<<计算物理学>>

图书基本信息

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内容概要

This Second Edition has been fully updated. The wide range of topics covered inthe First Edition has been extended with new chapters on finite element methodsand lattice Boltzmann simulation. New sections have been added to the chapters ondensity functional theory, quantum molecular dynamics, Monte Carlo simulationand diagonalisation of one-dimensional quantum systems.

The book covers many different areas of physics research and different computa-tional methodologies, with an emphasis on condensed matter physics and physicalchemistry. It includes computational methods such as Monte Carlo and moleculardynamics, various electronic structure methodologies, methods for solving par-tial differential equations, and lattice gauge theory. Throughout the book, therelations between the methods used in different fields of physics are emphas-ised. Several new programs are described and these can be downloaded fromwww.cambridge.org/9780521833462

The book requires a background in elementary programming, numerical analysisand field theory, as well as undergraduate knowledge of condensed matter theoryand statistical physics. It will be of interest to graduate students and researchers intheoretical, computational and experimental physics.Jos THIJSSEN is a lecturer at the Kavli Institute of Nanoscience at Delft Universityof Technology.

作者简介

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章节摘录

版权页：插图：Now we can define the problems in a more abstract way. It is convenient toconsider continuum problems. The candidate solutions （for example the possibleconformations） form a phase space, and the merit function has some complicatedshape on that space - it contains many valleys and mountains, which can be verysteep. The solution we seek corresponds to the lowest valley in the landscape. Notethat the landscape is high-dimensional. You may think, naively, that a standardnumerical minimum finder can solve this problem for you. However, this is notthe case as such an algorithm always needs a starting point, from which it findsthe nearest local minimum, which is not necessarily the best you can find in theconformation space. The set of points which would go to one particular local min-imum when fed into a steepest descent or other minimum-finder （see AppendixA4） is called the basin of attraction of that minimum. Once we are in the basinof attraction of the global minimum we can easily find this global minimum; theproblem is to find its basin of attraction.

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