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

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

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

- Rank: #2945366 in Books
- Published on: 2013-09-03
- Original language: English
- Number of items: 1
- Dimensions: 9.45" h x .55" w x 6.70" l, .0 pounds
- Binding: Paperback
- 296 pages

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 fï¿½r 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 Dï¿½ez Muino is Vice Director of the Centro de Fï¿½sica 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.

Users Review

From reader reviews:

John Krumm:

Book is actually written, printed, or descriptive for everything. You can learn everything you want by a e-book. Book has a different type. As we know that book is important issue to bring us around the world. Close to that you can your reading proficiency was fluently. A e-book Quantum Monte-Carlo Programming: For Atoms, Molecules, Clusters, and Solids will make you to become smarter. You can feel much more confidence if you can know about every little thing. But some of you think which open or reading a book make you bored. It is far from make you fun. Why they may be thought like that? Have you looking for best book or acceptable book with you?

Kevin Pennell:

What do you concerning book? It is not important along? Or just adding material when you require something to explain what yours problem? How about your spare time? Or are you busy individual? If you don't have spare time to try and do others business, it is gives you the sense of being bored faster. And you have free time? What did you do? Everyone has many questions above. The doctor has to answer that question due to the fact just their can do that. It said that about book. Book is familiar on every person. Yes, it is suitable. Because start from on pre-school until university need this kind of Quantum Monte-Carlo Programming: For Atoms, Molecules, Clusters, and Solids to read.

Alberto Alvarez:

This Quantum Monte-Carlo Programming: For Atoms, Molecules, Clusters, and Solids tend to be reliable for you who want to become a successful person, why. The reason of this Quantum Monte-Carlo Programming: For Atoms, Molecules, Clusters, and Solids can be among the great books you must have will be giving you more than just simple reading food but feed you actually with information that perhaps will shock your preceding knowledge. This book is usually handy, you can bring it all over the place and whenever your conditions at e-book and printed ones. Beside that this Quantum Monte-Carlo Programming: For Atoms, Molecules, Clusters, and Solids giving you an enormous of experience including rich vocabulary, giving you test of critical thinking that we realize it useful in your day pastime. So , let's have it and revel in reading.

Dorothy Saunders:

This Quantum Monte-Carlo Programming: For Atoms, Molecules, Clusters, and Solids is brand new way for you who has curiosity to look for some information as it relief your hunger info. Getting deeper you into it getting knowledge more you know or perhaps you who still having bit of digest in reading this Quantum

Monte-Carlo Programming: For Atoms, Molecules, Clusters, and Solids can be the light food to suit your needs because the information inside this particular book is easy to get by simply anyone. These books develop itself in the form which can be reachable by anyone, yes I mean in the e-book contact form. People who think that in guide form make them feel tired even dizzy this reserve is the answer. So there isn't any in reading a reserve especially this one. You can find actually looking for. It should be here for you. So , don't miss it! Just read this e-book sort for your better life along with knowledge.

Download and Read Online Quantum Monte-Carlo Programming: For Atoms, Molecules, Clusters, and Solids By Wolfgang Schattke, Ricardo Díez Muiño #WZ5EMX4OSH3

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

Quantum Monte-Carlo Programming: For Atoms, Molecules, Clusters, and Solids By Wolfgang Schattke, Ricardo Díez Muiño Free PDF d0wnl0ad, audio books, books to read, good books to read, cheap books, good books, online books, books online, book reviews epub, read books online, books to read online, online library, greatbooks to read, PDF best books to read, top books to read Quantum Monte-Carlo Programming: For Atoms, Molecules, Clusters, and Solids By Wolfgang Schattke, Ricardo Díez Muiño books to read online.

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

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

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

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

WZ5EMX4OSH3: Quantum Monte-Carlo Programming: For Atoms, Molecules, Clusters, and Solids By Wolfgang Schattke, Ricardo Díez Muiño