# The Potato and its dynamics

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# Abstract

This is an abstract text.

# Acknowledgements

I acknowledge my acknowledgements.

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# Chapter 1

# Introduction

Start your chapter by writing something smart. Then go get coffee.

# Part I

# Theory

# Chapter 2

# Hartree-Fock theory

Because its all about that energy, 'bout that energy, 'bout that energy!

# Part II

# Appendices

# Appendix A

# Hartree-Fock

Hartree-Fock appendix.

# Appendix B

# Reformulating the amplitude equations

We will in this appendix show how to formulate the tensor contractions occuring in the the coupled cluster equations from Gauss et al.[1] as matrix products. The reason we wish to do this is to be able to perform these contractions as dot products (or matrix products) as there exists highly optimized code performing these operations, e.g., BLAS[1].

To be able to treat tensors of rank $> 2$ as matrices we have to create *compound indices* by stacking the dimensions after one another. For instance, by looking at the tensor $g \in \mathbb{C}^{I \times J \times K \times L}$ where we denote a single element by $g_{ijkl}$. Here $g$ denotes a tensor of rank 4. By creating compound indices $\tilde{I} = IJ$ and $\tilde{K} = KL$ we can create a new tensor $\tilde{g} = \mathbb{C}^{\tilde{I} \times \tilde{K}}$ of rank 2 (represented as a matrix). Using the indices $\tilde{i} = iJ + j$ and $\tilde{k} = kL + l$ we now construct $\tilde{g}$ in such a way that $\tilde{g}_{\tilde{i}\tilde{k}} = g_{ijkl}$.

[1]BLAS can be found here: http://www.netlib.org/blas/

# Bibliography

[1] Jürgen Gauss and John F Stanton. "Coupled-cluster calculations of nuclear magnetic resonance chemical shifts". In: *The Journal of chemical physics* 103.9 (1995), pp. 3561–3577.