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The Quantum Mechanical Three-Body Problem

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Preface

One of the outstanding problems of classical physics was the three-body problem, namely, to solve Isaac Newton's equations of motion for three interacting bodies. There is a similar problem in modern quantum mechanics, namely, to describe the motion of three interacting atomic or subatomic particles by rigorous integral equations. L. D. Faddeev, in 1960, published the first work on this problem, *Scattering Theory for a Three-Particle System*, and since then a great deal of work has been done, the results of which are mainly available in original articles and reviews.

The present book originated from a course given by the authors in the summer semester of 1972. It was felt that the student who wants to acquaint himself with the field should no longer have to work his way through the review articles and the original literature. Therefore, the course lectures were revised and expanded into this volume.

It is not the aim of this book to cover the field completely. For example, there are different formulations of the abstract theory, any of which can equally well serve as a mathematical basis for the theory. Those of S. Weinberg, L. Rosenberg, J. V. Noble, R. G. Newton, R. Sugar and R. Blankenbecler, and P. A. Kazaks and K. R. Greider, however, have been omitted, while that of Faddeev has been dealt with extensively. Emphasis, instead, has been placed on the various ways of getting from the abstract operator equations to numerical solutions and to data which can be compared with experimental results.

We hope that this book will make the field of three-particle physics more readily accessible to the interested student. We also hope that it will help the experimentalist to understand better how the theoretical data are derived.

We thank Dr. J. Schwager and Dr. F. Sohre for their critical reading of the manuscript and Mrs. Ch. Stiller for the typing. We also thank the authors of original papers for giving us permission to reproduce their figures.

Erich W. Schmid / Horst Ziegelmann

1. Introduction

The quantum mechanical three-body problem deals with the motion of three particles under the influence of an interaction potential. Its fundament is the Schrödinger equation for three particles,

$$i\hbar\frac{\partial}{\partial t}\psi = H\psi \ ,$$

with

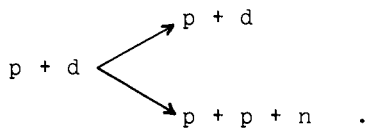
$$H = -\sum_{i=1}^{3}\frac{\hbar^2}{2m_i}\nabla_i^2 + \sum_{i>k=1}^{3} V(i,k)$$

where V(i,k) is a two-body potential; also a three-body potential V(i,k,j) is thinkable, but it is used very seldom.

In atomic-, nuclear-, and elementary-particle physics, there exists a large number of states and processes which demand to be treated as three-particle systems. Here are a few examples:

a) the scattering of electrons from hydrogen
b) the nuclei ^{3}H and ^{3}He
c) the nucleon-deuteron scattering
d) the photodisintegration of ^{3}H and ^{3}He
e) the scattering of mesons from deuterons
f) the scattering of a meson from a nucleon, where the latter is treated as a meson-nucleon bound state
g) multiparticle systems, which can be treated approximately as three-particle systems as, for instance, the scattering of deuterons from ^{4}He with breakup of the deuteron and the scattering of protons from ^{11}B with breakup into three α-particles.

Particular difficulties arise when a reaction leads to a final state with three free particles, as in the case of proton-deuteron scattering at a center-of-mass energy of more than 2.22 MeV,



Because of such processes, the three-particle problem becomes especially interesting. The three-particle scattering system is still simple enough to yield exact solutions, but it is also complicated enough to have channels other than the elastic one, namely, rearrangement and breakup channels.

We now shall discuss the difficulties of three-particle breakup and examine the experimental situation.

1. Scattering Experiments with Three-Particle Breakup

The three particles which participate in the reaction have 3 times 3 = 9 degrees of freedom in configuration space. The reaction also can be described in momentum space, and here we also have 9 degrees of freedom. Asymptotically, the momenta are sharp, i.e., they are measurable for every single event.

In a so-called complete experiment, all 9 momenta are determined. The difficulty arises from the multiplicity of data to be measured simultaneously and from the small number of events for each combination of data.

Let us look at the reaction

$$p + d \longrightarrow p + p + n \quad .$$

Four out of nine momentum components of the final state are determined by the initial state via momentum and energy conservation. Conservation of momentum means that the sum of momenta of the outgoing particles in the laboratory system must be equal to the momentum of the incoming proton. Conservation of energy means that the sum of the kinetic energies of the outgoing particles must be equal to the kinetic energy of the incoming proton minus the binding energy of the deuteron. In the notation of Fig. 1, this means

$$\vec{k}_1 = \sum_{i=3}^{5} \vec{k}_i \,,$$

$$\frac{k_1^2}{2m_1} - |E_B| = \sum_{i=3}^{5} \frac{k_i^2}{2m_i} \,.$$

There remain 9 minus 4 = 5 momentum components of the outgoing particles to be measured.

One can proceed in the following way. Two of the outgoing particles are detected, the third one remains undetected.

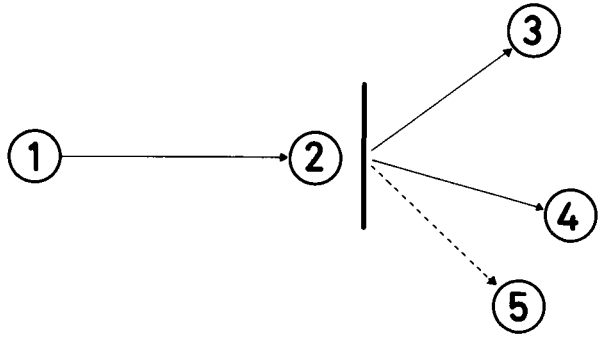


Fig. 1. Notation of a three-particle breakup reaction

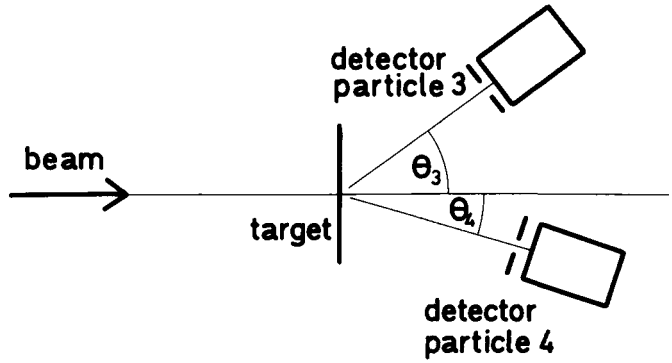


Fig. 2. Experimental setup

Each counter determines three parameters (see Fig. 2), namely energy and direction of momentum of one outgoing nucleon. The two counters together measure six parameters. One of them is redundant and the data, therefore, are not independent. They have to fulfill a kinematical condition. When, for a given position of the counters, all events are plotted in an E_3, E_4 diagram, they will lie, theoretically, on a certain curve, as shown in Fig. 3.

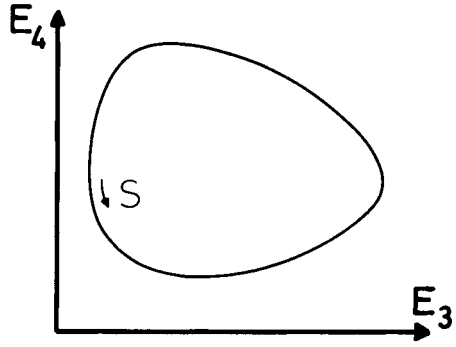


Fig. 3. Kinematically allowed curve in a three-particle breakup reaction

In practice, one uses scintillation counters of finite aperture, finite energy resolution and multichannel analyzers. The numbers of events are represented by more or less pronounced dots. When the background is suppressed by a complicated coincidence technique, a band appears along the kinematical curve (Fig. 4). Its width shows the finite resolution of the experimental setup. The picture changes for every location of the two counters. Usually, the intensity of the band along the kinematical curve is plotted against a curve parameter (Fig. 5). The angles θ_3 and θ_4 can be chosen so as to pick out interesting details of the scattering process, as in the process where two particles have very low relative velocity.

The described experiment is called c o m p l e t e because a maximum of information is determined (except for polarization). It is hard to perform since the counting rates are very low.

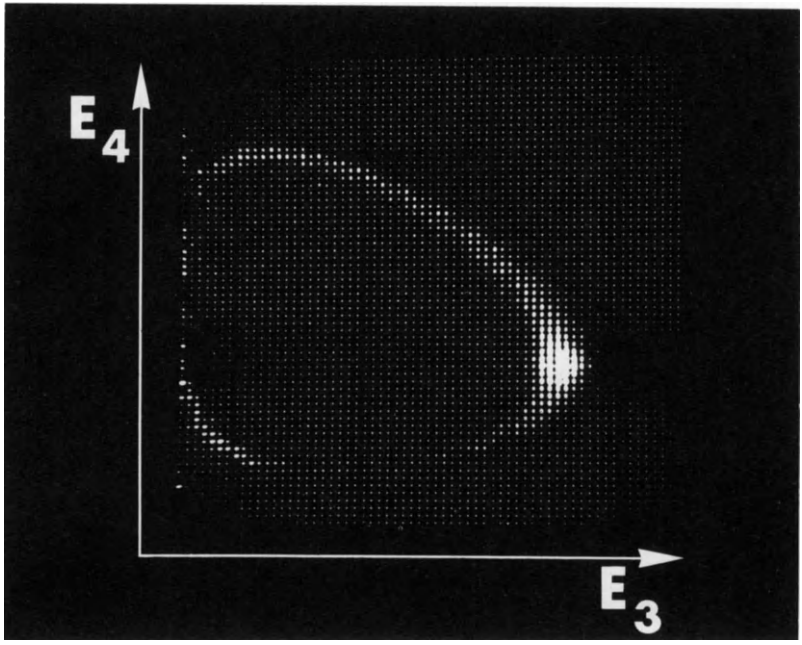


Fig. 4. Result of a coincidence experiment (H. Brückmann et al. [1])

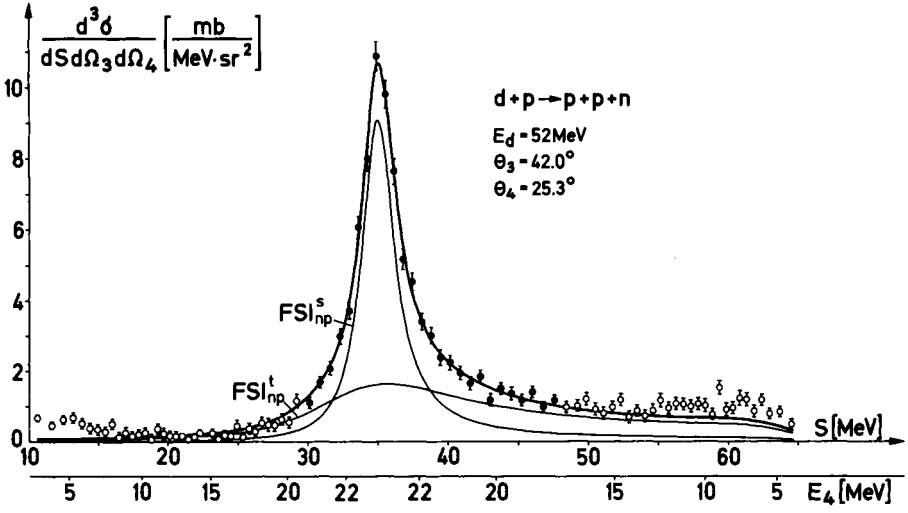


Fig. 5. Three-particle breakup cross section plotted versus curve parameter S (H. Brückmann et al. [1])

In the majority of scattering events, the outgoing particles miss either one or both of the counters. The rare events where both counters respond in coincidence are distributed over a whole kinematical curve. The statistic, therefore, is very bad. Earlier experiments always were incomplete because one had to achieve a reasonable intensity by measuring less than five parameters. One used, for instance, only one proton counter and received a cross section which represented an integral of the complete differential cross section over the undetermined parameters.

2. Difficulties of the Theory

When we ask for difficulties of the three-particle problem, it is advantageous to ask first why the two-particle problem is so simple.

a) Scattering of Two Elementary Particles

In the initial state, a wave packet - which describes the projectile - approaches a wave which describes the target in the laboratory system. In the center-of-mass system, a wave packet approaches the origin where the interaction takes place (Fig. 6).

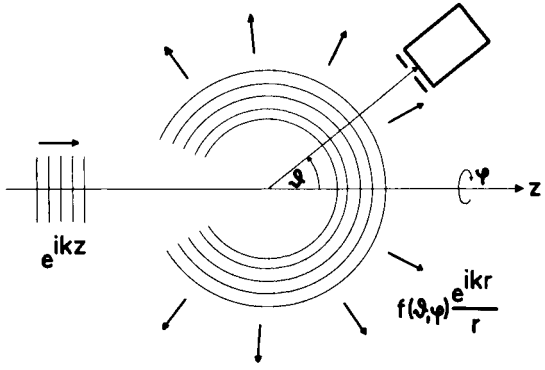


Fig. 6. Scattering of two particles in the center-of-mass system

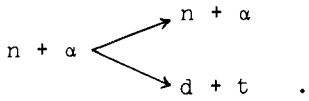
The initial condition or boundary condition is, basically, a condition in t i m e . One can now go over to the limit

where the energy of the wave packet is sharp and can separate out time dependence. The boundary condition, then, becomes a time-independent one. With some effort, this transition can be made with mathematical rigor [2]. What comes out is rather convincing.

The scattering solution consists of a plane wave e^{ikz} which describes the incoming flux and the flux of unscattered particles plus a spherical wave $f(\vartheta,\varphi)e^{ikr}/r$ which describes the flux of scattered particles. When spins are not involved, the amplitude $f(\vartheta,\varphi)$ does not depend on the azimuth φ, and the spherical wave has the form $f(\vartheta)e^{ikr}/r$. Particles emerge into a continuum of directions (ϑ) or (ϑ,φ) which, for short-ranged potentials, can easily be described by a superposition of a small number of partial waves. The relative momentum k is the same for every direction because of energy conservation.

b) Scattering of Composite Particles without Breakup

In contrast to (a), the reaction products can be different from the initial particles, for instance:



But also in this case, the scattering solution has an asymptotic form which is typical for a two-body problem. It consists of a plane wave and outgoing spherical waves,

$$\psi(\infty)=\phi(1)e^{ik_1z_1}+\phi(1)f(\vartheta_1,\varphi_1)\frac{e^{ik_1r_1}}{r_1}+\phi(2)g(\vartheta_2,\varphi_2)\frac{e^{ik_2r_2}}{r_2}\quad .$$

But there are two spherical waves now, according to the two decay possibilities, and every term is multiplied by a function $\phi(i)$ which describes the internal motion of the

fragments. When the spin of particles is taken into account, one has to combine spin and orbital angular momentum in such a way as to obtain partial waves of given total angular momentum. The boundary condition has still the simple time-independent form and, for short-ranged interaction potentials, a few partial waves are sufficient to describe the process of decay in all directions. Because of different energies of internal motion, the relative momenta k_1, k_2 of the decay channels are, in general, different, but they form a small set of discrete numbers.

c) Three-Body Breakup

In contrast to (b), we are now faced with the problem of infinitely many decay channels. Let us consider particles 2 and 3 as a subsystem of the final state, as shown in Fig. 7.

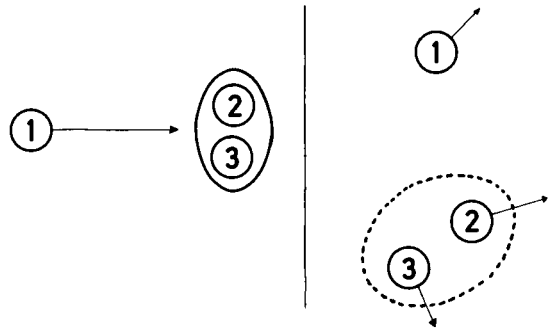


Fig. 7. Three-particle reaction with breakup into three free particles

This subsystem is now not in one of its bound states, as it was in case (b), but occupies one out of a continuum of two-particle scattering states. The continuum is characterized in particular by the relative momentum k which can assume a continuous variety of values and serves as a continuous channel index (recall the discussion on the degrees of freedom; the distribution of energy among the three free particles was one degree of freedom).

A second problem is the size of the reaction volume. While it was finite or even very small (for nuclear forces) in case (b), it becomes infinitely large now, as can be seen in the following way.

The scattering can proceed in three steps. In the first step, a subsystem (2, 3) is formed in an excited state (Fig. 8a).

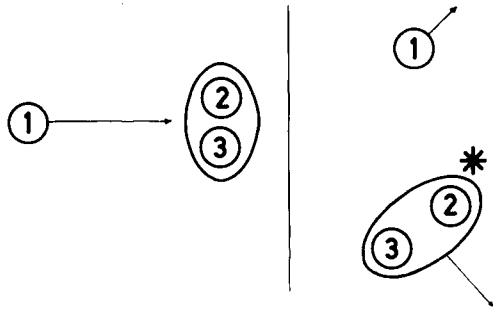


Fig. 8a. First step of a breakup reaction: production of a two-particle excited state

A little later, the excited state decays (Fig. 8b) and one of the particles, for instance particle 2, emerges in the direction of the outgoing particle 1. Particle 2 then catches up with particle 1 (Fig. 8c) and is scattered once more. This process is called "rescattering". It shows that the interaction which forms the final state is not confined to a small region around the center-of-mass, but can take place everywhere in three-dimensional space.

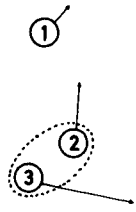


Fig. 8b. Second step: decay of the excited state

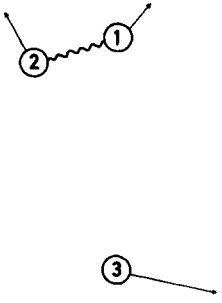


Fig. 8c. Third step: rescattering

From the two difficulties, namely continuum of channels and infinity of the reaction volume, a third one follows. There is no longer a simple way to postulate a time-independent boundary condition. In case of doubt, one has always to go back to the physical time-dependent boundary condition and make certain that a boundary condition is in agreement with it. The difficulty of a time-independent boundary condition can easily be understood by asking the following question: When two of the three particles recede from the common center-of-mass, and one particle approaches it, is this, then, an outgoing or an ingoing state ?

It is indeed possible to also construct outgoing states here (for instance by the use of "K - harmonics" or wave packets, Chapter 8, or by splitting the wave function into components, Chapter 3). But it is no longer as easy as in the two-body case.

3. Importance of the Three-Body Problem in Nuclear Physics

What is so interesting about the three-body problem in nuclear physics ? A still-unsolved problem of nuclear physics and, quite generally, of elementary particle physics is the problem of strong interaction. Experiments only furnish binding energies and cross sections. By help of the Schrödinger equation, one then derives phenomenological potentials which form the basis of theoretical nuclear physics. It is hoped that, at a later stage, these potentials can also be derived from a fundamental theory.

In order to determine a phenomenological potential, it is necessary to establish the relation between measurable data and interaction. In other words, it is necessary to solve the Schrödinger equation. For two nucleons, this is relatively easy. But the two-nucleon data do not contain enough information. Besides, not all two-nucleon experiments can be performed in practice as, for instance, neutron-neutron scattering. In order to get a fairly reliable nucleon-nucleon potential, one has to take into account at least the three-nucleon data in addition to the two-nucleon data.

The following details are of special interest.

a) The Neutron-Neutron Interaction

This interaction is needed to check charge symmetry and isospin invariance of nuclear forces. The interaction is contained in triton data, in the cross section of elastic n-d scattering, and, more sensitively, in some data of the n-d breakup reaction. In the latter, one can arrange the counters and choose the energies E_3, E_4 in such a way that events are measured for which the relative momentum of the two neutrons is very small. The neutrons interact for a rather long time ("final state interaction") which expresses itself in the scattering cross section.

b) The Off-Shell Behaviour of Nuclear Forces

In two-particle scattering, energy is conserved when, before and after scattering, long-enough time intervals are available for the determination of energy. The allowed momenta of the two particles are restricted by energy conservation as soon as the particles are outside of the region of interaction. All possible events are located on a hypersphere of momentum space which is called energy shell. The events are called "on-shell-events".

When the two-particle system can be considered as isolated only during a short time interval (Δt), while it interacts with its surrounding outside of this interval, then energy conservation no longer rigorously holds because of the uncertainty principle. Scattering processes which occur during the interval Δt and violate energy conservation have a nonzero probability. Such processes are called "off-the-energy-shell" or, briefly, "off-shell". Such a mechanism is typical for three-particle scattering where scattering within the two-particle subsystem is disturbed by the presence of the third particle (Fig. 9). When two particles interact in a three-particle process, the final state does not necessarily have the same energy as the initial state because it usually happens that the final state exists only

for a very short time before it is destroyed by the influence of the third particle.

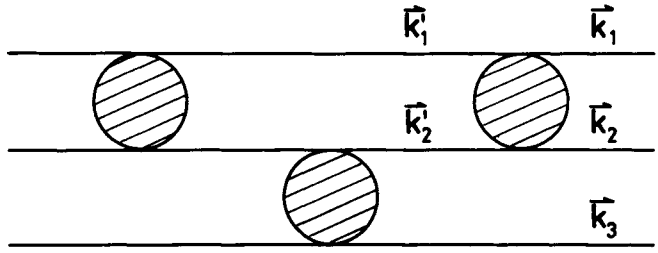


Fig. 9. Three-particle multiple scattering. The energy of the (1,2) subsystem in the intermediate state $(\vec{k}_1', \vec{k}_2')$ and in the initial state $(\vec{k}_1, \vec{k}_2)$ do not have to be equal; $k_1'^2/2m_1 + k_2'^2/2m_2 \neq k_1^2/2m_1 + k_2^2/2m_2$.

Off-shell effects are well described by the Schrödinger equation just as the uncertainty relation follows from the Schrödinger equation. In two-particle scattering, however, one usually does not pay any attention to off-shell effects because one assumes that the interaction potential is given. In this case, the Schrödinger equation defines the on-shell scattering amplitude as well as the off-shell amplitude. But as soon as the inverse scattering problem is considered, namely finding a potential which fits the scattering data, it becomes clear that the on-shell amplitude of two-particle scattering does not contain enough information to define the interaction potential uniquely [1]. There are infinitely many potentials which give the same on-shell but different off-shell amplitudes for two-particle scattering. It is said that such potentials have different "off-shell properties".

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1) Only under certain assumptions on the mathematical form of the potential does it become possible to fit certain parameters by two-particle scattering data.

In the three-particle problem, the off-shell properties of the interaction potential play an important role and, therefore, three-particle data are important for the inverse scattering problem. Some information is already contained in three-particle binding data and in scattering processes with two-body fragmentation as, for instance, elastic n-d scattering. The full information is present only in complete breakup results. It has been shown, however, by Brayshaw [128] that breakup experiments have to be extremely accurate to furnish such information.

2. Some Concepts of Quantum Mechanics

In this section, we first consider two-particle scattering in a more generalized formalism. It will then be shown which results can be used also for three-particle scattering and where the difficulties arise.

1. The Two-Particle Problem

1.1. The Hamiltonian

The Hamiltonian for two particles which interact via a potential v has the form

$$h' = \frac{k_1^2}{2m_1} + \frac{k_2^2}{2m_2} + V \quad , \tag{2.1}$$

where $\vec{k}_1, \vec{k}_2$ are the momenta and m_1, m_2 are the masses of the particles. For a translational invariant potential v, the center-of-mass motion can be separated by the introduction of a center-of-mass momentum $\vec{k}$ and a relative momentum $\vec{p}$,

$$\vec{k} = \vec{k}_1 + \vec{k}_2 \tag{2.2}$$

$$\vec{p} = \frac{m_2 \vec{k}_1 - m_1 \vec{k}_2}{m_1 + m_2} \tag{2.3}$$

$$h' = \frac{k^2}{2(m_1+m_2)} + \frac{p^2}{2\mu} + V \quad , \tag{2.4}$$

with the reduced mass,

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \quad . \tag{2.5}$$

Because of translation invariance, the center-of-mass motion is a free motion, i.e., a momentum eigenstate. We are not interested in it and confine ourselves to the Hamiltonian for the relative motion

$$h = \frac{p^2}{2\mu} + V \equiv h_0 + V \quad . \tag{2.6}$$

1.2. Boundary Condition of the Scattering State

The scattering of two particles is described by the time-dependent Schrödinger equation (we use units for which $\hbar = 1$),

$$i \frac{\partial}{\partial t} \psi_a^{(+)}(t) = h \psi_a^{(+)}(t) \quad . \tag{2.7}$$

The superscript (+) indicates that the system is an experimentally prepared state before scattering and is gradually scattered with increasing time. A superscript (-) would mean that a collimated beam is obtained after scattering, which is not experimentally verifiable. The index a denotes all properties of the initial state.

