

# FYS4411 - Project 1

## Variational Monte Carlo

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### Abstract

Abstract awesomeness

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## 1 Introduction

## 2 Theoretical model

## 3 Methods

### 3.1 Minimizing computation in the non-interacting case

For the non-interacting case ( $a = 0$ ), certain shortcuts are possible, to save FLOPS.

#### 3.1.1 Computing the numerical energy

From the Schrödinger equation:

$$\hat{H}\Psi_T = \left(-\frac{1}{2}\nabla^2 + V\right)\Psi_T = E\Psi_T \quad (1)$$

The kinetic energy is, numerically, given by (in dimensionless form):

$$T = -\frac{1}{2}\nabla^2\Psi_T \quad (2)$$

This gives, for particle  $i$  and component  $j$ :

$$T_{ij} \approx \frac{\Psi_T(\mathbf{r}_1, \dots, \mathbf{r}_{i,j} + h, \dots, \mathbf{r}_n) - 2\Psi_T(\mathbf{r}) + \Psi_T(\mathbf{r}_1, \dots, \mathbf{r}_{i,j} - h, \dots, \mathbf{r}_n)}{h^2} \quad (3)$$

Which gives, for the simplest trialfunction ( $a = 0$ ):

$$T_{ij} = -\frac{1}{2}\Psi_T \left( \frac{\exp(-\alpha_j(x_j + h)^2)}{\exp(-\alpha_j x_j^2)} - 2 + \frac{\exp(-\alpha_j(x_j - h)^2)}{\exp(-\alpha_j x_j^2)} \right) \frac{1}{h^2} = -\frac{1}{2h^2}\Psi_T (\exp(-2\alpha_j x_j h - \alpha_j h^2) + \exp(2\alpha_j x_j h - \alpha_j h^2)) \quad (4)$$

## 4 Results and discussion

## 5 Conclusion

### 5.1 Conclusion

### 5.2 Outlook

# Appendices

## A Finding the drift force

We wish to compute:

$$\vec{F} = 2 \frac{1}{\psi_T} \nabla \psi_T \quad (5)$$

## B Finding the analytic expression for the local energy

We wish to find:

$$E_L = \frac{1}{\Psi_T} \nabla^2 \Psi_T \quad (6)$$

Where  $\Psi_T$  is given by:

$$\exp \left[ -\alpha \sum_i^n (x_i^2 + y_i^2 + z_i^2) \right] \prod_{i < j} f(a, |\mathbf{r}_i - \mathbf{r}_j|) \quad (7)$$

Look first at  $a = 0$ . In this case, this reduces to the harmonic oscillator potential. The local energy is then:

$$\exp \left[ \alpha \sum_i^n (x_i^2 + y_i^2 + z_i^2) \right] \left( -\frac{\hbar^2}{2m_i} \nabla_i^2 + V \right) \exp \left[ -\alpha \sum_i^n (x_i^2 + y_i^2 + z_i^2) \right] \quad (8)$$

In the simple harmonic oscillator case, this gives:

$$E_L(\mathbf{r}, \alpha) = -\frac{\hbar^2}{2m} \sum_{i=1}^n 2\alpha (2\alpha(x_i^2 + y_i^2 + z_i^2) - 3) + \frac{1}{2} m \omega_{ho}^2 \sum_{i=1}^n (x_i^2 + y_i^2 + z_i^2) \quad (9)$$

**FIX FOR ONE/N PARTICLES AND LOWER DIMENSION** Similarly for the drift force:

$$F = \frac{2\nabla \Psi_T}{\Psi_T} \quad (10)$$

$$F = -2\alpha \sum_{i=1}^n (x_i + y_i + z_i) \quad (11)$$

Now for the ugly part:  
For one particle,  $\nabla_k$ :

$$\nabla_k \Psi_T = \nabla_k \left( \Psi_T(\mathbf{r}) = \nabla_k \prod_{i=1}^n \phi(\mathbf{r}_i) \exp \left( \sum_{i < j} u(r_{ij}) \right) \right) \quad (12)$$

Now apply the product rule. For the first term, all terms are unchanged except where  $i = k$ , giving the first term as:

$$\nabla_k \phi(\mathbf{r}_k) \left[ \prod_{i \neq k} \phi(\mathbf{r}_i) \right] \exp \left( \sum_{i < j} u(r_{ij}) \right) \quad (13)$$

The second term is trickier. We can rewrite it as follows:

$$\prod_i \phi(\mathbf{r}_i) \nabla_k \left[ \exp \left( \sum_{i < j} u(r_{ij}) \right) \right] = \prod_i \phi(\mathbf{r}_i) \nabla_k \left[ \exp \left( \sum_{j=1}^n \sum_{i=1}^{j-1} u(r_{ij}) \right) \right] \quad (14)$$

