Atomic Magnetism

Types of magnetism in atoms

$$\vec{M} = \frac{\chi}{\mu_0} \vec{B}$$

χ = susceptibility

μ_0 = permeability

Paramagnetism: $\chi > 0$ applied field results in magnetic moment aligned with field

Diamagnetism $\chi < 0$ magn. moment opposes applied field

$$H = H_0 + \underbrace{\mu_B \vec{B}(\vec{\ell} + g\vec{S})}_{\substack{\text{paramagnetic term} \\ \text{(Zeeman term)}}} + \underbrace{\frac{e^2}{2m}\vec{A}^2}_{\substack{\text{diamagnetic} \\ \text{term}}}$$

with $\nabla \times \vec{A} = \vec{B}$

$$\vec{\mu}_B \vec{B} (\vec{l} + g\vec{s}) = g_{eff} \mu_B \vec{B} \vec{j}$$

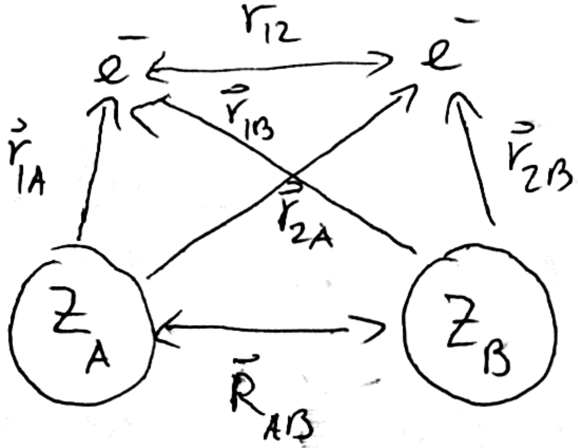
if $\vec{J} = 0 \rightarrow$ diamagnetic

if $\vec{J} \neq 0 \rightarrow$ paramagnetic

Diatomic Molecules

W. Demtroeder, "Atoms, Molecules and Photons", Chp 9.

H_2



in H_2

$Z_A = Z_B = 1$

$M_A = M_B = m_{p^+}$

$$H\Psi(r_1, r_2, R_A, R_B) = E\Psi(\sim)$$

$$H = \underbrace{-\frac{\hbar^2}{2M_A}\nabla_A^2 - \frac{\hbar^2}{2M_B}\nabla_B^2}_{T_N} \underbrace{- \frac{\hbar^2}{2m_e}\nabla_1^2 - \frac{\hbar^2}{2m_e}\nabla_2^2}_{T_{e^-}}$$

$$\underbrace{-\frac{Z_A e^2}{4\pi\varepsilon_0 r_{1A}} - \frac{Z_B e^2}{4\pi\varepsilon_0 r_{1B}} - \frac{Z_A e^2}{4\pi\varepsilon_0 r_{2A}} - \frac{Z_B e^2}{4\pi\varepsilon_0 r_{2B}}}_{V_{Ne^-}}$$

$$+ \frac{e^2}{4\pi\varepsilon_0 r_{12}} + \frac{Z_A Z_B e^2}{4\pi\varepsilon_0 R_{AB}}$$

in Hartree units:

$$H = \frac{1}{2M_A}\nabla_A^2 - \frac{1}{2M_B}\nabla_B^2 - \frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2$$

$$- \frac{Z_A}{r_{1A}} - \frac{Z_B}{r_{1B}} - \frac{Z_A}{r_{2A}} - \frac{Z_B}{r_{2B}} + \frac{1}{r_{12}} + \frac{Z_A Z_B}{R_{AB}}$$

because $M_N \gg m_e \rightarrow T_N \approx 0$

$\rightarrow$ fix nuclei in place

$$\Psi(r_1, r_2, R_A, R_B) = \Psi_e^{R_{AB}}(r_1, r_2)\, \Psi_N(R_A, R_B)$$

(Born - Oppenheimer Approximation)

$$H_{elec}\Psi_e = E_e(R_A, R_B)\Psi_e$$