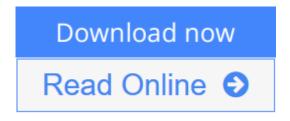# Quantum Monte-Carlo Programming: For Atoms, Molecules, Clusters, and Solids

By Wolfgang Schattke, Ricardo Díez Muiño

Quantum Monte-Carlo Programming: For Atoms, Molecules, Clusters, and Solids By Wolfgang Schattke, Ricardo Díez Muiño

Quantum Monte Carlo is a large class of computer algorithms that simulate quantum systems to solve many body systems in order to investigate the electronic structure of many-body systems. This book presents a numeric approach to determine the electronic structure of atoms, molecules and solids. Because of the simplicity of its theoretical concept, the authors focus on the variational Quantum-Monte-Carlo (VQMC) scheme. The reader is enabled to proceed from simple examples as the hydrogen atom to advanced ones as the Lithium solid. Several intermediate steps cover the Hydrogen molecule, how to deal with a two electron systems, going over to three electrons, and expanding to an arbitrary number of electrons to finally treat the three-dimensional periodic array of Lithium atoms in a crystal.
The exmples in the field of VQMC are followed by the subject of diffusion Monte-Calro (DMC) which covers a common example, the harmonic ascillator.

The book is unique as it provides both theory and numerical programs. It includes rather practical advices to do what is usually described in a theoretical textbook, and presents in more detail the physical understanding of what the manual of a code usually promises as result. Detailed derivations can be found at the appendix, and the references are chosen with respect to their use for specifying details or getting an deeper understanding .

The authors address an introductory readership in condensed matter physics, computational phyiscs, chemistry and materials science. As the text is intended to open the reader's view towards various possibilities of choices of computing schemes connected with the method of QMC, it might also become a welcome literature for researchers who would like to know more about QMC methods.

The book is accompanied with a collection of programs, routines, and data. To download the codes, please follow
http://www.wiley-vch.de/books/sample/3527408517_codes.tar.gz

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Editorial Review

Review

"The combination of both aspects allows the reader to assimilate the fundamentals of Quantum Monte Carlo not only by reading but also by practice." (*ETDE Energy Database*, 1 November 2013)

From the Back Cover

This is a book that initiates the reader into the basic concepts and practical applications of Quantum Monte Carlo. Because of the simplicity of its theoretical concept, the authors focus on the variational Quantum Monte Carlo scheme. The reader is enabled to proceed from simple examples as the Hydrogen atom to advanced ones as the Lithium solid. In between, several intermediate steps are introduced, including the Hydrogen molecule (2 electrons), the Lithium atom (3 electrons) and expanding to an arbitrary number of electrons to finally treat the three-dimensional periodic array of Lithium atoms in a crystal.

The book is unique because it provides both theory and numerical programs. It pedagogically explains how to transfer into computational tools what is usually described in a theoretical textbook. It also includes the detailed physical understanding of methodology that cannot be found in a code manual.

The combination of both aspects allows the reader to assimilate the fundamentals of Quantum Monte Carlo not only by reading but also by practice.

From the contents:

- A first Monte Carlo example
- Variational Quantum Monte Carlo for a One-Electron System
- Two electrons with two adiabatically decoupled nuclei: Hydrogen molecule
- Three electrons: Lithium Atom
- Many-electron confined systems
- Many-electron atomic aggregates: Lithium cluster
- Infinite number of electrons: Lithium solid
- Diffusion Quantum Monte Carlo: One-dimensional example

About the Author
Wolfgang Schattke is a retired member of the Institut f�r Theoretische Physik und Astrophysik der Christian-Albrechts-University Kiel where his teaching covered the branch of theoretical physics from the basic courses to advanced topics of the PhD curriculum. His research interests focus on material properties of the solid state and its surfaces investigated with ab-initio electronic structure methods. Besides studying numerical access to photoemission spectroscopy, his scientific efforts point to many-body theory where Quantum Monte-Carlo offers a central tool to complete the successful application of Density Functional Theory to material sciences.

Ricardo D�ez Muino is Vice Director of the Centro de F�sica de Materiales, a Joint Center between the University of the Basque Country UPV/EHU and the Spanish Research Council CSIC in San Sebastian.

Previously, he developed his research activity in the Donostia International Physics Center DIPC (Spain), the Lawrence Berkeley National Laboratory (USA), and the Universitï¿½ de Bordeaux (France). His main field of research is condensed matter theory, particularly electronic excitations in metallic systems, with some excursions into atomic and molecular physics.

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