LECTURE #7

Note Title 9/17/2008

- MAGNETIC PROPERTIES
- FULL HAMILTONIAN ATOM/ION WITH $\vec{H} \parallel z$
- $\mu_B(\vec{L} + g_0\vec{S})\cdot\vec{H} + \alpha H^2 \sum_i (x_i^2 + y_i^2)$ (I, II)

① FILLED SHELLS $\Rightarrow L = 0, S = 0$

ONLY II IS PRESENT

POSITIVE ENERGY SHIFT $\propto H^2$

$$\chi_M = -\frac{1}{V}\frac{\partial^2 E(H)}{\partial H^2} < 0$$

SMALL DIAMAGNETISM

② $L \neq 0$ / $S \neq 0$

I IS IMPORTANT AND "STRONG"

PARTIALLY FILLED SHELLS

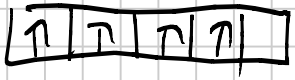
PARAMAGNETISM $\chi_M > 0$

$$\chi_M(T) \sim \frac{(\mu_B g)^2}{3} \frac{J(J+1)}{k_B T}$$

CURIE'S LAW STRONG FOR TRANSITION METALS (Mn^{2+}) RARE EARTH IONS

f ORBITALS PARTIALLY FILLED

(3) $L = S$ SHELL LESS THAN ½ FILLED



$\Rightarrow J = 0$

$\Rightarrow$ I TERM IS 0

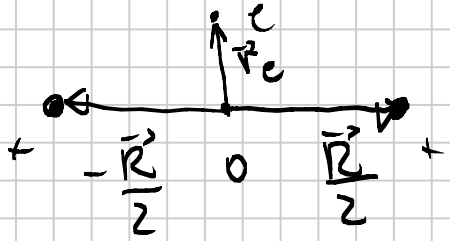
WEAK MAGNETIC PROPERTIES

2° ORDER PERTURBATION THEORY

$\Rightarrow$ WEAK PARAMAGNETISM (VAN VLECK PARAMAGNETISM)

MOLECULES

H_2^+ MOLECULE



$\vec{r}_e$ POSITION OF e

$\vec{R}$ RELATIVE POSITION OF 2 PROTONS

$$\psi(\vec{r}_e, \vec{R})$$

$$\left(-\frac{\hbar^2 \nabla_R^2}{2\mu_p} - \frac{\hbar^2 \nabla_r^2}{2m_e} + \underbrace{\frac{e^2}{|\vec{R}|}}_{V_{pp}} \underbrace{- \frac{e^2}{\left|\vec{r}_e + \frac{\vec{R}}{2}\right|} - \frac{e^2}{\left|\vec{r}_e - \frac{\vec{R}}{2}\right|}}_{V_{pe}} \right) \psi(r_e, R) = E\,\psi(r_e, R)$$

$$\mu_p \sim \frac{m_{PROTON}}{2} \gg m_e$$

BORN - OPPENHEIMER APPROXIMATION

$$\psi(\vec{r}_e, \vec{R}) = \psi_p(\vec{R})\,\psi_e^R(r_e) \longrightarrow \psi_e(r)$$ DEPENDS PARAMETRICALLY ON R

① CLAMP THE 2 PROTONS AT FIXED DISTANCE $\vec{R}$

$$\left[-\frac{\hbar\nabla_r^2}{2m} + \underline{V_{pp}(R)} + V_{pe}(r,R)\right] \cancel{\psi_p(R)}\;\psi_e(r) = E\,\cancel{\psi_p(R)}\,\psi_e(r)$$

SINGLE ELECTRON PROBLEM

$$\downarrow$$

$$\psi_{\ell,m}^R(r) \qquad E_{\ell,m}(R)$$

M LABLES THE EIGENSTATES OF THE SCHROEDINGER EQ.

②

I WANT TO RE-CONSIDER KINETIC ENERGY

OF PROTONS

$$\frac{\nabla_R^2}{\mu_p}\left(\psi_p(\vec{R})\,\psi_e^R(\vec{r}_e)\right)$$

$$\psi_e^R\,\nabla_R^2\,\psi_p(R)$$

$$\vec{\nabla}_R\psi_e^R \cdot \vec{\nabla}_R\psi_p(R)$$

$$\psi_p(R)\,\nabla_R^2\,\psi_e^R(r_e)$$

$\psi_p(R)$ VERY LOCALIZED

$\psi_e^R(r)$ DELOCALIZED $\Rightarrow$ DEPENDS WEAKLY ON THE RELATIVE POSITION OF PROTONS