This is calculated by using the chain-rule. To evaluate the innerfunction, we must look at  $1 \leq j \leq k$ ,  $j = k$  and  $j \geq k$ . Beginning with  $1 \leq j \leq k$ , the first sum is from 1 up the kth particle, meaning all terms differentiated before  $k$  vanishes and we are left with  $u(r_{ik})$ , thus leaving with us with:

$$\prod_i \phi(\mathbf{r}_i) \nabla_k \left[ \exp \left( \sum_{j=1}^k \sum_{i=1}^{j-1} u(r_{ij}) \right) \right] = \prod_i \phi(\mathbf{r}_i) \exp \left\{ \left( \sum_{i < j} u(r_{ij}) \right) \right\} \left[ \sum_{i=1}^{k-1} \nabla_k u(r_{ik}) \right] \quad (15)$$

For  $j = k$ , we see that the first sum goes from and end up at kth particle, meaning this sum vanishes, secondly, the second sum is evaluated at  $1 \leq i \leq k - 1$ , leaving with constants up to  $k - 1$ , thus this term becomes 0.

$$\prod_i \phi(\mathbf{r}_i) \nabla_k \left[ \exp \left( \sum_{j=1}^n \sum_{i=1}^{j-1} u(r_{ij}) \right) \right] = 0 \quad (16)$$

For  $j > k$ , the first sum goes from  $k + 1 \leq j \leq n$  and the second  $1 \leq i \leq k$ . The second sum vanishes, because all constants are differentiated away except the last term  $i = k$ . This leaves us with:

$$\prod_i \phi(\mathbf{r}_i) \nabla_k \left[ \exp \left( \sum_{j=k+1}^n \sum_{i=1}^k u(r_{ij}) \right) \right] = \prod_i \phi(\mathbf{r}_i) \exp \left\{ \left( \sum_{i < j} u(r_{ij}) \right) \right\} \left[ \sum_{j=k+1}^n \nabla_k u(r_{kj}) \right] \quad (17)$$

We can now write the second term as 14):

$$\prod_i \phi(\mathbf{r}_i) \exp \left\{ \left( \sum_{i < j} u(r_{ij}) \right) \right\} \left[ \sum_{j=k+1}^n \nabla_k u(r_{kj}) + \left[ \sum_{i=1}^{k-1} \nabla_k u(r_{ik}) \right] \right] \quad (18)$$

This can be rewritten to:

$$\prod_i \phi(\mathbf{r}_i) \exp \left\{ \left( \sum_{i < j} u(r_{ij}) \right) \right\} \left[ \sum_{j \neq k} \nabla_k u(r_{kj}) \right] \quad (19)$$

FORKLAR denne delen litt. Thus the first derivative of the trial wavefunction can be written as:

$$\nabla_k \Psi_T = \nabla_k \phi(\mathbf{r}_k) \left[ \prod_{i \neq k} \phi(\mathbf{r}_i) \right] \exp \left( \sum_{i < j} u(r_{ij}) \right) + \prod_i \phi(\mathbf{r}_i) \exp \left\{ \left( \sum_{i < j} u(r_{ij}) \right) \right\} \left[ \sum_{j \neq k} \nabla_k u(r_{kj}) \right] \quad (20)$$

Lastly we will calculate the second derivative of the trial function, where we use the product rule and the chain rule. We will then obtain the following:

$$\begin{aligned}
\nabla_k^2 \Psi_T = & \underbrace{\nabla_k^2 \phi(\mathbf{r}_k) \left[ \prod_{i \neq k} \phi(\mathbf{r}_i) \right] \exp \left( \sum_{i < j} u(r_{ij}) \right)}_{\text{I}} + \\
& \underbrace{2 \left( \nabla_k \phi(\mathbf{r}_k) \left[ \prod_{i \neq k} \phi(\mathbf{r}_i) \right] \exp \left\{ \left( \sum_{i < j} u(r_{ij}) \right) \right\} \left[ \sum_{j \neq k} \nabla_k u(r_{kj}) \right] \right)}_{\text{II}} + \\
& \underbrace{\prod_i \phi(\mathbf{r}_i) \exp \left\{ \left( \sum_{i < j} u(r_{ij}) \right) \right\} \left[ \sum_{j \neq k} \nabla_k u(r_{kj}) \right]^2}_{\text{III}} + \\
& \underbrace{\prod_i \phi(\mathbf{r}_i) \exp \left\{ \left( \sum_{i < j} u(r_{ij}) \right) \right\} \left[ \sum_{j \neq k} \nabla_k \nabla_k u(r_{kj}) \right]}_{\text{IV}}
\end{aligned}$$

