

The local energy for the helium molecule trial wavefunction. The trial wavefunction has the form

$$\Psi_{(1,2)} = e^{-2r_1} e^{-2r_2} e^{\frac{r_{12}^2}{2(1+\alpha r_{12})}}.$$

We abbreviate this as follows

$$\Psi_{(1,2)} = \phi_1 \phi_2 f_{12}$$

where $\phi_1 = e^{-2r_1}$ etcetera.

Now we use the following rules

$$\nabla_1 \phi_1 = \hat{1} \phi_1',$$

where $\phi_1'(1) = \partial \phi_1 / \partial r_1$, and $\hat{1}$ is a unit vector along r_1 .

Furthermore

$$\nabla^2 \phi_1 = \frac{2}{r_1} \phi_1' + \frac{\partial^2 \phi_1}{\partial r_1^2}.$$

Similarly, we have

$$\nabla_1 f_{12} = \hat{1}_2 f'(r_{12}) \text{ and}$$

$$\nabla^2 f_{12} = \frac{2}{r_{12}} f'_{12} + \frac{\partial^2 f_{12}}{\partial r_{12}^2}.$$

We now can write immediately

$$\begin{aligned} (\nabla_1^2 + \nabla_2^2) \Psi_{(1,2)} &= \frac{2}{r_1} \phi_1' \phi_2 f_{12} + \frac{2}{r_2} \phi_1 \phi_2' f_{12} + \\ &\phi_1'' \phi_2 f_{12} + \phi_1 \phi_2'' f_{12} + 2[(\hat{1}_1 \phi_1' \phi_2 - \hat{2} \phi_1 \phi_2') \cdot \hat{1}_2] f'_{12} + \\ &\frac{4}{r_{12}} \phi_1 \phi_2 f'_{12} + 2 \phi_1 \phi_2 f''_{12}. \end{aligned}$$

Now work out the derivatives:

$$\phi_1' = -2\phi_1; \quad \phi_1'' = -2,$$

and similarly for ϕ_2 . Furthermore

$$f'_{12} = \frac{1}{2(1 + \alpha r_{12})^2} f_{12}$$

$$f''_{12} = \left[\frac{1}{4(1 + \alpha r_{12})^4} - \frac{\alpha}{(1 + \alpha r_{12})^3} \right] f_{12}.$$

Putting all the pieces together, and putting the factor $-1/2$ in front of the expression, we then obtain for the kinetic energy K :

$$K = \frac{2}{r_1} + \frac{2}{r_2} - 4 + \frac{(\hat{1} - \hat{2}) \cdot \hat{1}_2}{(1 + \alpha r_{12})^2} - \frac{1}{r_{12}(1 + \alpha r_{12})^3} - \frac{1}{4(1 + \alpha r_{12})^4}.$$