The solution of Eq. (2.7) is given by

$$\psi_a^{(+)}(t) = e^{-iht} \psi_a^{(+)} \tag{2.8}$$

where $\psi_a^{(+)}$ is a time-independent wave packet.

The initial or boundary condition can be expressed verbally as this: The scattering state $\psi_a^{(+)}(t)$ has to develop from a wave packet which is free in the infinite past and whose properties are characterized by the index a ; free means that the amplitude vanishes in the region of interaction, where $v \neq 0$.

Mathematically, this condition is formulated in the following way. A reference wave packet is introduced which has the form ϕ_a at $t = 0$ and whose time dependence is described by the free Hamiltonian h_o ,

$$\phi_a(t) = e^{-ih_o t} \phi_a \tag{2.9}$$

It is demanded that the wave packet $\psi_a^{(+)}$ coincides with the free packet ϕ_a in the limit of the infinite past. Since wave packets dissolve in the course of time, it would not make sense to demand a pointwise agreement of the two functions.

Instead, one demands that the norm [1] of the difference becomes zero,

$$\lim_{t \to -\infty} \| e^{-iht} \psi_a^{(+)} - e^{-ih_0 t} \phi_a \| = 0 \quad . \tag{2.10}$$

The limit of the norm is called a strong limit. We denote it by "s-lim" in the following. Our verbal demand has the disadvantage that a wave packet which is confined to the laboratory at a finite time becomes a rather diffuse subject at the infinite past (unless its production is included in the formalism). By use of a free reference wave packet ϕ_a, which is also confined to the laboratory at t = 0, this difficulty is circumvented.

It should be noted that the verbal demand implies a certain restriction as to the range of the potential. Mathematically, this restriction is expressed by the fact that the limit (2.10) does not exist for every potential [3].
Equation (2.10) can also be written as

$$\psi_a^{(+)} = \text{s-}\lim_{t \to -\infty} e^{iht} e^{-ih_0 t} \phi_a \equiv \Omega^{(+)} \phi_a \quad , \tag{2.11}$$

where the limit has the meaning of a strong limit (vanishing norm of the difference of the left-hand and the right-hand side). Equation (2.11) defines the so-called Møller operator $\Omega^{(+)}$.

1.3. The Møller Operator

The Møller operator $\Omega^{(+)}$, when applied to a free state, produces the scattering state $\psi_a^{(+)}$. According to Eq. (2.11), it is given by

$$\Omega^{(\pm)} = \text{s-}\lim_{t \to \mp \infty} e^{iht} e^{-ih_0 t} \quad . \tag{2.12}$$

---

[1] The norm implies an integration over all space and, therefore, Eq. (2.10) is a meaningful condition.

We have included here the definition of the Møller operator $\Omega^{(-)}$. This operator produces the scattering state $\psi_a^{(-)}(t)$ which goes over into the free state $\phi_a(t)$ for $t \longrightarrow +\infty$. Although the states $\psi_a^{(-)}(t)$ cannot be prepared experimentally, they are needed for the precise description of a measurement (because they are "seen" by the counters).

It follows from the definition (2.12) that for any finite time τ

$$\underset{t\to\mp\infty}{s\text{-}\lim} e^{ih(t+\tau)} e^{-ih_0(t+\tau)} = \Omega^{(\pm)} = e^{ih\tau}\,\Omega^{(\pm)}\, e^{-ih_0\tau} \qquad (2.13)$$

is also valid. By differentiation, we get

$$0 = \frac{d\Omega^{(\pm)}}{d\tau} = e^{ih\tau}\left(h\Omega^{(\pm)} - \Omega^{(\pm)}h_0\right)e^{-ih_0\tau} ,$$

and have the "commutation relation"

$$h\,\Omega^{(\pm)} = \Omega^{(\pm)}h_0 \quad . \qquad (2.14)$$

The domain of the Møller operator is the Hilbert space of free states or, more precisely, the space of square integrable free states. The domain, however, can be extended to include states of sharp momentum. For this, a limiting procedure toward sharp energy has to be performed on the wave packets. This extension brings about some conceptual difficulties because the wave packet now becomes infinitely large and interaction is a l w a y s present. Accordingly, the mathematical treatment becomes difficult. One should not be deceived by the fact that application of a Møller operator on a non-normalizable state does apparently not lead to convergence problems. The extension is justified by the work of Faddeev [4], who showed that correct results are obtained for a large class of potentials. We are thus allowed to use momentum eigenstates $|\vec{p}\rangle$ instead of wave packets ϕ_a and to apply the operators $\Omega^{(\pm)}$ on them. In this way we get scattering states $|\vec{p}\rangle^{(\pm)}$, where $|\vec{p}\rangle^{(+)}$ corresponds to the state which has been discussed in the introduction,

namely the state which consists of a plane wave plus an outgoing spherical wave. The scattering states $|\vec{p}\rangle^{(\pm)}$ have a sharp energy E just as the free states $|\vec{p}\rangle$ have the sharp energy $p^2/2\mu$. The two energies are the same, as can be shown by use of the "commutation relation" (2.14),

$$h|\vec{p}\rangle^{(\pm)} = h\Omega^{(\pm)}|\vec{p}\rangle = \Omega^{(\pm)} h_0 |\vec{p}\rangle$$
$$= \Omega^{(\pm)} \frac{p^2}{2\mu}|\vec{p}\rangle = \frac{p^2}{2\mu}|\vec{p}\rangle^{(\pm)} . \qquad (2.15)$$

We can now generally state that the Møller operators map the proper and improper free Hilbert space on the corresponding scattering states of h. The bound states of h are not reached by this mapping; they do not belong to the range of the Møller operators. The Møller operators, therefore, are not unitary but only isometric. The Hermitean conjugate operators $\Omega^{(\pm)\dagger}$ reverse the mapping when applied to scattering states. When applied to the bound states $|\psi_n\rangle$ of h, they give zero. This can be seen from the relation

$$\langle \Omega^{(\pm)\dagger} \psi_n | \vec{p}\rangle = \langle \psi_n | \Omega^{(\pm)} \vec{p}\rangle = \langle \psi_n | \vec{p}\rangle^{(\pm)} = 0 .$$

The expression on the right-hand side is zero because $|\psi_n\rangle$ and $|\vec{p}\rangle^{(\pm)}$ are eigenstates of h with different energies. Since the expression on the left-hand side is zero and the states $|\vec{p}\rangle$ form a complete set, we have

$$\Omega^{(\pm)\dagger}|\psi_n\rangle = 0 .$$

The time limit in Eq. (2.12) can be replaced by an Euler limit

$$\Omega^{(\pm)} = \text{s-}\lim_{t\to\mp\infty} e^{iht} e^{-ih_0 t} = \text{s-}\lim_{\epsilon\to 0} \pm\epsilon \int_{\mp\infty}^{0} e^{\pm\epsilon t} e^{iht} e^{-ih_0 t}\, dt . \qquad (2.16)$$

This has been shown by Jauch [5] under the assumption that the strong time limit on the left-hand side exists.

The procedure of an Euler limit can be understood by applying it to an ordinary function f(t) which goes to f_∞ for $t \longrightarrow -\infty$. It is readily seen that

$$\int_{-\infty}^{0} \epsilon e^{\epsilon t} dt = 1 \quad ,$$

and that finite time intervals do not contribute to the integral

$$\lim_{\epsilon \to 0} \int_{-\infty}^{0} \epsilon\, e^{\epsilon t} f(t)\, dt \quad .$$

The contribution of infinitely distant times is just f_∞, as can be seen by substituting

$$\epsilon t = x$$

$$\int_{-\infty}^{0} \epsilon\, e^{\epsilon t} f(t)\, dt = \int_{-\infty}^{0} e^{x} f\left(\frac{x}{\epsilon}\right) dx \quad .$$

When ϵ goes to zero, $f(\frac{x}{\epsilon})$ goes to f_∞ and can be put in front of the integral.

The introduction of an Euler limit is the point where time disappears from our two-particle theory. We shall see in the next section that by this procedure a time-independent integral equation is obtained which incorporates exactly the boundary condition that has been discussed in the introduction.

1.4. Resolvent Equation and Lippmann-Schwinger Equation

The expression (2.16) for the Møller operator does not help much, as it stands, because we cannot carry out the integration [1].

---

[1] Since h and h_0 do not commute, the two exponential functions in the integrand cannot be put together,

$$e^{iht}\, e^{-ih_0 t} \neq e^{i(h-h_0)t} \quad .$$

But, since we are allowed to apply the Møller operators on plane waves, we can write

$$
\begin{aligned}
|p\rangle^{(\pm)} &= \lim_{\epsilon \to 0} \pm\epsilon \int_{\mp\infty}^{0} dt\, e^{\pm\epsilon t}\, e^{iht}\, e^{-iEt}\, |\vec{p}\rangle \\
&= \lim_{\epsilon \to 0} \pm\epsilon \int_{\mp\infty}^{0} dt\, e^{i(h - E \mp i\epsilon)t}\, |\vec{p}\rangle \qquad (2.17) \\
&= \lim_{\epsilon \to 0} \pm i\epsilon \left(E \pm i\epsilon - h\right)^{-1} |\vec{p}\rangle \quad .
\end{aligned}
$$

We have found an important relation between the scattering solutions $|\vec{p}\rangle^{(\pm)}$ and the resolvent or Green's function

$$
g(z) \equiv (z - h)^{-1} \quad . \qquad (2.18)
$$

The relation

$$
|\vec{p}\rangle^{(\pm)} = \lim_{\epsilon \to 0} \pm i\epsilon\, g(E \pm i\epsilon)\, |\vec{p}\rangle \quad , \qquad (2.19)
$$

marks the transition from time-dependent to time-independent theory.
From $z - z' = g^{-1}(z) - g^{-1}(z')$ we get, by multiplication with $g(z)g(z')$, the first resolvent equation

$$
g(z') - g(z) = (z - z')\, g(z)\, g(z') \quad , \qquad (2.20a)
$$

$$
= (z - z')\, g(z')\, g(z) \quad . \qquad (2.20b)
$$

With the definition of the free resolvent

$$
g_0(z) \equiv (z - h_0)^{-1} \quad , \qquad (2.21)
$$

and the relation

$$V = h - h_0 = g_0^{-1}(z) - g^{-1}(z) \quad ,$$

we get, by multiplication with $g(z) g_0(z)$, the second resolvent equation

$$g(z) = g_0(z) + g_0(z) V g(z) \quad , \tag{2.22a}$$

$$= g_0(z) + g(z) V g_0(z) \quad . \tag{2.22b}$$

We now use this operator identity to derive an integral equation for scattering states from Eq. (2.19)

$$|\vec{p}\rangle^{(\pm)} = \lim_{\epsilon \to 0} \pm i\epsilon \left(g_0(E \pm i\epsilon) + g_0(E \pm i\epsilon) V g(E \pm i\epsilon) \right) |\vec{p}\rangle \quad . \tag{2.23}$$

Using the relation

$$\pm i\epsilon \, g_0(E \pm i\epsilon) |\vec{p}\rangle = \pm i\epsilon (E \pm i\epsilon - h_0)^{-1} |\vec{p}\rangle = |\vec{p}\rangle \quad , \tag{2.24}$$

for the first term of Eq. (2.23), and Eq. (2.19) for the second term, we get

$$|\vec{p}\rangle^{(\pm)} = |\vec{p}\rangle + g_0(E \pm i0) V |\vec{p}\rangle^{(\pm)} \quad . \tag{2.25}$$

This is the Lippmann-Schwinger equation for the scattering states $|\vec{p}\rangle^{(\pm)}$. The ε-limit, which has to be performed in $g_0(E \pm i\varepsilon)$, is indicated by the notation $E \pm i0$. In configuration space representation [6] this limit leads to

$$\langle \vec{r} | g_0(E \pm i0) | \vec{r}' \rangle = -\frac{\mu}{2\pi} \frac{e^{\pm i\sqrt{2\mu E}\,|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|} \quad . \tag{2.26}$$

The free resolvent $g_0(E)$ has a cut along the positive real E-axis. The ε-limit tells us on which side of the cut we have to stay in order to fulfill the boundary condition. The (+) sign corresponds to the physical boundary condition (see p. 15).

By writing the Lippmann-Schwinger equation in configuration space representation [1],

$$\langle \vec{r}|\vec{p}\rangle^{(+)} = \langle \vec{r}|\vec{p}\rangle - \int d\vec{r}\,' \frac{\mu}{2\pi} \frac{e^{i\sqrt{2\mu E}\,|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} V(\vec{r}\,')\langle \vec{r}\,'|\vec{p}\rangle^{(+)}, \quad (2.27)$$

we see that the first term on the right-hand side is a plane wave, and the second term is (for large values of r) an outgoing spherical wave. The physical, time-dependent boundary condition has led to an integral equation which incorporates the time-independent boundary condition which has been described in the introduction.

We now have to find out whether the kernel of our integral equation is a compact operator [7]. If it is compact, the Fredholm theory and all the standard methods of solution, which will be discussed in Chapter 4, can be applied. The simplest way to learn something about compactness is to investigate whether the Schmidt norm is finite, which is a sufficient condition. The Schmidt norm of an operator $K(\vec{r},\vec{r}\,')$ is defined as

$$\|K\|_S = \left[\mathrm{Tr}\,(K^\dagger K)\right]^{1/2} = \left[\iint d\vec{r}\, d\vec{r}\,' |K(\vec{r},\vec{r}\,')|^2\right]^{1/2} . \quad (2.28)$$

---

[1] The operator product of Eq. (2.25) is evaluated by insertion of the complete set $1 = \int d\vec{r}\,' |\vec{r}\,'\rangle\langle \vec{r}\,'|$ under the assumption of a local potential $\langle \vec{r}|V|\vec{r}\,'\rangle = V(\vec{r})\,\delta(\vec{r}-\vec{r}\,')$.

In our integral equation (2.27), the kernel is

$$K(\vec{r},\vec{r}') = -\frac{\mu}{2\pi}\,\frac{e^{i\sqrt{2\mu z}\,|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}\,V(\vec{r}')\quad , \tag{2.29}$$

with $z = E + i\varepsilon$.

The square of the Schmidt norm is given by

$$\begin{aligned}\|K\|_S^2 &= \frac{\mu^2}{4\pi^2}\iint d\vec{r}\,d\vec{r}'\,\frac{e^{-2\,\mathrm{Im}(\sqrt{2\mu z})\,|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|^2}\,|V(\vec{r}')|^2 \\ &= \frac{\mu^2}{4\pi^2}\int d\vec{R}\,\frac{e^{-2\,\mathrm{Im}(\sqrt{2\mu z})\,R}}{R^2}\int d\vec{r}'\,|V(\vec{r}')|^2 \qquad (2.30)\\ &= \frac{\mu^2}{2\pi\,\mathrm{Im}(\sqrt{2\mu z})}\int d\vec{r}'\,|V(\vec{r}')|^2\quad .\end{aligned}$$

Apparently, the Schmidt norm can only be finite when, firstly, the integral over the absolute square of the potential exists (which excludes Coulomb and hard-core potentials), and when, secondly, the imaginary part of $\sqrt{2\mu z}$ is unequal to zero (which exactly excludes the scattering energies we are interested in). The fact that the Schmidt norm diverges in the limit $\varepsilon \longrightarrow 0$ is closely related to the fact that we have left the Hilbert space L_2 of square integrable functions (compare with p. 17). But, as has been previously stated, a finite Schmidt norm is only a sufficient condition for compactness and not a necessary one. Lovelace [8] could show that the kernel of our integral equation is compact in the Banach space C_1 of continuous bounded functions with continuous bounded derivatives, despite divergence of the Schmidt norm. This answers the question of whether the Lippmann-Schwinger equation has a unique solution. For compact operators, the Fredholm alternative is valid: An inhomogeneous integral equation with compact kernel has e i t h e r a unique solution for any inhomogeneity, while the corresponding homogeneous equation has only the trivial solution

(identical to zero), o r the homogeneous integral equation has at least one non-trivial solution, while the inhomogenous equation is either not solvable or its solution is not unique.

We now shall show that the first alternative applies to our case. Let us look at the homogeneous equation which corresponds to Eq. (2.27) :

$$|\psi\rangle = g_0(E + i0)V|\psi\rangle \quad . \tag{2.31}$$

If there were a solution $|\psi\rangle$ for positive energies $E > 0$, it would have to fulfill the Schrödinger equation. The latter can be verified easily by multiplying Eq. (2.31) with $g_0(E + i0)^{-1}$ from the left. As a solution of the Schrödinger equation $|\psi\rangle$ would have to conserve probability, which it cannot do because it contains only outgoing waves (compare with remarks made after Eq. (2.27)). Therefore, the homogeneous equation has no solution [1] for $E > 0$, and the solution of the inhomogeneous equation (2.27) is unique.

As we shall see, there will be a difficulty in the three-particle problem at this point.

To complete the discussion on the Lippmann-Schwinger equation (2.25), we write down its representation in momentum space,

$$\langle \vec{k}|\vec{p}\rangle^{(\pm)} = \langle \vec{k}|\vec{p}\rangle + \left(E \pm i\epsilon - \frac{k^2}{2\mu}\right)^{-1} \int d\vec{k}' \langle \vec{k}|V|\vec{k}'\rangle \langle \vec{k}'|\vec{p}\rangle^{(\pm)} \quad . \tag{2.32}$$

In this representation, the kernel has the form

$$K(\vec{k}, \vec{k}') = \left(E \pm i\epsilon - \frac{k^2}{2\mu}\right)^{-1} \langle \vec{k}|V|\vec{k}'\rangle \quad . \tag{2.33}$$

For $\epsilon \longrightarrow 0$, the kernel has a pole on the real axis which leads to divergence of the Schmidt norm. Apparently, such a singularity is relatively harmless because Lovelace [8] could show that the kernel is, nevertheless, compact.

---

[1] For $E < 0$, solutions are possible and represent bound states.

As another example of a singular operator, we consider the unity operator, which also seems to be harmless,

$$\langle \vec{p} \mid \mathbb{1} \mid \vec{p}' \rangle = \delta(\vec{p} - \vec{p}') \quad . \tag{2.34}$$

It has no finite Schmidt norm because the integral of the square of a δ-function diverges. In contrast to Eq. (2.33), however, the singularity here is strong enough to prevent compactness; this will have severe consequences in the three-particle problem.

1.5. The S-Matrix

The S-matrix is the link between scattering solutions and measurable data.

We consider the scattering state $\psi_a^{(+)}(t)$ which has evolved, according to Eq. (2.8), from a free wave packet $\phi_a(t)$, and ask for the probability of finding in $\psi_a^{(+)}(t)$ another free wave packet $\phi_b(t)$ in the limit $t \longrightarrow +\infty$. Just as $\phi_a(t)$ describes the initial situation, $\phi_b(t)$ describes the final situation, namely, the reaction products in a configuration which is selected by the setting of the counters.

What we are looking for is the (absolute square of the) matrix element

$$S_{ba} = \lim_{t \to \infty} \langle \phi_b(t) \mid \psi_a^{(+)}(t) \rangle \quad , \tag{2.35}$$

$$= \lim_{t \to \infty} \langle e^{-ih_0 t} \phi_b \mid e^{-iht} \psi_a^{(+)} \rangle \quad , \tag{2.36}$$

$$= \lim_{t \to \infty} \langle e^{iht} e^{-ih_0 t} \phi_b \mid \psi_a^{(+)} \rangle \quad . \tag{2.37}$$

Using Eqs. (2.11) and (2.12), we get

$$S_{ba} = \langle \Omega^{(-)} \phi_b | \Omega^{(+)} \phi_a \rangle \quad , \tag{2.38}$$

or

$$S_{ba} = \langle \psi_b^{(-)} | \psi_a^{(+)} \rangle \quad , \tag{2.39}$$

or

$$S_{ba} = \langle \phi_b | \Omega^{(-)\dagger} \Omega^{(+)} | \phi_a \rangle \quad . \tag{2.40}$$

With momentum eigenstates instead of wave packets, we get

$$S_{\vec{p}'\vec{p}} = \langle \vec{p}' | \Omega^{(-)\dagger} \Omega^{(+)} | \vec{p} \rangle \quad . \tag{2.41}$$

Hence, the S-matrix is the momentum representation of the S-operator

$$S = \Omega^{(-)\dagger} \Omega^{(+)} \quad . \tag{2.42}$$

To carry out the limits which are contained in the S-matrix, we go back to Eq. (2.36) which reads, for sharp energy,

$$S_{\vec{p}'\vec{p}} = \lim_{t \to \infty} e^{i(E'-E)t} \langle \vec{p}' | \vec{p} \rangle^{(+)} \quad . \tag{2.43}$$

For the sake of generality, we assume that the two energies are different,

$$E' = \frac{p'^2}{2\mu} \neq E = \frac{p^2}{2\mu} \quad . \tag{2.44}$$

We can express the scattering state $|\vec{p}\rangle^{(+)}$ by the resolvent, according to Eq. (2.19), and get

$$S_{\vec{p}'\vec{p}} = \lim_{t \to \infty} \lim_{\epsilon \to 0} i\epsilon \, e^{i(E'-E)t} \langle \vec{p}' | g(E + i\epsilon) | \vec{p} \rangle \quad . \tag{2.45}$$

The resolvent satisfies an integral equation which is very similar to the Lippmann-Schwinger equation (compare Eqs. (2.22a) and (2.25)). Its momentum representation, therefore, has poles (compare with Eq. (2.32)). We shall now extract these poles from the matrix element and carry out the limit.

