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# An Introduction to Quantum Monte Carlo Methods



# An Introduction to Quantum Monte Carlo Methods

**Tao Pang**

*University of Nevada, Las Vegas, USA*

Morgan & Claypool Publishers

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*To Yunhua, for her love and care*



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# 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  ${}^4\text{He}$  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*  
*August, 2016*

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# Author biography

## **Tao Pang**

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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.