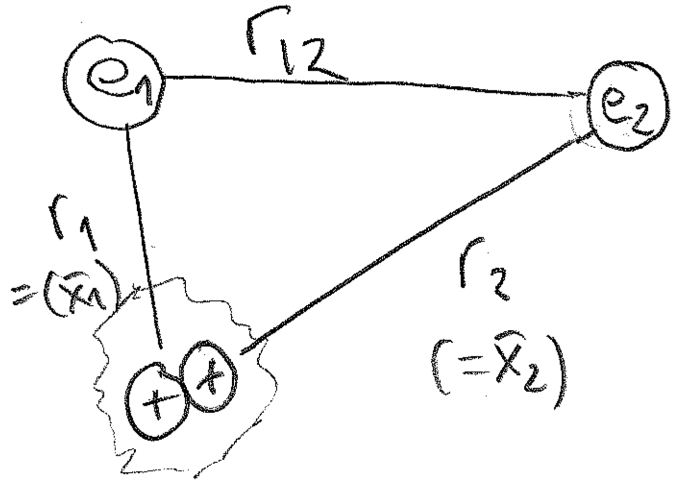
HELIUM ATOM

- 2 ELECTRONS, IDENTITY QUESTIONS ARISE

$$\boxed{H = \frac{\bar{p}_1^2}{2m} + \frac{\bar{p}_2^2}{2m} - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{r_{12}}}$$

- WITHOUT INTERACTION TERM $\frac{e^2}{r_{12}}$ EXACT SOLUTION SEPARABLE AND WELL KNOWN: $\Psi_{He} = \Psi_H(Z=2, r_1, \bar{p}_1)\,\Psi_H(Z=2, r_2, \bar{p}_2)$



LET US CONSIDER A STATE IN WHICH ONE ELECTRON IS IN THE GROUND STATE AND THE OTHER IN STATE $\psi_{n\ell m}$

WAVE FUNCTION READS

$$\varphi(\bar{x}_1, \bar{x}_2)_{SPAT} = \frac{1}{\sqrt{2}}\left[\psi_{100}(\bar{x}_1)\psi_{n\ell m}(\bar{x}_2) \pm \psi_{100}(\bar{x}_2)\psi_{n\ell m}\right]$$

+ SIGN SPIN SINGLET ← (ASYM)

− SIGN SPIN TRIPLET ← (SYMM)

<u>GROUND STATE:</u>

$$\varphi = \frac{1}{\sqrt{2}}\left[\psi_{100}(x_1)\psi_{100}(x_2) + \psi_{100}\psi_{100}\right]$$

NECESSARILY SPACE-SYMMETRIC

→ $\chi_{GROUND} = \chi_1$ = SPIN SINGLET

$$\psi_{100}(\bar{x}_1)\psi_{100}(\bar{x}_2)\chi_1 = \frac{Z^3}{\pi a_0^3} e^{-Z(r_1+r_2)/a_0}\chi_1 \quad (*)$$

THIS GIVES GROUND STATE ENERGY

$$E = 2 \cdot 4\left(\frac{-e^2}{2a_0}\right)$$ WHICH IS

30% TOO LARGE, BUT WE IGNORED MUTUAL INTERACTION

LET US TAKE (*) AS UNPERTURPED ψ AND CALCULATE THE CORRECTION (1ST ORDER) BY TAKING THE INTERACTION TERM AS A PERTURBATION

$$\Delta_1^n = E_n^{(1)} - E_n^{(0)} = \langle n|V|n\rangle$$

$$= \int \langle n|V|x_1\rangle\langle x_1|n\rangle dx_1$$

$$= \iint \langle n|x_2\rangle \underset{(3)}{\langle x_2|V|x_1\rangle} \psi_n(x_1)\, dx_1 dx_2$$

$$= \iint \psi_n^*(x_2)\langle x_2|V|x_1\rangle \psi_n(x_1)\,dx_1 dx_2$$

$$= \frac{Z^6}{\pi^2 a_0^6}\int e^{-2Z(r_1+r_2)/a_0}|\chi_1|^2 \frac{e^2}{r_{12}}\,d^3x_1 d^3x_2$$

