FYS4411 Project 1

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1 Analytical calculation of the local energy

Calculating the kinetic energy numerically is costly. One can considerably reduce computational time by using a closed form expression for the energy.

We have trial wavefunction

$$\Psi = e^{-\alpha(r_1+r_2)}$$

and we want to calculate the local energy given by

$$E_L = \frac{1}{\Psi}\hat{H}\Psi$$

where

$$\hat{H} = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}$$

Rewriting

$$T_{L1} = \frac{1}{\Psi}\left(-\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2}\right)\Psi$$

$$V_{L1} = \frac{1}{\Psi}\left(-\frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}\right)\Psi$$

Doing the calculations, we find that

$$T_{L1} = -\frac{1}{2}\frac{1}{\Psi}\left(\frac{1}{r_1^2}\frac{\partial}{\partial r_1}\left(r_1^2\frac{\partial}{\partial r_1}\Psi\right) + \frac{1}{r_2^2}\frac{\partial}{\partial r_2}\left(r_2^2\frac{\partial}{\partial r_2}\Psi\right)\right)$$

$$T_{L1} = -\frac{1}{2}\left(-\frac{2}{r_1}\alpha + \alpha^2 - \frac{2}{r_2} + \alpha^2\right)$$

Adding T_{L1} and V_{L1}

$$E_{L1} = (\alpha - 2)\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{1}{r_{12}} - \alpha^2$$

Introducing the Jastrow factor, one can rewrite the wavefunction as a product of the direct term and the corrolation term.

$$\Psi = \Psi_D\Psi_C$$

We want to calculate the kinetic energy and divide by the wavefunction.

$$T_{L2} = \frac{1}{\Psi}\frac{-\nabla^2}{2}\Psi$$

Using the chain rule. This equation must be calculated for both particles.

$$T_{L2} = -\frac{1}{2}\left(\frac{1}{\Psi_D}\nabla^2\Psi_D + 2\frac{1}{\Psi_D\Psi_C}\nabla\Psi_D \cdot \nabla\Psi_C + \nabla^2\Psi_C\right) \tag{1}$$

The first term is easily calculated, as it is the same as for E_{L1}

$$\frac{1}{\Psi_D}\nabla^2\Psi_D = -\frac{2}{r_1}\alpha + \alpha^2$$

Calculating the second term

$$\frac{1}{\Psi_D}\nabla\Psi_D = \frac{1}{\Psi_D}\frac{\partial}{\partial r}\Psi_D\hat{e}_r$$

$$\frac{1}{\Psi_D}\nabla\Psi_D = -\alpha\hat{e}_r \tag{2}$$

When differentiating the corrolation term, given by

$$e^{\frac{r_{12}}{2(1+\beta r_{12})}}$$

One must use that

$$\frac{\partial}{\partial r_i}r_{12} = (-1)^{i+1}\frac{\vec{r}_1 - \vec{r}_2}{r_{12}}\hat{e}_{ri} \tag{3}$$

$$\frac{1}{\Psi_C}\nabla\Psi_C = \frac{1}{\Psi_C}\frac{\partial}{\partial r}\Psi_C\hat{e}_r$$

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$$\frac{1}{\Psi_C}\nabla\Psi_C = (-1)^{i+1}\frac{\vec{r}_1 - \vec{r}_2}{2r_{12}\left(1+\beta r_{12}\right)}$$

Finally multiplying and adding both particles.

$$\frac{\nabla_1\Psi_D}{\Psi_D}\cdot\frac{\nabla_1\Psi_C}{\Psi_C} + \frac{\nabla_2\Psi_D}{\Psi_D}\cdot\frac{\nabla_2\Psi_C}{\Psi_C} = \frac{-1}{(1+\beta r_{12})}\left(\frac{\alpha(r_1+r_2)}{r_{12}}\left(1 - \frac{\vec{r}_1\cdot\vec{r}_2)}{r_1 r_2}\right)\right) \tag{4}$$

Now, to calculate the last term in (1).

$$\frac{\nabla^2\Psi_C}{\Psi_C} = \frac{1}{\Psi_C}\left(\frac{2}{r}\frac{\partial}{\partial r}\Psi_C + \frac{\partial^2}{\partial r^2}\Psi_C\right) \tag{5}$$

Looking at the first part for both particles

$$\frac{2}{r_1}\frac{\vec{r}_1 - \vec{r}_2}{2r_{12}\left(1+\beta r_{12}\right)}\frac{\vec{r}_1}{r_1} + \frac{2}{r_1}\frac{\vec{r}_2 - \vec{r}_1}{2r_{12}\left(1+\beta r_{12}\right)}\frac{\vec{r}_2}{r_2}$$

Sorting this gives

$$\frac{2}{r_{12}(1+\beta r_{12})^2} - \frac{\vec{r}_1\cdot\vec{r}_2}{r_{12}r_1^2(1+\beta r_{12})^2} - \frac{\vec{r}_1\cdot\vec{r}_2}{r_{12}r_2^2(1+\beta r_{12})^2}$$

The second part for particle 1

$$\frac{1}{\Psi_C}\frac{\partial^2}{\partial r^2}\Psi_C = \left(\frac{\vec{r}_1 - \vec{r}_2}{2r_{12}\left(1+\beta r_{12}\right)}\hat{e}_{r1}\right)^2 + \frac{\partial}{\partial r_1}\left(\frac{\vec{r}_1 - \vec{r}_2}{2r_{12}\left(1+\beta r_{12}\right)}\hat{e}_{r1}\right)$$

$$\frac{1}{4(1+\beta r_{12})^4} + \frac{\beta}{(1+\beta r_{12})^3}$$

Combining these calculations

$$\frac{\nabla^2 \Psi_C}{\Psi_C} = \frac{1}{r_{12}(1+\beta r_{12})^2} + \frac{1}{4(1+\beta r_{12})^4} - \frac{\beta}{(1+\beta r_{12})^3}$$

Combining, we get the T_{L2}

Giving the total local energy

$$E_{L2} = E_{L1} + \frac{1}{2(1+\beta r_{12})^2} \left[\frac{\alpha(r1+r2)}{r_{12}} \left(1 - \frac{\vec{r}_1 \cdot \vec{r}_2}{r_1 r_2}\right) - \frac{1}{2(1+\beta r_{12})^2} - \frac{2}{r_{12}} + \frac{2\beta}{1+\beta r_{12}} \right]$$