I. ENERGY

The normalized wavefunction is

$$\psi(r_1, r_2) = \alpha^3 \exp(-\alpha r_1) \exp(-\alpha r_2). \tag{1}$$

Using the expression of laplacian from the previous section, the kinetic energy is

$$\begin{aligned}
\langle K \rangle &= -\frac{1}{2}\int \frac{\nabla^2_{r_1}\psi}{\psi}|\psi|^2 d^3r_1 d^3r_2 - \frac{1}{2}\int \frac{\nabla^2_{r_2}\psi}{\psi}|\psi|^2 d^3r_1 d^3r_2 && (2)\\
&= -\frac{1}{2}\int_0^\infty \left(-\frac{2\alpha}{r_1} + \alpha^2\right)\alpha^6 \exp(-2\alpha r_1) 4r_1^2 dr_1 \int_0^\infty \exp(-2\alpha r_2) 4r_2^2 dr_2 + \cdots && (3)\\
&= -\frac{1}{2}\left(-\frac{1}{\alpha}\right)\frac{1}{\alpha^3}\alpha^6 - \frac{1}{2}\left(-\frac{1}{\alpha}\right)\frac{1}{\alpha^3}\alpha^6 && (4)\\
&= \boxed{\alpha^2}. && (5)
\end{aligned}$$

The electron-nuclear potential is

$$\begin{aligned}
\langle V_{\text{en}} \rangle &= -Z\int \frac{\alpha^6}{r_1}\exp(-2\alpha r_1)\exp(-2\alpha r_2) d^3r_1 d^3r_2 - \cdots && (6)\\
&= -Z\int_0^\infty \frac{1}{r_1}\exp(-2\alpha r_1) 4r_1^2 dr_1 \int_0^\infty \exp(-2\alpha r_2) 4r_2^2 dr_2 - \cdots && (7)\\
&= -Z\left(\frac{1}{\alpha^2}\right)\left(\frac{1}{\alpha^3}\right)\alpha^6 - Z\left(\frac{1}{\alpha^2}\right)\left(\frac{1}{\alpha^3}\right) && (8)\\
&= \boxed{-2Z\alpha}. && (9)
\end{aligned}$$

The electron-electron potential is

$$\begin{aligned}
\langle V_{\text{ee}} \rangle &= \int \frac{\alpha^6}{r_1 - r_2}\exp(-2\alpha r_1)\exp(-2\alpha r_2) d^3r_1 d^3r_2 && (10)\\
&= \alpha^6 \int_0^\infty \int_0^\infty \frac{1}{r_1 - r_2}\exp(-2\alpha r_1)\exp(-2\alpha r_2) 4r_1^2 dr_1 4r_2^2 dr_2. && (11)\\
&= 16\alpha^6 \int_0^\infty \int_0^\infty \frac{1}{r_1 - r_2}\exp(-2\alpha r_1)\exp(-2\alpha r_2) r_1^2 dr_1 r_2^2 dr_2. && (12)\\
&= 16\alpha^6 \int_0^\infty \exp(-2\alpha r_1) r_1^2 dr_1 \int_0^\infty \frac{1}{r_1 - r_2}\exp(-2\alpha r_2) r_2^2 dr_2. && (13)\\
& && (14)
\end{aligned}$$

II. GRADIENT

The (unnormalized) wavefunction is

$$\psi(r_1, r_2) = \exp(-\alpha r_1)\exp(-\alpha r_2). \tag{15}$$

$$\psi(x_1, y_1, z_1, x_2, y_2, z_2) = \exp\left(-\alpha\sqrt{x_1^2 + y_1^2 + z_1^2}\right)\exp\left(\alpha\sqrt{x_2^2 + y_2^2 + z_2^2}\right). \tag{16}$$

The gradient is

$$\nabla\psi = \left[\frac{\partial\psi}{\partial x_1}, \frac{\partial\psi}{\partial y_1}, \frac{\partial\psi}{\partial z_1}, \frac{\partial\psi}{\partial x_2}, \frac{\partial\psi}{\partial y_2}, \frac{\partial\psi}{\partial z_2}\right]^T. \tag{17}$$

Evaluate each element.

$$\frac{\partial\psi}{\partial x_1} = -\alpha\exp\left(-\alpha\sqrt{x_1^2 + y_1^2 + z_1^2}\right)\frac{1}{2}(x_1^2 + y_1^2 + z_1^2)^{-1/2}2x_1\exp\left(\alpha\sqrt{x_2^2 + y_2^2 + z_2^2}\right) \quad = -\alpha\frac{x_1}{r_1}\psi \tag{18}$$

