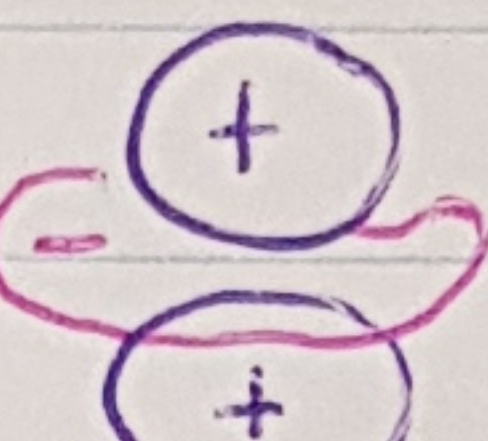
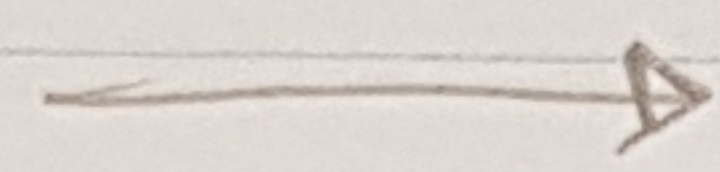
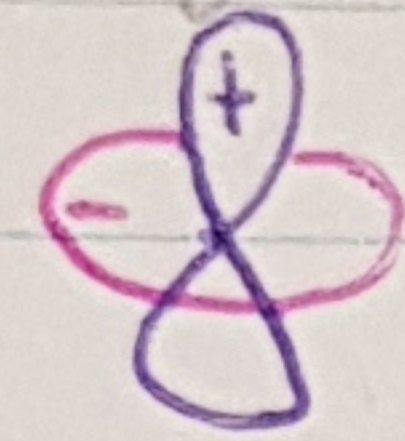
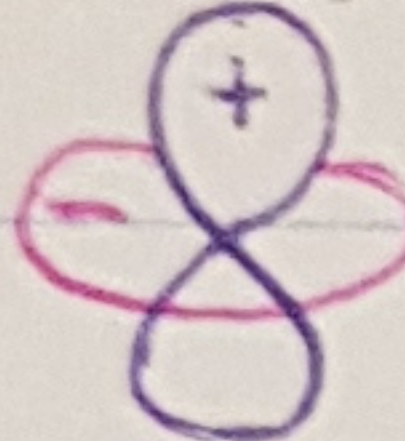
$\pi_u^+$

d)  $\psi_{2p_z}^{(l)}(\vec{r}) - \psi_{2p_z}^{(r)}(\vec{r})$



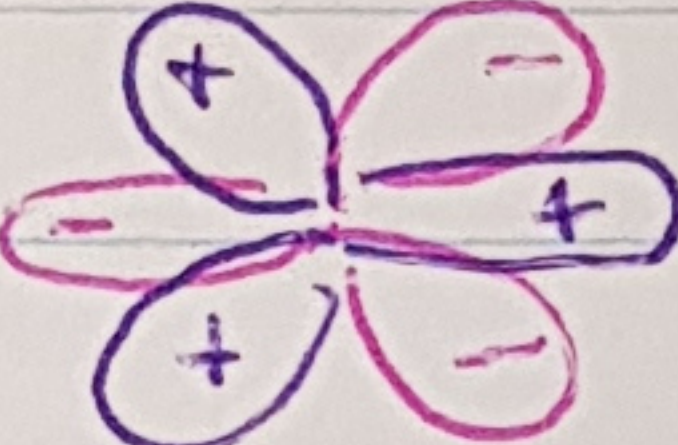
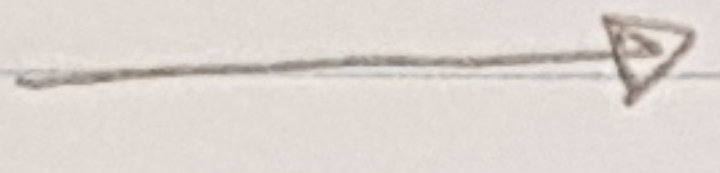
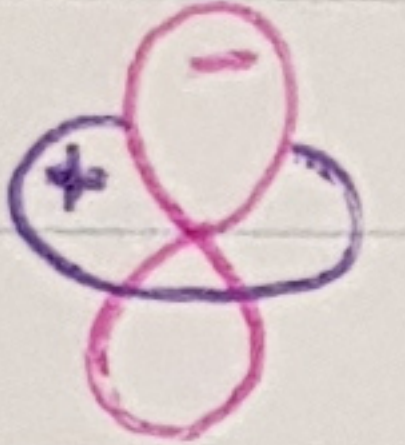
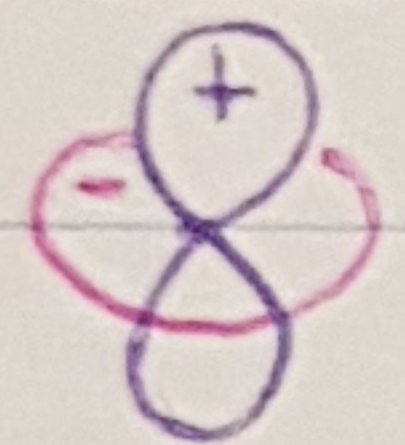
$\pi_g^+$