We insert version (b) of the resolvent Eq. (2.22) into version (a) and get

$$\begin{aligned} g(z) &= g_0(z) + g_0(z)Vg_0(z) + g_0(z)Vg(z)Vg_0(z) \\ &= g_0(z) + g_0(z)\left[V + V\,g(z)\,V\right]g_0(z) \qquad (2.46) \\ &\equiv g_0(z) + g_0(z)\,t(z)\,g_0(z) \quad . \end{aligned}$$

The resolvent, thus, has been related to an operator t(z) which is less singular than g(z),

$$t(z) \equiv V + V\,g(z)\,V \quad . \qquad (2.47)$$

The kinematic singularities of g(z) now show up explicitly,

$$\langle \vec{p}' | g(z) | \vec{p} \rangle = \frac{\delta(\vec{p}'-\vec{p})}{z - p^2/2\mu} + \frac{\langle \vec{p}' | t(z) | \vec{p} \rangle}{(z - p'^2/2\mu)(z - p^2/2\mu)} \quad . \qquad (2.48)$$

We insert this result with $z = E + i\varepsilon$, $E = \frac{p^2}{2\mu}$ into the expression (2.45) for the S-matrix and get

$$S_{\vec{p}'\vec{p}} = \lim_{t\to\infty}\lim_{\epsilon\to 0} i\epsilon\, e^{i(E'-E)t}\left\{\frac{\delta(\vec{p}'-\vec{p})}{i\epsilon} + \frac{\langle \vec{p}' | t(E+i\epsilon) | \vec{p} \rangle}{(E+i\epsilon-E')\,i\epsilon}\right\} \qquad (2.49)$$

$$= \delta(\vec{p}'-\vec{p}) - \lim_{t\to\infty}\lim_{\epsilon\to 0} \frac{e^{i(E'-E)t}}{E'-E-i\epsilon} \langle \vec{p}' | t(E+i\epsilon) | \vec{p} \rangle \quad .$$

In the second term, the limits can be carried out using the symbolic relation [1]

$$\lim_{t\to\infty}\lim_{\epsilon\to 0}\frac{e^{i\omega t}}{\omega - i\epsilon} = 2\pi i\,\delta(\omega) \quad . \tag{2.50}$$

We finally get

$$S_{\vec{p}'\vec{p}} = \delta(\vec{p}' - \vec{p}) - 2\pi i\,\delta(p'^2/2\mu - p^2/2\mu)\langle\vec{p}'|t(E+i0)|\vec{p}\rangle \quad . \tag{2.51}$$

1.6. The T-Matrix

The singularities of the resolvent have led to two δ-functions in the S-matrix. One of them describes "no-scattering", since $\vec{p}' = \vec{p}$. (Because of the infinite extension of a plane wave, infinitely many particles pass the scattering center without deflection.) The second δ-function stands for energy conservation. All information on the scattering process is contained in the T-matrix. It yields the differential cross section by

$$\frac{d\sigma}{d\Omega} = (2\pi)^4\mu^2\,|\langle\vec{p}'|t(E+i0)|\vec{p}\rangle|^2 \quad . \tag{2.52}$$

The state $|\vec{p}\rangle$ defines energy and direction of the beam; $|\vec{p}'\rangle$ contains the direction under which the counter is placed. Because of energy conservation, we have, of course,

$$\frac{p'^2}{2\mu} = \frac{p^2}{2\mu} = E \quad . \tag{2.53}$$

---

[1] This relation is easily verified by multiplication with a testfunction and contour integration. In the present scattering theory, such an integration means transition from energy eigenstates to wave packets.

But we have to point out that Eq. (2.47) also defines the T-matrix off-shell, where

$$\frac{p'^2}{2\mu} \neq \frac{p^2}{2\mu} \neq E \quad . \tag{2.54}$$

However, there are no two-particle data which are related to the off-shell T-matrix; in three-particle scattering, though, (see Introduction and Chapter 3) the situation is different.

Since the cross section follows directly from the T-matrix, it becomes desirable to have an integral equation for t itself. Inserting Eq. (2.46) into the second resolvent equation (2.22a), we get

$$\begin{aligned} (g(z) =)\ & g_0(z) + g_0(z)\, t(z)\, g_0(z) \\ = & g_0(z) + g_0(z) V g_0(z) + g_0(z) V g_0(z) t(z) g_0(z) \ , \end{aligned} \tag{2.55}$$

or,

$$t(z) = V + V g_0(z) t(z) \quad . \tag{2.56a}$$

Using Eq. (2.22b) instead of Eq. (2.22a), one obtains

$$t(z) = V + t(z) g_0(z) V \tag{2.56b}$$

In a representation space, these equations are integral equations for the T-matrix. All integral equations of this chapter (Eqs. (2.22), (2.25), (2.56)) have the same kernel

$$K(z) = g_0(z) V \ ,$$

or, respectively,

$$K^{+}(z^*) = V g_0(z) \quad .$$

Some usefull relations for the T-matrix are the following:

Comparison of Eq. (2.56) with Eq. (2.47) leads to

$$g_0(z)\,t(z) = g(z)\,v \quad , \tag{2.57a}$$

$$t(z)\,g_0(z) = v\,g(z) \quad . \tag{2.57b}$$

It is also easily verified that

$$t(z) = (1 - v\,g_0(z))^{-1}\,v \quad , \tag{2.58a}$$

$$t(z) = v\,(1 - g_0(z)\,v)^{-1} \quad , \tag{2.58b}$$

$$(1 - g_0(z)\,v)^{-1} = 1 + g_0(z)\,t(z) \quad , \tag{2.59a}$$

$$(1 - v\,g_0(z))^{-1} = 1 + t(z)\,g_0(z) \quad . \tag{2.59b}$$

1.7. The Unitarity Relation

For a Hermitian potential, there is a conservation law for probability flux. As a consequence, the S-matrix must be unitary

$$S^{+}S = \mathbb{1} \quad . \tag{2.60}$$

By Eq. (2.51), one can derive the consequences of this relation for the T-matrix. We want to look at another way [9], however, which is also suitable for the three-particle problem.

From Eq. (2.56a), the following equation can easily be derived (multiply by $t^{-1}(z)$ from the right and by v^{-1} from the left),

$$t^{-1}(z) = v^{-1} - g_0(z) \quad . \tag{2.61}$$

As mentioned in connection with Eq. (2.26), $g_0(z)$ has a cut along the positive real energy axis. According to Eq. (2.61), t^{-1} and, consequently, t have the same cut. The unitarity relation and the discontinuity of t at the cut are equivalent to each other.

We write Eq. (2.61) for $z = E + i\varepsilon$,

$$t^{-1}(E+i\epsilon) = v^{-1} - g_0(E+i\epsilon) \quad , \tag{2.62a}$$

and for $z = E - i\varepsilon$,

$$t^{-1}(E-i\epsilon) = v^{-1} - g_0(E-i\epsilon) \quad , \tag{2.62b}$$

and get the discontinuity by subtraction and multiplication by $t(E+i\varepsilon)$, $t(E-i\varepsilon)$ from the left and right, respectively,

$$t^{-1}(E+i\epsilon) - t^{-1}(E-i\epsilon) = -g_0(E+i\epsilon) + g_0(E-i\epsilon) \tag{2.63}$$

$$t(E-i\epsilon) - t(E+i\epsilon) = t(E+i\epsilon)\left\{-g_0(E+i\epsilon) + g_0(E-i\epsilon)\right\} t(E-i\epsilon) \, .$$

Using the first resolvent equation, the difference in parentheses becomes

$$\begin{aligned} -g_0(E+i\epsilon) + g_0(E-i\epsilon) &= 2i\epsilon\, g_0(E+i\epsilon) g_0(E-i\epsilon) \\ &= 2i\epsilon \left((E-h_0)^2 + \epsilon^2\right)^{-1} \quad . \end{aligned} \tag{2.64}$$

By the relation

$$\pi \delta(x) = \lim_{\epsilon \to 0} \epsilon \, (x^2 + \epsilon^2)^{-1} \quad , \tag{2.65}$$

we get in the limit $\varepsilon \to 0$ the unitarity relation ,

$$t(E-i0) - t(E+i0) = 2\pi i \, t(E+i0) \, \delta(E-h_0) \, t(E-i0) \, ,$$

or (compare with Eq. (2.47)),

$$t(E+i0)-t^{\dagger}(E+i0)=-2\pi i\, t(E+i0)\,\delta(E-h_0)\,t^{\dagger}(E+i0) \quad . \qquad (2.66)$$

In momentum representation, we get for the forward direction

$$\mathrm{Im}\langle\vec{p}\,|\,t(E+i0)\,|\,\vec{p}\rangle = -\pi\int d\vec{p}\,''\,\delta\left(E-\frac{p''^{2}}{2\mu}\right)\left|\langle\vec{p}\,|\,t(E+i0)\,|\,\vec{p}\,''\rangle\right|^{2}$$

$$= -\pi\mu p\int d\hat{p}''\left|\langle\vec{p}\,|\,t(E+i0)\,|\,\vec{p}\,''\rangle\right|^{2}, \quad |\vec{p}\,| = |\vec{p}\,''| = \sqrt{2\mu E} \qquad (2.67)$$

$$= -\frac{p}{16\pi^{3}\mu}\,\sigma_{\mathrm{total}} \quad . \qquad (2.68)$$

This is the well-known optical theorem [10] which relates the imaginary part of the forward amplitude to the total cross section.

2. The Three-Particle Problem

2.1. The Hamiltonian

When three-particle potentials are disregarded, the Hamiltonian for three particles with masses m_1, m_2, m_3 has the form

$$H' = \frac{k_1^2}{2m_1} + \frac{k_2^2}{2m_2} + \frac{k_3^2}{2m_3} + V_1 + V_2 + V_3 \quad . \qquad (2.69)$$

The potentials describe the two-particle interaction v(i,k) in the following notation

$$V_1 = V(2,3) \;,\; V_2 = V(3,1) \;,\; V_3 = V(1,2) \quad . \qquad (2.70)$$

We shall use this kind of notation rather frequently for various two-body quantities.

We want to separate out the center-of-mass motion and introduce Jacobi coordinates. The cartesian space coordinates are $\vec{r}_1$, $\vec{r}_2$, $\vec{r}_3$. The Jacobi coordinates for which particles 2 and 3 appear explicitly as a subsystem are denoted by $\vec{\xi}_1$, $\vec{\eta}_1$, $\vec{r}$. The transformation reads

$$\begin{aligned}
\vec{\xi}_1 &= \vec{r}_2 - \vec{r}_3 \\
\vec{\eta}_1 &= \vec{r}_1 - \frac{m_2\vec{r}_2 + m_3\vec{r}_3}{m_2 + m_3} \\
\vec{r} &= \frac{m_1\vec{r}_1 + m_2\vec{r}_2 + m_3\vec{r}_3}{m_1 + m_2 + m_3} \quad .
\end{aligned} \tag{2.71}$$

The corresponding transformation for momentum coordinates becomes

$$\begin{aligned}
\vec{p}_1 &= \frac{m_3\vec{k}_2 - m_2\vec{k}_3}{m_2 + m_3} \\
\vec{q}_1 &= \frac{(m_2 + m_3)\vec{k}_1 - m_1(\vec{k}_2 + \vec{k}_3)}{m_1 + m_2 + m_3} \\
\vec{k} &= \vec{k}_1 + \vec{k}_2 + \vec{k}_3 \quad .
\end{aligned} \tag{2.72}$$

The coordinate $\vec{p}_1$, which is the canonical conjugate to $\vec{\xi}_1$, is the momentum of particle 2 in the center-of-mass system of particles 2 and 3, and $\vec{q}_1$, which is the canonical conjugate to $\vec{\eta}_1$, is the momentum of particle 1 in the center-of-mass system of all three particles.

The Jacobi coordinates with indices 2 and 3, where the subsystems (1,3) and (1,2) appear explicitly, are obtained by an appropriate interchange of indices in the transformations (2.71) and (2.72).

In Jacobi coordinates, the Hamilton operator has the form

$$H' = \frac{k^2}{2(m_1 + m_2 + m_3)} + \frac{p_1^2}{2\mu_1} + \frac{q_1^2}{2M_1} + \sum_{\gamma=1}^{3} V_\gamma \quad , \tag{2.73}$$

with the reduced masses

$$\mu_1 = \frac{m_2 m_3}{m_2 + m_3} \qquad M_1 = \frac{m_1 (m_2 + m_3)}{m_1 + m_2 + m_3} \quad . \tag{2.74}$$

Because of translation invariance of the two-body potentials, the total center-of-mass motion becomes a momentum eigenstate, which does not interest us. We leave it and write (α = 1,2 or 3)

$$H = \frac{p_\alpha^2}{2\mu_\alpha} + \frac{q_\alpha^2}{2M_\alpha} + \sum_{\gamma=1}^{3} V_\gamma \equiv h_0 + \sum_{\gamma=1}^{3} V_\gamma \quad . \tag{2.75}$$

2.2. Two-Particle Subsystems in Three-Particle Space

Two-particle subsystems play an important role in the three-particle problem. We have already chosen Jacobi coordinates, in consideration of this fact, and we now introduce the so-called channel Hamiltonians h_α,

$$h_\alpha = \frac{p_\alpha^2}{2\mu_\alpha} + \frac{q_\alpha^2}{2M_\alpha} + V_\alpha \quad . \tag{2.76}$$

Asymptotic states with two particles in a bound state, as in elastic scattering, for instance, are eigenstates of such an h_α, and that is where the name "channel Hamiltonian" comes from. For the full Hamiltonian we have

$$H = h_\alpha + \overline{V}_\alpha \quad , \tag{2.77}$$

with

$$\overline{V}_\alpha = V - V_\alpha = \sum_{\gamma \neq \alpha} V_\gamma \quad . \tag{2.78}$$

It is useful to designate the breakup channel (all particles free) by the index α = o. With the definition

$$V_0 \equiv 0 \quad , \tag{2.79}$$

the relations (2.76 - 2.78) become valid also for $\alpha = o$. Along with channel Hamiltonians, we introduce channel resolvents,

$$g_\alpha(z) \equiv (z - h_\alpha)^{-1} \quad . \tag{2.80}$$

For the notation of operators, we use the following convention. All operators which act in three-particle Hilbert space and contain only one two-particle interaction (as h_α, v_α, g_α) or no two-particle interaction (as h_o, v_o, g_o) are denoted by small letters. Their matrix elements can be expressed by matrix elements of two-particle operators in two-particle space. When a confusion with two-particle operators in two-particle space is possible, the latter will be labeled by a hat ($\wedge$). For instance,

$$\langle \vec{p}_\alpha, \vec{q}_\alpha | V_\alpha | \vec{p}'_\alpha, \vec{q}'_\alpha \rangle = \delta(\vec{q}_\alpha - \vec{q}'_\alpha) \langle \vec{p}_\alpha | \hat{V}_\alpha | \vec{p}'_\alpha \rangle \quad . \tag{2.81}$$

Genuine three-particle operators (like $H, V, \overline{V}_\alpha$) are denoted by capital letters.

The matrix elements of the above mentioned channel resolvents are

$$\langle \vec{p}_\alpha, \vec{q}_\alpha | g_\alpha(z) | \vec{p}'_\alpha, q'_\alpha \rangle = \delta(q_\alpha - q'_\alpha) \langle \vec{p}_\alpha | \hat{g}_\alpha(z - \frac{q_\alpha^2}{2M_\alpha}) | \vec{p}'_\alpha \rangle \quad . \tag{2.82a}$$

These matrix elements are related to the matrix elements of the two-particle resolvents (2.18). The resolvent g_α carries the channel index because different potentials v_α can act in different channels. The δ-function comes from the fact that g_α contains only the interaction of subsystem α and particle α is free. The argument of $\hat{g}_\alpha$ is the energy of subsystem α, which is obtained by subtracting the kinetic energy of particle α from the three-particle energy z. For g_o we have

$$\langle \vec{p}_\alpha, \vec{q}_\alpha | g_o(z) | \vec{p}'_\alpha, \vec{q}'_\alpha \rangle = \frac{\delta(\vec{q}_\alpha - \vec{q}'_\alpha)\, \delta(\vec{p}_\alpha - \vec{p}'_\alpha)}{z - q_\alpha^2/2M_\alpha - p_\alpha^2/2\mu_\alpha} \quad . \tag{2.82b}$$

The scattering in subsystem α is described by the T-matrix (compare with Eq. (2.47))

$$t_\alpha(z) = V_\alpha + V_\alpha g_\alpha(z) V_\alpha \quad . \tag{2.83}$$

In analogy to Eqs. (2.56) and (2.58), we have

$$t_\alpha(z) = V_\alpha + V_\alpha g_0(z) t_\alpha(z) \tag{2.84a}$$

$$= V_\alpha + t_\alpha(z) g_0(z) V_\alpha \quad , \tag{2.84b}$$

and

$$t_\alpha(z) = \left(1 - V_\alpha g_0(z)\right)^{-1} V_\alpha \tag{2.85a}$$

$$= V_\alpha \left(1 - g_0(z) V_\alpha\right)^{-1} \quad . \tag{2.85b}$$

The matrix elements become

$$\langle \vec{p}_\alpha, \vec{q}_\alpha | t_\alpha(z) | \vec{p}'_\alpha, \vec{q}'_\alpha \rangle = \delta(\vec{q}_\alpha - \vec{q}'_\alpha) \langle \vec{p}_\alpha | \hat{t}_\alpha(z - \frac{q_\alpha^2}{2M_\alpha}) | \vec{p}'_\alpha \rangle \quad . \tag{2.86}$$

The operator t_α will be needed, for instance, to describe three-particle scattering as two-particle multiple scattering. Figure 10 shows a graphical representation of expression (2.86).

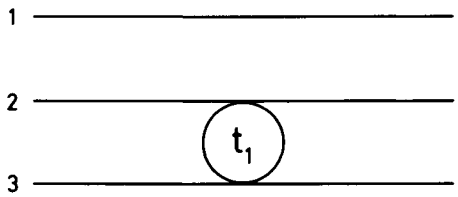


Fig. 10. Three-particle process with scattering in the two-particle subsystem

2.3. Boundary Conditions and Møller Operators

The discussion of boundary conditions and Møller operators, which has been presented in the previous sections (1.2 and 1.3) for two-particle scattering, can be generalized without difficulty to three-particle scattering.

The time development of a three-particle wave packet is given by

$$\psi_{\alpha m}^{(+)}(t) = e^{-iHt}\,\psi_{\alpha m}^{(+)} \quad , \tag{2.87}$$

while the reference wave packets develop according to

$$\phi_{\alpha m}(t) = e^{-ih_\alpha t}\,\phi_{\alpha m} \quad . \tag{2.88}$$

The wave packet $\phi_{\alpha m}$ describes the free motion of particle α (α = 1,2,3) relative to the other two particles which are in their m^{th} bound state. For α = o, we have a wave packet ϕ_o with three free particles which, however, is not very useful as an initial state (except for the description of a gas).

The boundary condition is formulated analogously to the two-particle case. One demands that the norm of the difference $\psi_{\alpha m}^{(+)}(t) - \phi_{\alpha m}(t)$ vanishes in the distant past,

$$\lim_{t \to -\infty} \| e^{-iHt}\,\psi_{\alpha m}^{(+)} - e^{-ih_\alpha t}\,\phi_{\alpha m} \| = 0 \quad . \tag{2.89}$$

This leads to the following representation of scattering states

$$\psi_{\alpha m}^{(\pm)} = \underset{t \to \mp\infty}{s\text{-}\lim}\; e^{iHt}\, e^{-ih_\alpha t}\,\phi_{\alpha m} \equiv \Omega_\alpha^{(\pm)}\,\phi_{\alpha m} \quad , \tag{2.90}$$

and to the definition of Møller operators

$$\Omega_\alpha^{(\pm)} = \underset{t \to \mp\infty}{s\text{-}\lim}\; e^{iHt}\, e^{-ih_\alpha t} \quad , \quad \alpha = 0,1,2,3 \quad , \tag{2.91}$$

where we have included the limit $t \longrightarrow +\infty$ which is important for the construction of the S-matrix.

Despite the formal analogy, it should not be overlooked that the three-particle problem is much more difficult to handle. This can already be seen from the fact that a separate Møller operator is needed for every partition α. A problem by itself is the proof that the Møller operators exist [11] and the proof that they can be applied to non-normalizable states of sharp

energy [12]. Such states are channel states with two-body fragmentation,

$$|\phi_{\alpha m}\rangle = |\vec{q}_\alpha, \psi_{\alpha m}\rangle = |\vec{q}_\alpha\rangle |\psi_{\alpha m}\rangle \quad , \tag{2.92}$$

where

$$h_\alpha |\phi_{\alpha m}\rangle = E_{\alpha m} |\phi_{\alpha m}\rangle \quad ,$$

and channel states with three free particles,

$$|\phi_0\rangle = |\vec{q}_\alpha, \vec{p}_\alpha\rangle = |\vec{q}_\alpha\rangle |\vec{p}_\alpha\rangle \quad , \tag{2.93}$$

where

$$h_0 |\phi_0\rangle = \left(q_\alpha^2 / 2M_\alpha + p_\alpha^2 / 2\mu_\alpha \right) |\phi_0\rangle \quad .$$

In Eq. (2.93), the index α is arbitrary and indicates only one out of three possible systems of Jacobi coordinates.
The domain of the Møller operators (2.91) is the space of channel states. Their range is the space of scattering states,

$$|\psi^{(\pm)}_{\alpha m}\rangle = \Omega^{(\pm)}_\alpha |\phi_{\alpha m}\rangle \quad . \tag{2.94}$$

Also in the three-particle case, a "commutation relation"

$$H \Omega^{(\pm)}_\alpha = \Omega^{(\pm)}_\alpha h_\alpha \quad , \alpha = 0,1,2,3 \, , \tag{2.95}$$

is valid, in analogy to Eq. (2.14). It follows from this relation that scattering states have the same energy as the free initial and final states, despite the fact that all these states are eigenstates of different Hamiltonians.

It can be shown [13] that scattering states which belong to different initial (or different final) states are orthogonal

$$\langle \psi^{(\pm)}_{\alpha m} | \psi^{(\pm)}_{\beta n} \rangle = \delta_{\alpha\beta} \delta_{mn} \delta(\vec{q}'_\alpha - \vec{q}_\beta) \tag{2.96}$$

(for free channel states this is not true unless $\alpha = \beta$!).

As in the two-particle case, the Hermitian conjugate Møller operators $\Omega_\alpha^{(\pm)\dagger}$ exist. They lead back from scattering states to free channel states (when channel indices match),

$$\Omega_\alpha^{(\pm)\dagger} |\psi_{\beta u}^{(\pm)}\rangle = \delta_{\alpha\beta} |\phi_{\beta u}\rangle \quad . \tag{2.97}$$

When applied to a three-particle bound state, they give zero,

$$\Omega_\alpha^{(\pm)\dagger} |\psi_\nu^B\rangle = 0 \quad . \tag{2.98}$$

Note that those states which are annihilated by the Hermitian conjugate Møller operator and those states which are not annihilated are separated energetically ($E < 0$, $E > 0$) in the two-particle case (see page 18). For three particles, this is no longer true (compare with Eq. (2.97) for $\alpha \neq \beta$: $\Omega_\alpha^{(\pm)\dagger} |\psi_{\beta u}^{(\pm)}\rangle = 0$ for $E > 0$).

2.4. Resolvent Equation and Lippmann-Schwinger Equation

We shall try now to make a connection between the time-dependent theory and the time-independent theory.