Thus, the gradient is

$$\boxed{\frac{\nabla\psi}{\psi} = -\alpha\left[\frac{x_1}{r_1}, \frac{y_1}{r_1}, \frac{z_1}{r_1}, \frac{x_2}{r_2}, \frac{y_2}{r_2}, \frac{z_2}{r_2}\right]^T.} \tag{19}$$

III. LAPLACIAN

$$\frac{\partial^2\psi}{\partial x_1^2} = -\alpha\exp\left(-\alpha\sqrt{x_2^2 + y_2^2 + z_2^2}\right)\frac{\partial}{\partial x_1}\left[x_1\frac{1}{\sqrt{x_1^2 + y_1^2 + z_1^2}}\exp\left(-\alpha\sqrt{x_1^2 + y_1^2 + z_1^2}\right)\right] \tag{20}$$

$$= -\alpha\exp\left(-\alpha\sqrt{x_2^2 + y_2^2 + z_2^2}\right)\frac{\partial}{\partial x_1}A. \tag{21}$$

$$\tag{22}$$

$$\frac{\partial A}{\partial x_1} = \frac{1}{\sqrt{x_1^2 + y_1^2 + z_1^2}}\exp\left(-\alpha\sqrt{x_1^2 + y_1^2 + z_1^2}\right) \tag{23}$$

$$+ x_1\left(-\frac{1}{2}\right)(x_1^2 + y_1^2 + z_1^2)^{-\frac{3}{2}}2x_1\exp\left(-\alpha\sqrt{x_1^2 + y_1^2 + z_1^2}\right) \tag{24}$$

$$+ x_1\frac{1}{\sqrt{x_1^2 + y_1^2 + z_1^2}}(-\alpha)\frac{1}{2}\frac{2x_1}{\sqrt{x_1^2 + y_1^2 + z_1^2}}\exp\left(-\alpha\sqrt{x_1^2 + y_1^2 + z_1^2}\right) \tag{25}$$

$$= \left[\frac{1}{r_1} - \frac{x_1^2}{r_1^3} - \alpha\frac{x_1^2}{r_1^2}\right]\exp(-\alpha r_1). \tag{26}$$

$$\tag{27}$$

$$\frac{\partial^2\psi}{\partial x_1^2} = -\alpha \exp\left(-\alpha r_2\right)\left[\frac{1}{r_1} - \frac{x_1^2}{r_1^3} - \alpha\frac{x_1^2}{r_1^2}\right]\exp(-\alpha r_1) \tag{28}$$

$$= -\frac{\alpha}{r_1}\psi\left[1 - \frac{x_1^2}{r_1^2} - \alpha\frac{x_1^2}{r_1}\right]. \tag{29}$$

Thus, the laplacian is

$$\frac{\nabla^2\psi}{\psi} = \left[\frac{\partial^2\psi}{\partial x_1^2} + \frac{\partial^2\psi}{\partial y_1^2} + \frac{\partial^2\psi}{\partial z_1^2}, \frac{\partial^2\psi}{\partial x_2^2} + \frac{\partial^2\psi}{\partial y_2^2} + \frac{\partial^2\psi}{\partial z_2^2}\right] \tag{30}$$

$$= \left[-\frac{\alpha}{r_1}\left(3 - \frac{x_1^2 + y_1^2 + z_1^2}{r_1^2} - \alpha\frac{x_1^2 + y_1^2 + z_1^2}{r_1}\right), -\frac{\alpha}{r_2}\left(3 - \frac{x_2^2 + y_2^2 + z_2^2}{r_2^2} - \alpha\frac{x_2^2 + y_2^2 + z_2^2}{r_2}\right)\right] \tag{31}$$

$$= \left[-\frac{\alpha}{r_1}(2 - \alpha r_1), -\frac{\alpha}{r_2}(2 - \alpha r_2)\right] \tag{32}$$

$$= \boxed{\left[-\frac{2\alpha}{r_1} + \alpha^2, -\frac{2\alpha}{r_2} + \alpha^2\right].} \tag{33}$$

IV. JASTROW

The Jastrow factor is

$$\psi(r_1, r_2) = \exp(\beta r_{12}) = \exp(\beta |r_1 - r_2|) \tag{34}$$

$$\psi(x_1, y_1, z_1, x_2, y_2, z_2) = \exp\left[\beta\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}\right] \tag{35}$$