e)  $\psi_{3d_{z^2}}^{(l)}(\vec{r}) + \psi_{3d_{z^2}}^{(r)}(\vec{r})$



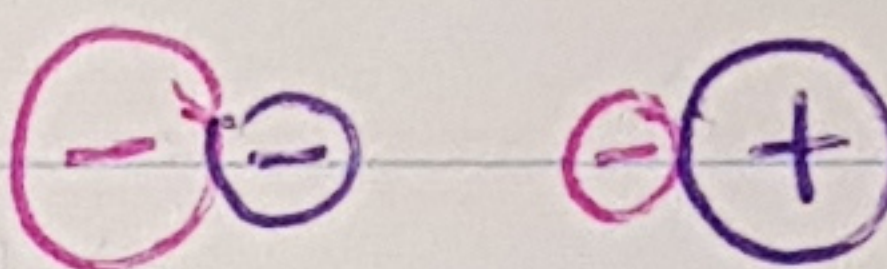
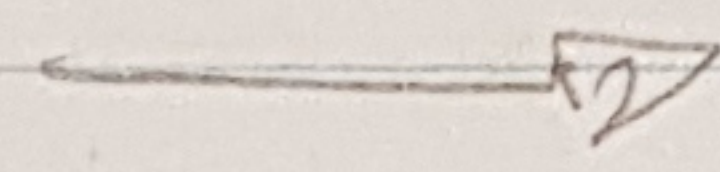
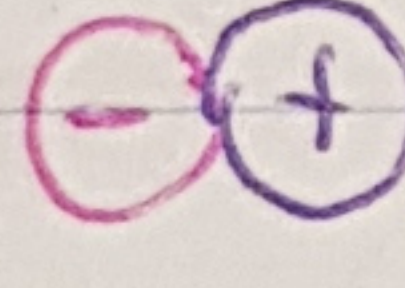
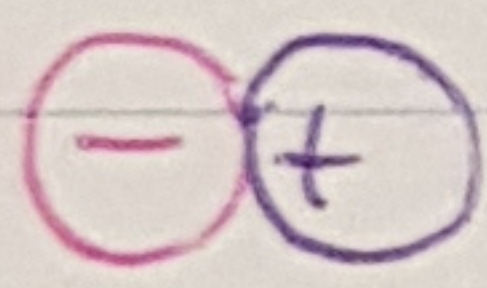
$\sigma_g^+$

f)  $\psi_{3d_{z^2}}^{(l)}(\vec{r}) - \psi_{3d_{z^2}}^{(r)}(\vec{r})$



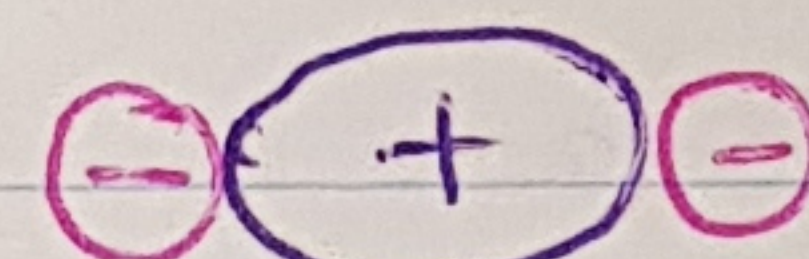
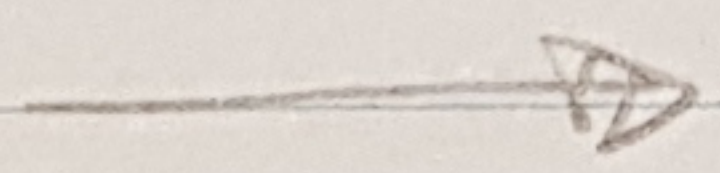
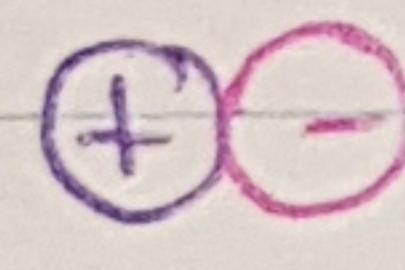
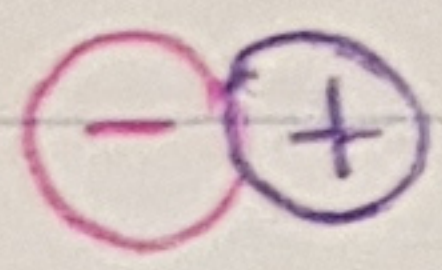
$\sigma_u^+$

