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An Introduction to Quantum Monte Carlo Methods

An Introduction to Quantum Monte Carlo Methods

Tao Pang

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To Yunhua, for her love and care

Contents

Preface	ix
Acknowledgements	x
Author biography	xi
1 Introduction	1-1
1.1 Sampling	1-2
1.2 Random-number generators	1-4
Uniform random-number generators	1-5
Other distributions	1-9
Percolation in two dimensions	1-11
Exercises	1-12
Bibliography	1-14
2 The Metropolis algorithm	2-1
2.1 Importance sampling	2-1
2.2 Classical liquids	2-5
2.3 Block algorithms	2-8
Exercises	2-13
Bibliography	2-14
3 Variational Monte Carlo	3-1
3.1 Variational principle	3-2
3.2 The Metropolis step	3-2
3.3 Kinetic energy and wavefunction	3-4
3.4 Quantum dots	3-7
Exercises	3-7
Bibliography	3-9
4 Diffusion Monte Carlo	4-1
4.1 The algorithm	4-1
4.2 Evaluation of physical quantities	4-3
Energy	4-3
Structural analysis	4-4
4.3 ^4He clusters on a graphite surface	4-5

The model Hamiltonian	4-5
The guide/trial wavefunction	4-6
Some preliminary simulation results	4-8
Exercises	4-11
Bibliography	4-13
5 Path-integral Monte Carlo	5-1
5.1 Introduction	5-1
5.2 The propagation of a quantum state	5-2
5.3 Single-particle system	5-5
5.4 Quantum many-body systems	5-8
5.5 Physical properties of extended systems	5-9
5.6 Cold atoms	5-10
Exercises	5-15
Bibliography	5-16

Preface

In nearly a century, we have witnessed steady progress in the computational study of scientific problems. Now many complex issues in all the technical fields are analyzed and tackled on computers. New paradigms of global-scale computing have emerged, such as the cloud or grid computing. Computers are faster and bigger than ever and come with many more functionalities and applications. There has never been a better time to study scientific problems on computers. Amongst all the computer techniques used in scientific studies, the Monte Carlo approach appears to be most prominent.

This book provides a concise but complete introduction to two computer simulation methods, the diffusion quantum Monte Carlo and the path-integral quantum Monte Carlo, primarily used in research of the many-body problem. There is no assumption of previous experience in computer simulation of the readers but a minimum knowledge of physics typically possessed by an upper-division student or a beginning graduate in physics is required.

To make this book practical, two complete programs in Java, one for the diffusion quantum Monte Carlo simulation of ^4He clusters on a graphite surface and the other for the path-integral quantum Monte Carlo simulation of cold atoms in a potential trap, are ready to be downloaded and altered for any research project that the reader wants. These programs will be maintained and improved over time. There will also be additions to the existing programs and they are all accessible through my web page: <http://www.physics.unlv.edu/~pang>.

Tao Pang
Las Vegas, Nevada, USA
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Many colleagues from all over the world have made contributions to this book either through collaborating with me on some of the projects described here or communicating with me on the subjects discussed in this book. My deepest gratitude goes to those who have worked or communicated with me over the years regarding the topics covered in the book, especially to those inspired young scholars who have constantly reminded me that the effort of writing this book will be worthwhile and the students who have taken courses from me on related matters.

Author biography

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Tao Pang is Professor of Physics at the University of Nevada, Las Vegas (UNLV). Following his higher education at Fudan University, one of the most prestigious institutions in China, he obtained his PhD in condensed matter theory from the University of Minnesota in 1989. He then spent two years as a Miller Research Fellow at the University of California, Berkeley, before joining the UNLV physics faculty in the fall of 1991. He has been Professor of Physics at UNLV since 2002. His main areas of research include condensed matter theory and computational physics.