V. GRADIENT

Take the derivative.

$$\frac{\partial \psi}{\partial x_1} = \beta \frac{1}{2}[(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2]^{-1/2} 2(x_1 - x_2) \exp\left[\beta\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}\right] \tag{36}$$

$$= \beta \frac{x_1 - x_2}{\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}} \exp\left[\beta\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}\right] \tag{37}$$

$$= \beta \frac{x_1 - x_2}{r_{12}} \exp(\beta r_{12}) \tag{38}$$

$$= \beta \frac{x_1 - x_2}{r_{12}} \psi. \tag{39}$$

The gradient is

$$\frac{\nabla \psi}{\psi} = \frac{\beta}{r_{12}}[x_1 - x_2, y_1 - y_2, z_1 - z_2, x_2 - x_1, y_2 - y_1, z_2 - z_1]^T \tag{40}$$

$$= \frac{\beta}{r_{12}}[\mathbf{r}_{12}, -\mathbf{r}_{12}]^T \tag{41}$$

$$= \boxed{\frac{\beta}{r_{12}}[1, -1]^T \mathbf{r}_{12}}. \tag{42}$$

VI. LAPLACIAN

Take the derivative using `sympy` to reduce pain.

$$\frac{\partial^2 \psi}{\partial x_1^2} = \beta \left[\frac{\beta (x_1 - x_2)^2}{r_{12}^2} - \frac{(x_1 - x_2)^2}{r_{12}^3} + \frac{1}{r_{12}}\right] \psi \tag{43}$$

Thus, the laplacian is

$$\frac{\nabla^2\psi}{\psi} = \frac{\beta}{r_{12}}\Bigg[\frac{\beta(x_1-x_2)^2}{r_{12}} - \frac{(x_1-x_2)^2}{r_{12}^2} + 1 + \frac{\beta(y_1-y_2)^2}{r_{12}} - \frac{(y_1-y_2)^2}{r_{12}^2} + 1 + \frac{\beta(z_1-z_2)^2}{r_{12}} - \frac{(z_1-z_2)^2}{r_{12}^2} + 1, \tag{44}$$

$$\frac{\beta(x_2-x_1)^2}{r_{12}} - \frac{(x_2-x_1)^2}{r_{12}^2} + 1 + \frac{\beta(y_2-y_1)^2}{r_{12}} - \frac{(y_2-y_1)^2}{r_{12}^2} + 1 + \frac{\beta(z_2-z_1)^2}{r_{12}} - \frac{(z_2-z_1)^2}{r_{12}^2} + 1\Bigg]^T \tag{45}$$

$$= \frac{\beta}{r_{12}}\left[\frac{\beta r_{12}^2}{r_{12}} - \frac{r_{12}^2}{r_{12}^2} + 3, \frac{\beta r_{12}^2}{r_{12}} - \frac{r_{12}^2}{r_{12}^2} + 3\right]^T \tag{46}$$

$$= \frac{\beta}{r_{12}}[\beta r_{12} + 2, \beta r_{12} + 2]^T \tag{47}$$

$$= \frac{\beta}{r_{12}}(\beta r_{12} + 2)[1, 1]^T \tag{48}$$

$$\tag{49}$$

VII. MULTIPLYING WAVEFUNCTIONS

The value of the wavefunction is

$$\psi = \psi_1\psi_2. \tag{50}$$

The gradient is

$$\nabla\psi = (\nabla\psi_1)\psi_2 + \psi_1(\nabla\psi_2) \tag{51}$$

$$\frac{\nabla\psi}{\psi} = \frac{\nabla\psi_1}{\psi_1} + \frac{\nabla\psi_2}{\psi_2}. \tag{52}$$

The laplacian is

$$\nabla^2\psi = (\nabla^2\psi_1)\psi_2 + \nabla\psi_1\nabla\psi_2 + \nabla\psi_1\nabla\psi_2 + \psi_1(\nabla^2\psi_2) \tag{53}$$

$$= (\nabla^2\psi_1)\psi_2 + 2\nabla\psi_1\nabla\psi_2 + \psi_1(\nabla^2\psi_2). \tag{54}$$

$$\frac{\nabla^2\psi}{\psi} = \frac{\nabla^2\psi_1}{\psi_1} + 2\frac{\nabla\psi_1}{\psi_1}\frac{\nabla\psi_2}{\psi_2} + \frac{\nabla^2\psi_2}{\psi_2}. \tag{55}$$