The transition from time limit to Euler limit (compare with Eq. (2.16)) is also possible for three-particle scattering. Integration over time leads, in analogy to Eq. (2.19), to the relation

$$|\psi_{\alpha u}^{(\pm)}\rangle = \lim_{\epsilon \to 0} \pm i\epsilon \, G(E \pm i\epsilon) |\phi_{\alpha u}\rangle \quad , \tag{2.99}$$

where $G(z)$ is the full resolvent of the three-particle system

$$G(z) \equiv (z - H)^{-1} \quad . \tag{2.100}$$

With the channel resolvent (2.80), the two resolvent equations

$$G(z) = g_\alpha(z) + g_\alpha(z) \bar{V}_\alpha G(z) \quad , \tag{2.101a}$$

and

$$= g_\alpha(z) + G(z) \bar{V}_\alpha g_\alpha(z) \quad , \tag{2.101b}$$

can be written down; they are verified easily by use of the identity

$$\bar{V}_\alpha = g_\alpha^{-1}(z) - G^{-1}(z) \quad . \tag{2.102}$$

The Lippmann-Schwinger equation for the scattering state is obtained by insertion of the resolvent equation (2.101a) into Eq. (2.99)

$$|\psi_{\alpha m}^{(\pm)}\rangle = \lim_{\epsilon \to 0} \pm i\epsilon \left(g_\alpha(E \pm i\epsilon) + g_\alpha(E \pm i\epsilon) \bar{V}_\alpha G(E \pm i\epsilon) \right) |\phi_{\alpha m}\rangle \quad . \tag{2.103}$$

Since the free channel state $|\phi_{\alpha m}\rangle$ is an eigenstate of h_α with energy E, we have

$$\lim_{\epsilon \to 0} \pm i\epsilon\, g_\alpha(E \pm i\epsilon) |\phi_{\alpha m}\rangle = |\phi_{\alpha m}\rangle \quad . \tag{2.104}$$

With this result, we obtain from Eq. (2.103), using Eq. (2.99) for the second term,

$$|\psi_{\alpha m}^{(\pm)}\rangle = |\phi_{\alpha m}\rangle + g_\alpha(E \pm i0)\, \bar{V}_\alpha |\psi_{\alpha m}^{(\pm)}\rangle \quad . \tag{2.105}$$

In contrast to the two-particle problem (see remarks made in connection with Eq. (2.31)), the solution of the Lippmann-Schwinger equation is now not uniquely determined, because the homogeneous equation,

$$|\psi\rangle = g_\alpha(E \pm i0)\, \bar{V}_\alpha |\psi\rangle \quad , \tag{2.106}$$

has solutions for energies in the scattering region. The latter can be seen by choosing another channel state $|\phi_{\beta u}\rangle, \beta \neq \alpha$, in Eq. (2.103). We then get [14]

$$\lim_{\epsilon \to 0} \pm i\epsilon\, g_\alpha(E \pm i\epsilon) |\phi_{\beta u}\rangle = 0 \quad , \tag{2.107}$$

because the state $|\phi_{\beta n}\rangle$ is not an eigenstate of h_α ; the product $g_\alpha |\phi_{\beta n}\rangle$ remains finite for $\varepsilon \longrightarrow 0$ and, therefore, expression (2.107) vanishes. We obtain the equation

$$|\psi_{\beta u}^{(\pm)}\rangle = g_\alpha(E \pm i0)\bar{V}_\alpha |\psi_{\beta u}^{(\pm)}\rangle \quad . \tag{2.108}$$

This equation tells us that the homogeneous equation, which belongs to the inhomogeneous Lippmann-Schwinger equation (2.105), has as non-trivial solutions the scattering states $|\psi_{\beta u}^{(\pm)}\rangle$ of other channels with $\beta \neq \alpha$.

In the two-particle problem, the homogeneous equation had non-trivial solutions, too, but only at discrete binding energies where no scattering takes place. In the three-particle problem, the homogeneous equation has non-trivial solutions (besides at three-particle binding energies) at a continuum of energies which covers the region of scattering energies.

This property of the Lippmann-Schwinger equation in the three-particle case is closely related to the projection properties of the Hermitian conjugate Møller operators, Eq. (2.97) [9].

In order to get unique solutions for the Lippmann-Schwinger equation, one has to introduce additional conditions which select from the multifold of solutions those which obey the physical boundary condition or its representative, Eq. (2.99). Glöckle [15] has shown that the following system of equations has unique solutions

$$|\psi_{\alpha u}^{(+)}\rangle = |\phi_{\alpha u}\rangle + g_\alpha(E + i0)\bar{V}_\alpha |\psi_{\alpha u}^{(+)}\rangle \tag{2.109a}$$

$$|\psi_{\alpha u}^{(+)}\rangle = g_\beta(E + i0)\bar{V}_\beta |\psi_{\alpha u}^{(+)}\rangle \tag{2.109b}$$

$$|\psi_{\alpha u}^{(+)}\rangle = g_\gamma(E + i0)\bar{V}_\gamma |\psi_{\alpha u}^{(+)}\rangle \quad . \tag{2.109c}$$

In addition to the Lippmann-Schwinger equation, he demands that there are only outgoing waves in channels β, γ and no incoming waves (the latter would be possible according to Eq. (2.108),

if only Eq. (2.109a) were demanded). By introduction of a suitable approximation, Glöckle succeeded in transforming the system of Eqs. (2.109a,b,c) into a system of integral equations with a finite Schmidt norm.

As they stand, neither the kernel of Eq. (2.105) nor the kernel of Eqs. (2.109a,b,c) have a finite Schmidt norm. Also the kernels are not compact [7] and, therefore, standard methods of the theory of integral equations cannot be applied. The kernel of the Lippmann-Schwinger equation is

$$K_\alpha(z) = g_\alpha(z)\bar{V}_\alpha \quad . \tag{2.110}$$

Using Eq. (2.22a), one gets

$$K_\alpha(z) = g_0(z)\bar{V}_\alpha + g_0(z)V_\alpha g_\alpha(z)\bar{V}_\alpha \quad . \tag{2.111}$$

The δ-functions which come from the two-body potentials in the first term are the reason for the divergence of the Schmidt norm (see remark made in connection with Eq. (2.34));

$$\langle \vec{k}_1 \vec{k}_2 \vec{k}_3 | g_0(z)\bar{V}_\alpha | \vec{k}_1' \vec{k}_2' \vec{k}_3' \rangle \sim \left(z - \sum_{i=1}^{3} k_i^2/2m_i\right)^{-1} \sum_{\gamma \neq \alpha} \delta(\vec{q}_\gamma - \vec{q}_\gamma') \langle \vec{p}_\gamma | \hat{V}_\gamma | \vec{p}_\gamma' \rangle \, . \tag{2.112}$$

In Eq. (2.112), the δ-function belonging to the total center-of-mass motion has been omitted on the right-hand side.

A graphical representation (see Fig. 11) of the operator g_0V shows that this operator has disconnected parts.

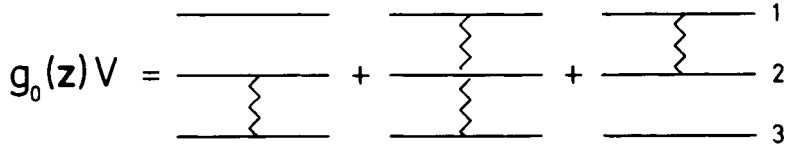


Fig. 11. Kernel of the three-particle Lippmann-Schwinger equation in graphical representation

Only two particles interact in each term, while the third one moves freely, which means that there is a δ-function in momentum space. When looking for useful integral equations, one should try to avoid disconnected parts in the kernel.

3. The Faddeev Equations

1. The Faddeev Equations for the T-Matrix

After Faddeev had shown [16] in 1960 that the Lippmann-Schwinger equation (2.105) does not have a unique solution, he studied the properties of the operator

$$T(z) = V + VG(z)V \quad . \tag{3.1}$$

Although this operator is the formal analogue of the two-particle T-operator (Eq. (2.47)), it is not related to a scattering cross section as directly as in the two-particle case. In analogy to Eq. (2.46), we have

$$G(z) = g_0(z) + g_0(z)T(z)g_0(z) \quad . \tag{3.2}$$

The operator T(z) is less singular than the resolvent G(z) since the singular operators $g_0(z)$ are split off. As in the two-particle case (Eq. (2.56)), we have the equations

$$T(z) = V + Vg_0(z)T(z) \quad , \tag{3.3a}$$

$$T(z) = V + T(z)g_0(z)V \quad . \tag{3.3b}$$

These integral equations for the T-operator suffer from the same disadvantage as the Lippmann-Schwinger equation (2.105) and the resolvent equations (2.101) since they have the same kernels.

Faddeev arrives at a new equation by the following manipulation: He splits Eq. (3.3a) into three equations (we omit, in the following, the z-dependence of operators)

$$T_i = v_i + v_i g_0 T \quad . \tag{3.4}$$

Because of $V = v_1 + v_2 + v_3$, the T-operator is the sum of the three new operators T_i,

$$T = T_1 + T_2 + T_3 \quad . \tag{3.5}$$

By this splitting, Eq. (3.3a) is blown up into a system of equations for the components T_i.
In matrix form,

$$\begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix} = \begin{pmatrix} V_1 \\ V_2 \\ V_3 \end{pmatrix} + \begin{pmatrix} V_1 & V_1 & V_1 \\ V_2 & V_2 & V_2 \\ V_3 & V_3 & V_3 \end{pmatrix} g_0 \begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix} \quad . \tag{3.6}$$

So far, nothing has been gained. Equation (3.6) still has a non-compact kernel, and the same is true also for all equations which are derived from it by iteration. The splitting, however, brings about a partial solution which leaves the kernel less singular. In the first line of the matrix equation (3.6), we bring the term $(v_1 g_0 T_1)$ to the left-hand side,

$$T_1 - V_1 g_0 T_1 = V_1 + V_1 g_0 (T_2 + T_3) \quad . \tag{3.7}$$

Multiplication by $(1-v_1 g_0)^{-1}$ from the left yields

$$T_1 = t_1 + t_1 g_0 (T_2 + T_3) \quad , \tag{3.8}$$

where (see Eq. (2.85a))

$$t_1 = (1 - V_1 g_0)^{-1} V_1 \quad , \tag{3.9}$$

has been used. When line 2 and 3 are transformed in the same way, we get the matrix equation

$$\begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix} = \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} + \begin{pmatrix} 0 & t_1 & t_1 \\ t_2 & 0 & t_2 \\ t_3 & t_3 & 0 \end{pmatrix} g_0 \begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix} \quad . \tag{3.10}$$

This equation is called Faddeev equation for the T-matrix. It is sometimes written as

$$T_i(z) = t_i(z) + \sum_{j=1}^{3} F_{ij}(z)\, g_0(z)\, T_j(z) \quad ,$$

or, in matrix notation,

$$\mathcal{T}(z) = \mathcal{t}(z) + \mathcal{K}_F(z)\, \mathcal{T}(z) \quad ,$$

with

$$\left(\mathcal{K}_F(z)\right)_{ij} \equiv F_{ij}(z)\, g_0(z) \equiv (1 - \delta_{ij})\, t_i(z)\, g_0(z) \quad .$$

Instead of the potentials v_i, the new equations (3.10) contain the two-particle T-matrices t_i, which are now to be understood as operators in three-particle space (see Eq. (2.86)). The quantities t_i enter into the Faddeev equation off-shell because of the energy shift $z - q_i''^2/2M_i$ and because of the fact that the evaluation of the operator product $t_i g_0 T_j$ implies an integration over all possible intermediate states $|\vec{p}_i''\rangle\,|\vec{q}_i''\rangle$ with

$$\frac{p_i^2}{2\mu_i} \neq z - \frac{q_i''^2}{2M_i} \neq \frac{p_i''^2}{2\mu_i} \quad .$$

We have here the mathematical formulation of the phenomenon mentioned in the introduction, according to which two-particle scattering amplitudes enter into the three-particle amplitude off the energy-shell with the consequence that three-particle scattering data contain more information than two-particle data alone.

Since the operators t_i act only in subsystem i, the kernel of Eq. (3.10) still contains δ-functions,

$$\langle \vec{p}_i \vec{q}_i | t_i(z) | \vec{p}_i' \vec{q}_i' \rangle = \delta(\vec{q}_i - \vec{q}_i')\, \langle \vec{p}_i | \hat{t}_i\left(z - \frac{q_i^2}{2M_i}\right) | \vec{p}_i' \rangle \quad . \qquad (3.11)$$

Consequently, the kernel does not have a finite Schmidt norm. Nevertheless, Eq. (3.10) has an advantage over Eqs. (3.3) and (3.6). In its first iteration, the dangerous δ-functions are already gone (by integration),

$$\begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix} = \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} + \begin{pmatrix} t_1 g_0 (t_2 + t_3) \\ t_2 g_0 (t_3 + t_1) \\ t_3 g_0 (t_1 + t_2) \end{pmatrix}$$

(3.12)

$$+ \begin{pmatrix} t_1 g_0 (t_2+t_3) & t_1 g_0 t_3 & t_1 g_0 t_2 \\ t_2 g_0 t_3 & t_2 g_0 (t_3+t_1) & t_2 g_0 t_1 \\ t_3 g_0 t_2 & t_3 g_0 t_1 & t_3 g_0 (t_1+t_2) \end{pmatrix} g_0 \begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix} .$$

There are only operator products $t_i g_0 t_j$ with $i \neq j$ and, therefore, the kernel contains only terms where all three particles are linked together. Figure 12 shows a graphical representation of such a term; compare this with the graphical representation of a Lippmann-Schwinger kernel (Fig. 11).

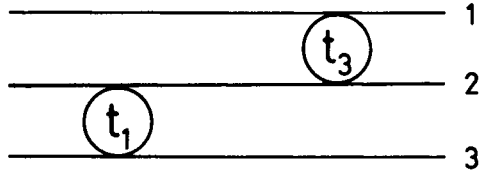


Fig. 12. Graphical representation of a typical term of the iterated Faddeev kernel

The Schmidt norm of the kernel of the iterated Faddeev equations (3.12) exists when the potentials vanish fast enough and when Im z ≠ o.

This sounds rather promising, but we have not yet reached our goal. There are two problems to be investigated.

a) The Schmidt norm of the iterated kernel does not exist for Im z = o and Re z > E^B_{min} (where E^B_{min} is the lowest energy level

of the subsystems) and, therefore, it is uncertain whether the kernel is compact for physical energies.

b) The Faddeev equations have been derived from the "sick" equation (3.6) which does not have a unique solution for Im z = o. It is questionable, therefore, whether Eqs. (3.10) or (3.12) have unique solutions.

The major part of the work of Faddeev [17] is concerned with these two questions.
The Schmidt norm of an expression of the form

$$t_i(z)\,g_0(z)\,t_j(z) \qquad i \neq j \quad , \tag{3.13}$$

diverges for Im $z \longrightarrow o$ and Re $z > E^B_{min}$ because the T-matrices as well as the free propagator are singular (the latter only for Re $z > o$, see Eqs. (2.82) and (5.28)). A second iteration leads to operator products of the form

$$t_i(z)\,g_0(z)\,t_j(z)\,g_0(z)\,t_k(z) \qquad i \neq j \quad j \neq k \quad . \tag{3.14}$$

These expressions are again less singular than the expressions (3.13) because integrations over intermediate states tend to smooth out singularities, and there are more integrations in (3.14). After the fourth iteration, which leads to the kernel K_F^5, the remaining singularities become as harmless as those of the two-particle problem (compare with remark made after Eq. (2.33)). Faddeev could show [18] that the fifth power K_F^5 of the kernel of Eq. (3.10) is compact in a suitable Banach space for real energies greater than E^B_{min} .

It follows as a consequence that the kernel K_F of the non-iterated Faddeev equation has, despite δ-functions and despite singularities of t_i and g_o on the real energy axis, some important properties which are known from compact operators:

a) The Fredholm alternative is valid [18] (see also page 23).

b) The kernel has only a discrete sprectrum η_ν ,

$$K_T \psi_\nu = \eta_\nu \psi_\nu \tag{3.15}$$

c) The resolvent $R(\lambda) = (\lambda - K_T)^{-1}$ exists [19] and is a meromorphic function of the parameter λ.

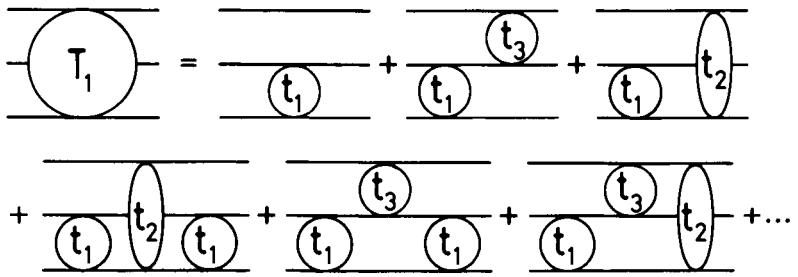
Since the homogeneous part of Eq. (3.10) has as solutions only three-particle bound states [18], it follows from point (a) that Eq. (3.10) has unique solutions at scattering energies. And it follows from point (c) that a practical solution for our problem does not have to start at the fourth iteration but can handle the original equation directly.

This solves our three-particle problem in principle. There are difficulties with charged particles because of the long-ranged Coulomb force, but also here progress has been made [20].

To get a feeling for the Faddeev equations, we write the Neumann series of Eq. (3.10), which is obtained by continued iteration,

$$T(z) = \sum_{\nu=0}^{\infty} t(z) \left(K_T(z)\, t(z) \right)^\nu \tag{3.16}$$

The question of convergence does not concern us here. In graphical representation, we get for T_1 , for instance,



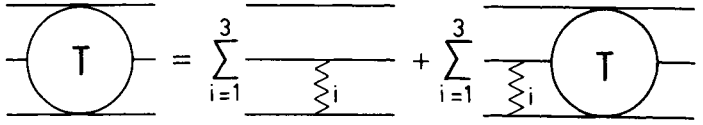
(3.17)

Because of the special form of the Faddeev kernel, only T-matrices of different subsystems follow each other (compare also Eq. (3.12) and Fig. 12). The graphs are to be read by the following rules: Straight lines represent free states (eigenstates of h_o). The operators g_o do not appear explicitly because they only give numerical factors when they are applied to free states. For the translation from graphical to operator representation, we only have to keep in mind that every interaction

is followed by a free propagation and that we have to insert the free propagator g_o . We let the time sequence run from right to left; the initial state is the state at the right-hand side of a graph; the final state is the one at the left-hand side.

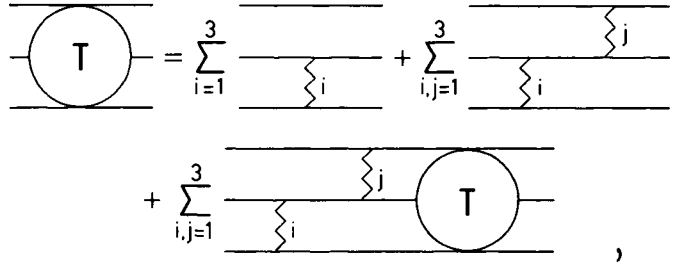
The meaning of the Faddeev equations can be seen now from the graphical representation of its Neumann series. The equations describe the three-particle scattering process as a two-particle multiple scattering process where the individual two-particle events can be on-shell or off-shell. A description of three-particle scattering as two-particle multiscattering has already been introduced by Watson [21] in 1953.

We now want to compare the graphical representation, Eq. (3.17), with a graphical representation of the Lippmann-Schwinger equation in order to see once more the non-compactness of the kernel of Eq. (3.3) and to further clarify the role of the two-particle T-matrices in the Faddeev equations. The potentials which occur in Eq. (3.3) are represented by wavy lines



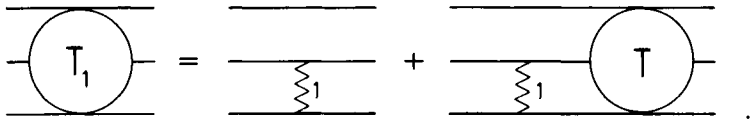
(3.18)

We see, once again, what the expression "disconnected kernel" means: In each term of the second sum, one particle does not interact; its state does not change, which is expressed by a δ-function in the integration over intermediate states. The situation is the same after one iteration,



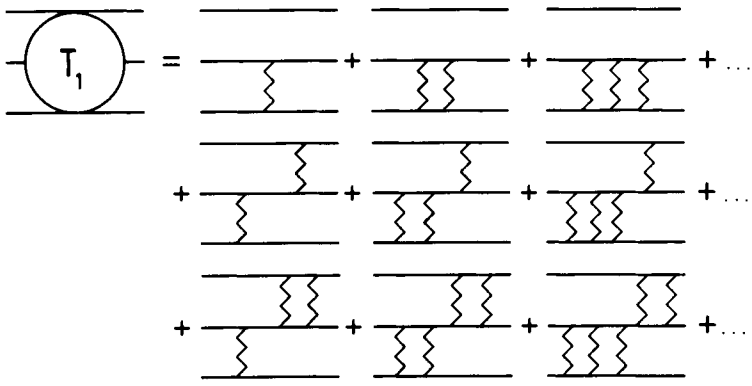
(3.19)

since the third sum contains terms with $i = j$.
At first sight, the splitting of T in T_1, T_2, T_3 does not seem to bring an advantage. In graphical representation Eq. (3.4) reads



(3.20)

But the continued iteration leads to subseries,

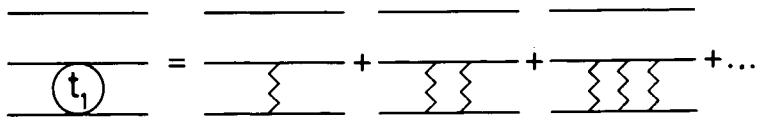


(3.21)

which can be added up. According to Eq. (3.9), we have the expansion

$$t_i = \sum_{\nu=0}^{\infty} v_i (g_0 v_i)^{\nu} , \tag{3.22}$$

or, in graphical representation,



(3.23)

Adding up the various subseries of Eq. (3.21) by this expression, we arrive at the Neumann series of the Faddeev equations, Eq. (3.17). Since only a few graphs are shown in Eq. (3.21), some imagination is needed to verify this from our plot; it is clearly visible, however, how the first two graphs on the right-hand side of Eq. (3.17) evolve.

It is evident that the series (3.21) becomes less divergent by the partial summation since the subseries (3.23), which can be divergent, has been replaced by the two-particle T-matrix.

The partial summation of the Neumann series has lead Faddeev to the splitting of the three-particle T-matrix into components T_i. As we have seen, this splitting leads after one iteration to an integral equation with a connected kernel.

We now want to derive other versions of the Faddeev equations. According to Eq. (3.2), the resolvent G(z) can be calculated when the T-operator is known. It is possible, however, to write down Faddeev equations for the resolvent directly or, more precisely, for a splitting of the resolvent into components. With the resolvent G(z), the scattering solution is known, according to Eq. (2.99). Also, here it is possible to find Faddeev equations which can yield the scattering solution directly. From the scattering solution, one can read off the elements of the S-matrix, especially the physical interesting transition amplitudes. For the latter, again there are Faddeev equations of their own.

2. The Faddeev Equations for the Resolvent

We insert the splitting of the T-operators, Eq. (3.5), into the expression (3.2) for the resolvent,

$$G(z) = g_0(z) + \sum_{i=1}^{3} g_0(z)\, T_i(z)\, g_0(z) \quad . \tag{3.24}$$

Defining components $G_i(z)$ by

$$G_i(z) = g_0(z)\, T_i(z)\, g_0(z) \quad , \tag{3.25}$$

the resolvent becomes

$$G(z) = g_0(z) + \sum_{i=1}^{3} G_i(z) \quad . \tag{3.26}$$

Integral equations for the components $G_i(z)$ are derived by inserting the Faddeev equations (3.10) into Eq. (3.25),

$$G_i = g_0 t_i g_0 + g_0 \sum_{j=1}^{3} F_{ij}\, g_0 T_j g_0 \quad . \tag{3.27}$$

By extending Eq. (2.46) to three-particle space, we get

$$g_0 t_i g_0 = g_i - g_0 \quad , \tag{3.28}$$

and, together with Eq. (3.25), Eq. (3.27) becomes,

$$G_i(z) = g_i(z) - g_0(z) + \sum_{j=1}^{3} g_0(z) F_{ij}(z) G_j(z) \quad . \tag{3.29}$$

These are the Faddeev equations [14] for the resolvent. Again, the typical Faddeev operator $F_{ij}(z)$ appears in the kernel, and what has been said about the kernel on page 47 remains valid in the present case.