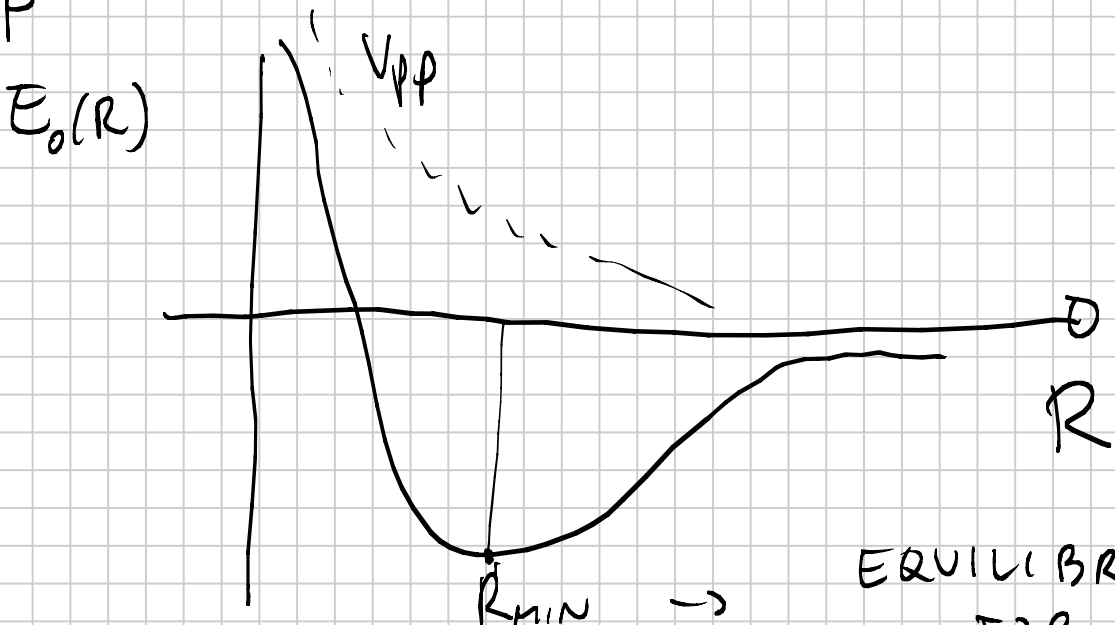
$$\nabla_R\,\psi_e^R(r) \ll 1$$

$$-\frac{\hbar^2}{2\mu_p}\psi_e^R(r)\nabla_R^2\psi_p(\vec{R}) + \left[-\frac{\hbar^2}{2m_e}\nabla_r^2 + V_{pp}(R) + V_{ep}(R)\right]\psi_e^R(r)\psi_p(R) = E\psi_e\psi_p$$

$$E_0(R)\ \psi_{e_0}^R(r)$$

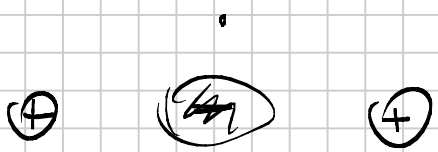
ENERGY OF e AT FIXED R IS AN EFFECTIVE POTENTIAL FOR THE PROTONS

$$-\frac{\hbar^2}{2\mu_p}\nabla_R^2\psi_p(R) + \underbrace{V(R)}_{=E_0(R)}\psi_p(R) = E_p\,\psi_p(R)$$

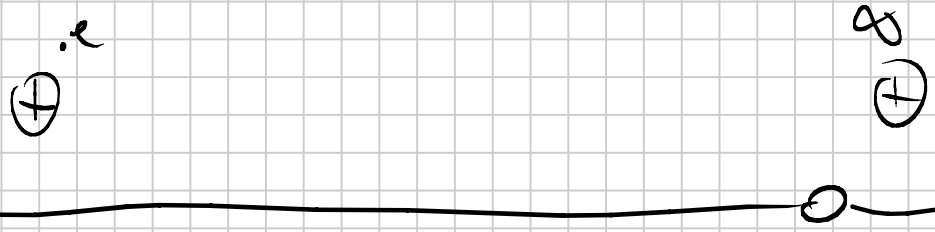


$\rightarrow$ EQUILIBRIUM POSITION FOR THE MOLECULE

COVALENT BONDING



HAS LOWER ENERGY THAN



GROUP WORK

LAST QUESTION # 5

VARIATIONAL 2-BODY PROBLEM.