Squeezing Atoms Using a Confinement Potential

A Thesis presented in fulfillment of the requirements for the degree of

Master of Science in Mathematical Physics

Massey University, Albany
New Zealand

Julianne Neilson Coxe
Supervisor: Peter Schwerdtfeger

2010

Abstract

Understanding the complexities of the interior of planets and stars requires the help of analyzing the effects of high pressures on certain elements believed to be found within. The Hartree-Fock method uses the Schrödinger equation, Kummer's differential equations and a confinement potential to simulate an atom being squeezed to high pressures. The Hartree-Fock method was used to calculate the total energies of atoms. After being compared to Gaussian03 and VASP, the results were deemed accurate. It was also observed that the pressure versus density data closely approximated those pairs found in outer space in the interiors of, for example, Jupiter.

Acknowledgments

To Massey University and Gaven Martin for allowing me the privilege of studying at this fine institution. ⋆ To Peter Schwerdtfeger for his vision, his help and his suggestion for me to complete a Masters degree. ⋆ To Christian Thierfelder for his patience, thorough explanations, encouragement and assistance. ⋆ To Detlev, Andreas and Matthias for their help, patience and stimulating lunch conversations. ⋆ To Elke for proofreading my thesis more than one time. ⋆ To Thomas Proffen and Tony Burrell without whom I would not be in New Zealand. ⋆ To my parents for their unending love and encouragement. ⋆ And to God for his wonderful love and mercy in giving me all of the courage, patience and perseverance I needed to complete this challenge.

Contents

List of Figures

List of Tables