3. The Faddeev Equations for Scattering States

For scattering states we have, according to Eq. (2.99),

$$|\psi^{(\pm)}_{\alpha m}\rangle = \lim_{\epsilon \to 0} \pm i\epsilon\, G(E \pm i\epsilon) |\phi_{\alpha m}\rangle \quad . \tag{3.30}$$

With the splitting (3.26) of the resolvent, this becomes

$$\begin{aligned} |\psi^{(\pm)}_{\alpha m}\rangle &= \lim_{\epsilon \to 0} \pm i\epsilon\, g_0(E \pm i\epsilon) |\phi_{\alpha m}\rangle \\ &+ \lim_{\epsilon \to 0} \pm i\epsilon \sum_{i=1}^{3} G_i(E \pm i\epsilon) |\phi_{\alpha m}\rangle \quad . \end{aligned} \tag{3.31}$$

With the definitions

$$|\chi^{(\pm)}_{i\alpha m}\rangle = \lim_{\epsilon \to 0} \pm i\epsilon\, g_i(E \pm i\epsilon) |\phi_{\alpha m}\rangle \quad i = 0,1,2,3 \quad , \tag{3.32a}$$

and,

$$|\psi^{(\pm)}_{\alpha m}\rangle_i = \lim_{\epsilon \to 0} \pm i\epsilon\, G_i(E \pm i\epsilon) |\phi_{\alpha m}\rangle \quad i = 1,2,3 \quad , \tag{3.32b}$$

we get the following splitting of the scattering state into components

$$|\psi^{(\pm)}_{\alpha m}\rangle = |\chi^{(\pm)}_{0\alpha m}\rangle + \sum_{i=1}^{3} |\psi^{(\pm)}_{\alpha m}\rangle_i \quad . \tag{3.33}$$

We insert the Faddeev equations (3.29) into Eq. (3.32b) and get

$$|\psi^{(\pm)}_{\alpha m}\rangle_i = \lim_{\epsilon\to 0} \pm i\epsilon \Big\{ g_i(E\pm i\epsilon) - g_0(E\pm i\epsilon) + \sum_{j=1}^{3} g_0(E\pm i\epsilon) F_{ij}(E\pm i\epsilon) G_j(E\pm i\epsilon) \Big\} |\phi_{\alpha m}\rangle \quad . \tag{3.34}$$

Using the definitions (3.32) once more, this becomes

$$|\psi^{(\pm)}_{\alpha m}\rangle_i = |\chi^{(\pm)}_{i\alpha m}\rangle - |\chi^{(\pm)}_{0\alpha m}\rangle + \sum_{j=1}^{3} g_0(E\pm i\epsilon) F_{ij}(E\pm i\epsilon) |\psi^{(\pm)}_{\alpha m}\rangle_j \quad . \tag{3.35}$$

The limit which is contained in the definition (3.32a) can be carried out. For $\alpha \neq o$ (when we have a bound pair in the entrance channel), we get

$$|\chi^{(\pm)}_{i\alpha m}\rangle = \delta_{i\alpha} |\phi_{\alpha m}\rangle \quad , \quad i = 0,1,2,3 \quad , \tag{3.36}$$

(compare with the remark made after Eq. (2.107)). For $\alpha = o$ (the scattering state evolves from a free state $|\phi_o\rangle$), we get,

$$|\chi^{(\pm)}_{io}\rangle = \begin{cases} \lim_{\epsilon\to 0} \pm i\epsilon\, g_0(E\pm i\epsilon)|\phi_o\rangle = |\phi_o\rangle & i=o \\ \lim_{\epsilon\to 0} \pm i\epsilon\, g_i(E\pm i\epsilon)|\phi_o\rangle = \Omega^{(\pm)}_i |\phi_o\rangle & i\neq o \end{cases} , \tag{3.37}$$

where $\Omega^{(\pm)}_i$ is the two-particle Møller operator in three-particle space (compare Eqs. (2.11) and (2.17)).
With Eqs. (3.36) and (3.37), the Faddeev equations, see Eq. (3.35), for scattering states [14] become:

a) when there is a bound pair in the entrance channel, $\alpha \neq o$,

$$|\psi^{(\pm)}_{\alpha m}\rangle_i = \delta_{i\alpha} |\phi_{\alpha m}\rangle + \sum_{j=1}^{3} g_0(E\pm i0) F_{ij}(E\pm i0) |\psi^{(\pm)}_{\alpha m}\rangle_j \, , \tag{3.38}$$

$$|\psi^{(\pm)}_{\alpha m}\rangle = \sum_{i=1}^{3} |\psi^{(\pm)}_{\alpha m}\rangle_i \, ,$$

b) when there are three free particles in the entrance channel, $\alpha = o$,

$$|\psi_o^{(\pm)}\rangle_i = |\psi_i^{(\pm)}\rangle + \sum_{j=1}^{3} g_o(E \pm io)\, \bar{T}_{ij}(E \pm io)\, |\psi_o^{(\pm)}\rangle_j \qquad (3.39)$$

$$|\psi_o^{(\pm)}\rangle = |\phi_o\rangle + \sum_{i=1}^{3} |\psi_o^{(\pm)}\rangle_i \quad .$$

The quantity $|\psi_i^{(\pm)}\rangle$ is defined as (compare with Eq. (3.37))

$$|\psi_i^{(\pm)}\rangle = \Omega_i^{(\pm)} |\phi_o\rangle - |\phi_o\rangle \ ,$$

and represents a spherical wave (out- or ingoing, respectively).

4. The S-Matrix

We define as S-matrix the amplitude which is obtained when we let a free state $e^{-ih_\alpha t}|\phi_{\alpha m}\rangle$ or $e^{-ih_o t}|\phi_o\rangle$ develop into a scattering state $e^{-iHt}|\psi_{\alpha m}^{(+)}\rangle$ or $e^{-iHt}|\psi_o^{(+)}\rangle$, respectively, and analyze the scattering state for free states $e^{-ih_\beta t}|\phi_{\beta n}\rangle$ or $e^{-ih_o t}|\phi_o\rangle$ in the limit $t \to \infty$,

$$S_{\beta n, \alpha m}(\vec{q}'_\beta, \vec{q}_\alpha) = \lim_{t\to\infty} \langle e^{-ih_\beta t} \phi_{\beta n} | e^{-iHt} \psi_{\alpha m}^{(+)} \rangle \qquad (3.40a)$$

($\alpha, \beta \neq o$, rearrangement scattering),

$$S_{o, \alpha m}(\vec{q}'_\alpha, \vec{p}'_\alpha, \vec{q}_\alpha) = \lim_{t\to\infty} \langle e^{-ih_o t} \phi_o | e^{-iHt} \psi_{\alpha m}^{(+)} \rangle \qquad (3.40b)$$

($\alpha \neq o$, breakup),
and,

$$S_{o,o}(\vec{q}'_\alpha, \vec{p}'_\alpha, \vec{q}_\alpha, \vec{p}_\alpha) = \lim_{t\to\infty} \langle e^{-ih_o t} \phi_o | e^{-iHt} \psi_o^{(+)} \rangle \qquad (3.40c)$$

(free-free scattering).

By help of Eqs. (2.90) and (2.91), we get

$$S_{\beta u,\alpha m}(\vec{q}'_\beta;\vec{q}_\alpha) = \langle \phi_{\beta u}|\Omega_\beta^{(-)\dagger}\Omega_\alpha^{(+)}|\phi_{\alpha m}\rangle \qquad (3.41a)$$

($\alpha, \beta \neq o$),

$$S_{o,\alpha m}(\vec{q}'_\alpha,\vec{p}'_\alpha;\vec{q}_\alpha) = \langle \phi_o|\Omega_o^{(-)\dagger}\Omega_\alpha^{(+)}|\phi_{\alpha m}\rangle \qquad (3.41b)$$

($\alpha \neq o$),

and,

$$S_{o,o}(\vec{q}'_\alpha,\vec{p}'_\alpha;\vec{q}_\alpha,\vec{p}_\alpha) = \langle \phi_o|\Omega_o^{(-)\dagger}\Omega_o^{(+)}|\phi_o\rangle . \qquad (3.41c)$$

In contrast to the two-particle case, Eq. (2.42), we have a 4 x 4 matrix of operators in the three-particle case,

$$S_{\beta\alpha} = \Omega_\beta^{(-)\dagger}\Omega_\alpha^{(+)} . \qquad (3.42)$$

The matrix elements of this set of operators, taken with channel states $|\phi_{\alpha m}\rangle$ or $|\phi_o\rangle$, form the S-matrix.

The channel states $|\phi_{1m}\rangle$ do not form a complete set because m denotes a bound state of the subsystem (2,3), and the continuum of this subsystem is missing, similarly for $|\phi_{2n}\rangle$ and $|\phi_{3e}\rangle$. Only the states $|\phi_o\rangle$ form a complete set of functions. The set of functions spanned by all channel states $|\phi_o\rangle, |\phi_{1m}\rangle$, $|\phi_{2n}\rangle$ and $|\phi_{3e}\rangle$ on the other hand, is non-orthogonal and overcomplete.

From Eq. (3.41), we get, by help of Eq. (2.94),

$$S_{\beta u,\alpha m}(\vec{q}'_\beta;\vec{q}_\alpha) = \langle \psi_{\beta u}^{(-)}|\psi_{\alpha m}^{(+)}\rangle \qquad (3.43a)$$

($\alpha, \beta \neq o$),

$$S_{o,\alpha m}(\vec{q}'_\alpha,\vec{p}'_\alpha;\vec{q}_\alpha) = \langle \psi_o^{(-)}|\psi_{\alpha m}^{(+)}\rangle \qquad (3.43b)$$

($\alpha \neq o$),

and,

$$S_{0,0}(\vec{q}'_\alpha, \vec{p}'_\alpha, \vec{q}_\alpha, \vec{p}_\alpha) = \langle \psi_0^{(-)} | \psi_0^{(+)} \rangle \quad . \tag{3.43c}$$

We could stop here because we can consider the scattering states as being given by Eqs. (3.38) and (3.39). But we want to separate out the δ-functions from the S-matrix and derive Faddeev equations for the remaining transition amplitudes. We could proceed similarly as in the two-particle case, Eqs. (2.39 - 51), but then we would have to know the form of the transition operators which allows a separation of the kinematic singularities of the resolvent (analogous to Eq. (2.48)). Not having this knowledge, we proceed in the following way. Let us first consider only rearrangement scattering.

We insert the resolvent equation (2.101b) into equation (2.99),

$$|\psi_{\alpha m}^{(\pm)}\rangle = |\phi_{\alpha m}\rangle + G(E_{\alpha m} \pm i0)\bar{V}_\alpha |\phi_{\alpha m}\rangle \quad . \tag{3.44}$$

From this we get

$$|\psi_{\alpha m}^{(+)}\rangle = |\psi_{\alpha m}^{(-)}\rangle + \left(G(E_{\alpha m} + i0) - G(E_{\alpha m} - i0)\right)\bar{V}_\alpha |\phi_{\alpha m}\rangle \quad . \tag{3.45}$$

The difference of the resolvents is calculated in the same way as in Eqs. (2.64) and (2.65),

$$G(E_{\alpha m} + i0) - G(E_{\alpha m} - i0) = -2\pi i\, \delta(E_{\alpha m} - H) \quad . \tag{3.46}$$

With Eqs. (3.43), (3.45), and (3.46), the S-matrix becomes

$$S_{\beta u, \alpha m}(\vec{q}'_\beta, \vec{q}_\alpha) = \langle \psi_{\beta u}^{(-)} | \psi_{\alpha m}^{(-)} \rangle - 2\pi i \langle \psi_{\beta u}^{(-)} | \delta(E_{\alpha m} - H)\, \bar{V}_\alpha | \phi_{\alpha m} \rangle \quad . \tag{3.47}$$

The scattering states $|\psi_{\alpha m}^{(-)}\rangle$ and $|\psi_{\beta u}^{(-)}\rangle$ are orthogonal for $\alpha \neq \beta$ because they are eigenstates of the same Hamiltonian with different boundary conditions (see Eq. (2.96)). We also have, of course,

$$\langle \psi_{\beta u}^{(-)} | \delta(E_{\alpha m} - H) = \delta(E_{\alpha m} - E_{\beta u}) \langle \psi_{\beta u}^{(-)} | \quad ,$$

and get

$$S_{\beta u,\alpha m}(\vec{q}'_\beta,\vec{q}_\alpha) = \delta(\vec{q}'_\beta-\vec{q}_\alpha)\,\delta_{\beta\alpha}\,\delta_{mu} \qquad (3.48a)$$

$$-2\pi i\,\delta(E_{\alpha m}-E_{\beta u})\langle\psi^{(-)}_{\beta u}|\bar{V}_\alpha|\phi_{\alpha m}\rangle$$

$(\alpha,\ \beta \neq o)$.

Turning to the breakup case we can repeat our derivation in an analogous way and obtain

$$S_{o,\alpha m}(\vec{q}'_\alpha,\vec{p}'_\alpha;\vec{q}_\alpha) = \qquad (3.48b)$$

$$-2\pi i\,\delta\Big(E_{\alpha m}-\frac{q'^2_\alpha}{2M_\alpha}-\frac{p'^2_\alpha}{2\mu_\alpha}\Big)\langle\psi^{(-)}_o|\bar{V}_\alpha|\phi_{\alpha m}\rangle$$

$(\alpha \neq o)$.

For free-free scattering the result is

$$S_{o,o}(\vec{q}'_\alpha,\vec{p}'_\alpha;\vec{q}_\alpha,\vec{p}_\alpha) = \delta(\vec{q}'_\alpha-\vec{q}_\alpha)\,\delta(\vec{p}'_\alpha-\vec{p}_\alpha) \qquad (3.48c)$$

$$-2\pi i\,\delta\Big(\frac{q^2_\alpha}{2M_\alpha}+\frac{p^2_\alpha}{2\mu_\alpha}-\frac{q'^2_\alpha}{2M_\alpha}-\frac{p'^2_\alpha}{2\mu_\alpha}\Big)\langle\psi^{(-)}_o|V|\phi_o\rangle\,.$$

The S-matrix now has the same form as in Eq. (2.51). The part of the scattering process where "nothing happens" is split off. The rest describes transitions of the system by a transition matrix

$$R^{(-)}_{\beta u,\alpha m}(\vec{q}'_\beta,\vec{q}_\alpha) = \langle\psi^{(-)}_{\beta u}|\bar{V}_\alpha|\phi_{\alpha m}\rangle\,, \qquad (3.49a)$$

and by corresponding matrices taken from Eqs. (3.48b and c).

In analogy to Eq. (3.45), we could have written down an equation for $\langle\psi^{(-)}_{\beta u}|$ and would have obtained an expression for $S_{\beta\alpha}$ with another transition matrix

$$R^{(+)}_{\beta u,\alpha m}(\vec{q}'_\beta,\vec{q}_\alpha) = \langle\phi_{\beta u}|\bar{V}_\beta|\psi^{(+)}_{\alpha m}\rangle\,. \qquad (3.49b)$$

Summarizing, we can write

$$S_{\beta u,\alpha m}(\vec{q}'_\beta;\vec{q}_\alpha)=\delta(\vec{q}'_\beta-\vec{q}'_\alpha)\delta_{\beta\alpha}\delta_{mn} \qquad (3.50a)$$

$$-2\pi i\,\delta(E_{\alpha m}-E_{\beta n})R^{(\pm)}_{\beta u,\alpha m}(\vec{q}'_\beta;\vec{q}_\alpha)\,,$$

$$S_{0,\alpha m}(\vec{q}'_\alpha,\vec{p}'_\alpha;\vec{q}_\alpha)= \qquad (3.50b)$$

$$-2\pi i\,\delta(E_{\alpha m}-\frac{q'^2_\alpha}{2M_\alpha}-\frac{p'^2_\alpha}{2\mu_\alpha})R^{(\pm)}_{0,\alpha m}(\vec{q}'_\alpha,\vec{p}'_\alpha;\vec{q}_\alpha)\,,$$

$$S_{0,0}(\vec{q}'_\alpha,\vec{p}'_\alpha;\vec{q}_\alpha,\vec{p}_\alpha)=\delta(\vec{q}'_\alpha-\vec{q}_\alpha)\delta(\vec{p}'_\alpha-\vec{p}_\alpha) \qquad (3.50c)$$

$$-2\pi i\,\delta(\frac{q^2_\alpha}{2M_\alpha}+\frac{p^2_\alpha}{2\mu_\alpha}-\frac{q'^2_\alpha}{2M_\alpha}-\frac{p'^2_\alpha}{2\mu_\alpha})R^{(\pm)}_{0,0}(\vec{q}'_\alpha,\vec{p}'_\alpha;\vec{q}_\alpha,\vec{p}_\alpha)\,.$$

Lovelace has shown [22] that the two transition matrices $R^{(+)}_{\beta\alpha}$ and $R^{(-)}_{\beta\alpha}$ are different only off-shell, and, therefore, the two possibilities (±) in Eq. (3.50) are equivalent.

5. The Faddeev Equations for Transition Operators

We want to consider the transition matrices $R^{(\pm)}_{\beta\alpha}$ as representations of transition operators in the space of channel states $|\phi_\alpha\rangle$. Using relation (3.44), the scattering states in Eq. (3.49) can be expressed by channel states,

$$R^{(+)}_{\beta u,\alpha m}=\langle\phi_{\beta u}|\bar{V}_\beta+\bar{V}_\beta G(E_{\alpha m}+i0)\bar{V}_\alpha|\phi_{\alpha m}\rangle \qquad (3.51a)$$

$$R^{(+)}_{0,\alpha m}=\langle\phi_0|V+V\,G(E_{\alpha m}+i0)\bar{V}_\alpha|\phi_{\alpha m}\rangle$$

$$R^{(+)}_{0,0} = \langle \phi_0 | V + V G\left(\frac{q_\alpha^2}{2M_\alpha} + \frac{p_\alpha^2}{2\mu_\alpha} + i0\right) V | \phi_0 \rangle ,$$

and

$$R^{(-)}_{\beta u,\alpha w} = \langle \phi_{\beta u} | \bar{V}_\alpha + \bar{V}_\beta G(E_{\beta u} + i0) \bar{V}_\alpha | \phi_{\alpha w} \rangle \qquad (3.51b)$$

$$R^{(-)}_{0,\alpha w} = \langle \phi_0 | \bar{V}_\alpha + V G\left(\frac{q_\alpha'^2}{2M_\alpha} + \frac{p_\alpha'^2}{2\mu_\alpha} + i0\right) \bar{V}_\alpha | \phi_{\alpha w} \rangle$$

$$R^{(-)}_{0,0} = \langle \phi_0 | V + V G\left(\frac{q_\alpha'^2}{2M_\alpha} + \frac{p_\alpha'^2}{2\mu_\alpha} + i0\right) V | \phi_0 \rangle$$

As transition operators, we define for $\alpha, \beta = 0,1,2,3$ [1]

$$U^{(+)}_{\beta\alpha}(z) \equiv \bar{V}_\beta + \bar{V}_\beta G(z) \bar{V}_\alpha \qquad (3.52a)$$

and

$$U^{(-)}_{\beta\alpha}(z) \equiv \bar{V}_\alpha + \bar{V}_\beta G(z) \bar{V}_\alpha \; ; \qquad (3.52b)$$

note that for the S-matrix we have to take the limit (in both cases) where z approaches the real energy axis from the upper half plane.

In the S- and R-matrices the range of the indices is the number of different channels (counting the breakup channel as o n e channel), while in case of the transition operator the indices label the different partitions 0,1,2,3. It can happen that there is no bound state at all for a certain subsystem. In this case the corresponding value of α or β does not appear among the channel indices. It does, however, appear as index of the operator matrices in Eq. (3.52). The corresponding operators even contribute to the scattering in other channels by the coupling of all operators via the Faddeev equations (compare Eq. (3.56)).

---

[1] Note that $\bar{V}_0 = V$.

Faddeev equations for the transition operators $U_{\beta\alpha}^{(\pm)}(z)$ are derived in the following way. In Eq. (3.52a), we use the definition (2.78) for $\bar{V}_\alpha$,

$$U_{\beta\alpha}^{(+)} = \bar{V}_\beta + \bar{V}_\beta \sum_{\delta \neq \alpha} G V_\delta \quad , \tag{3.53}$$

and insert the resolvent equation (2.101b),

$$U_{\beta\alpha}^{(+)} = \bar{V}_\beta + \bar{V}_\beta \sum_{\delta \neq \alpha} (g_\delta + G \bar{V}_\delta g_\delta) V_\delta \quad . \tag{3.54}$$

With

$$g_\delta V_\delta = g_0 t_\delta$$

(compare with Eqs. (2.83) and (2.84a)), we get

$$U_{\beta\alpha}^{(+)} = \bar{V}_\beta + \bar{V}_\beta \sum_{\delta \neq \alpha} (1 + G \bar{V}_\delta) g_0 t_\delta \quad . \tag{3.55}$$

With the definition (3.52a), this becomes

$$\begin{aligned} U_{\beta\alpha}^{(+)} &= \bar{V}_\beta + \sum_{\delta \neq \alpha} U_{\beta\delta}^{(+)} g_0 t_\delta \\ &= \bar{V}_\beta + \sum_{\delta=0}^{3} U_{\beta\delta}^{(+)} g_0 \bar{F}_{\delta\alpha} \quad . \end{aligned} \tag{3.56}$$

We thus obtain again a Faddeev-like system of equations. The Faddeev kernel of Eq. (3.10) has been enlarged by one line and one column

$$\bar{F}_{\beta\alpha} = t_\beta (1 - \delta_{\beta\alpha}) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ t_1 & 0 & t_1 & t_1 \\ t_2 & t_2 & 0 & t_2 \\ t_3 & t_3 & t_3 & 0 \end{pmatrix} , \tag{3.57}$$

(α, β = 0,1,2,3 and $t_0 \equiv 0$).

It is not obvious that we get a Faddeev kernel in our equation for $U_{\beta\alpha}$. For instance with $\beta = \alpha$, the following equation can be derived

$$U^{(+)}_{\alpha\alpha} = \bar{V}_\alpha + U^{(+)}_{\alpha\alpha} g_\alpha \bar{V}_\alpha \quad . \tag{3.58}$$

This equation has a Lippmann-Schwinger kernel and, thus, all the disadvantages which have been discussed on pp. 40 - 42. It is obviously important to derive c o u p l e d equations and thus take into account that channel states overlap and that transitions between different channels occur during the time of interaction [9].

Analogously, we get Faddeev equations for the operators $U^{(-)}_{\beta\alpha}$,

$$U^{(-)}_{\beta\alpha} = \bar{V}_\alpha + \sum_{\delta=0}^{3} F_{\delta\beta} g_0 U^{(-)}_{\delta\alpha} \quad . \tag{3.59}$$

Equations (3.56) and (3.59) have been introduced by Lovelace [8]. They have a slight flaw because, in contrast to Eqs. (3.10), (3.29), (3.38), and (3.39), they contain two-body T-matrices a n d potentials. This disadvantage can be overcome by a slight modification of the transition operators [23]. We introduce the operators

$$\begin{aligned} U_{\beta\alpha} &= (1 - \delta_{\beta\alpha}) g_\alpha^{-1} + U^{(+)}_{\beta\alpha} \\ &= (1 - \delta_{\beta\alpha}) g_\beta^{-1} + U^{(-)}_{\beta\alpha} \quad . \end{aligned} \tag{3.60}$$

On-shell, these operators lead to the same S-matrix as the operators $U^{(\pm)}_{\beta\alpha}$, and they obey the equations

$$U_{\beta\alpha} = (1 - \delta_{\beta\alpha}) g_0^{-1} + \sum_{\delta=0}^{3} F_{\delta\beta} g_0 U_{\delta\alpha} \quad , \tag{3.61a}$$

and

$$U_{\beta\alpha} = (1 - \delta_{\beta\alpha}) g_0^{-1} + \sum_{\delta=0}^{3} U_{\beta\delta} g_0 F_{\delta\alpha} \tag{3.61b}$$

(α, β = 0,1,2,3) .

The Faddeev equations (3.56), (3.59), and (3.61) do not couple together a l l transition operators. We show this in case of Eq. (3.61); the other equations can be treated similarly.

