

# FYS4411 - Project 2

## The restricted Boltzmann machine applied to the quantum many body problem

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**Abstract**

NICE ABSTRACT

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# **1 Introduction**

COOL INTRO

# **2 Theoretical model**

MUCH THEORY

# **3 Methods**

MUCHO METHOD

# **4 Results**

GROUNDBREAKING RESULTS

# **5 Discussion**

EXCELLENT DISCUSSION

# **6 Conclusion**

BRILLIANT CONCLUSION

## **6.1 Outlook**

MAGNIFICENT OUTLOOK

# **References**

# Appendices

## A Finding the derivatives

In this section, we derive the expressions for the various derivatives stated in section **SECTION**. We begin with the local energy.

### A.1 The local energy

The local energy is given by:

$$E_L = \frac{1}{\Psi} \hat{H} \Psi = \sum_{i=1}^N \left( -\frac{1}{2\Psi} \nabla_i^2 \Psi + \frac{1}{2} \omega^2 r_i^2 \right) + \sum_{i < j} \frac{1}{r_{ij}} \quad (1)$$

Thus, we must compute:

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

This may be rewritten as:

$$\frac{1}{\Psi} \nabla \left( \Psi \frac{1}{\Psi} \nabla \Psi \right) = \left( \frac{1}{\Psi} \nabla \Psi \right)^2 + \nabla \left( \frac{1}{\Psi} \nabla \Psi \right) = [\nabla \log \Psi]^2 + \nabla^2 \log \Psi \quad (3)$$

The logarithm of our trial wavefunction is given by:

$$\log \Psi = -\log Z - \sum_{i=1}^M \left( \frac{(X_i - a_i)^2}{2\sigma^2} \right) + \sum_{j=1}^N \log \left( 1 + \exp \left( b_j + \sum_{i=1}^M \frac{X_i w_{ij}}{\sigma^2} \right) \right) \quad (4)$$

The derivative with respect to one coordinate is now given by:

$$\begin{aligned} \frac{\partial \log \Psi}{\partial X_k} &= \frac{(a_k - X_k)}{\sigma^2} + \sum_{j=1}^N \frac{w_{kj} \exp \left( b_j + \sum_{i=1}^M \frac{X_i w_{ij}}{\sigma^2} \right)}{\sigma^2 \left( 1 + \exp \left( b_j + \sum_{i=1}^M \frac{X_i w_{ij}}{\sigma^2} \right) \right)} \\ &= \frac{a_k - X_k}{\sigma^2} + \sum_{j=1}^N \frac{w_{kj}}{\sigma^2 \left( 1 + \exp \left( -b_j - \sum_{i=1}^M \frac{X_i w_{ij}}{\sigma^2} \right) \right)} \end{aligned} \quad (5)$$

Whereas the second derivative is:

$$\frac{\partial^2 \log \Psi}{\partial X_k^2} = -\frac{1}{\sigma^2} + \sum_{j=1}^N \frac{w_{kj}^2 \exp \left( -b_j - \sum_{i=1}^M \frac{X_i w_{ij}}{\sigma^2} \right)}{\sigma^4 \left( 1 + \exp \left( -b_j - \sum_{i=1}^M \frac{X_i w_{ij}}{\sigma^2} \right) \right)^2} \quad (6)$$

The local energy can now be found by using equation 3, and inserting equation 5 and equation 6.

### A.2 The derivatives with respect to the parameters

For our optimization method, we require:

$$\frac{1}{\Psi} \frac{\partial \Psi}{\partial \alpha_k} = \frac{\partial}{\partial \alpha_k} \log \Psi \quad (7)$$

Where  $\alpha_k$  is any of the variational parameters  $a$ ,  $b$  or  $w$ . These derivatives are given by:

$$\frac{\partial \log \Psi}{\partial a_k} = \frac{X_k - a_k}{\sigma^2} \quad (8)$$

$$\frac{\partial \log \Psi}{\partial b_k} = \frac{\exp\left(b_k + \sum_{i=1}^M \frac{X_i w_{ik}}{\sigma^2}\right)}{1 + \exp\left(b_k + \sum_{i=1}^M \frac{X_i w_{ik}}{\sigma^2}\right)} = \frac{1}{1 + \exp\left(-b_k - \sum_{i=1}^M \frac{X_i w_{ik}}{\sigma^2}\right)} \quad (9)$$

Finally, the derivative with respect to the weights,  $w_{kl}$  is given by:

$$\frac{\partial \log \Psi}{\partial w_{kl}} = \frac{X_k \exp\left(b_l + \sum_{i=1}^M \frac{X_i w_{il}}{\sigma^2}\right)}{\sigma^2 \left(1 + \exp\left(b_l + \sum_{i=1}^M \frac{X_i w_{il}}{\sigma^2}\right)\right)} = \frac{X_k}{\sigma^2 \left(1 + \exp\left(-b_l - \sum_{i=1}^M \frac{X_i w_{il}}{\sigma^2}\right)\right)} \quad (10)$$