Confined Atomic Systems

A thesis presented in partial fulfilment of the

requirements for the degree of

Doctor of Philosophy

in

Mathematical Physics

at Massey University, Albany,

New Zealand

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2015

Abstract

In this thesis, we investigate physical properties of various atomic systems such as hydrogen, helium and argon confined in a soft–wall potential of the form $V_s(r) = (r/r_0)^N$, where r_0 is the radius of the spherical confinement and N is the stiffness controlling variable. Our main purpose is to introduce a confinement for atomic systems that is flexible in terms of stiffness of the confining walls. However, this brings its complications such as non–existence of analytic solutions to the non–relativistic Schrödinger equation for this particular problem, and non–availability of good basis sets for studying electronic properties of such systems. Therefore, at first, we treat the problem in pure numerical fashion. Based on our experience on the numerical data, we then attempt to design basis sets that can be used in quantum chemical software packages. We compare our results to known theoretical and experimental results and, in return, make a decision on the quality of the basis sets. To our knowledge, systems confined in this type of potential has not yet been studied, and, we believe that this study will open up new research areas in this field. Possible applications are in high–pressure simulations of atomic, or molecular systems.

Acknowledgements

This research project would not have been successful without the support of many people. I would like to express my deep gratitude towards my supervisor Distinguished Prof. Peter Schwerdtfeger for all his support, help, guidance and vision. He was always within reach when I needed his help. I would also like to thank my co–supervisor Prof. Boris Pavlov for all the exciting discussions on Mathematics. In addition, my thanks to the old and new members of the CTCP for all the lunch breaks and our awesome challenging discussions, specially Dr. Michael Wormit, Dr. Andreas Hauser and Dr. Florian Senn. One special thanks goes to Dr. Jonas Kortner. If it wasn't for him, I wouldn't be able to make it this far. He repeatedly explained very trivial concept without losing his patience. And, thanks to him I was able to grasp the basics. I would also like to thank Nik Harris for his support, courage, patience and care. Without him, this journey would be a very difficult one. Last but not least, I am grateful to have the love, respect and appreciation of my mother and sisters.

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