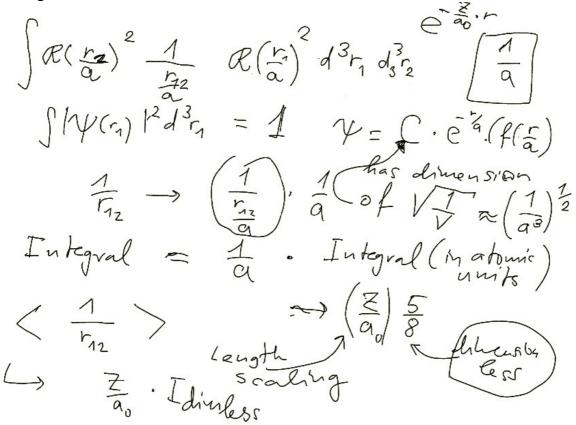
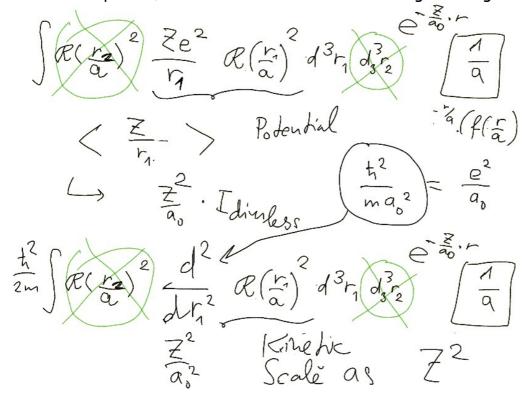
## Lecture Thursday 6. September 2007

Topics Helium atom part 4: Ground State; Variational Methods

Scaling - how to transform to dimensionless



How do the repulsion, nuclear atraction and kinetic energies change with Z



Variational methods

ariational methods Variational methods, first time (Y(X) | H IY(X) > -> H(X) function of parameter X > physidea -> Screening 23 ez Z-screen (Horexample) In helinn

General on variational method; Expansion - analogy to vector spaces

$$\Psi(\vec{r}) = \sum_{i} c_{i} q_{i}(\vec{r})$$
  
 $= \frac{i}{2} q_{i} are \left[ H(q_{i} = E_{i} q_{i} \right]$   
Soluhous of H form a  
complete set  
Nectors in 3-div space  
 $R = xe_{x} + ge_{y} + ze_{z}(ANY)$  Libeas "Spaces"  
Genevalizedous  
All Hungs we rando with  
coordinates  
we can generalize to "functions"  
Sdim space... 3 base vectors  
Functional space  
 $Q = C_{i} q_{i} (c_{i}' components)$ 

General proof; Expansion in eigenstates; Complete set of basis functins;

$$\begin{split} \psi(\vec{r}) &= \sum_{i} c_{i} \varphi_{i}(\vec{r}) \\ &= \frac{\lambda}{2} \varphi_{i}(\vec{r}) \\ \varphi_{i}(\vec{r}) \varphi_{i}(\vec{r}) d^{3}r = 1 \\ \int \varphi_{i}(\vec{r}) \varphi_{i}(\vec{r}) d^{3}r = 0 \quad R_{2r} i \neq 1 \\ f(\alpha) &= \int \psi_{\alpha}(r_{n}) H \psi_{\alpha}(\dots) d \dots \\ H(\alpha) &= \int \psi_{\alpha}(r_{n}) H \psi_{\alpha}(\dots) d \dots \\ H(\alpha) &= \sum_{i} \sum_{i} \int c_{i}^{*} \varphi_{i}^{*} H c_{i} \varphi_{i} d^{*}r \dots \\ f(\alpha) &= \sum_{i} \sum_{i} \int c_{i}^{*} c_{j}^{*} E_{i} \varphi_{i} d^{*}r \dots \\ \int \varphi_{\alpha}(\alpha) = \sum_{i} \sum_{i} \int c_{i}^{\alpha} c_{j}^{*} E_{i} \varphi_{i} d^{*}r \dots \\ \int \varphi_{\alpha}(\alpha) = \sum_{i} \sum_{i} \int c_{i}^{\alpha} c_{j}^{*} E_{i} \varphi_{i} d^{*}r \dots \\ \int \varphi_{\alpha}(\alpha) = \sum_{i} |e_{i}^{\alpha}|^{2} E_{i} A^{*}r \dots \\ \int \sum_{i} |e_{i}^{\alpha}|^{2} E_{i} A^{*}r \dots \\ \int \sum_{i} |e_{i}^{\alpha}|^{2} E_{i} E_{i} E_{i} A^{*}r \dots \\ \int \sum_{i} |e_{i}^{\alpha}|^{2} E_{i} E_{i} E_{i} A^{*}r \dots \\ \int \sum_{i} |e_{i}^{\alpha}|^{2} E_{i} E_{i} E_{i} A^{*}r \dots \\ \int \sum_{i} |e_{i}^{\alpha}|^{2} E_{i} E_{i} E_{i} E_{i} A^{*}r \dots \\ \int \sum_{i} |e_{i}^{\alpha}|^{2} E_{i} E_{i} E_{i} A^{*}r \dots \\ \int \sum_{i} |e_{i}^{\alpha}|^{2} E_{i} E_{i} E_{i} A^{*}r \dots \\ \int \sum_{i} |e_{i}^{\alpha}|^{2} E_{i} E_{i} E_{i} E_{i} A^{*}r \dots \\ \int \sum_{i} |e_{i}^{\alpha}|^{2} E_{i} E_{i} E_{i} E_{i} A^{*}r \dots \\ \int \sum_{i} |e_{i}^{\alpha}|^{2} E_{i} E_{i} E_{i} E_{i} E_{i} A^{*}r \dots \\ \int \sum_{i} |e_{i}^{\alpha}|^{2} E_{i} E_{i$$