THIS IS ANALYTICALLY INTEGRABLE

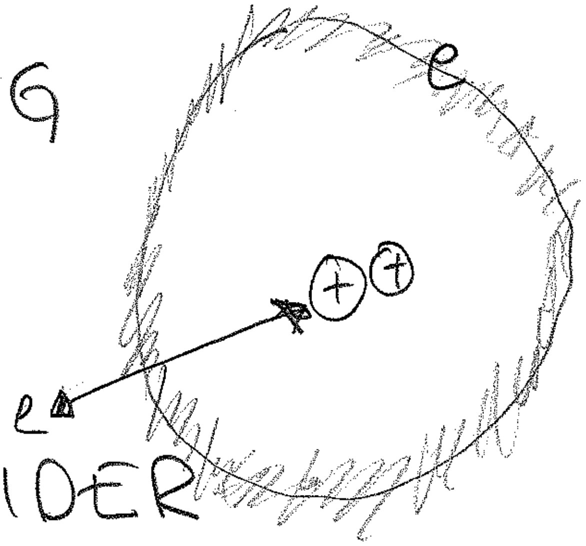
$$\Delta_1^{n=1} = \frac{5}{2}\left(\frac{e^2}{2a_0}\right)$$

THUS $E_{n=1}^{n=1} = \left(-8+5/2\right)\left(\frac{e^2}{2a_0}\right) = -74,8\,eV$

EXPERIMENTALLY $E_{n=1} = -78,8\,eV$

- VARIATIONAL METHOD CAN BE USED TO GET IMPROVEMENT

NAMELY, ELECTRONS ARE SCREENING EACH OTHER



LET US CONSIDER THE EFFECTIVE CHARGE SEEN BY THE ELECTRONS ($Z_{eff} < +2$) AS A VARIATIONAL PARAMETER

· TRIAL WAVE FUNCTION:

$$\frac{Z_{eff}^3}{\pi a_0^3} e^{-Z_{eff}(r_1+r_2)/a_0} = \psi(\bar{x}_1, \bar{x}_2 | \bar{0}\rangle)$$

$$\bar{H} = \langle \bar{0} | \frac{\bar{p}_1^2 + \bar{p}_2^2}{2m} | \bar{0} \rangle + \langle \bar{0} | \frac{Z_{eff} e^2}{r_1} + \frac{Z_{eff} e^2}{r_2} | \bar{0} \rangle$$

$$+ \langle \bar{0} | \frac{e^2}{r_{12}} | \bar{0} \rangle$$

EVALUATION LEADS

$$\left(\frac{e^2}{a_0}\right)\left[\frac{2Z_{eff}^2}{2} - 2ZZ_{eff} + \frac{5}{8}Z_{eff}\right] \equiv 0$$

$\rightarrow Z_{eff} = 1,69$

$\rightarrow E_{n=1} = -77,5\,eV \approx -78,8\,eV$

LET US CONSIDER THE $\frac{e^2}{r_{12}}$ TERM, SUCH THAT

$$\psi = \psi_{100}^{(x_1)}\psi_{n\ell m}^{(x_2)} \pm \psi_{n\ell m}^{(x_2)}\psi_{100}(x_1)$$

WE NEED TO INTEGRATE OVER THE PROBABILITY $\psi^*\psi\, d^3x_1\, d^3x_2$ THE $\frac{e^2}{r_{12}}$ TERM TO GET THE ENERGY CORRECTION $E = E_{100} + E_{n\ell m} + \Delta E$

WE SAW BEFORE

$$|\Psi| = \frac{1}{2}\left(|\psi_{100}(x_1)|^2 |\psi_{nlm}(x_2)|^2 + |\psi_{nlm}(x_1)|^2 |\psi_{100}(x_2)|^2\right.$$

$$\left. + \frac{2}{2} \mathrm{Re}\left[\psi_{100}^*(x_1)\psi_{nlm}^*(x_2)\psi_{100}(x_2)\psi_{nlm}(x_1)\right]\right)$$

