The local energy is

$$E_L(x) = \frac{\hat{H}\Psi_T(x)}{\Psi_T(x)} = \frac{1}{\Psi_T(x)}\left[-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2\right]\Psi_T(x) = -e^{\alpha x^2}\frac{1}{2}\frac{d^2}{dx^2}e^{-\alpha x^2} + \frac{1}{2}x^2 \tag{27}$$

in which $\frac{d^2}{dx^2}e^{\alpha x^2} = -2\alpha e^{-\alpha x^2} + 4\alpha^2 x^2 e^{-\alpha x^2}$, so

$$E_L(x) = -e^{\alpha x^2}\frac{1}{2}\frac{d^2}{dx^2}e^{-\alpha x^2} + \frac{1}{2}x^2 = \alpha + x^2\left(\frac{1}{2} - 2\alpha^2\right) \tag{28}$$

4.1.2 Hydrogen molecule H_2

$$\hat{H} = -\frac{\hbar}{2m}\left(\nabla_1^2 + \nabla_2^2\right) - \left[\frac{ke^2}{\left|\vec{r}_1 + \frac{s}{2}\hat{i}\right|} + \frac{ke^2}{\left|\vec{r}_1 - \frac{s}{2}\hat{i}\right|} + \frac{ke^2}{\left|\vec{r}_2 + \frac{s}{2}\hat{i}\right|} + \frac{ke^2}{\left|\vec{r}_2 - \frac{s}{2}\hat{i}\right|}\right] + \frac{ke^2}{|\vec{r}_1 + \vec{r}_2|} \tag{29}$$

in which the first term is the kinetic energy of the two electrons, the part in the square brackets is the attraction between the nucleus and the electrons and the last term is the Coulomb interaction between the electrons. Setting the constants to unity, and setting $\vec{r}_{1L} = \vec{r}_1 + \frac{s}{2}\hat{i}$, $\vec{r}_{1R} = \vec{r}_1 - \frac{s}{2}\hat{i}$, $\vec{r}_{2L} = \vec{r}_2 + \frac{s}{2}\hat{i}$, $\vec{r}_{1R} = \vec{r}_2 - \frac{s}{2}\hat{i}$ and $\vec{r}_{12} = \vec{r}_1 - \vec{r}_2$ we obtain

$$\hat{H} = -\frac{1}{2}\left(\nabla_1^2 + \nabla_2^2\right) - \left[\frac{1}{|\vec{r}_{1L}|} + \frac{1}{|\vec{r}_{1R}|} + \frac{1}{|\vec{r}_{2L}|} + \frac{1}{|\vec{r}_{2R}|}\right] + \frac{1}{|\vec{r}_{12}|} \tag{30}$$

In the light of the solvability of this Hamiltonian we split it up in two non-interacting Hamiltonians and a interaction term.

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{ee} \tag{31}$$

in which $\hat{H}_1 = -\frac{1}{2}\nabla_1^2 - \frac{1}{|\vec{r}_{1L}|} - \frac{1}{|\vec{r}_{1R}|}$, $\hat{H}_2 = -\frac{1}{2}\nabla_2^2 - \frac{2}{|\vec{r}_{1L}|} - \frac{2}{|\vec{r}_{2R}|}$ and $\hat{H}_{ee} = \frac{1}{|\vec{r}_{12}|}$
We have chosen our trail variational wave function $\Psi_{T,\alpha}$ to be

$$\Psi_T(\vec{r}_1, \vec{r}_2) = \phi(\vec{r}_1)\phi(\vec{r}_2)\psi(\vec{r}_1, \vec{r}_2) \tag{32}$$

where $\psi(\vec{r}_1, \vec{r}_2)$ is the Jastrow function

$$\psi(\vec{r}_1, \vec{r}_2) = \psi_{12} = e^{\frac{|\vec{r}_{12}|}{\alpha(1+\beta|\vec{r}_{12}|)}} \tag{33}$$

and $\phi(\vec{r}_1)$ and $\phi(\vec{r}_2)$ are

$$\phi(\vec{r}_1) = e^{-|\vec{r}_{1L}|/a} + e^{-|\vec{r}_{1R}|/a} = \phi_1 = \phi_{1L} + \phi_{1R} \tag{34}$$

$$\phi(\vec{r}_2) = e^{-|\vec{r}_{2L}|/a} + e^{-|\vec{r}_{2R}|/a} = \phi_2 = \phi_{2L} + \phi_{2R} \tag{35}$$

$$E_L(R) = \frac{\hat{H}\Psi_T(R)}{\Psi_T(R)} = \frac{1}{\phi_1\phi_2\psi_{12}}\hat{H}\phi_1\phi_2\psi_{12} \tag{36}$$

