• Se $H = T + V$ dove $T = -\sum_{a=1}^{Z} \frac{\hbar^2}{2m} \nabla_a^2 + V$

inserito in 3) si ha:

$$\sum_M \sum_f (E_f - E_i) |\langle f | Q_{\sigma M} | i \rangle|^2 =$$

$$\sum_M \Big\{ -\frac{\hbar^2}{2m} \frac{1}{2} \langle i | \sum_a e_a r_a^{\sigma} Y^*_{\sigma M}(\hat r_a) \sum_q \nabla_q^2 \sum_b r_b^{\sigma} Y_{\sigma M}(\hat r_b) e_b$$

$$- \sum_q \nabla_q^2 \sum_a e_a r_a^{\sigma} Y^*_{\sigma M}(\hat r_a) \sum_b e_b r_b^{\sigma} Y_{\sigma M}(\hat r_b)$$

$$+ \sum_a e_a r_a^{\sigma} Y^*_{\sigma M}(\hat r_a) \sum_q \nabla_q^2 \sum_b r_b^{\sigma} Y_{\sigma M}(\hat r_b) e_b$$

$$- \sum_a e_a r_a^{\sigma} Y^*_{\sigma M}(\hat r_a) \sum_b e_b r_b^{\sigma} Y_{\sigma M}(\hat r_b) \sum_q \nabla_q^2 | i \rangle \Big\}$$ 4

• Si ha che:

$$\vec\nabla_a \left(\phi(r_i) Y_{l\mu}(\hat r_i) \right) = \vec\nabla_a \left(\phi(r_a) Y_{l\mu}(\hat r_a) \right) \delta_{ai}$$ 5a

$$\nabla^2 \left(r^l Y_{l\mu}(\hat r) \right) = 0$$ 5b

$$\sum_a \nabla_a^2 | i \rangle = 0 .$$ 5c

• Dimostrazione 5b)

Uso le formule dell'Edmonds:

$$\vec\nabla \phi(r) Y_{l\mu} = -\left(\frac{l+1}{2l+1}\right)^{1/2} \left(\frac{d}{dr} - \frac{l}{r}\right) \phi \vec Y^{\mu}_{l,l+1,1} + \left(\frac{l}{2l+1}\right)^{1/2} \left(\frac{d}{dr} + \frac{l+1}{r}\right) \phi \vec Y^{\mu}_{l,l-1,1}$$

(E 5.9.17)

$$\vec\nabla \cdot \left(\phi \vec Y^{\mu}_{l,l+1,1} \right) = -\left(\frac{l+1}{2l+1}\right)^{1/2} \left(\frac{d}{dr} + \frac{l+2}{r}\right) \phi Y_{l\mu}$$ (E 5.9.21)

$$\vec\nabla \cdot \left(\phi \vec Y^{\mu}_{l\,l-1\,1} \right) = \left(\frac{l}{2l+1}\right)^{1/2} \left(\frac{d}{dr} - \frac{l-1}{r}\right) \phi Y_{l\mu}$$ (E 5.9.23)

con

$$\vec Y^{M}_{l\sigma 1} = \sum_{\mu\sigma} \langle l \mu 1 \sigma | \sigma M \rangle Y_{l\mu} \vec e_{\sigma}$$ (E 5.9.10)