FYS4411 - Computational quantum mechanics

Spring 2016

Project 1

temporary report

Sean Bruce Sangolt Miller
s.b.s.miller@fys.uio.no

Filip Henrik Lasren
filiphenriklarsen@gmail.com

Date: February 1, 2016

Abstract

Some text that is abstact

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1 Introduction

2 Theory and methods

$$E_L(\mathbf{R}) = \frac{1}{\Psi_T(\mathbf{R})} H \Psi_T(\mathbf{R}), \tag{1}$$

$$E_L(\mathbf{R}) = \frac{1}{\Psi_T(\mathbf{R})} \sum_i^N \left(\frac{-\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} m \omega_{ho}^2 r_i^2 \right) \Psi_T(\mathbf{R}), \tag{2}$$

The potential term is trivial since this is a scalar. A more challenging problem is to find an expression for $\nabla_i^2 \Psi_T(\mathbf{R})$. With our wavefunction given as

$$\Psi_T(\mathbf{R}) = \prod_i e^{-\alpha r_i^2} \tag{3}$$

we may start by taking the first derivatives

$$\nabla_j \prod_i e^{-\alpha r_i^2} = -2\alpha r_j e^{-\alpha r_j^2} \prod_{i \neq j} e^{-\alpha r_i^2} \tag{4}$$

$$= -2\alpha r_j \prod_i e^{-\alpha r_i^2}. \tag{5}$$

The second derivatives are then

$$\nabla_j^2 \prod_i e^{-\alpha r_i^2} = \nabla_j \left(-2\alpha r_j \prod_i e^{-\alpha r_i^2} \right) \tag{6}$$

$$= \left(4\alpha^2 r_j^2 - 2\alpha \right) \prod_i e^{-\alpha r_i^2}. \tag{7}$$

Inserting this into our local energy (2) we have

$$E_L(\mathbf{R}) = \frac{1}{\Psi_T(\mathbf{R})} \sum_i^N \left(\frac{-\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} m \omega_{ho}^2 r^2 \right) \Psi_T(\mathbf{R}), \tag{8}$$

2.1 Preliminary derivations

3 Results

4 Conclusions

5 Appendix