Computational Physics II
FYS-4411

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Abstract

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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

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

$$E_L = \frac{1}{\Psi_T}\hat{H}\Psi_T \tag{1}$$

$$= \exp\{\alpha(r_1 + r_2)\}\left(-\frac{nabla_1^2}{2} - \frac{nabla_2^2}{2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}\right)\exp\{-\alpha(r_1 + r_2)\} \tag{2}$$

3 Results and discussion

4 Conclusions and perspectives

The local energy for the simple trialfunct

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