

The trial wavefunction for the Helium atom is:

$$\Psi_T(\vec{r}_1, \vec{r}_2) = \exp \left[-2r_1 - 2r_2 + \frac{r_{12}}{2(1 + \alpha r_{12})} \right], \quad (1)$$

where \vec{r}_1 and \vec{r}_2 denote the vectorial positions of the two electrons, $r_{12} = \|\vec{r}_1 - \vec{r}_2\|$, and α the variational parameter. The local energy is given by the expression:

$$E_L(\vec{r}_1, \vec{r}_2) = -4 + (\hat{r}_1 - \hat{r}_2)(\vec{r}_1 - \vec{r}_2) \frac{1}{r_{12}(1 + \alpha r_{12})^2} - \frac{1}{r_{12}(1 + \alpha r_{12})^3} - \frac{1}{4(1 + \alpha r_{12})^4} + \frac{1}{r_{12}}, \quad (2)$$

where \hat{r}_1 and \hat{r}_2 are the normalised unit vectors in the respective directions of \vec{r}_1 and \vec{r}_2 .

To update the variational parameter α , we need to compute:

$$\ln(\Psi_T) = -2r_1 - 2r_2 + \frac{r_{12}}{2(1 + \alpha r_{12})} \implies \frac{d \ln(\Psi_T)}{d\alpha} = -\frac{r_{12}^2}{2(1 + \alpha r_{12})^2}. \quad (3)$$

We then get that α is updated accordingly to the expression $\alpha_{new} = \alpha_{old} - \gamma \left(\frac{dE}{d\alpha} \right)_{old}$, where

$$\frac{dE}{d\alpha} = 2 \left(\langle E_L \rangle \left\langle \frac{r_{12}^2}{2(1 + \alpha r_{12})^2} \right\rangle - \left\langle E_L \cdot \frac{r_{12}^2}{2(1 + \alpha r_{12})^2} \right\rangle \right). \quad (4)$$

Jos Thijssen found in his book the values shown in the table [1](#).

Figure 1: $\langle E \rangle$ and $\text{Var}(\langle E \rangle)$ in terms of the variational parameter α .

Helium atom		
α	$\langle E \rangle$	$\text{var}(\langle E \rangle)$
0.05	$-2.8713(4)$	$0.1749(2)$
0.075	$-2.8753(4)$	$0.1531(2)$
0.10	$-2.8770(3)$	$0.1360(2)$
0.125	$-2.8780(4)$	$0.1223(2)$
0.15	$-2.8778(3)$	$0.1114(2)$
0.175	$-2.8781(3)$	$0.1028(2)$
0.20	$-2.8767(4)$	$0.0968(2)$
0.25	$-2.8746(10)$	$0.0883(2)$