Where the derivatives of the different parts are obtained from previous. We will now divide the second derivative by the trial wavefunction, and obtain:

$$\frac{1}{\Psi_T} \nabla_k^2 \Psi_T = \underbrace{\frac{\nabla_k^2 \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)}}_{\text{I}} + \underbrace{2 \frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \sum_{j \neq k} \nabla_k u(r_{kj})}_{\text{II}} + \underbrace{\left( \sum_{j \neq k} \nabla_k u(r_{kj}) \right)^2}_{\text{III}} + \underbrace{\left[ \sum_{j \neq k} \nabla_k \nabla_k u(r_{kj}) \right]}_{\text{IV}} \quad (21)$$

We will now carry out the differentiation in term (II), (III) and (IV). Beginning with the (II), by using the chain rule we can rewrite (II) as:

$$2 \frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \sum_{j \neq k} \frac{\partial u(r_{kj})}{\partial r_{kj}} \frac{\partial r_{kj}}{\partial \mathbf{r}_k} = 2 \frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \left( \sum_{j \neq k} \frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} u'(r_{kj}) \right)$$

Where we have used  $\nabla_k r_{kj} = (\mathbf{r}_k - \mathbf{r}_j)/r_{kj}$ . Looking at (III), we can write out the square into two factors. The second paranthese the summation index is replaced by a dummy index  $i$ . Thus will look as:

$$\left( \sum_{j \neq k} \nabla_k u(r_{kj}) \right)^2 = \left( \sum_{j \neq k} \nabla_k u(r_{kj}) \right) \left( \sum_{i \neq k} \nabla_k u(r_{ki}) \right) \quad (22)$$

From (II) we found the derivative of this function. Thus this can be expressed as (combining also the double sum):

$$\left( \sum_{j \neq k} \nabla_k u(r_{kj}) \right)^2 = \sum_{i, j \neq k} \left( \frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} \right) \left( \frac{\mathbf{r}_k - \mathbf{r}_i}{r_{ki}} \right) u'(r_{kj}) u'(r_{ki}) \quad (23)$$

The last part (IV), we must use the chain rule and product rule together. We will obtain the following term:

$$\sum_{j \neq k} \nabla_k \nabla_k u(r_{kj}) = \sum_{j \neq k} \nabla_k \left( \left( \frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} \right)^2 u''(r_{kj}) + u'(r_{kj}) \nabla_k \left( \frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} \right) \right) \quad (24)$$

Note that this is a unit vector squared:

$$\left(\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}}\right)^2 = 1 \quad (25)$$

and the last part is found by using the quotient rule. This is the divergence to the vectors, since we are evaluating for specific particle  $k$ , and gradient to scalar (we must look for all combination of  $k$  particle):

$$\nabla_k \left( \frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} \right) = \frac{r_{kj} (\nabla_k \cdot \mathbf{r}_k - \nabla_k \cdot \mathbf{r}_j) - (\mathbf{r}_k - \mathbf{r}_j) \nabla_k r_{kj}}{r_{kj}^2} \quad (26)$$

This simply becomes:

$$\nabla_k \left( \frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} \right) = \frac{3r_{kj}^2 - \mathbf{r}_k^2 + 2(\mathbf{r}_k \cdot \mathbf{r}_j) - \mathbf{r}_j^2}{r_{kj}^3} \quad (27)$$

Note that  $r_{kj}^2 - \mathbf{r}_k^2 + 2(\mathbf{r}_k \cdot \mathbf{r}_j) - \mathbf{r}_j^2 = 0$ , this leaves us with:

$$\nabla_k \left( \frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} \right) = \frac{2}{r_{kj}} \quad (28)$$

Thus expression (IV) can be expressed as:

$$\sum_{j \neq k} \nabla_k \nabla_k u(r_{kj}) = \sum_{j \neq k} \nabla_k \left( u''(r_{kj}) + \frac{2}{r_{kj}} u'(r_{kj}) \right) \quad (29)$$

Combining (I), (II), (III) and (IV), we we will get that the second derivative of the trial function is:

$$\begin{aligned} \frac{1}{\Psi_t} \nabla_k^2 \Psi_T &= \frac{\nabla_k^2 \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + 2 \frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \left( \sum_{j \neq k} \frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} u'(r_{kj}) \right) + \\ &\sum_{i, j \neq k} \left( \frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} \right) \left( \frac{\mathbf{r}_k - \mathbf{r}_i}{r_{ki}} \right) u'(r_{kj}) u'(r_{ki}) + \sum_{j \neq k} \nabla_k \left( u''(r_{kj}) + \frac{2}{r_{kj}} u'(r_{kj}) \right) \end{aligned} \quad (30)$$