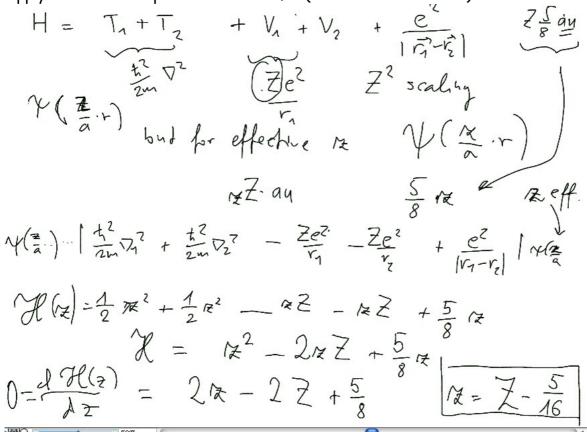
The Ground state is smallest in energy

$$I \text{ Leep Ma} = \Lambda \quad \int c_{i}^{*} c_{j} E_{j} q_{i} q_{j} d \dots$$

$$J \text{ Hange Ma} = \Lambda \quad \int c_{i}^{*} c_{j} E_{i} q_{i} q_{j} d \dots$$

$$J \text{ Hange Ma} = \sum_{i} |e_{i}^{\alpha}|^{2} E_{i} A^{\prime\prime\prime} + E_{i} \sum_{i} (\sum_{i} |e_{i}^{\alpha}|^{2} + E_{i} \sum_{i} \sum_{$$

Apply this to our expectation value of z (lower case z variable)



Here we evaluate the actual H(z) with z=Z - 5/16

$$\begin{aligned} \mathcal{H}(z) &= z^{2} - 2z Z + \frac{5}{8} rz \\ rz - Z - \frac{1}{2} \frac{5}{8} \\ \frac{Z^{2}}{r} - \frac{5}{2} Z + \left(\frac{1}{2} \frac{5}{8}\right)^{2} - 2ZZ \\ -\frac{2}{7} \frac{5}{9}^{2} + \frac{5}{8} Z \\ -\frac{2}{7} - \frac{7}{4} \frac{5}{9}^{2} + \frac{5}{8} Z \\ \frac{7}{2} - \frac{7}{2} \frac{1}{8} \frac{5}{8} Z + \frac{5}{8} Z - \frac{1}{2} \left(\frac{5}{8}\right)^{2} \\ \frac{7}{4} \frac{1}{2} \frac{1}{2} \frac{7}{7} - \frac{2e^{2}}{r_{1}} + \frac{e^{2}}{r_{2}} - \frac{7}{2} \frac{e^{2}}{r_{1}} \\ \frac{7}{2} \frac{1}{r_{1}} \frac{1}{r_{1}} \frac{1}{r_{1}} \frac{1}{r_{1}} \frac{1}{r_{1}} \frac{1}{r_{1}} \frac{1}{r_{2}} \frac{1}{r_{2}} - \frac{2e^{2}}{r_{1}} + \frac{e^{2}}{r_{2}} \frac{1}{r_{1}} \frac{1}{r_{1}} \frac{1}{r_{1}} \frac{1}{r_{1}} \\ \frac{7}{4} \frac{1}{2} \frac{1}{r_{2}} \frac{1}{r_{2}} \frac{2}{r_{2}} - \frac{2e^{2}}{r_{1}} + \frac{5}{8} rz \\ \frac{7}{4} \frac{1}{r_{1}} \frac{1}{r_{2}} \frac{1}{r_{2}}$$

How to make variation more efficient

Other variational methods  

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