Computational Physics II
FYS-4411

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Abstract

Fill in abstract

1 Introduction

2 Methods

2.1 Derivation of local energies

2.1.1 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

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

$$E_L = \frac{1}{\Psi_T(\mathbf{r_i}, \mathbf{r_{ij}})} \hat{H} \Psi_T \Psi_T(\mathbf{r_i}, \mathbf{r_{ij}}) \tag{1}$$

$$= \frac{1}{\Psi_T(\mathbf{r_i}, \mathbf{r_{ij}})} \left(-\frac{\partial^2}{\partial x_k^2} - \frac{Z}{r_i} - \frac{Z}{r_j} + \frac{1}{r_{ij}} \right) \Psi_T(\mathbf{r_i}, \mathbf{r_{ij}}) \tag{2}$$

$$= -\frac{1}{2\Psi_T(\mathbf{r_i}, \mathbf{r_{ij}})} \left(\frac{\partial^2 \Psi_T(\mathbf{r_i}, \mathbf{r_{ij}})}{\partial x_k^2} \right) - \frac{Z}{r_i} - \frac{Z}{r_j} + \frac{1}{r_{ij}} \tag{3}$$

Let us focus on one of the terms that will be different for each type of trial function

$$-\frac{1}{2\Psi_T} \frac{\partial^2 \Psi_T}{\partial x_k^2} = -\frac{1}{2\Psi_T} \frac{\partial}{\partial x_k} \left(\frac{\partial \Psi_T}{\partial x_k} \right) \tag{4}$$

$$= -\frac{1}{2\Psi_T} \frac{\partial}{\partial x_k} \left(\frac{\partial \Psi_T}{\partial r_i} \frac{\partial r_i}{\partial x_k} \right) \tag{5}$$

$\frac{\partial r_i}{\partial x_k}$

$$g \tag{6}$$

3 Results and discussion

4 Conclusions and perspectives

The local energy for the simple trialfunct

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