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Singletní a tripletní stavy pro konfiguraci $1s^1 2s^1$ atomu He

Literatura: John P. Löwe, Quantum Chemistry

Kapitola 5: 5-5

5-5 Singletní a tripletní stavy pro konfiguraci $1s^1 2s^1$ atomu He

$$\psi_{s,a}(1,2) = (1/\sqrt{2})\left[1s(1)2s(2) + 2s(1)1s(2)\right](1/\sqrt{2})\left[\alpha(1)\beta(2) - \beta(1)\alpha(2)\right] \quad (5\text{-}42)$$

$$\psi_{a,s}(1,2) = (1/\sqrt{2})\left[1s(1)2s(2) - 2s(1)1s(2)\right] \begin{cases} \alpha(1)\alpha(2) & (5\text{-}43a) \\ (1/\sqrt{2})\left[\alpha(1)\beta(2) + \beta(1)\alpha(2)\right] & (5\text{-}43b) \\ \beta(1)\beta(2) & (5\text{-}43c) \end{cases}$$

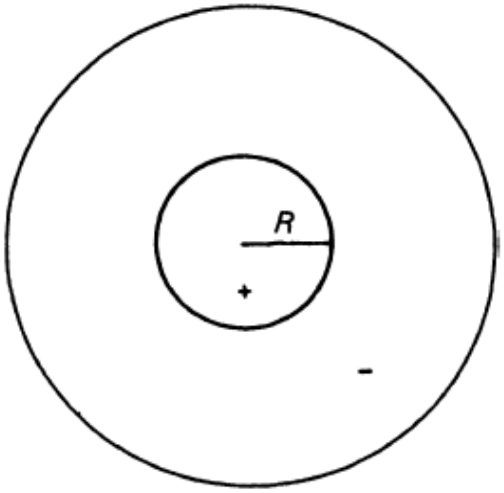

Figure 5-2 ▶ The function produced by multiplying together hydrogenlike 1s and 2s orbitals. R is the radius of the spherical nodal surface.

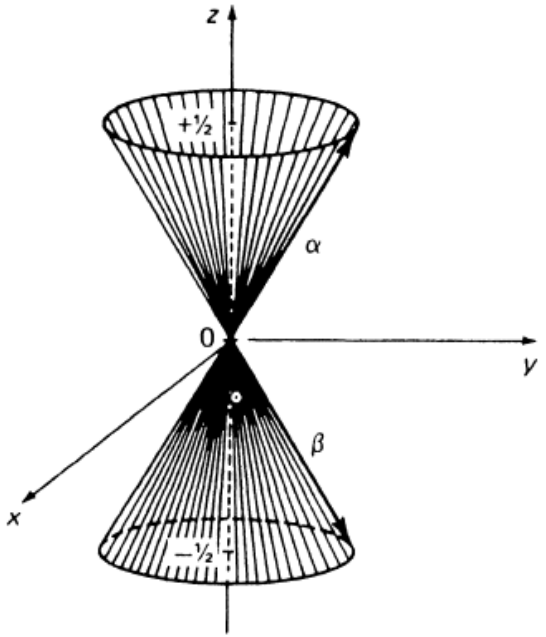

Figure 5-3 ▶ The angular momentum vectors for α and β precess around the magnetic field axis z. The z components of these vectors are constant and have values of $+\frac{1}{2}$ and $-\frac{1}{2}$ a.u. respectively.

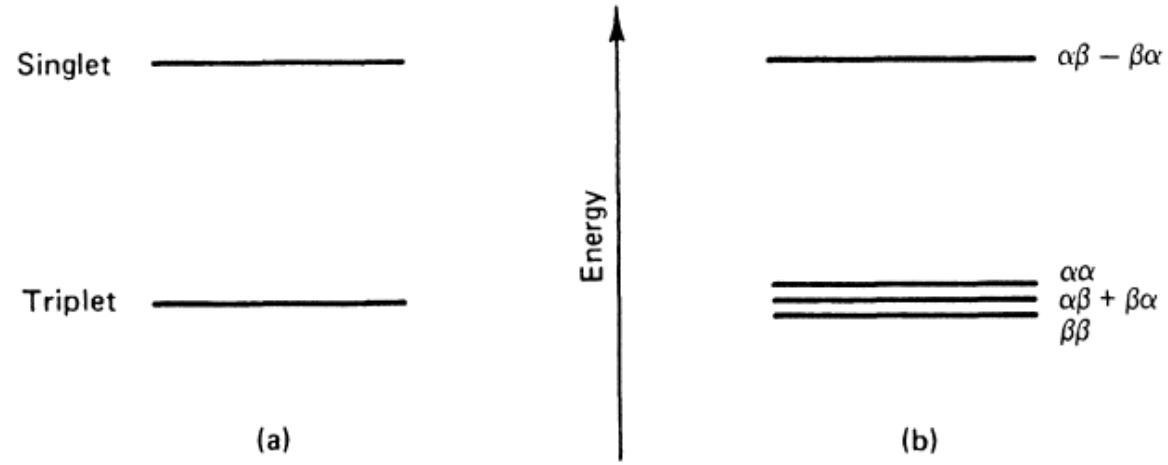

Figure 5-4 ▶ Energy levels for singlet and triplet levels of 1s2s helium in (a) absence, and (b) presence of an external magnetic field.