

Using the trial wavefunction

$$\Psi_T(\mathbf{r}_1, \mathbf{r}_2) = e^{-\alpha\omega(r_1^2+r_2^2)/2} e^{ar_{12}/(1+\beta r_{12})}$$

where $r_i = \sqrt{r_{ix}^2 + r_{iy}^2}$, $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$, redefining the exponentials as

$$e^{-\alpha\omega(r_1^2+r_2^2)/2} = e^{O_\alpha}, \quad e^{ar_{12}/(1+\beta r_{12})} = e^{O_\beta}$$

$$\nabla_{i_x} \Psi_T = e^{O_\alpha} e^{O_\beta} \left(-\alpha\omega x_i + (-1)^{i+1} (x_1 - x_2) \frac{a}{r_{12}(1+\beta r_{12})^2} \right)$$

where i and j are particle number. This will look the same for the y -coordinate and one sign change for the second term depending on the particle number. Defining the parenthesis as $[\cdot]$, taking the Laplacian and dividing with Ψ_T to get the local energy E_L .

$$\frac{\nabla_{i_x}^2 \Psi_T}{\Psi_T} = [\cdot]^2 - \alpha\omega + \frac{a}{r_{12}^2(1+\beta r_{12})^2} \left(r_{12} - \frac{(x_1 - x_2)(1 - \beta r_{12})}{r_{12}(1 + \beta r_{12})} \right)$$

.1 Calculations

.1.1 Local Energy E_L

Derivative of first exponential

$$\begin{aligned} \frac{\partial}{\partial x_1} e^{-\alpha\omega(r_1^2+r_2^2)/2} &= -\alpha\omega x_1 e^{-\alpha\omega(r_1^2+r_2^2)/2} \\ \frac{\partial}{\partial x_2} e^{-\alpha\omega(r_1^2+r_2^2)/2} &= -\alpha\omega x_2 e^{-\alpha\omega(r_1^2+r_2^2)/2} \end{aligned}$$

Derivative of second exponential

$$\begin{aligned} \frac{\partial}{\partial x_1} e^{ar_{12}/(1+\beta r_{12})} &\Rightarrow \\ \text{with change of variables} & \\ \frac{\partial r_{12}}{\partial x_1} = \frac{x_1 - x_2}{r_{12}}, \quad \frac{\partial r_{12}}{\partial x_2} = -\frac{x_1 - x_2}{r_{12}} & \\ \frac{\partial r_{12}}{\partial x_1} \frac{\partial}{\partial r_{12}} e^{ar_{12}/(1+\beta r_{12})} = e^{ar_{12}/(1+\beta r_{12})} \frac{(x_1 - x_2)a}{r_{12}(1 + \beta r_{12})^2} & \\ \frac{\partial r_{12}}{\partial x_2} e^{ar_{12}/(1+\beta r_{12})} = -e^{ar_{12}/(1+\beta r_{12})} \frac{(x_1 - x_2)a}{r_{12}(1 + \beta r_{12})^2} & \end{aligned}$$

The result will be the same for other dimensions too. Collected the term is

$$e^{-\alpha\omega(r_1^2+r_2^2)/2} e^{ar_{12}/(1+\beta r_{12})} \left(-\alpha\omega x_1 + (-1)^{i+1} \frac{a(x_1 - x_2)}{r_{12}(1 + \beta r_{12})^2} \right)$$

Defining the parenthesis as $[\cdot]$

$$\begin{aligned} \frac{\partial}{\partial x_1} [\cdot] &= a \left(\frac{1}{r_{12}(1 + \beta r_{12})^2} - \frac{(x_1 - x_2)^2}{r_{12}^3(1 + \beta r_{12})^2} - \frac{2(x_1 - x_2)^2}{r_{12}^2(1 + \beta r_{12})^3} \right) \\ &= \frac{a}{r_{12}^2(1 + \beta r_{12})^2} \left(r_{12} - (x_1 - x_2)^2 \left(\frac{1}{r_{12}} - \frac{2\beta}{r_{12}(1 + \beta r_{12})} \right) \right) \\ &= \frac{a}{r_{12}^2(1 + \beta r_{12})^2} \left(r_{12} - (x_1 - x_2)^2 \left(\frac{1 - \beta r_{12}}{r_{12}(1 + \beta r_{12})} \right) \right) \end{aligned}$$

Comibining these calculations gives the gradient and local energy E_L

$$\frac{\nabla_{i_x} \Psi_T}{\Psi_T} = -\alpha\omega x_1 + (-1)^{i+1} \frac{a(x_1 - x_2)}{r_{12}(1 + \beta r_{12})^2} \quad (1)$$

$$\frac{\nabla_{i_x}^2 \Psi_T}{\Psi_T} = [\cdot]^2 - \alpha\omega + \frac{a}{r_{12}^2(1 + \beta r_{12})^2} \left(r_{12} - (x_1 - x_2)^2 \left(\frac{1 - \beta r_{12}}{r_{12}(1 + \beta r_{12})} \right) \right) \quad (2)$$