NOW THE FIRST 2 TERMS

ARE SYMMETRICAL

$$\int \psi_{100}^*(x_1)\frac{e^2}{r_{12}}\psi_{nlm}(x_2)\,dx_1\,dx_2$$

WHEN INTEGRATED OVER

ALL SPACE

$$\rightarrow \left\langle \frac{e}{r_{12}} \right\rangle = I \pm J$$

$$I = \int d^3x_1 \int d^3x_2 \, |\psi_{100}(x_1)|^2 |\psi_{nlm}(x_2)|^2$$

= DIRECT INTEGRAL

EXCHANGE DENSITY TERM

J COMES WITH

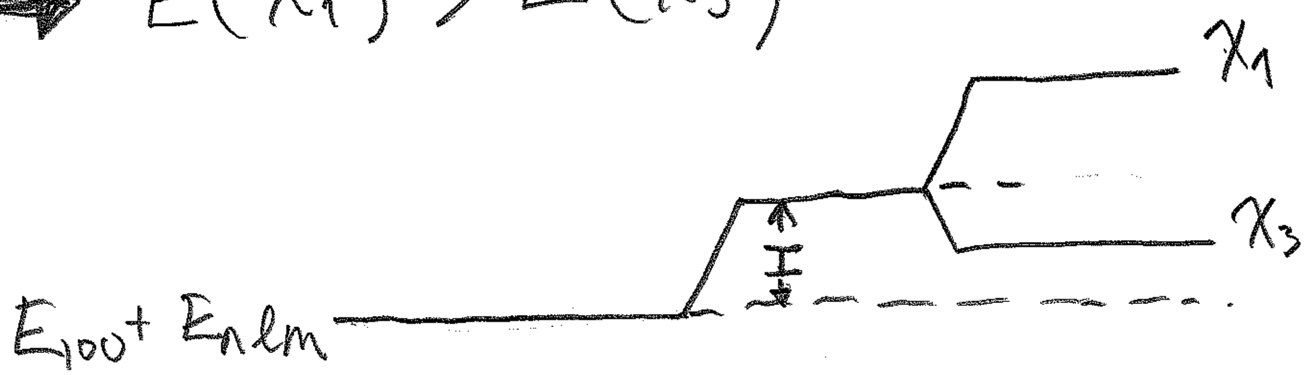
+ SIGN FOR SPIN SINGLET

– SIGN FOR SPIN TRIPLET

$I > 0$ ALWAYS

$J > 0$ ALSO

$\Rightarrow E(\chi_1) > E(\chi_3)$



INTERPRETATION:

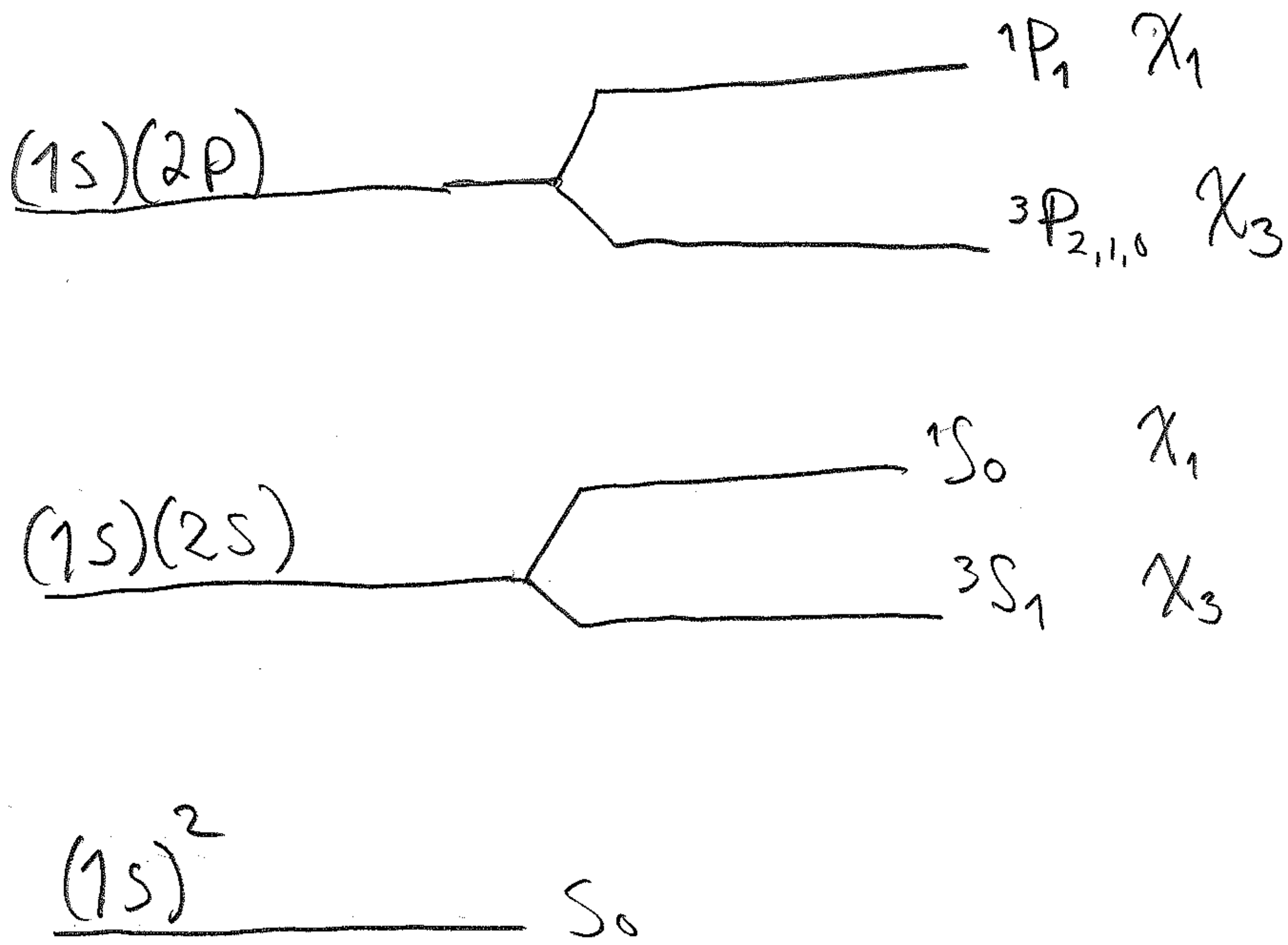
IN χ_1 (ASYM) $\rightarrow \psi$ (SYMM)

