

NB: The graded, first version of the report must be returned if you hand in a second time!

H2b: Variational Monte Carlo

Victor Nilsson and Simon Nilsson

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Task N ^o	Points	Avail. points
Σ		

Introduction

Problem 1

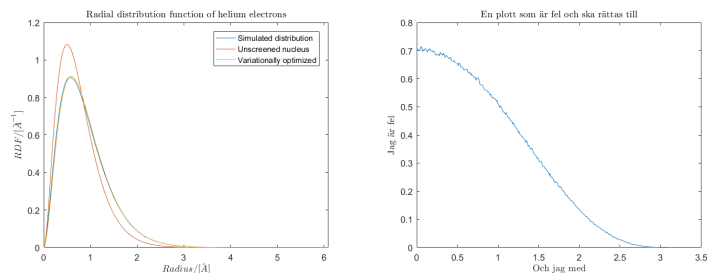


Figure 1: Simulated and calculated radial distribution function for the two electrons in the helium atom. The distribution of the relative θ angle for the two electrons.

As we can see in (Fig. 1) we can see that our radial distribution looks like the variationally optimized distribution.

Problem 2

Problem 3

Problem 4

$$\psi_t(r_1, r_2) = e^{-2r_1} e^{-2r_2} e^{\frac{r_{12}}{2(1+\alpha r_{12})}} \quad (1)$$

$$\nabla \alpha \ln \psi_t(r_1, r_2) = -\frac{r_{12}^2}{2(1 + \alpha r_{12})^2} \quad (2)$$

$$\beta = 0.75 \quad \alpha_{min} = 0.142553129000000 \quad E_{min} = -2.891044220000000$$

Problem 5

$$E_{min} = -2.878146$$

A Source code

A.1 Task1/main.c