

FYS-4411: Computational Physics II

Project 1

Gullik Vetvik Killie
Håkon Sebastian Bakke Mørk
Jose Emilio Ruiz Navarro

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Abstract

0.1 Efficient calculation of derivatives

Calculating the derivatives involved in the VMC calculation numerically is slow in that they entail several calls to the wavefunctions in addition to introducing an extra numerical error. Here we will show how we have found divided up the derivatives and found analytic expressions for all the parts.

The trialfunction can be factorized as

$$\Psi_T(\mathbf{x}) = \Psi_D \Psi_C = |D_\uparrow| |D_\downarrow| \Psi_C \quad (1)$$

where D_\uparrow , D_\downarrow and Ψ_C is the spin up and down part of the Slater determinant and the Jastrow factor respectively.

0.1.1 Kinetic Energy

From the Hamiltonian the expectation value of kinetic energy for each electron is given by

$$K_i = -\frac{1}{2} \frac{\nabla_i^2 \Psi}{\Psi} \quad (2)$$

Using the factorization of of the trialfunction from (1) we can calculate the ratio needed for the kinetic energy.

$$\frac{1}{\Psi_T} \frac{\partial^2 \Psi_T}{\partial x_k^2} = \frac{1}{\Psi_D \Psi_C} \frac{\partial^2 (\Psi_D \Psi_C)}{\partial x_k^2} = \frac{1}{\Psi_D \Psi_C} \frac{\partial}{\partial x_k} \left(\frac{\partial \Psi_D}{\partial x_k} \Psi_C + \Psi_D \frac{\partial \Psi_C}{\partial x_k} \right) \quad (3)$$

$$= \frac{1}{\Psi_D \Psi_C} \left(\frac{\partial^2 \Psi_D}{\partial x_k^2} \Psi_C + 2 \frac{\partial \Psi_D}{\partial x_k} \frac{\partial \Psi_C}{\partial x_k} + \Psi_D \frac{\partial^2 \Psi_C}{\partial x_k^2} \right) \quad (4)$$

$$= \frac{1}{\Psi_D} \frac{\partial^2 \Psi_D}{\partial x_k^2} + 2 \frac{1}{\Psi_D} \frac{\partial \Psi_D}{\partial x_k} \cdot \frac{1}{\Psi_C} \frac{\partial \Psi_C}{\partial x_k} + \frac{1}{\Psi_C} \frac{\partial^2 \Psi_C}{\partial x_k^2} \quad (5)$$

Since the Slater determinant part of the trialfunction is separable into a spin up and down part we can simplify it further.

$$\frac{1}{\Psi_D} \frac{\partial^2 \Psi_D}{\partial x_k^2} = \frac{1}{|D_\uparrow||D_\downarrow|} \frac{\partial^2 |D_\uparrow||D_\downarrow|}{\partial x_k^2} = \frac{1}{|D_\uparrow|} \frac{\partial^2 |D_\uparrow|}{\partial x_k^2} + \frac{1}{|D_\downarrow|} \frac{\partial^2 |D_\downarrow|}{\partial x_k^2} \quad (6)$$

$$\frac{1}{\Psi_D} \frac{\partial \Psi_D}{\partial x_k} = \frac{1}{|D_\uparrow||D_\downarrow|} \frac{\partial |D_\uparrow||D_\downarrow|}{\partial x_k} = \frac{1}{|D_\uparrow|} \frac{\partial |D_\uparrow|}{\partial x_k} + \frac{1}{|D_\downarrow|} \frac{\partial |D_\downarrow|}{\partial x_k} \quad (7)$$

Inserting equations (7) and (6) into (5) we get

$$\frac{\nabla^2 \Psi_T}{\Psi_T} = \frac{\nabla^2 |D_\uparrow|}{|D_\uparrow|} + \frac{\nabla^2 |D_\downarrow|}{|D_\downarrow|} + 2 \left(\frac{\nabla |D_\uparrow|}{|D_\uparrow|} + \frac{\nabla |D_\downarrow|}{|D_\downarrow|} \right) \cdot \frac{\nabla \Psi_C}{\Psi_C} + \frac{\nabla^2 \Psi_C}{\Psi_C} \quad (8)$$

Now we have 4 different types of ratios we need to find an expression for, $\frac{\nabla^2 |D|}{|D|}$, $\frac{\nabla |D|}{|D|}$, $\frac{\nabla^2 \Psi_C}{\Psi_C}$ and $\frac{\nabla \Psi_C}{\Psi_C}$.