Chapter 1

Introduction

Few-body systems have played a crucial role in the development of the understanding of the nucleon–nucleon interaction. This is most clearly illustrated by the establishment of the nonzero-range character of the nucleon–nucleon interaction (a zero-range interaction leads to a collapse of the three-nucleon system, \textit{i.e.}, the ground-state energy would be minus infinity [Thomas, 1935]), and its noncentral character (a purely central potential cannot fit the two-, three-, and four-nucleon binding energies simultaneously [Rarita and Present, 1937]). After these initial successes, failure dominated for a long time. Progress was hampered by a lack of computational power, mathematical formalism, and numerical techniques. Much has changed since then: computers, mathematics, and numerics have reached a high level of sophistication, and the field of few-body physics has widened dramatically. This thesis describes very efficient numerical techniques based on a sound mathematical formalism and presents results obtained using modern powerful computers, for a wide range of few-body systems.

1.1 Historical overview

Few-body physics has developed into a field with a wide range of applications. Many important physical systems consist of a small number of constituents and are open to investigation by the tools of few-body physics. The field developed initially as a part of nuclear physics, as the name of the first few-body conference (“Nuclear forces and the few-nucleon problem”, [Griffith and Power, 1960]), held in London in 1959, suggests. Since then, the field has widened to include atomic and (meso-) molecular, as well as quark systems.\footnote{Actually, the atomic two-electron atoms had already been attacked by Hylleraas [1929] and conquered by Pekeris [1958, 1959]. However, at that time, there was a clear separation between atomic and nuclear few-body physics. (One of the reasons being the differences in the numerical methods and the successes achieved between both fields, due to the differences in the two-body interaction.)}

The pivotal point in the theory of few-body systems was 1960. In that year
Faddeev published his mathematically rigorous scattering theory for three particles. Formal scattering theory had initially been developed for the scattering of two elementary particles only [Lippmann and Schwinger, 1950; Gell-Mann and Goldberger, 1953], but soon attempts were being made to extend the formalism to processes in which the reaction products may differ from the initial particles (i.e., multichannel scattering) [Ekstein, 1956; Gerjuoy, 1958]. These formalisms were mathematically unsound for three-particle scattering and suffered from spurious solutions. This was first pointed out by Foldy and Tobocman [1957]. It was Faddeev [1960] who fully grasped the difficulties at hand, and proposed a set of three coupled integral equations, which do have a unique solution.

By that time, Mitra [1962] had realized that by decomposing the wave function into three components, and by assuming separable interactions, the three-body equations could be reduced to one-dimensional integral equations. Soon it was realized that Faddeev’s and Mitra’s formalisms coincide, even though Mitra merely intended to find a useful approximation to the three-body equations, whereas Faddeev had set out to put three-body scattering on a firm mathematical basis. In some sense, the use of separable interactions was a breakthrough in few-body physics since it allowed for direct, i.e., nonvariational, solutions of the three-body problem, but it was of limited practical use, since the nucleon–nucleon interaction is difficult to approximate by a separable interaction due to its repulsive core.

Slowly, it was realized that the Faddeev equations not only give a correct description of three-body scattering, but that they can simplify solving the three-body bound-state problem as well. Humberston et al. [1968] were the first to solve the Faddeev integral equations directly for three spinless particles interacting via local potentials. After that, other solution techniques were rapidly developed, with some success (among these were hyperspherical harmonic expansions [Simonov, 1966; Erens et al., 1971; Fabre de la Ripelle, 1972] and the Padé method [Malfliet and Tjon, 1969]), but the real breakthrough came when the configuration-space Faddeev equations were first solved (without the use of a hyperspherical expansion) by Gignoux and Laverne [Gignoux and Laverne, 1972; Laverne and Gignoux, 1973], and the solution of the momentum-space equations had become sufficiently reliable [Malfliet and Tjon, 1972; Harper et al., 1972]. By that time, hyperspherical and variational methods lagged severely behind [Bruinsma et al., 1972].

