Computational Physics II
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Abstract

Fill in abstract

1 Introduction

2 Methods

2.1 Monte Carlo of the Helium Atom

In a quantum mechanical system the energy is given by the expectation value of the Hamiltonian.

$$E[H] = \langle \Psi | \tag{1}$$

2.2 Derivation of local energies

The local energy of is dependant on the Hamiltonian and the wavefunction describing the system, the Hamiltonian incorporates both a kinetic energy part given by $\frac{\nabla_i^2}{2}$ for each particle and a potential energy part given by $\frac{Z}{r_i}$ and $\frac{1}{r_{ij}}$, where Z is the charge of the center, r_i is the distance for electron i to the atom center and r_{ij} is the distance between electron l and m. Then the local energy is given by the following:

$$\begin{aligned}
E_L &= \sum_{i,i<j} \frac{1}{\Psi_T(\mathbf{r_i}, \mathbf{r_{ij}})} \hat{H} \Psi_T(\mathbf{r_i}, \mathbf{r_{ij}}) && (2) \\
&= \sum_{i,i<j} \frac{1}{\Psi_T(\mathbf{r_i}, \mathbf{r_{ij}})} \left(-\frac{\nabla_i^2}{2} - \frac{Z}{r_i} - \frac{Z}{r_j} + \frac{1}{r_{ij}} \right) \Psi_T(\mathbf{r_i}, \mathbf{r_{ij}}) && (3) \\
&= \sum_{i,i<j} -\frac{1}{2\Psi_T} \left(\nabla_i^2 \Psi_T \right) - \frac{Z}{r_i} - \frac{Z}{r_j} + \frac{1}{r_{ij}} && (4)
\end{aligned}$$

Let us change derivation variables:

$$
\begin{aligned}
-\frac{1}{2\Psi_T}\left(\nabla_i^2\Psi_T\right) &= \sum_{m=1}^{3} -\frac{1}{2\Psi_T}\left(\frac{\partial^2\Psi_T}{\partial x_m^2}\right)_i && (5)\\
&= \sum_{m=1}^{3} -\frac{1}{2\Psi_T}\left(\frac{\partial}{\partial x_m}\left(\frac{\partial\Psi_T}{\partial r_i}\frac{\partial r_i}{\partial x_m}\right)\right)_i && (6)
\end{aligned}
$$

Since $r_i = \left(x_1^2 + x_2^2 + x_3^2\right)^{1/2}$ then $\frac{\partial r_i}{\partial x_m} = \frac{\partial\left(x_1^2+x_2^2+x_3^2\right)^{1/2}}{\partial x_m} = \frac{x_m}{r_i}$

$$
\begin{aligned}
&= \sum_{m=1}^{3} -\frac{1}{2\Psi_T}\left(\frac{\partial}{\partial x_m}\left(\frac{\partial\Psi_T}{\partial r_i}\frac{x_m}{r_i}\right)\right)_i && (7)\\
&= \sum_{m=1}^{3} -\frac{1}{2\Psi_T}\left(\frac{\partial^2\Psi_T}{\partial x_m\partial r_i}\frac{x_m}{r_i} + \frac{\partial\Psi_T}{\partial r_i}\frac{\partial}{\partial x_m}\left(\frac{x_m}{r_i}\right)\right)_i && (8)
\end{aligned}
$$

The term $\frac{\partial}{\partial x_m}\left(\frac{x_m}{r_i}\right)$ becomes for the different values for m, $\frac{\partial}{\partial x_1}\left(\frac{x_1}{\left(x_1^2+x_2^2+x_3^2\right)^{1/2}}\right) = \frac{x_2^2+x_3^2}{r_i^3}$ so all the values for m term it should sum up to $\frac{2(x_1^2+x_2^2+x_3^2)}{r_i^3}$

$$
\begin{aligned}
&= -\frac{1}{2\Psi_T}\left(\frac{\partial^2\Psi_T}{\partial r_i^2}\frac{x_1^2+x_2^2+x_3^2}{r_i^2} + \frac{\partial\Psi_T}{\partial r_i}\frac{2(x_1^2+x_2^2+x_3^2)}{r_i^3}\right)_i && (9)\\
&= -\frac{1}{2\Psi_T}\left(\frac{\partial^2\Psi_T}{\partial r_i^2} + \frac{\partial\Psi_T}{\partial r_i}\frac{2}{r_i}\right) && (10)
\end{aligned}
$$

Then the local energy becomes:

$$
E_L = \sum_{i,i<j} -\frac{1}{2\Psi_T}\left(\frac{\partial^2\Psi_T}{\partial r_i^2} + \frac{\partial\Psi_T}{\partial r_i}\frac{2}{r_i}\right) - \frac{Z}{r_i} - \frac{Z}{r_j} + \frac{1}{r_{ij}} \tag{11}
$$

2.2.1 Helium: Simple trialfunction

The simple version of the trial function is only dependant on one parameter α and does not take into account interaction between the two electrons, it is of the form

$$
\Psi_T(\mathbf{r_1},\mathbf{r_2}) = \exp\{-\alpha(r_1+r_2)\}
$$

Let us set this trialfunction into the equation for the local energy (11).

$$
E_L = \sum_{i,i<j} -\frac{1}{2\Psi_T}\left(\frac{\partial^2 e^{-\alpha(r_i+r_j)}}{\partial r_i^2} + \frac{\partial e^{-\alpha(r_i+r_j)}}{\partial r_i}\frac{2}{r_i}\right) - \frac{Z}{r_i} - \frac{Z}{r_j} + \frac{1}{r_{ij}} \tag{12}
$$

$$
E_L = -\frac{1}{2\Psi_T}\sum_{i=1}^{2}\left(\alpha^2 - \alpha\frac{2}{r_i}\right)\Psi_T - \frac{Z}{r_i} + \frac{1}{r_{ij}} \tag{13}
$$

$$
E_L = -\alpha^2 + (\alpha - Z)\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{1}{r_{12}} \tag{14}
$$

3 Results and discussion

4 Conclusions and perspectives

The local energy for the simple trialfunct

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