g)  $\psi_{2p_z}^{(l)}(\vec{r}) + \psi_{2p_z}^{(r)}(\vec{r})$



$\sigma_u^+$

h)  $\psi_{2p_z}^{(l)}(\vec{r}) - \psi_{2p_z}^{(r)}(\vec{r})$



$\sigma_g^+$

2)  $Li_2^{2+} : (1\sigma_g^+)^2 (1\sigma_u^+)^2 \rightarrow |\phi_{1\sigma_g^+} \alpha \phi_{1\sigma_g^+} \beta \phi_{1\sigma_u^+} \alpha \phi_{1\sigma_u^+} \beta|$

$$= \frac{1}{\sqrt{4!}} \begin{vmatrix} \phi_{1\sigma_g^+}(\vec{r}_1) \alpha(1) & \phi_{1\sigma_g^+}(\vec{r}_1) \beta(1) & \phi_{1\sigma_u^+}(\vec{r}_1) \alpha(1) & \phi_{1\sigma_u^+}(\vec{r}_1) \beta(1) \\ \phi_{1\sigma_g^+}(\vec{r}_2) \alpha(2) & \phi_{1\sigma_g^+}(\vec{r}_2) \beta(2) & \phi_{1\sigma_u^+}(\vec{r}_2) \alpha(2) & \phi_{1\sigma_u^+}(\vec{r}_2) \beta(2) \\ \phi_{1\sigma_g^+}(\vec{r}_3) \alpha(3) & \phi_{1\sigma_g^+}(\vec{r}_3) \beta(3) & \phi_{1\sigma_u^+}(\vec{r}_3) \alpha(3) & \phi_{1\sigma_u^+}(\vec{r}_3) \beta(3) \\ \phi_{1\sigma_g^+}(\vec{r}_4) \alpha(4) & \phi_{1\sigma_g^+}(\vec{r}_4) \beta(4) & \phi_{1\sigma_u^+}(\vec{r}_4) \alpha(4) & \phi_{1\sigma_u^+}(\vec{r}_4) \beta(4) \end{vmatrix}$$

3)  $\psi_{Li^{2+}}(\vec{r}) = -(\frac{1}{3})^{1/2} R_{4,2}(r) Y_{2,-1}(\theta, \phi) + (\frac{2i}{3}) R_{3,2}(r) Y_{2,1}(\theta, \phi) - (\frac{2}{9})^{1/2} R_{1,0}(r) Y_{0,0}(\theta, \phi)$

a)  $E = \{E_4, E_3, E_1\} = \{-\frac{3^2}{2(4)^2}, -\frac{3^2}{2(3)^2}, -\frac{3^2}{2(1)^2}\} = \{-\frac{9}{32}, -\frac{1}{2}, -\frac{9}{2}\}$

b)  $P(E_4) = |\langle -(\frac{1}{3})^{1/2} R_{4,2} Y_{2,-1} | \psi_{Li^{2+}} \rangle| = |(-\frac{11}{3})^{1/2}|^2 = \frac{1}{3}$

$P(E_3) = |\langle (\frac{2i}{3}) R_{3,2} Y_{2,1} | \psi_{Li^{2+}} \rangle| = |(\frac{2i}{3})|^2 = \frac{4}{9}$

$P(E_1) = |\langle (\frac{2}{9})^{1/2} R_{1,0} Y_{0,0} | \psi_{Li^{2+}} \rangle| = |(-\frac{2}{9})^{1/2}|^2 = \frac{2}{9}$

$\langle E \rangle = \frac{3}{9}(-\frac{9}{32}) + \frac{4}{9}(-\frac{1}{2}) + \frac{2}{9}(-\frac{9}{2}) = \frac{-27-64-288}{288} = -1.316$

c)  $L^2 = \{h^2(2)(2+1), h^2(2)(2+1), h^2(0)(0+1)\} = \{6h^2, 6h^2, 0h^2\}$

d)  $P(6h^2) = (\frac{1}{3})^{1/2})^2 + |(\frac{2i}{3})|^2 = \frac{7}{9}$