Equation (3.61a) disintegrates into different types of equations, namely in

a) a system of equations for rearrangement transition operators (a scattering process in which a bound state is produced which consists of other particles than the original bound state is called rearrangement scattering),

$$\begin{aligned} U_{1\alpha} &= (1-\delta_{1\alpha})\, g_0^{-1} + t_2 g_0 U_{2\alpha} + t_3 g_0 U_{3\alpha} \\ U_{2\alpha} &= (1-\delta_{2\alpha})\, g_0^{-1} + t_1 g_0 U_{1\alpha} + t_3 g_0 U_{3\alpha} \\ U_{3\alpha} &= (1-\delta_{3\alpha})\, g_0^{-1} + t_1 g_0 U_{1\alpha} + t_2 g_0 U_{2\alpha} \end{aligned} \qquad (3.62)$$

$(\alpha = 1,2,3)$,

b) a system of equations for breakup operators,

$$\begin{aligned} U_{10} &= g_0^{-1} + t_2 g_0 U_{20} + t_3 g_0 U_{30} \\ U_{20} &= g_0^{-1} + t_1 g_0 U_{10} + t_3 g_0 U_{30} \\ U_{30} &= g_0^{-1} + t_1 g_0 U_{10} + t_2 g_0 U_{20} \,, \end{aligned} \qquad (3.63)$$

c) equations which relate the breakup operators to the rearrangement operators,

$$\begin{aligned} U_{01} &= g_0^{-1} + t_1 g_0 U_{11} + t_2 g_0 U_{21} + t_3 g_0 U_{31} \\ U_{02} &= g_0^{-1} + t_1 g_0 U_{12} + t_2 g_0 U_{22} + t_3 g_0 U_{32} \\ U_{03} &= g_0^{-1} + t_1 g_0 U_{13} + t_2 g_0 U_{23} + t_3 g_0 U_{33} \,, \end{aligned} \qquad (3.64)$$

d) an equation which relates the operator for free-free transitions to the breakup operators,

$$U_{00} = t_1 g_0 U_{10} + t_2 g_0 U_{20} + t_3 g_0 U_{30} \quad . \tag{3.65}$$

The equations (3.62) are, for $\alpha = 1, 2$ or 3, closed systems of integral equations, and the same is true for system (3.63). The following is remarkable. When the integral equations for rearrangement scattering (3.62) have been solved, there is no longer any need to solve the integral equations for breakup, for, according to Eq. (3.64), the breakup amplitudes then can be obtained from the known amplitudes by a simple integration, i.e., without solving an integral equation. From the breakup amplitudes, one then gets the amplitudes of transitions from the three-particle continuum into the three-particle continuum again by integration (Eq. (3.65)). Hence, the rearrangement amplitudes already contain the full information on three-particle scattering. However, they have to be known completely and not only on the energy shell. In Eqs. (3.64) and (3.65), the amplitudes enter off-shell because energy is not conserved for the intermediate states which are introduced to evaluate the operator products.

There is a formal analogy between Eq. (3.62) and the Lippmann-Schwinger equation [24]. To show this, we rewrite Eq. (3.62)

$$U_{\beta\alpha} = (1-\delta_{\beta\alpha}) g_0^{-1} + \sum_{\delta} (1-\delta_{\beta\delta}) g_0^{-1} g_0 t_\delta g_0 U_{\delta\alpha} \quad , \tag{3.66}$$

and identify the inhomogeneity by the matrix element of a "potential" operator $\mathbf{V}$,

$$(\mathbf{V})_{\beta\alpha} = (1-\delta_{\beta\alpha}) g_0^{-1} \quad , \quad \alpha, \beta = 1, 2, 3 \, . \tag{3.67}$$

We also introduce a "propagator" $\mathbf{G_0}$,

$$(\mathbf{G_0})_{\beta\alpha} = \delta_{\beta\alpha} g_0 t_\beta g_0 \quad , \quad \alpha, \beta = 1, 2, 3 \quad , \tag{3.68}$$

and a "T-matrix" $\mathbf{T}$,

$$(T)_{\beta\alpha} = U_{\beta\alpha} \quad , \quad \alpha, \beta = 1,2,3 \; . \tag{3.69}$$

With these quantities, Eq. (3.66) becomes

$$T = V + VG_0T \quad , \tag{3.70}$$

in complete analogy to Eq. (2.56). The present equation, however, is a matrix equation with respect to partition indices, α, β = 1,2,3 , which expresses the fact that we now have a multichannel problem. At first sight, Eq. (3.70) seems to be no more than a formal pastime. It is even confusing to have t_β associated with G_0 and g_0^{-1} with V . But, when we recall that the transition matrix is obtained by taking matrix elements of $U_{\beta\alpha}$ with channel states, and write, for $z = E_{\alpha m} + i\varepsilon$,

$$\begin{aligned} \langle \phi_{\beta n} | (V)_{\beta\alpha} | \phi_{\alpha m} \rangle &= (1 - \delta_{\beta\alpha}) \langle \phi_{\beta n} | E_{\alpha m} - h_0 | \phi_{\alpha m} \rangle \\ &= (1 - \delta_{\beta\alpha}) \langle \phi_{\beta n} | v_\alpha | \phi_{\alpha m} \rangle \; , \end{aligned} \tag{3.71}$$

we see the connection between V and an interaction. We shall use Eq. (3.70) later to formulate the three-particle problem as an effective two-particle problem, namely, as a problem of interaction of a particle with a bound pair of particles. It will become clear, then, why the interaction of the subsystem has to be present in the propagator G_0 .

The formulation (3.70) is of great heuristic value: algebraic manipulations can be performed in analogy to the two-particle problem. We can ask, for instance, for the matrix operator which corresponds to the two-particle resolvent. In analogy to Eq. (2.46), it must have the form

$$G = G_0 + G_0 T G_0 \quad . \tag{3.72}$$

Using the definitions (3.68) and (3.69), we get

$$(G)_{\rho\alpha} = g_0 (\delta_{\rho\alpha} v_\alpha + v_\beta G v_\alpha) g_0 \quad . \tag{3.73}$$

In analogy to Eq. (2.22), there exists a "resolvent" equation

$$G = G_0 + G_0 V G \,. \tag{3.74}$$

Inserting Eq. (3.73) and defining the abbreviation

$$M_{\beta\alpha} = \delta_{\beta\alpha} V_\alpha + V_\beta G V_\alpha \,, \tag{3.75}$$

we get

$$M_{\beta\alpha} = \delta_{\beta\alpha} t_\alpha + t_\beta g_0 \sum_{\gamma \neq \beta} M_{\gamma\alpha} \,. \tag{3.76}$$

This equation has been used by Faddeev to study the resolvent G [25]. In terms of $M_{\beta\alpha}$, the resolvent G is

$$G = g_0 + g_0 \sum_{\beta,\alpha} M_{\beta\alpha} g_0 \,. \tag{3.77}$$

6. The Unitarity Relation

A further application of version (3.70) of the Faddeev equation (3.62) is the derivation of an unitarity relation for the transition operators $U_{\beta\alpha}$ [24]. Proceeding similarly as in Chapter 2, section 1.7, the influence of the various channels is distinctly taken into account.

From Eq. (3.70), the following analogue of Eq. (2.61) is easily derived,

$$T^{-1}(z) = V^{-1}(z) - G_0(z) \,. \tag{3.78}$$

The inverse of the "potential" V is, for $\alpha, \beta = 1,2,3$,

$$\left(V^{-1}(z)\right)_{\beta\alpha} = (1/2 - \delta_{\beta\alpha})\, g_0(z) \,, \tag{3.79}$$

as can be verified by multiplication with the definition (3.67). The inverse of the potential is energy-dependent in the present case. For the discontinuity of T along the real energy axis, we

therefore get, in contrast to Eq. (2.63),

$$T(E+i\epsilon) - T(E-i\epsilon) = \tag{3.80}$$

$$-T(E+i\epsilon)\left\{V^{-1}(E+i\epsilon) - V^{-1}(E-i\epsilon) - G_0(E+i\epsilon) + G_0(E-i\epsilon)\right\} T(E-i\epsilon) \ .$$

The expression in curly brackets becomes by means of Eqs. (3.68) and (3.79)

$$(1/2 - \delta_{\beta\alpha})\Delta q_0 - \delta_{\beta\alpha}\Delta(q_0 t_\alpha q_0) \tag{3.81}$$

$$= 1/2\,\Delta q_0 - \delta_{\beta\alpha}\Delta q_\alpha \quad , \quad \alpha,\beta = 1,2,3 \ ,$$

where Δ marks the discontinuity, and, in the second line, Eq. (2.46) has been used in three-particle space. The discontinuity of g_γ becomes (compare with Eqs. (2.64) and (2.65))

$$\Delta q_\gamma = \lim_{\epsilon \to 0} \left(q_\gamma(E+i\epsilon) - q_\gamma(E-i\epsilon)\right) = -2\pi i\,\delta(E-h_\gamma) \ , \tag{3.82}$$

$\gamma = 0,1,2,3$.

The discontinuity Δg_γ with $\gamma \neq 0$ contains contributions from bound states of the subsystems and from the three-particle continuum as well. They can be separated in the following way

$$\delta(E-h_\gamma) = \tag{3.83}$$

$$\sum_n \Delta_{\gamma n}(E) + \left(1 + q_0(E+i0)\,t_\gamma(E+i0)\right)\Delta_0(E)\left(1 + t_\gamma(E-i0)\,q_0(E-i0)\right),$$

where

$$\Delta_{\gamma n}(E) = |\vec{q}_\gamma\rangle|\psi_{\gamma n}\rangle\,\delta\left(E - \frac{q_\gamma^2}{2M_\gamma} - E^B_{\gamma n}\right)\langle\psi_{\gamma n}|\langle\vec{q}_\gamma|$$

and

$$\Delta_0(E) = |\vec{q}_\gamma\rangle|\vec{p}_\gamma\rangle\,\delta\left(E - \frac{q_\gamma^2}{2M_\gamma} - \frac{p_\gamma^2}{2\mu_\gamma}\right)\langle\vec{p}_\gamma|\langle\vec{q}_\gamma| \ .$$

This splitting is verified by operating with $\delta(E - h_\gamma)$ on the representation of the unit matrix

$$1 = \sum_n \int d\vec{q}_\gamma \, |\psi_{\gamma n}\rangle |\vec{q}_\gamma\rangle \langle \vec{q}_\gamma| \langle \psi_{\gamma n}| + \int d\vec{p}_\gamma \int d\vec{q}_\gamma \, |\vec{p}_\gamma^{\,(+)}\rangle |\vec{q}_\gamma\rangle \langle \vec{q}_\gamma| \langle \vec{p}_\gamma|^{(+)} \,, \tag{3.84}$$

using

$$\begin{aligned} |\vec{p}_\gamma^{\,(+)}\rangle |\vec{q}_\gamma\rangle &= \lim_{\epsilon \to 0} i\epsilon \, g_\gamma \left(\frac{p_\gamma^2}{2\mu_\gamma} + \frac{q_\gamma^2}{2M_\gamma} + i\epsilon\right) |\vec{p}_\gamma\rangle |\vec{q}_\gamma\rangle \\ &= \left[1 + g_0\left(\frac{p_\gamma^2}{2\mu_\gamma} + \frac{q_\gamma^2}{2M_\gamma} + i0\right) t_\gamma \left(\frac{p_\gamma^2}{2\mu_\gamma} + \frac{q_\gamma^2}{2M_\gamma} + i0\right)\right] |\vec{p}_\gamma\rangle |\vec{q}_\gamma\rangle \end{aligned} \tag{3.85}$$

(compare with Eqs. (2.17) and (2.46)).

Inserting Eqs. (3.82 - 3.83) into Eq. (3.80) and returning to the explicit notation, we obtain for $\alpha, \beta = 1,2,3$

$$\begin{aligned} &U_{\beta\alpha}(E+i0) - U_{\beta\alpha}(E-i0) = \\ &-2\pi i \Bigg\{ \sum_{\gamma=1}^{3} \sum_n U_{\beta\gamma}(E+i0) \, \Delta_{\gamma n}(E) \, U_{\gamma\alpha}(E-i0) \\ &+ \sum_{\gamma=1}^{3} U_{\beta\gamma}(E+i0) \left(1 + g_0(E+i0) t_\gamma(E+i0)\right) \Delta_0(E) \left(1 + t_\gamma(E-i0) g_0(E-i0)\right) U_{\gamma\alpha}(E-i0) \\ &- \sum_{\gamma,\delta=1}^{3} U_{\beta\gamma}(E+i0) \, \tfrac{1}{2} \, \Delta_0(E) \, U_{\delta\alpha}(E-i0) \Bigg\} \,. \end{aligned} \tag{3.86}$$

Using the relations

$$\begin{aligned} (1 + t_\gamma g_0) U_{\gamma\alpha} &= U_{0\alpha} - \delta_{\gamma\alpha} g_0^{-1} \quad , \alpha \neq 0 \,, \\ U_{\beta\gamma}(1 + g_0 t_\gamma) &= U_{\beta 0} - \delta_{\beta\gamma} g_0^{-1} \quad , \beta \neq 0 \,, \\ \sum_{\delta=1}^{3} U_{\delta\alpha} &= 2 U_{0\alpha} \quad , \alpha \neq 0 \,, \end{aligned} \tag{3.87}$$

which are easily verified by help of Eq. (3.61), Eq. (3.86) reduces to

$$U_{\beta\alpha}(E+i0) - U_{\beta\alpha}(E-i0) =$$

$$-2\pi i\Big\{\sum_{\gamma=1}^{3}\sum_{n} U_{\beta\gamma}(E+i0)\,\Delta_{\gamma n}(E)\,U_{\gamma\alpha}(E-i0) \qquad (3.88)$$

$$+\; U_{\beta 0}(E+i0)\,\Delta_{0}(E)\,U_{0\alpha}(E-i0)\Big\}\,, \quad \alpha,\beta = 1,2,3\,.$$

This is the unitarity relation for the three-particle transition operators $U_{\beta\alpha}$. The optical theorem is derived by specializing to the forward direction and to $\beta = \alpha$. Using the projection properties of $\Delta_{\gamma n}$, we get,

$$\langle\phi_{\alpha m}|U_{\alpha\alpha}(E+i0) - U_{\alpha\alpha}(E-i0)|\phi_{\alpha m}\rangle = \qquad (3.89)$$

$$-2\pi i\Big\{\sum_{\gamma,n}\int d\vec{q}_\gamma \langle\phi_{\alpha m}|U^{(E+i0)}_{\alpha\gamma}|\phi_{\gamma n}\rangle\,\delta\Big(E-\frac{q_\gamma^2}{2M_\gamma}-E^B_{\gamma n}\Big)\langle\phi_{\gamma n}|U_{\gamma\alpha}(E-i0)|\phi_{\alpha m}\rangle$$

$$+\int d\vec{q}_1\, d\vec{p}_1 \langle\phi_{\alpha m}|U^{(E+i0)}_{\alpha 0}|\vec{q}_1,\vec{p}_1\rangle\,\delta\Big(E-\frac{q_1^2}{2M_1}-\frac{p_1^2}{2\mu_1}\Big)\langle\vec{q}_1,\vec{p}_1|U^{(E-i0)}_{0\alpha}|\phi_{\alpha m}\rangle\,.$$

Because of

$$\langle\phi_{\gamma n}|U_{\gamma\alpha}(E-i0)|\phi_{\alpha m}\rangle = \langle\phi_{\alpha m}|U_{\alpha\gamma}(E+i0)|\phi_{\gamma n}\rangle^{*}\,, \qquad (3.90)$$

(compare with Eq. (3.52)), Eq. (3.89) becomes

$$\mathrm{Im}\,\langle\phi_{\alpha m}|U_{\alpha\alpha}(E+i0)|\phi_{\alpha m}\rangle =$$

$$=-\pi\Big\{\sum_{\gamma,n}\int d\vec{q}_\gamma\,\delta\Big(E-\frac{q_\gamma^2}{2M_\gamma}-E^B_{\gamma n}\Big)\big|\langle\phi_{\alpha m}|U_{\alpha\gamma}(E+i0)|\phi_{\gamma n}\rangle\big|^2 \qquad (3.91)$$

$$+\int d\vec{q}_1\, d\vec{p}_1\,\delta\Big(E-\frac{q_1^2}{2M_1}-\frac{p_1^2}{2\mu_1}\Big)\big|\langle\phi_{\alpha m}|U_{\alpha 0}(E+i0)|\vec{q}_1,\vec{p}_1\rangle\big|^2\Big\}\,.$$

This is the optical theorem for three-particle scattering. It relates the total cross section (i.e., the sum of elastic, rearrangement, and breakup cross section) to the amplitude of elastic scattering in forward direction

$$\mathrm{Im}\,\langle\phi_{\alpha m}|U_{\alpha\alpha}(E+i0)|\phi_{\alpha m}\rangle = -\frac{q_\alpha}{16\pi^3 M_\alpha}\Big\{\sum_{\gamma=1}^{3}\sum_{n}\sigma_{\gamma n} + \sigma_{\text{breakup}}\Big\}\,. \qquad (3.92)$$

4. Solution Methods for the Faddeev Equations

In this chapter, we want to investigate how the Faddeev equations can be solved in practice. We first move from abstract operator equations to integral equations. Then we will study some methods of the theory of integral equations and see whether they can be applied to Faddeev equations.

1. Partial Wave Decomposition of the Faddeev Equations

From the Faddeev equations for the operators T_i, G_i, $U_{\beta\alpha}$, $U_{0\alpha}$ or the state vectors $|\psi_{\alpha n}\rangle_i$, integral equations are obtained by choosing a representation space. In momentum space $|\vec{p}_\alpha, \vec{q}_\alpha\rangle$, the integral equations become six-dimensional. Since the total angular momentum L and its z-component M are conserved, it is sensible to choose a representation space whose vectors are eigenstates of L and M. In this way, the integral equations become four-dimensional. This is still too much for numerical calculations. Although there are no more conserved quantities, the dimension can be further reduced at the cost of getting more coupled equations.

For this purpose, we use a space of states which are characterized by the total angular momentum L, its z-component M, the angular momentum l_α of subsystem α, the angular momentum λ_α of particle α, and by the absolute values of the momenta p_α, q_α [26,27]. There are three spaces of this kind, depending on which subsystem is preferred,

$$|\psi\rangle = \begin{cases} |\mathrm{I}\rangle = |L M \ell_1 \lambda_1 p_1 q_1\rangle \\ |\mathrm{II}\rangle = |L M \ell_2 \lambda_2 p_2 q_2\rangle \\ |\mathrm{III}\rangle = |L M \ell_3 \lambda_3 p_3 q_3\rangle \end{cases} . \qquad (4.1)$$

At first sight, the preference of a certain subsystem seems to be inappropriate because all three particles should be treated on the same footing [28]. But, since our operators t_α, $U_{\beta\alpha}$ prefer certain subsystems, anyway, this can even be an advantage. Now, our integral equations are only two-dimensional, since there are only two continuous variables p_α, q_α. But the number of coupled equations becomes infinite because there is an

infinite number of ways for a given angular momentum L to decompose into angular momenta l_α and λ_α .

Nevertheless, it makes sense to proceed in this way. For short-ranged potentials, interaction will be effective only for a small number of angular momenta, and, therefore, the infinite system of equations can be approximated to high accuracy by a finite one. We now are going to perform the partial wave decomposition in the case of the Faddeev equations (3.61).
First, we have to find the transformation between the states (4.1) and the momentum states $|\vec{p}_\alpha,\vec{q}_\alpha\rangle$. A basis which diagonalizes energies, angular momenta, and z-components of angular momenta of individual Jacobi coordinates is obtained by the unitary transformation

$$|q_\alpha \lambda_\alpha \mu_\alpha)|p_\alpha l_\alpha m_\alpha\rangle = \int d\hat{q}_\alpha\, d\hat{p}_\alpha\, Y_{\lambda_\alpha \mu_\alpha}(\hat{q}_\alpha)\, Y_{l_\alpha m_\alpha}(\hat{p}_\alpha)\, |\vec{p}_\alpha, \vec{q}_\alpha\rangle \quad . \tag{4.2}$$

The functions $Y_{\lambda\mu}$, Y_{lm} are the well-known spherical harmonics. The integration ranges over the directions of the vectors $\vec{q}_\alpha$, $\vec{p}_\alpha$. The quantum numbers μ_α , m_α denote the z-components of angular momenta λ_α , l_α . A second unitary transformation leads to the basis given by Eq. (4.1) with defined total angular momentum,

$$|LM l_\alpha \lambda_\alpha p_\alpha q_\alpha\rangle = \sum_{\mu_\alpha, m_\alpha} \langle \lambda_\alpha l_\alpha \mu_\alpha m_\alpha | LM\rangle\, |q_\alpha \lambda_\alpha \mu_\alpha, p_\alpha l_\alpha m_\alpha\rangle \quad . \tag{4.3}$$

The matrix elements $\langle \lambda l \mu m | LM\rangle$ are the well-known Clebsch-Gordan coefficients.
It follows from the normalization of the momentum states $|\vec{p}_\alpha,\vec{q}_\alpha\rangle$ that

$$\langle I | I'\rangle = \frac{\delta(q_1-q_1')}{q_1^2}\,\frac{\delta(p_1-p_1')}{p_1^2}\,\delta_{LL'}\,\delta_{MM'}\,\delta_{\lambda_1\lambda_1'}\,\delta_{l_1 l_1'} \quad . \tag{4.4}$$

In the new representation, the two-body T-matrix (2.86) has the form (for γ = I ; similarly for γ = II,III)

$$\langle I | t_1(z) | I'\rangle = \tag{4.5}$$

$$\frac{\delta(q_1-q_1')}{q_1^2}\,\delta_{LL'}\,\delta_{MM'}\,\delta_{l_1 l_1'}\,\delta_{\lambda_1\lambda_1'}\,\hat{t}_{1,l_1}\left(z-\frac{q_1^2}{2M_{1,1}}; p_1, p_1'\right) .$$

The quantity $\hat{t}_{1,l_1}$ is the contribution of the l_1^{th} partial wave to the T-matrix $\hat{t}_1$,

$$\langle \vec{p}_1 | \hat{t}_1 (z - \frac{q_1^2}{2M_1}) | \vec{p}_1' \rangle = \sum_{\ell_1=0}^{\infty} (2\ell_1+1) P_{\ell_1}(\hat{p}_1 \cdot \hat{p}_1') \hat{t}_{1,\ell_1}(z - \frac{q_1^2}{2M_1}; p_1, p_1') \quad . \tag{4.6}$$

The free resolvent $g_0(z)$, which also appears in the Faddeev equations, becomes (for γ = I ; similarly for γ = II,III)

$$\langle I | g_0(z) | I' \rangle = \langle I | I' \rangle (z - \frac{q_1^2}{2M_1} - \frac{p_1^2}{2\mu_1})^{-1} \quad . \tag{4.7}$$

A representation of operators like $U_{\beta\alpha}$, t_γ has a simple form only when the representation space prefers the same subsystem as the operator, as in $\langle \beta | U_{\beta\alpha} | \alpha \rangle$, $\langle \gamma | t_\gamma | \gamma' \rangle$. The Faddeev equations, on the other hand, couple all different subsystems. We have to use, therefore, all three spaces (4.1) and to switch from one to the other. For the switching, we need the overlap $\langle \beta' | \alpha \rangle$. To calculate this overlap is rather complicated because the calculation implies an 8-fold integration $\int d\hat{q}_\alpha \, d\hat{p}_\alpha \, d\hat{q}_\beta' \, d\hat{p}_\beta'$ and a 4-fold summation $\sum(\mu_\alpha, m_\alpha, \mu_\beta, m_\beta)$ over a product of Clebsch-Gordan coefficients and spherical harmonics. The result, which we quote from Balian and Brezin [27], is accordingly complicated,

$$\langle \beta' | \alpha \rangle = f(w_1, w_2, w_3) \, \delta_{L'L} \, \delta_{M'M} \cdot \tag{4.8}$$

$$\cdot \frac{\delta(p_\beta'^2/2\mu_\beta + q_\beta'^2/2m_\beta - p_\alpha^2/2\mu_\alpha - q_\alpha^2/2m_\alpha)}{p_\beta' q_\beta' p_\alpha q_\alpha} A_{\beta'\alpha}\left(\frac{p_\alpha}{q_\beta'}, \frac{p_\beta'}{q_\beta'}, L, \ell_\beta, \lambda_\beta, \ell_\alpha, \lambda_\alpha\right) .$$

The angular momenta of one Jacobi coordinate system do not uniquely determine the mixture of angular momenta in another Jacobi coordinate system. One needs, in addition, the absolute values of the linear momenta. This dependence is essentially expressed by the function $A_{\beta'\alpha}$ which contains that part of the above-mentioned summation which cannot be performed explicitly in the general case. We may assume, however, the function $A_{\beta'\alpha}$

to be known. In many practical applications (see Chapter 6, section 1, and Chapter 7, section 3), interaction is assumed to be effective only for relative orbital angular momentum zero, which greatly simplifies matters.