$\rightarrow$ ELECTRONS TEND TO COME CLOSER TO EACH OTHER : $E_{COULOMB}$ LARGER

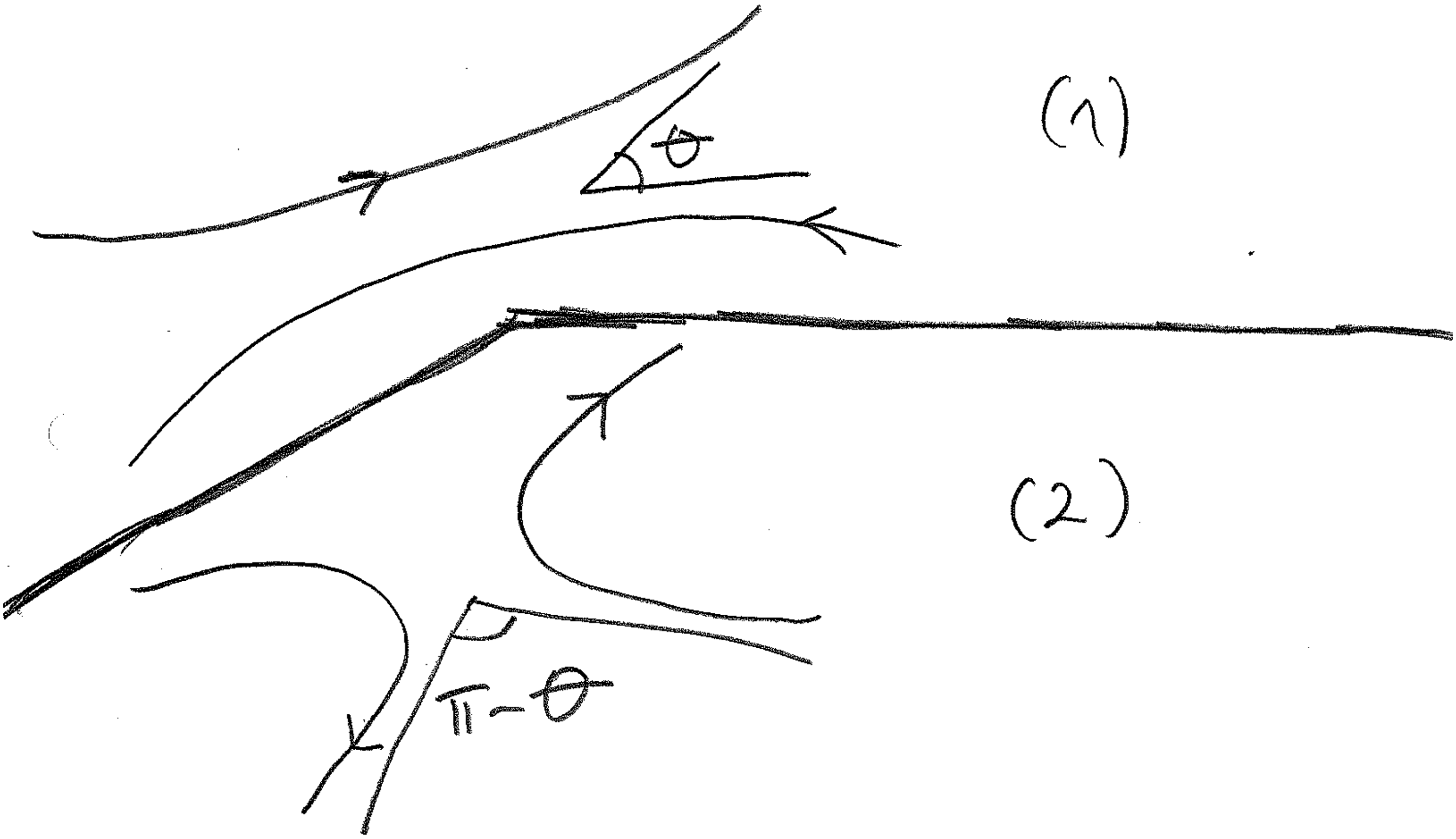
χ_1: PARAHELIUM

χ_3: ORTOHELIUM

GROUND STATE: PARA ONLY



SCATTERING OF 2 IDENTICAL PRTCLS



• 2 SPINLESS BOSONS

• ψ SYMMETRIC: (IN CM-FRAME:)

$$\psi(\bar{r}) = e^{i\bar{k}\cdot\bar{r}} + e^{-i\bar{k}\cdot\bar{r}} + [f(\theta)+f(\pi-\theta)]\frac{e^{ik\cdot r}}{|\bar{r}|}$$

• $f(\theta)+f(\pi-\theta)$ = SCATTERING AMPLITUDE = SUM OF THE 2 POSSIBLE GRAPHS

DIFFERENTIAL CROSS-SECTION

$$\frac{d\sigma}{d\Omega} = |f(\theta) + f(\pi - \theta)|^2 \quad \text{(BOSONS)}$$

$$= |f(\theta)|^2 + |f(\pi-\theta)|^2 + 2\,\mathrm{Re}\left[f(\theta) f^*(\pi-\theta)\right]$$

FOR DISTINQUISHABLE PARTICLES THERE WOULD NOT BE ANY INTERFERENCE TERM, INSTEAD

$$\frac{d\sigma}{d\Omega} = P(\text{graph } 1) + P(\text{graph } 2)$$

$$= |f(\theta)|^2 + |f(\pi-\theta)|^2 \quad \text{(CLASSICAL)}$$

SIMILAR CONSIDERATION, FOR FERMIONS

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |f(\pi-\theta)|^2 - 2\,\mathrm{Re}\left[f(\theta) f^*(\pi-\theta)\right]$$

(FERMION)

CONSIDER 90° SCATTERING

$$\left.\frac{d\sigma}{d\Omega}\right|_B = |f(\pi/2)|^2 + |f(\pi/2)|^2 + 2|f(\pi/2)|^2$$

$$= \underline{\underline{4A}}$$

$$\left.\frac{d\sigma}{d\Omega}\right|_{CLASS} = |f(\pi/2)|^2 + |f(\pi/2)|^2 = \underline{\underline{2A}}$$

$$\left.\frac{d\sigma}{d\Omega}\right|_F = |f(\pi/2)|^2 + |f(\pi/2)|^2 - 2|f(\pi/2)|^2 = \underline{\underline{0}}$$

- ALL ABOVE HAVE BEEN VERIFIED EXPERIMENTALLY