Preface

The variational method is one of the most widely used techniques to solve the eigenvalue problems of quantum-mechanical Hamiltonians. Its popularity is due to its simplicity and flexibility. The most crucial point in the variational approach is the choice of a variational trial function. One usually attempts to construct the trial function from some adequate basis functions which contain a number of nonlinear parameters. The direct method of diagonalizing the Hamiltonian matrix on such a basis set may not be feasible, except for simple systems, because of the large number of degrees of freedom involved in specifying the system. One thus faces a problem of selecting the most suitable basis set. It is by the stochastic variational method, that is, by a trial and error procedure with an admittance test that we give an answer to this problem. The stochastic variational method has been developed through the search for precise solutions of nuclear few-body problems. In this method we set up the basis element one after the other because it enables us to test many parameters as fast as possible and moreover to monitor the energy convergence.

The aim of this book is to give a unified and reasonably simple recipe for solutions of few-body bound-state problems with the use of the stochastic variational method and to present its application to various few-body problems which one encounters in atomic, molecular, nuclear, subnuclear and solid state physics.

Though a unified approach to the diverse quantum systems is in general extremely difficult and challenging, great advances have been made in recent years, especially for systems of a few particles and it has become possible to obtain accurate solutions for the eigenvalue problem of various quantum-mechanical Hamiltonians. The main interest in the few-body problems lies in, e.g., finding an accurate solution for the system so as to understand the dynamics of its constituents, test-

ing the equation of motion and the conservation laws and symmetries, or looking for unknown interactions governing the system.

Quantum mechanics plays a fundamental role in atomic and subatomic physics. It is via quantum mechanics that one can understand the binding mechanism of atoms, molecules and atomic nuclei, that is, the structure of the building blocks of matter. The interaction between the particles depends on the system: For example, the long-range Coulomb interaction dominates in atoms and molecules but the very different mass ratio of the electrons and the atomic nucleus plays a key role as well. In contrast, the protons and neutrons in nuclei have almost equal masses and the interaction between them is short-ranged.

The variational foundation for the time-independent Schrödinger equation provides a solid and arbitrarily improvable framework for the solution of diverse bound-state problems. As mentioned above, the most crucial point in the variational approach is the choice of the trial function. There are two widely applied strategies for this choice: One is to use the most appropriate functional form to describe the short-range as well as the long-range correlations among the particles. Such calculations, however, are fairly complex for systems of more than three particles, and the integration involved is performed by the Monte Carlo method. Another way is to approximate the solution as a combination of a number of simple basis states which facilitate the analytical calculation of matrix elements. We follow the latter course in this book and show that the stochastic variational method selects the most important basis set without any bias, keeps the dimension of the basis low and, most importantly, provides a very accurate solution.

The book is conceptually divided into two parts. The first seven chapters present the basic concepts of the variational method and the formulation using Gaussian basis functions. The latter four chapters of the book cover applications of the formulation to various quantum-mechanical few-body bound-state problems. In Chap. 2 a general formulation is developed to express the physical operators which are needed to specify the Hamiltonian in terms of an arbitrary set of independent relative coordinates. The linear transformation of the relative coordinates induced by the permutation of identical particles is also established in this chapter. In Chap. 3 we review the basic principles of the variational method with particular emphasis on the case where the variational trial function is given as a linear combination of nonorthogonal basis functions. We introduce in Chap. 4 a key algorithm used in this book, the stochastic variational method, and show

that its trial and error search procedure makes it possible to select the most important basis functions without any bias in the function space spanned by the basis functions. Some other methods to solve few-body problems are briefly introduced in Chap. 5. Chapter 6 defines the type of variational trial functions used extensively in the book, the correlated Gaussians and the correlated Gaussian-type geminals. They are chosen because they enable us to evaluate matrix elements analytically and because they provide us with precise solutions for most problems of real interest. A simple but powerful angular function is introduced to describe orbital motion with nonzero orbital angular momentum. To facilitate the systematic and unified evaluation of matrix elements, it is shown that the above Gaussian basis functions are all obtained from a generating function. In Chap. 7 we show that the generating function plays a vital role in deriving the matrix elements of the Gaussian basis functions for an N-body system of essentially any interaction. Explicit formulas are given in this chapter for the simplest possible Gaussian basis functions, because they are already found to be very useful. The matrix elements for a general case are detailed in the appendix. We show also in this chapter that the method can be extended to evaluate the matrix elements of nonlocal potentials and the semirelativistic kinetic energy as well. Chapters 8–11 present application of the stochastic variational method to various systems: small atoms and molecules (Chap. 8), baryon spectroscopy (Chap. 9), excitonic complexes and quantum dots in solid state physics (Chap. 10), and nuclear few-body problems (Chap. 11).

We hope that this book will be found useful by students who want to understand and make use of the variational approach to quantum-mechanical few-body problems, while it may also be of interest to researchers who are familiar with the subjects. It will be our pleasure if this book serves to bridge the gap between graduate lectures and the literature in scientific journals, as well as to give impetus to further development in the deeper understanding of quantum-mechanical few-body systems. We assume that readers have taken courses on quantum mechanics and mathematical physics at an undergraduate level. No special knowledge is assumed of, e.g., atomic physics or nuclear physics. To help readers to understand the text, we have attempted to make the book self-contained, put as much emphasis as possible on clarity, and given several Complements of an explanatory nature. The Complements are intended to further develop or to reinforce the arguments and ideas presented in the text. We have collected the derivation

of formulas that may possibly be difficult for readers as exercises with solutions at the end of the chapters.

Depending on their interest, readers may adopt several reading strategies. A thorough-going reader is advised to read all of the text including the Complements. A reader who wants to understand only the basic formulation can omit the Complements. Anyone who is familiar with the variational method may skip Chaps. 2 and 3. Experts, or those readers who are only interested in the performance of the stochastic variational approach or the physical consequences of the results, may skip Chaps. 2–7.

The Gaussian basis has long been used in many areas of physics. The correlated Gaussians were first introduced in quantum chemistry by S.F. Boys and K. Singer. The application of the Gaussian basis is one of the key elements of the success of the ab initio calculations in quantum chemistry. The stochastic variational method is actually very similar to the so-called "random tempering", that has been used to find the optimal parameters of the basis in quantum chemistry. In the random tempering pseudo-random parameters are generated, and the best basis functions are selected by sorting out the states which improve the energy. There exists another method which is also similar to the stochastic variational method, called the stochastic diagonalization. This method, originally developed in solid state physics, attempts to find the lowest eigenvalue of huge eigenvalue problems by randomly testing the contributions of different states. The random selection of the parameters of a Gaussian basis, named the stochastic variational method, was first used by V.I. Kukulin and V.M. Krasnopol'sky in nuclear physics.

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