We have now all the tools needed to write down the Faddeev equations in the new representation. We first take matrix elements of Eq. (3.61a) according to the "natural" representation of $U_{\beta\alpha}$

$$\langle\beta|U_{\beta\alpha}|\alpha'\rangle = \tag{4.9}$$

$$(1-\delta_{\beta\alpha})\langle\beta|\alpha'\rangle\left(z-\frac{p_\beta^2}{2\mu_\beta}-\frac{q_\beta^2}{2M_\beta}\right)+\sum_{\gamma\neq\beta}\langle\beta|t_\gamma q_0 U_{\gamma\alpha}|\alpha'\rangle \quad .$$

The operator product on the right-hand side is evaluated by inserting the complete set of states (γ = I,II or III)

$$\sum_{(\gamma)}\int|\gamma\rangle\langle\gamma| = \mathbb{1} \quad . \tag{4.10}$$

(Note that γ as a state index denotes all variables which appear in Eq. (4.1).) Using Eq. (4.7), we get

$$\langle\beta|t_\gamma q_0 U_{\gamma\alpha}|\alpha'\rangle = \sum_{(\gamma)}\int\frac{\langle\beta|t_\gamma|\gamma\rangle\langle\gamma|U_{\gamma\alpha}|\alpha'\rangle}{z-\frac{p_\gamma^2}{2\mu_\gamma}-\frac{q_\gamma^2}{2M_\gamma}} \quad . \tag{4.11}$$

In order to get the transition matrix t_γ in its natural representation, we insert expression (4.10) once more,

$$\langle\beta|t_\gamma = \sum_{(\gamma')}\int\langle\beta|\gamma'\rangle\langle\gamma'|t_\gamma \quad . \tag{4.12}$$

The Faddeev equations finally become

$$\langle\beta|U_{\beta\alpha}|\alpha'\rangle = (1-\delta_{\beta\alpha})\langle\beta|\alpha'\rangle\left(z-\frac{p_\beta^2}{2\mu_\beta}-\frac{q_\beta^2}{2M_\beta}\right)$$

$$+\sum_{\gamma\neq\beta}\sum_{(\gamma')}\int\sum_{(\gamma)}\int\frac{\langle\beta|\gamma'\rangle\langle\gamma'|t_\gamma|\gamma\rangle\langle\gamma|U_{\gamma\alpha}|\alpha'\rangle}{z-\frac{p_\gamma^2}{2\mu_\gamma}-\frac{q_\gamma^2}{2M_\gamma}} \quad . \tag{4.13}$$

Two of the four integrations can be carried out by the δ-functions which are contained in the transition matrix (4.5) and in the overlap (4.8). For a given total angular momentum, the overlap $\langle\beta|\gamma'\rangle$ couples infinitely many angular momenta of the subsystems. Equation (4.13) thus becomes an infinite system of coupled integral equations in two dimensions for the matrix elements $\langle\gamma|U_{\gamma\alpha}|\alpha'\rangle$. The energy z and the state α' enter as parameters. The limit $z \to E + i0$ serves, essentially, as a prescription of how to choose the path of integration in the neighborhood of singularities.

The infinite system of equations (4.13) becomes finite when it is assumed that only a finite number of partial waves contribute in expansion (4.6), which is justified for short-ranged potentials. The number of equations depends upon the total angular momentum L and upon the maximum angular momentum l_0 , for which interaction is effective. In the literature [27,29] there is a slight discrepancy about this number, which may serve as an indication of how complicated angular momentum coupling is in the three-particle system.

Up to now, we were concerned with distinguishable particles without spin. The inclusion of spin does not bring any major difficulties, in principle. Only the angular momentum coupling becomes more difficult, and the number of equations is increased. The Pauli principle is taken into account by using symmetric or antisymmetric states only, for the representation of operators [30,31]. For identical particles, the Faddeev equations are less complicated because identical particles mean identical channels, which reduces the number of coupled equations.

It should be mentioned that the Faddeev equations can also be transformed into a set of integro-differential equations in configuration space [32]. Also in this representation, they have been solved successfully in the three-nucleon bound state problem [33]. In most applications, however, a momentum representation, as in Eq. (4.13), is used.

2. Some Concepts of the Theory of Integral Equations

The Faddeev equations in momentum representation are Fredholm integral equations of the second kind,

$$f = h + Kf \quad . \tag{4.14a}$$

They can be solved, formally, by introduction of a resolvent [1]

$$R = (1 - K)^{-1} \rightsquigarrow \quad f = Rh \quad .$$

To discuss the methods of solution we consider, for simplicity, a one-dimensional equation of this type,

$$f(x) = h(x) + \int_a^b K(x,y) f(y)\, dy \quad . \tag{4.14b}$$

A generalization to Faddeev equations, which are systems of two-dimensional integral equations, can be made without difficulty. A more detailed discussion of the methods which are mentioned in the following can be found in two papers of Weinberg [7,34] and textbooks on integral equations [35].

a) Solution by Iteration

When Kf is small compared to h, the solution of Eq. (4.14a) is, in zeroth order,

$$f^{(0)} = h \quad .$$

It becomes, by continued iteration

$$f = \sum_{i=0}^{\infty} K^i h \quad . \tag{4.15}$$

The resolvent is

$$R = \sum_{i=0}^{\infty} K^i \quad . \tag{4.16}$$

---

[1] The resolvent defined in scattering theory differs from this resolvent by a factor g_0 .

This so-called Neumann series converges if and (for arbitrary h) only if the eigenvalues η_ν of the kernel K,

$$K\psi_\nu = \eta_\nu \psi_\nu \quad , \tag{4.17a}$$

all have absolute values smaller than one,

$$|\eta_\nu| < 1 \quad . \tag{4.17b}$$

b) Degenerate Kernel

When the kernel has the form

$$K(x,y) = \bar{\varphi}(x)\,\varphi(y) \quad , \tag{4.18}$$

the integral equation (4.14b) can be solved easily because the x-dependence of the integrand can be put in front of the integral which then becomes a constant c,

$$f(x) = h(x) + c\,\bar{\varphi}(x) \quad . \tag{4.19}$$

For the constant, we have

$$c = \int_a^b \varphi(y) f(y)\,dy = \int_a^b \varphi(y) h(y)\,dy + c \int_a^b \varphi(y)\,\bar{\varphi}(y)\,dy \quad ,$$

and get

$$C = \frac{\int_a^b \varphi(y) h(y)\,dy}{1 - \int_a^b \varphi(y)\,\bar{\varphi}(y)\,dy} \quad . \tag{4.20}$$

c) Expansion of a Compact Kernel into Degenerate Kernels

The simple method of solution in case (b) suggests the expansion of a non-degenerate kernel into degenerate kernels. Indeed, it is possible for every compact kernel to find a series of degenerate kernels which approximates it in such a way that the norm

of the difference becomes arbitrarily small. For a complete biorthogonal system $\{\bar{\varphi}_\mu \otimes \varphi_\nu\}$, $\int \bar{\varphi}_\mu(x)\varphi_\nu^*(x)dx = \delta_{\mu\nu}$, we have,

$$K(x,y) = \sum_{\mu,\nu=1}^{\infty} a_{\mu\nu}\, \bar{\varphi}_\mu(x)\, \varphi_\nu^*(y) \quad , \tag{4.21}$$

with

$$a_{\mu\nu} = \int_a^b \int_a^b K(x,y)\, \varphi_\mu^*(x)\, \bar{\varphi}_\nu(y)\, dx\, dy \quad . \tag{4.22}$$

When Eq. (4.21) is inserted into the integral equation (4.14b), we get

$$f(x) = h(x) + \sum_{\mu,\nu=1}^{\infty} a_{\mu\nu}\, c_\nu\, \bar{\varphi}_\mu(x) \quad , \tag{4.23}$$

with an infinite number of constants c_ν . The constants are determined by the equation

$$c_\kappa = \int_a^b \varphi_\kappa^*(y) f(y)\, dy = \int_a^b \varphi_\kappa^*(y) h(y)\, dy + \sum_{\mu,\nu=1}^{\infty} a_{\mu\nu}\, c_\nu \int_a^b \varphi_\kappa^*(y)\, \bar{\varphi}_\mu(y)\, dy \quad , \tag{4.24}$$

which is a set of linear equations,

$$\sum_{\nu=1}^{\infty} (\delta_{\kappa\nu} - a_{\kappa\nu})\, c_\nu = \int_a^b \varphi_\kappa^*(y) h(y)\, dy \quad . \tag{4.25}$$

For practical calculations, the expansion (4.21) has to be truncated after a finite number of terms,

$$K(x,y) = \sum_{\mu,\nu=1}^{N} a_{\mu\nu}\, \bar{\varphi}_\mu(x)\, \varphi_\nu^*(y) + K_N(x,y) \quad . \tag{4.26}$$

The rest $K_N(x,y)$ is either ignored or approximately taken into account by the method of Schmidt.

d) <u>The Schmidt Method</u> [36]

With the expansion (4.26), the integral equation (4.14b) becomes,

$$f(x) = h(x) + \sum_{\mu,\nu=1}^{N} a_{\mu\nu} c_\nu \bar{\varphi}_\mu(x) + \int_a^b K_N(x,y) f(y)\, dy \quad . \tag{4.27}$$

Only a finite number of terms $a_{\mu\nu}\bar{\varphi}_\mu \varphi_\nu^*$ has to be split off from the original kernel in order to achieve convergence of the Neumann series for the rest $K_N(x,y)$. This is so because, for compact kernels, there is only a finite number of eigenvalues, at most, which do not fulfill condition (4.17b).
The resolvent R_N of the rest kernel $K_N(x,y)$, therefore, can be calculated by

$$R_N = \sum_{i=0}^{\infty} K_N^i \quad . \tag{4.28}$$

With the resolvent R_N, Eq. (4.27) can be brought to a form which is similar to Eq. (4.23),

$$\begin{aligned} f(x) &= h'(x) + \sum_{\mu,\nu=1}^{N} a_{\mu\nu} c_\nu \bar{\varphi}'_\mu(x) \quad , \\ h'(x) &= \int_a^b R_N(x,y) h(y)\, dy \quad , \\ \bar{\varphi}'_\mu(x) &= \int_a^b R_N(x,y) \bar{\varphi}_\mu(y)\, dy \quad . \end{aligned} \tag{4.29}$$

As has been shown, (Eqs. (4.23 - 4.25)), such an equation can be solved by algebraic methods.

e) Padé Approximation

A non-convergent Neumann series becomes convergent when the kernel is multiplied by a complex parameter λ which fulfills the condition

$$|\lambda| < |\eta_{Max}^{-1}| < 1 \quad . \tag{4.30}$$

The series defines a function

$$f(\lambda) = \sum_{i=0}^{\infty} (\lambda K)^i h = h + \lambda K f(\lambda) \quad , \tag{4.31}$$

which is analytic in the region given by condition (4.30). Outside of this region, the function $f(\lambda)$ is still defined by the coefficients $K^i h$, but it can no longer be calculated by its Taylor series (4.31) since it is meromorphic with poles at $\lambda_i = \eta_i^{-1}$. The solution of the integral equation (4.14)

$$f = f(1) \quad , \tag{4.32}$$

can be calculated, however, by an ansatz which is a rational function of λ . This method, named after the French mathematician Padé [37,38], will be studied in more detail in Chapter 7.

Closely related to the Padé method is the method of moments [39]. The (eventually non-convergent) iteration of Eq. (4.14) generates a system of functions

$$f_\nu = \sum_{i=0}^{\nu} K^i h \quad , \tag{4.33}$$

from which an approximate solution

$$f^N = \sum_{\nu=0}^{N} a_\nu f_\nu \quad , \tag{4.34}$$

is constructed. It is then demanded that the approximate solution satisfies the integral equation (4.14) in the space spanned by the functions f_ν ,

$$\sum_{\nu=0}^{N} a_\nu (f_\mu, f_\nu) = (f_\mu, h) + \sum_{\nu=0}^{N} a_\nu (f_\mu, K f_\nu) \quad . \tag{4.35}$$

This is a set of linear equations which determines the coefficients a_ν . The set of functions f_ν does not have to be complete. The iteration generates just those functions which are relevant. Also, it is unnecessary to start the iteration with the inhomogeneity h. As a starting point, one can choose the solution of a related problem, for instance, or an approximate solution which has been obtained by another method.

f) Numerical Integration

Finally we want to mention a method which seems to be the most obvious one. Using an integration rule with mesh points y_j and weights w_j , Eq. (4.14b) becomes

$$f(x) = h(x) + \sum_{j=1}^{N} w_j K(x, y_j) f(y_j) + \text{rest} \quad . \tag{4.36}$$

Ignoring the rest and putting $x = y_i$, we get the set of linear equations

$$\sum_{j=1}^{N} \left(\delta_{ij} - w_j K(y_i, y_j) \right) f(y_j) = h(y_i) \quad , \tag{4.37}$$

which determines f(x) at the mesh points. The full function f(x) is then given by Eq. (4.36).

3. Application to the Faddeev Equations

We have to investigate now which one of the above-listed methods can be used to solve the Faddeev equations.

Method (a) can be ruled out, for instance, when the three-particle system has a bound state. In this case, the homogeneous equation (4.17a) has a solution at the energy of the bound state with eigenvalue $\eta = 1$. For energies above the binding energy, we even have $|\eta| > 1$, which means that we cannot expect the Neumann series to converge, (see Eq. (4.17b)). We obtain convergence only at very high energies (except for hard-core potentials), since the kernel then becomes less and less effective [40].

Method (b) also can be ruled out. As we see from Eqs. (4.5) and (4.8), none of the matrix elements $\langle \gamma' | t_\gamma | \gamma \rangle$ or $\langle \beta | \gamma' \rangle$ factorizes

$$\langle \gamma' | t_\gamma | \gamma \rangle \neq h(\gamma') \, i(\gamma) \quad , \tag{4.38a}$$

$$\langle \beta | \gamma' \rangle \neq j(\beta) \, k(\gamma') \quad , \tag{4.38b}$$

and, therefore, the β-dependence in Eq. (4.13) cannot be put in front of the integral.

A direct application of methods (c) and (d) is not practicable because one cannot find a series of degenerate kernels which approximates the Faddeev kernel fast enough. The reason is that the Faddeev kernel is four-dimensional and has various singularities arising from the operators t_γ and g_o .

Method (e) can be applied directly (see Chapter 7) because the solutions of the Faddeev equations can be approximated to arbitrary accuracy by rational functions (compare with statement (c) on page 48).

Method (f) has been applied directly to the Faddeev equations only once. The reason is that the capacity of computers is exceeded rather fast (see Chapter 6). When in each dimension an integration mesh of 30 points is used, we get a two-dimensional mesh of N = 900 points. The matrix which has to be inverted, according to Eq. (4.37), is a N x N = 900 x 900 matrix in the simplest case of identical, spinless particles which interact only for $l = o$.

Successful calculations have been performed in the early days of three-particle theory by a combination of methods (c) and (f), and later by a combination of (d) and (f). In these calculations, the method (c), or (d), is not applied to the whole Faddeev equations but only to the equations for the subsystems. The kernels of these equations are much easier to approximate. Also, it is easier to study the quality of an approximation in a subsystem than in the whole three-particle system [8]. In this way, however, the Faddeev equations do not reduce to an algebraic equation, as Eq. (4.25). They remain integral equations but only one-dimensional ones, which can be solved by method (f).

The combination of methods (c) and (f) corresponds to an introduction of separable potentials [41] which will be discussed in the next chapter.

5. Separable Potentials

1. Separable Potentials in the Two-Particle Problem

Let us look again at Eq. (2.56) for the two-particle T-matrix in two-particle space,

$$t(z) = V + V g_0(z) t(z) \quad ,$$

or, explicitly,

$$\langle \vec{p}' | t(z) | \vec{p} \rangle = \langle \vec{p}' | V | \vec{p} \rangle + \int d\vec{p}'' \frac{\langle \vec{p}' | V | \vec{p}'' \rangle \langle \vec{p}'' | t(z) | \vec{p} \rangle}{z - \frac{p''^2}{2\mu}} \tag{5.1}$$

The kernel of this integral equation,

$$K(\vec{p}', \vec{p}'') = \frac{\langle \vec{p}' | V | \vec{p}'' \rangle}{z - p''^2/2\mu} \quad , \tag{5.2}$$

degenerates when the potential has the form

$$\langle \vec{p}' | V | \vec{p}'' \rangle = \lambda \chi(\vec{p}') \chi^*(\vec{p}'') \quad . \tag{5.3}$$

Such a potential is called separable. With it, the integral equation (5.1) is as easy to solve as Eq. (4.19). Before we show this, we introduce an operator notation for the separable potential,

$$V^S = \lambda |\chi\rangle\langle\chi| \quad . \tag{5.4}$$

The separable potential, hence, is a projection operator. In configuration space, it has the form

$$\begin{aligned} \langle \vec{r} | V^S | \vec{r}' \rangle &= \lambda \langle \vec{r} | \chi \rangle \langle \chi | \vec{r}' \rangle \\ &= \lambda \chi(\vec{r}) \chi^*(\vec{r}') \end{aligned} \tag{5.5}$$

Thus, a separable potential is non-local [1].

---

[1] A local potential in configuration space has the form,

$$\langle \vec{r} | V | \vec{r}' \rangle = V(\vec{r}) \delta(\vec{r} - \vec{r}') \quad .$$

For a separable potential, Eq. (5.1) becomes in operator form

$$t = \lambda |\chi\rangle\langle\chi| + \lambda |\chi\rangle\langle\chi| g_0 t \quad . \tag{5.6}$$

It can be solved right away. We multiply by $\langle\chi| g_0$ from the left,

$$\langle\chi| g_0 t = \lambda \langle\chi| g_0 |\chi\rangle\langle\chi| + \lambda \langle\chi| g_0 |\chi\rangle \langle\chi| g_0 t \quad , \tag{5.7}$$

and get,

$$\langle\chi| g_0 t = \frac{\langle\chi| g_0 |\chi\rangle \langle\chi|}{\lambda^{-1} - \langle\chi| g_0 |\chi\rangle} \quad . \tag{5.8}$$

Inserted into Eq. (5.6), we get

$$t(z) = \lambda |\chi\rangle\langle\chi| + \frac{\lambda |\chi\rangle\langle\chi| g_0(z) |\chi\rangle\langle\chi|}{\lambda^{-1} - \langle\chi| g_0(z) |\chi\rangle} \quad ,$$

or,

$$t(z) = |\chi\rangle \tau(z) \langle\chi| \quad , \tag{5.9}$$

with

$$\tau(z) = \left(\lambda^{-1} - \langle\chi| g_0(z) |\chi\rangle\right)^{-1} \quad .$$

Thus, the T-matrix for a separable potential is separable itself. This property of the T-matrix is important for the solution of the Faddeev equations. As we shall see, the dimension of the equations is reduced from two to one when the two-particle T-matrix is separable. In momentum representation, the T-matrix becomes, according to Eq. (5.9),

$$\langle \vec{p}' | t(z) | \vec{p} \rangle = \frac{\chi(\vec{p}\,') \chi^*(\vec{p})}{\lambda^{-1} - \int d\vec{p}\,'' \frac{|\chi(\vec{p}\,'')|^2}{z - p''^2/2\mu}} \quad . \tag{5.10}$$

We now want to find out under what conditions the separable

potential (5.4) has a bound state with energy E^B [1]. For this purpose we consider the left eigenfunction of the kernel of Eq. (5.1),

$$\langle\psi| = \langle\psi| V g_0(E^B) \quad . \tag{5.11}$$

This equation is equivalent to the Schrödinger equation, as can be verified by multiplication with $g_0^{-1}(E^B)$ from the right. With the separable potential (5.4), we get

$$\langle\psi| = \lambda \langle\psi|\chi\rangle \langle\chi| g_0(E^B) \quad . \tag{5.12}$$

The eigensolution is proportional to $\langle\chi| g_0(E^B)$,

$$\langle\psi| = N \langle\chi| g_0(E^B) \quad . \tag{5.13}$$

The factor N follows from the normalization condition,

$$N^{-2} = \langle\chi| g_0^2(E^B) |\chi\rangle \quad . \tag{5.14}$$

We assume, in the following, the state $|\chi\rangle$ to be normalized in such a way that $N = 1$.
A solution of Eq. (5.12) does not exist for every energy E^B. Multiplying Eq. (5.12) by $|\chi\rangle$ from the right, we get

$$\langle\psi|\chi\rangle = \lambda \langle\psi|\chi\rangle \langle\chi| g_0(E^B) |\chi\rangle \quad , \tag{5.15}$$

and, since $\langle\psi|\chi\rangle = N \langle\chi| g_0(E^B) |\chi\rangle \neq 0$, we have

$$\lambda^{-1} = \langle\chi| g_0(E^B) |\chi\rangle \quad , \tag{5.16a}$$

or,

$$\lambda^{-1} = \int d\vec{p}\, \frac{|\chi(\vec{p})|^2}{E^B - p^2/2\mu} \quad . \tag{5.16b}$$

---

[1] There can be one bound state, at most, because of the projection property of the separable potential.