We let the Hamiltonians only work on correct terms, which results in

$$\frac{1}{\phi_1\phi_2\psi_{12}}(\hat{H}_1+\hat{H}_2+\hat{H}_{ee})\phi_1\phi_2\psi_{12} = \frac{1}{\phi_1\psi_{12}}\hat{H}_1\phi_1\psi_{12} + \frac{1}{\phi_2\psi_{12}}\hat{H}_2\phi_2\psi_{12} + \frac{1}{|\vec{r}_{12}|} \tag{37}$$

Now we first consider

$$\frac{1}{\phi_1\psi_{12}}\hat{H}_1\phi_1\psi_{12} = -\frac{1}{\phi_1\psi_{12}}\frac{1}{2}\nabla_1^2(\phi_1\psi_{12}) - \frac{1}{|\vec{r}_{1L}|} - \frac{1}{|\vec{r}_{1R}|} \tag{38}$$

from which we first consider $\nabla_1^2(\phi_1\psi_{12})$, using the chain rule

$$\nabla_1^2(\phi_1\psi_{12}) = \psi_{12}\nabla_1^2\phi_1 + 2\nabla_1\phi_1\cdot\nabla_1\psi_{12} + \phi_1\nabla_1^2\psi_{12} \tag{39}$$

where

$$\nabla_1\phi_1 = -\frac{1}{a}\left(e^{-|\vec{r}_{1L}|/a} + e^{-|\vec{r}_{1R}|/a}\right) = -\frac{1}{a}\left(e^{-|\vec{r}_{1L}|/a}\hat{r}_{1L} + e^{-|\vec{r}_{1R}|/a}\hat{r}_{1R}\right) \tag{40}$$

and [4]

$$\nabla_1^2\phi_1 = \left[\frac{1}{a^2} - \frac{2}{ar_{1L}}\right]e^{-r_{1L}/a} + \left[\frac{1}{a^2} - \frac{2}{ar_{1R}}\right]e^{-r_{1R}/a} \tag{41}$$

Similarly we find

$$\nabla_1\psi_{12} = \nabla_1\left(e^{\frac{r_{12}}{\alpha(1+\beta r_{12})}}\right) = \frac{e^{\frac{r_{12}}{\alpha(\beta r_{12}+1)}}}{\alpha(\beta r_{12}+1)^2}\hat{r}_{12} = \frac{\psi_{12}}{\alpha(\beta r_{12}+1)^2}\hat{r}_{12} \tag{42}$$

and

$$\nabla_1^2\psi_{12} = e^{\frac{r_{12}}{\alpha(1+\beta r_{12})}}\frac{2\alpha\beta r_{12}+2\alpha+r_{12}}{r_{12}\alpha^2(\beta r_{12}+1)^4} = \frac{(1+2\alpha\beta)r_{12}+2\alpha}{r_{12}\alpha^2(\beta r_{12}+1)^4}\psi_{12} \tag{43}$$

Now substituting equations 40, 41, 42 and 43 into 39.

$$\begin{aligned}\nabla_1^2(\phi_1\psi_{12}) = \psi_{12}&\left(\left[\frac{1}{a^2} - \frac{2}{ar_{1L}}\right]e^{-r_{1L}/a} + \left[\frac{1}{a^2} - \frac{2}{ar_{1R}}\right]e^{-r_{1R}/a}\right) + \\ &\frac{2}{a}\left(e^{-r_{1L}/a}\hat{r}_{1L} + e^{-r_{1R}/a}\hat{r}_{1R}\right)\frac{\psi_{12}}{\alpha(\beta r_{12}+1)^2}\hat{r}_{12} \\ &+\left(e^{-|\vec{r}_{1L}|/a} + e^{-|\vec{r}_{1R}|/a}\right)\left(\frac{(1+2\alpha\beta)r_{12}+2\alpha}{r_{12}\alpha^2(\beta r_{12}+1)^4}\psi_{12}\right)\end{aligned} \tag{44}$$

shuffle to get

$$\begin{aligned}\frac{\nabla_1^2(\phi_1\psi_{12})}{\phi_1\psi_{12}} = \frac{1}{\phi_1}&\left(\left[\frac{1}{a^2} - \frac{2}{ar_{1L}}\right]e^{-r_{1L}/a} + \left[\frac{1}{a^2} - \frac{2}{ar_{1R}}\right]e^{-r_{1R}/a}\right) + \\ \frac{1}{\phi_1}&\left(e^{-r_{1L}/a}\hat{r}_{1L} + e^{-r_{1R}/a}\hat{r}_{1R}\right)\cdot\frac{2\hat{r}_{12}}{\alpha a(\beta r_{12}+1)^2} + \frac{(1+2\alpha\beta)r_{12}+2\alpha}{r_{12}\alpha^2(\beta r_{12}+1)^4}\end{aligned} \tag{45}$$