Soon after that, the three-nucleon bound-state problem was solved to a very high degree of precision, which is sufficient for most purposes. This was mainly due to the excellent work of Payne, Friar, and Gibson, who use splines (a technique widely used in structural mechanics), to solve the configuration-space Faddeev equations (see, for example, [Payne et al., 1980; Chen et al., 1985]). On the other hand, the nucleon–deuteron scattering problem was solved to an excellent degree of precision by Glöckle and coworkers [Witala et al., 1989]. At the time this thesis was written, even the four-body problem has come close to a satisfactory numerical solution [Zabolitzky et al., 1982; Kamada and Glöckle, 1992; Schellingerhout et al., 1992; Schellingerhout, 1994].
1.2 About this thesis

This thesis contains a summary of the work that I have done in the course of my PhD research on the few-body problem in general, and configuration-space three- and four-body calculations in particular. Much of what is written here, can be found in previous publications [Schellingerhout et al., 1989; Schellingerhout and Kok, 1990; Kok and Schellingerhout, 1991; Schellingerhout et al., 1992; 1993; Schellingerhout, 1994], although there is a large amount of unpublished material.

This thesis contains substantial amounts of textbook material, which are partially intended as a reference, partially reflect the efforts put into understanding the theory and the physics, and are partially used as a starting point for numerical investigations. The central theme of this thesis is the search for the “best” numerical techniques for solving the three- and four-body problem, by exploiting factorizability in the matrices representing the discretized few-body equations.

The numerical method I have developed in the course of my PhD research is based on the existing method of piecewise cubic Hermite approximation and orthogonal collocation, often referred to as “the spline method.” This method was introduced in few-body physics by Payne et al. [1980]. It leads to a very large matrix eigenvalue equation, which can be solved using iterative techniques. The size of the matrices involved is a serious difficulty, so that very large computers are needed for solving the problem. However, it is possible to reduce the size of the matrices which must be handled by recognizing that the matrices can be built up from sums of direct products, and realizing that the product matrix itself is never really needed. These ideas can be applied to any of the usual formulations of the three- and four-body equations, and are worked out for various cases in Secs. 5.3.3, 5.3.4, 5.3.6, 6.2, and 7.3.2.

Note that the use of a separable, or factorizable, interaction has no relation whatsoever to the method discussed in this thesis. Exploiting the direct-product structure reduces the numerical problem to something comparable in size with the problem obtained when a separable expansion for the interaction is used, but it does not involve approximations.

1.3 Layout

This introductory chapter is followed by seven more chapters and six appendices. I will give a short description of their contents:

Chapter 2 contains a short introduction to the theory of the two-body bound system, a discussion of the spline method, and extensive numerical studies.

Chapter 3 contains a detailed description of two-body scattering theory, a discussion of the differences with the bound-state problem, and numerical studies.
Chapter 4 contains a detailed description of $N$-body scattering theory, following Faddeev and Yakubovsky, the angular-momentum analysis of the configuration-space Faddeev–Yakubovsky equations, and derivations of the boundary conditions.

Chapter 5 contains a detailed description of configuration-space Faddeev equation (including discussions regarding symmetries, spin, and isospin), the numerical solution by the spline method, the efficient solution of the remaining matrix problem exploiting factorizability, the evaluation of observables, numerical studies, and results for a wide range of systems.

Chapter 6 contains a short description of the equations and boundary conditions for three-body scattering below the breakup threshold, the numerical solution, and a comparison with other results.

Chapter 7 contains a detailed discussion of the four-body Yakubovskyy equations, a study of the coordinate transformations involved, numerical studies, and results for simple potentials.

Chapter 8 contains some concluding remarks.

Appendix A contains a detailed description of the numerical techniques used throughout this thesis.

Appendix B contains a collection of exactly solvable few-body systems, and a description of the potentials used throughout this thesis.

Appendix C contains formulas related to angular momentum in quantum mechanics.

Appendix D contains a discussion and definitions of the special functions used throughout this thesis.

Appendix E contains miscellaneous three- and four-body formulas.

Appendix F contains a short description of some of the implementation details of the methods described in this thesis.