[4] from now on we will omit the vector signs when it's not ambiguous

replace the exponents for the corresponding ϕ to obtain

$$\frac{\nabla_1^2(\phi_1\psi_{12})}{\phi_1\psi_{12}} = \left(\left[\frac{1}{a^2} - \frac{2}{ar_{1L}}\right]\frac{\phi_{1L}}{\phi_1} + \left[\frac{1}{a^2} - \frac{2}{ar_{1R}}\right]\frac{\phi_{1R}}{\phi_1}\right) + \left(\frac{\phi_{1L}}{\phi_1}\hat{r}_{1L} + \frac{\phi_{1R}}{\phi_1}\hat{r}_{1R}\right)\cdot\frac{2\hat{r}_{12}}{\alpha a(\beta r_{12}+1)^2} + \frac{(1+2\alpha\beta)r_{12}+2\alpha}{r_{12}\alpha^2(\beta r_{12}+1)^4} \tag{46}$$

in which

$$\left[\frac{1}{a^2} - \frac{2}{ar_{1L}}\right]\frac{\phi_{1L}}{\phi_1} + \left[\frac{1}{a^2} - \frac{2}{ar_{1R}}\right]\frac{\phi_{1R}}{\phi_1} = \frac{1}{a^2}\left[\frac{\phi_{1L}}{\phi_1} + \frac{\phi_{1R}}{\phi_1}\right] - \frac{2}{a\phi_1}\left[\frac{\phi_{1L}}{r_{1L}} + \frac{\phi_{1R}}{r_{1R}}\right] = \frac{1}{a^2} - \frac{2}{a\phi_1}\left[\frac{\phi_{1L}}{r_{1L}} + \frac{\phi_{1R}}{r_{1R}}\right] \tag{47}$$

Now adding the equations for the second electron, which are the same [5] because of the symmetry of the problem, multiplying with 1/2 and adding the Coulomb interaction terms to get

$$E_L = -\frac{1}{a^2} + \frac{1}{a\phi_1}\left[\frac{\phi_{1L}}{r_{1L}} + \frac{\phi_{1R}}{r_{1R}}\right] + \frac{1}{a\phi_2}\left[\frac{\phi_{2L}}{r_{2L}} + \frac{\phi_{2R}}{r_{2R}}\right] + \left(\frac{\phi_{1L}}{\phi_1}\hat{r}_{1L} + \frac{\phi_{1R}}{\phi_1}\hat{r}_{1R} - \frac{\phi_{2L}}{\phi_2}\hat{r}_{2L} - \frac{\phi_{2R}}{\phi_2}\hat{r}_{2R}\right)\cdot\frac{\hat{r}_{12}}{\alpha a(\beta r_{12}+1)^2} - \frac{(1+2\alpha\beta)r_{12}+2\alpha}{r_{12}\alpha^2(\beta r_{12}+1)^4} - \left[\frac{1}{|\vec{r}_{1L}|} + \frac{1}{|\vec{r}_{1R}|} + \frac{1}{|\vec{r}_{2L}|} + \frac{1}{|\vec{r}_{2R}|}\right] + \frac{1}{|\vec{r}_{12}|} \tag{48}$$

with $\alpha = 2$

$$E_L = -\frac{1}{a^2} + \frac{1}{a\phi_1}\left[\frac{\phi_{1L}}{r_{1L}} + \frac{\phi_{1R}}{r_{1R}}\right] + \frac{1}{a\phi_2}\left[\frac{\phi_{2L}}{r_{2L}} + \frac{\phi_{2R}}{r_{2R}}\right] + \left(\frac{\phi_{1L}\hat{r}_{1L} + \phi_{1R}\hat{r}_{1R}}{\phi_1} - \frac{\phi_{2L}\hat{r}_{2L} + \phi_{2R}\hat{r}_{2R}}{\phi_2}\right)\cdot\frac{\hat{r}_{12}}{2a(\beta r_{12}+1)^2} - \frac{(1+4\beta)r_{12}+4}{4r_{12}(\beta r_{12}+1)^4} - \left[\frac{1}{|\vec{r}_{1L}|} + \frac{1}{|\vec{r}_{1R}|} + \frac{1}{|\vec{r}_{2L}|} + \frac{1}{|\vec{r}_{2R}|}\right] + \frac{1}{|\vec{r}_{12}|} \tag{49}$$

4.2 Coulomb cusp condition

When two Coulomb particles get close, the potential has $1/r$ singularity. We want modify the wave function in such a way to cancel this singularity. Let

[5] up to one minus sign