This relates the binding energy E^B to the potential strength λ. When a bound state $E^B < o$ exists, λ is necessarily negative because the integrand in Eq. (5.16b) is negative. This is obvious since the potential is only attractive for $\lambda < o$. But even when $\lambda < o$, we do not always get a bound state. Because of $E^B < o$, the parameter λ must fulfill the inequality

$$\lambda^{-1} > -\int d\vec{p}\, \frac{|\chi(\vec{p})|^2}{p^2/2\mu} \equiv \left(\lambda^{-1}\right)_{Min} \qquad (5.17)$$

Let us consider once more the T-matrix for separable potential. We now assume that the potential has a bound state, i.e., the parameter λ follows from Eq. (5.16) with $E^B < o$. We then get from Eq. (5.9)

$$t(z) = \frac{|\chi\rangle\langle\chi|}{\langle\chi| g_o(E^B) - g_o(z) |\chi\rangle} \qquad (5.18)$$

Using the resolvent equation (2.20), we see that the T-matrix has a pole at the energy E^B of the bound state,

$$t(z) = \frac{|\chi\rangle\langle\chi|}{(z - E^B)\langle\chi| g_o(E^B)\, g_o(z) |\chi\rangle} \qquad (5.19)$$

The residuum can be expressed by the wave function of the bound state. From Eqs. (5.13), (5.14), and the Schrödinger equation $g_o^{-1}(E^B)|\psi\rangle = v|\psi\rangle$, we get

$$\mathrm{Res}(t) = v|\psi\rangle\langle\psi|v \qquad (5.20)$$

For the special case of a separable potential, we have thus verified the general rule that the two-particle T-matrix has poles at the energies of bound states and that the residua factorize. To generalize our result, we expand the kernel of Eq. (5.1) into the biorthogonal system of its eigenfunctions (compare with method (c), page 75). As the set of functions $\bar{\varphi}$, we take the right eigenfunctions,

$$v(z)|\bar{\varphi}_\nu(z)\rangle = v g_o(z)|\bar{\varphi}_\nu(z)\rangle = \eta_\nu(z)|\bar{\varphi}_\nu(z)\rangle \quad , \qquad (5.21)$$

and as set ψ , we take the left eigenfunctions,

$$\langle\varphi_\nu(z)|\,\mathcal{V}(z)=\langle\varphi_\nu(z)|\,V g_0(z)=\eta_\nu(z)\,\langle\varphi_\nu(z)| \quad . \tag{5.22}$$

It can be shown easily that corresponding eigenvalues are equal in both cases and that

$$\langle\varphi_\nu(z)|\,\bar{\varphi}_\mu(z)\rangle=\delta_{\mu\nu} \quad , \tag{5.23}$$

and,

$$|\bar{\varphi}_\nu(z)\rangle=V|\varphi_\nu(z^*)\rangle \quad , \tag{5.24}$$

are valid. From Eqs. (4.21) and (4.22), we then get the expansion

$$\mathcal{V}(z)=V g_0(z)=\sum_{\nu=1}^{\infty}\eta_\nu(z)\,|\bar{\varphi}_\nu(z)\rangle\langle\varphi_\nu(z)| \quad . \tag{5.25}$$

Multiplying Eq. (5.25) by $g_0^{-1}(z)$ from the right, we get the following expansion for the potential

$$V=\sum_{\nu=1}^{\infty}\eta_\nu(z)\,|\bar{\varphi}_\nu(z)\rangle\langle\varphi_\nu(z)|\,g_0^{-1}(z) \quad , \tag{5.26}$$

which can be simplified with the aid of Eqs. (5.22) and (5.24) in the following way

$$V=\sum_{\nu=1}^{\infty}|\bar{\varphi}_\nu(z)\rangle\langle\bar{\varphi}_\nu(z^*)| \quad . \tag{5.27}$$

With the so-called ideal choice [34] of expansion functions (Eqs. (5.21) and (5.22)), the solution of Eq. (4.25) can be written down explicitly, and the T-matrix becomes

$$t(z)=\sum_{\nu=1}^{\infty}\frac{V|\varphi_\nu(z^*)\rangle\langle\varphi_\nu(z)|V}{1-\eta_\nu(z)} \quad . \tag{5.28}$$

We realize that, in the general case, the T-matrix has poles at all energies z_p for which an eigenvalue $\eta_\nu(z)$ becomes equal to one,

$$\eta_\nu(z_p) = 1 \quad . \tag{5.29}$$

For $\mathrm{Im}\sqrt{z_p} > 0$, the energies z_p are energies of bound states, and the functions $\varphi_\nu(z_p)$ are the corresponding normalizable wave functions (because Eq. (5.22) becomes identical to the adjoint Schrödinger equation when $\eta_\nu(z_p) = 1$). Furthermore, we can see that the residuum factorizes in general, and that the pole term dominates the T-matrix in the vicinity of a pole,

$$t(z) \approx \frac{v|\varphi_\nu\rangle\langle\varphi_\nu|v}{1-\eta_\nu(z)} \quad . \tag{5.30}$$

The T-matrix is approximately separable in the vicinity of a pole and, since a separable T-matrix corresponds to a separable potential, we can say that any potential acts like a separable potential in the vicinity of a bound state. The same is true for the vicinity of a resonance pole (z_p complex) and for the vicinity of a so-called antibound state pole ($z_p < 0$). These poles are located in the so-called unphysical sheet, $\mathrm{Im}\sqrt{z_p} < 0$. Despite the name "unphysical", these poles can have a strong influence on the scattering process when they are close to the real positive energy axis.

At low energy, two-nucleon scattering is always dominated by poles. For triplet scattering, it is the deuteron bound state pole at -2.22 MeV, and for singlet scattering, it is the antibound state pole at -0.067 MeV. The interaction, therefore, can be approximated rather well by a separable potential. This would even be possible if the "true" potential were a local one. But anyway, a true potential is not known. We only know scattering and binding data, and we may claim that all potentials which represent these data are equally good. The "true" potential can then also be a separable one or a sum of separable terms. Only for large distances are there theoretical arguments (one-pion exchange) which say that the potential should be local. A local potential has the advantage of being effective in many angular momentum states, while a single separable term acts only in one state, which is not very realistic.

The first separable neutron-proton potential has been presented by Yamaguchi [41]. The form factor is

$$\chi(\vec{p}) = (p^2+\beta^2)^{-1} \quad . \tag{5.31}$$

The range parameter β and the coupling constant λ are fitted by low energy data; two values λ are used, one for the singlet and one for the triplet state. As Fig. 13 shows, the neutron-proton S-wave cross section is presented very well up to 14 MeV (Lab). Even more realistic are the potentials which also take into account scattering data of higher energy. These potentials have several separable terms and describe also Coulomb, tensor, and repulsion effects [42]. Figure 14 shows how well such a potential describes the neutron-proton $^1S_0$ phase shift up to 460 MeV (Lab).

In the following, we shall see how the Faddeev equations are solved for a separable potential. We should mention here that in 1962 Mitra [43] took advantage of separable potentials to solve the Schrödinger equation.

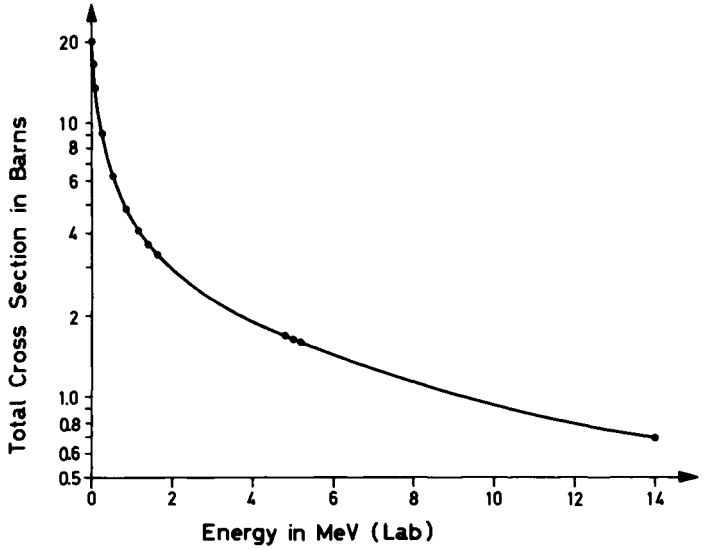


Fig. 13. Calculated n-p total cross section compared with experimental values (Y. Yamaguchi [41])

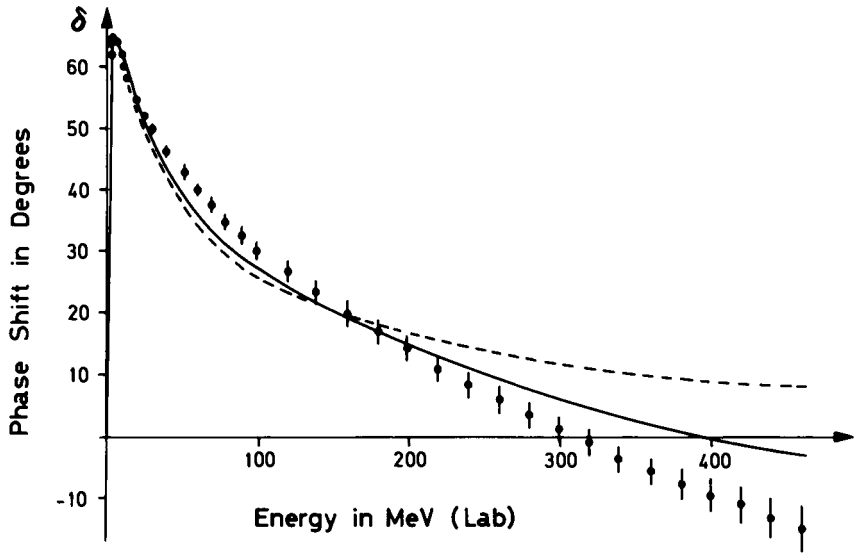


Fig. 14. Calculated $^1S_0$ n-p phase shift compared with experimental values. The full line represents the result of the two-term potential of L. Črepinšek et al. [42], whereas the broken line gives the result for the one-term Yamaguchi potential.

2. Solution of the Faddeev Equations for Separable Potentials

The two-particle T-operator in three-particle space, which enters into the Faddeev equations (3.61a,b), becomes for a separable potential

$$t_\gamma(z) = |\chi_\gamma\rangle \tau_\gamma\left(z - \frac{q_\gamma^2}{2M_\gamma}\right) \langle\chi_\gamma| \quad . \tag{5.32}$$

This equation generalizes the result (5.9) to the three-particle system. The index γ indicates the subsystem in which the form factors are effective. Since the function τ_γ depends on the energy of the subsystem, while z is the total energy of the three-particle system, we have to subtract the kinetic energy of the free particle. The right-hand side of Eq. (5.32) has the unit operator in the function space of particle γ as a factor, which is not explicitly written down.

2.1. Rearrangement Scattering

Let us review the S-matrix for rearrangement scattering. From Eqs. (3.50a), (3.51), (3.52), and (3.60), we have [1]

$$S_{\beta\alpha}(\vec{q}'_\beta;\vec{q}_\alpha) = \delta(\vec{q}'_\beta-\vec{q}_\alpha)\delta_{\beta\alpha} - 2\pi i\,\delta(E_\alpha-E_\beta)\langle\phi_\beta|U_{\beta\alpha}(E+i0)|\phi_\alpha\rangle \quad (5.33)$$

where,

$$|\phi_\gamma\rangle = |\vec{q}_\gamma\rangle|\psi_\gamma\rangle \quad . \quad (5.34)$$

For a separable potential with a duely normalized form factor, we have, according to Eq. (5.13),

$$|\phi_\gamma\rangle = g_0(E_\gamma)|\chi_\gamma\rangle|\vec{q}_\gamma\rangle \quad , \quad (5.35)$$

with $E_\gamma = E_\gamma^B + \frac{q_\gamma^2}{2M_\gamma}$.

The operator $g_0(z)$ acts in the three-particle space, here, in contrast to g_0 in Eq. (5.13). As a consequence, the argument of g_0 is a sum of the energy of the subsystem plus the energy of the free particle.

Combining Eqs. (5.33) - (5.35), we see that we only need a representation of the matrix operator,

$$X_{\beta\alpha}(z) = \langle\chi_\beta|g_0(z)\,U_{\beta\alpha}(z)\,g_0(z)|\chi_\alpha\rangle \quad , \quad (5.36)$$

in the momentum space $|\vec{q}_\beta\rangle$, $|\vec{q}_\alpha\rangle$ to get the S-matrix. An equation for the operator (5.36) follows from the Faddeev equations (3.61a), together with Eq. (5.32),

$$\langle\chi_\beta|g_0 U_{\beta\alpha} g_0|\chi_\alpha\rangle = (1-\delta_{\beta\alpha})\langle\chi_\beta|g_0|\chi_\alpha\rangle \quad (5.37)$$

$$+\sum_{\gamma=1}^{3}(1-\delta_{\beta\gamma})\langle\chi_\beta|g_0|\chi_\gamma\rangle\,\tau_\gamma\,\langle\chi_\gamma|g_0 U_{\gamma\alpha} g_0|\chi_\alpha\rangle \quad .$$

---

[1] In order to simplify the presentation we assume one bound state in each subsystem.

Equation (3.61a) has been multiplied by $\langle \chi_\beta | g_0$ and $g_0 | \chi_\alpha \rangle$ from the left and right, respectively. With the abbreviation (5.36) and

$$Z_{\beta\alpha}(z) = (1-\delta_{\beta\alpha}) \langle \chi_\beta | g_0(z) | \chi_\alpha \rangle \quad , \tag{5.38}$$

Eq. (5.37) becomes

$$X_{\beta\alpha}(z) = Z_{\beta\alpha}(z) + \sum_{\gamma=1}^{3} Z_{\beta\gamma}(z) \tau_\gamma \left(z - \frac{q_\gamma^2}{2M_\gamma}\right) X_{\gamma\alpha}(z) \quad . \tag{5.39}$$

After multiplication by $\langle \vec{q}_\beta |$ and $| \vec{q}'_\alpha \rangle$ from the left and right, respectively, and after introduction of intermediate states, Eq. (5.39) becomes an integral equation for the matrix elements of the operator $X_{\beta\alpha}$. Since this operator is already sandwiched between states of the subsystem by its definition (5.36), the integral equation is only three-dimensional and becomes one-dimensional after angular momentum decomposition.

To illustrate the meaning of Eq. (5.39), we compare it with equations (2.56a,b) for the two-particle T-operator

$$t(z) = V + V g_0(z) t(z) \quad . \tag{5.40}$$

We realize that Eq. (5.39) treats the three-particle problem as an effective two-body problem [1]. The degrees of freedom of the subsystem are integrated over and, therefore, the subsystem appears as o n e particle (in various channels). If we forget the channel indices, we can compare $X_{\beta\alpha}$ to the two-body T-operator and $Z_{\beta\alpha}$ to an effective two-body potential. As we shall see later in this chapter (section 2.4), the potential becomes complex for energies above the breakup threshold. For a complex potential, probability flux is not conserved. Particles disappear from the two-body system and reappear in the breakup channel. The operator τ_γ in Eq. (5.39) corresponds to the free two-particle propagator g_0 in Eq. (5.40). It describes the free motion of particle γ relative to the bound subsystem γ .

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[1] A similar analogy has already been worked out on page 63.

This correspondence can be seen even more clearly. In momentum representation, we have for the two-particle system

$$\langle \vec{q} | \hat{g}_0(z) | \vec{q}' \rangle = \frac{\delta(\vec{q}-\vec{q}')}{z - \frac{q^2}{2\mu}} \quad . \tag{5.41}$$

The free propagator $\hat{g}_0$ has a pole at the energy of the relative motion of the two particles. The same is true for τ_γ. According to Eqs. (5.9) and (5.19), we can write

$$\langle \vec{q}_\gamma | \tau_\gamma (z - \frac{q_\gamma^2}{2M_\gamma}) | \vec{q}_\gamma' \rangle = \frac{\delta(\vec{q}_\gamma - \vec{q}_\gamma')}{(z - E_\gamma^B - \frac{q_\gamma^2}{2M_\gamma}) \langle \chi_\gamma | \hat{q}_0(E_\gamma^B) \hat{q}_0 (z - \frac{q_\gamma^2}{2M_\gamma}) | \chi_\gamma \rangle} \quad . \tag{5.42}$$

The "propagator" τ_γ has a pole, too, when the energy [1] $z - E_\gamma^B$ becomes equal to the energy of the relative motion between the subsystem and the free particle.

2.2. Three-Particle Breakup

We do not have to solve another integral equation to get the breakup amplitudes. According to Eq. (3.64),

$$U_{0\alpha} = z - h_0 + \sum_{\gamma=1}^{3} t_\gamma g_0 U_{\gamma\alpha} \quad , \tag{5.43}$$

we can calculate them from the rearrangement amplitudes. For the S-matrix we need, in this case, the matrix elements

$$\langle \vec{q}_{1\alpha} \vec{p}_{1\alpha} | U_{0\alpha} | \phi_\alpha \rangle = \langle \vec{q}_{1\alpha} \vec{p}_{1\alpha} | U_{0\alpha} g_0 | \chi_\alpha \rangle | \vec{q}_\alpha' \rangle \equiv \langle \vec{q}_{1\alpha} | X_{0\alpha} | \vec{q}_\alpha' \rangle . \tag{5.44}$$

For the operator $X_{0\alpha}$ we get from Eq. (5.43)

$$\begin{aligned} X_{0\alpha} &= \langle \vec{p}_{1\alpha} | U_{0\alpha} g_0 | \chi_\alpha \rangle \\ &= \langle \vec{p}_{1\alpha} | \chi_\alpha \rangle + \sum_{\gamma=1}^{3} \langle \vec{p}_{1\alpha} | \chi_\gamma \rangle \tau_\gamma \langle \chi_\gamma | g_0 U_{\gamma\alpha} g_0 | \chi_\alpha \rangle \\ &= \sum_{\gamma=1}^{3} \langle \vec{p}_{1\alpha} | \chi_\gamma \rangle \tau_\gamma X_{\gamma\alpha} \quad . \end{aligned} \tag{5.45}$$

---

[1] We have to subtract, of course, the energy E_γ^B of the bound state, since z is the energy of the three-particle system. The residua are the same in Eqs. (5.41) and (5.42) since $\langle \chi | \hat{g}_0(E_\gamma^B) \hat{g}_0(z - q_\gamma^2/2M_\gamma) | \chi \rangle = 1$ for $z - q_\gamma^2/2M_\gamma = E_\gamma^B$ (see Eq. (5.14)).

It has been used, here, that $\langle \vec{q}_\gamma, \vec{p}_\gamma | \chi_\alpha \rangle | \vec{q}'_\alpha \rangle = 0$ on the energy shell. Equation (5.43) has, thus, led back to the rearrangement operators Eq. (5.36).

Also the result (5.45) for the breakup amplitude can be understood in the frame of an effective two-body reaction. One only has to realize that the rearrangement operators enter off-shell into Eq. (5.45), i.e., as a representation $\langle \vec{q}_\gamma | X_{\gamma\alpha} | \vec{q}_\alpha \rangle$ where $|\vec{q}_\gamma|$ can assume a continuum of values. In the initial state, we have

$$E = E_\alpha^B + \frac{q_\alpha^2}{2M_\alpha} ,$$

or,

$$|\vec{q}_\alpha| = \sqrt{2M_\alpha (E - E_\alpha^B)} . \tag{5.46}$$

In the final state, we have three free particles and the energy E becomes

$$E = \frac{p_\gamma^2}{2\mu_\gamma} + \frac{q_\gamma^2}{2M_\gamma} . \tag{5.47}$$

The total energy E can be conserved for any momentum $\vec{q}_\gamma$ within the range

$$0 \leq |\vec{q}_\gamma| \leq \sqrt{2M_\gamma E} . \tag{5.48}$$

For momenta $\vec{q}_\gamma$ which satisfy the on-shell condition,

$$E_\gamma^B + \frac{q_\gamma^2}{2M_\gamma} = E_\alpha^B + \frac{q_\alpha^2}{2M_\alpha} ,$$

the amplitude $\langle \vec{q}_\gamma | X_{\gamma\alpha} | \vec{q}_\alpha \rangle$ is the probability amplitude for the production of a rearranged final state. For momenta $\vec{q}_\gamma$ from the range (5.48), the amplitude $\langle \vec{q}_\gamma | X_{\gamma\alpha} | \vec{q}_\alpha \rangle$ becomes the probability amplitude for the production of a final state with subsystem γ in a state of positive energy $p_\gamma^2/2\mu_\gamma$ and particle γ in a momentum state $|\vec{q}_\gamma\rangle$. In the definition of $X_{\gamma\alpha}$, the operator $U_{\gamma\alpha}$ has been multiplied from the left by $g_0(E+i0)|\chi_\gamma\rangle|\vec{q}_\gamma\rangle$. This is a channel state if $\vec{q}_\gamma$ fulfills the on-shell condition $E = E_\gamma^B + q_\gamma^2/2M_\gamma$. If we take $\vec{q}_\gamma$ from the range (5.48), the state $g_0(E+i0)|\chi_\gamma\rangle|\vec{q}_\gamma\rangle$ is no longer a channel state. It describes positive energy

states of the subsystem with the energy $p_\gamma^2/2\mu_\gamma = E - q_\gamma^2/2M_\gamma$. Since we are not interested in the special positive energy state of subsystem γ but in the decay into three free particles, the operator $X_{\gamma\alpha}$ is multiplied, in Eq. (5.45), by $\langle \vec{p}_1 | \chi_\gamma \rangle \tau_\gamma$. This factor describes the decay of the subsystem. The main information on breakup, however, is contained in the operator $X_{\gamma\alpha}$.

2.3. Identical Particles

For identical particles, the rearrangement channels become indistinguishable and, therefore, the number of equations in the set (5.39) is reduced. It would not be right, however, to put $X_{11} = X_{12} = X_{13}$. The elastic amplitude X_{11} is not equal to the rearrangement amplitude X_{12} since the underlying scattering processes are completely different. This can already be seen from the Neumann series of Eq. (5.39): for X_{11} , the first term of the series is zero, while it is equal to $\langle \chi_1 | g_0 | \chi_2 \rangle$ for X_{12} . It is only impossible to distinguish the results of elastic scattering and of rearrangement scattering. It would be all right though, if we were able to calculate the sum of elastic and rearrangement scattering.

Up to now, the channel indices stood for different channels a n d different coordinate systems. For rearrangement scattering, there were exactly three channels, since we assumed spinless particles and one bound state per pair of particles. When particles are identical, these three channels become indistinguishable, and the channel index only stands for the coordinate system. All the form factors $|\chi_\gamma\rangle$ are identical. We still need the index γ , however, to tell in which subsystem the form factor acts.

Let us look at the effective potentials $Z_{\beta\alpha}$, Eq. (5.38). The non-diagonal elements, such as

$$Z_{12} = \langle \chi_1 | q_0 | \chi_2 \rangle \tag{5.49}$$

and

$$Z_{13} = \langle \chi_1 | q_0 | \chi_3 \rangle ,$$

differ only by a transformation of variables ($2 \leftrightarrow 3$). They are identical and will be denoted by Z ,

$$Z \equiv Z_{\beta\alpha} \quad , \quad \beta \neq \alpha \quad . \tag{5.50}$$

The diagonal elements of $Z_{\beta\alpha}$ are zero.

The situation is similar for the transition operators $X_{\beta\alpha}$. We only have diagonal elements,

$$X_D \equiv X_{\alpha\alpha} \quad , \tag{5.51a}$$

and non-diagonal elements,

$$X_N \equiv X_{\beta\alpha} \quad , \quad \beta \neq \alpha \quad . \tag{5.51b}$$

From Eq. (5.39), we get two different equations for the unknown amplitudes X_D and X_N ,

$$X_D = Z Z \tau X_N \tag{5.52a}$$

$$X_N = Z + Z \tau X_D + Z \tau X_N \quad . \tag{5.52b}$$

Adding Eq. (5.52b) twice to Eq. (5.52a), we get an equation for the quantity

$$X \equiv X_D + 2 X_N \quad , \tag{5.53a}$$

namely,

$$X = 2Z + 2Z \tau X \quad . \tag{5.53b}$$

The quantity X is the amplitude (in operator form) which alone determines the S-matrix for the scattering of identical, spinless particles with one two-particle bound state [8]. The rearrangement amplitude X_N enters with a factor of 2, according to the fact that there is only one possibility $\beta = \alpha$ for elastic scattering, while there are two possibilities $\beta \neq \alpha$ for rearrangement scattering.

The operators of Eqs. (5.53 a and b) act in the space of relative motion of bound state and free particle. In momentum representation, we get the integral equation

$$\langle \vec{q} | X(E+i\epsilon) | \vec{q}' \rangle = 2 \langle \vec{q} | Z(E+i\epsilon) | \vec{q}' \rangle \tag{5.54}$$

$$+2 \int d\vec{q}'' \langle \vec{q} | Z(E+i\epsilon) | \vec{q}'' \rangle \tau(E+i\epsilon - \frac{q''^2}{2M}) \langle \vec{q}'' | X(E+i\epsilon) | \vec{q}' \rangle .$$

For $m_1 = m_2 = m_3 = m$, the reduced masses become, according to Eq. (2.74),

$$\mu = \frac{m}{2} \qquad M = \frac{2}{3} m \quad . \tag{5.55}$$

For the calculation of the "potential" Z, we have to recall the definitions (5.38) and (5.50). According to these definitions, the "potential" is a matrix element of the free three-particle resolvent g_0 between form factors which act in different channels,

$$\langle \vec{q} | Z | \vec{q}' \rangle = \langle \vec{q} | \langle \chi_1 | g_0 | \chi_2 \rangle | \vec{q}' \rangle \quad . \tag{5.56}$$

The matrix element is evaluated by insertion of intermediate states $|\vec{q}_i, \vec{p}_i\rangle \langle \vec{q}_i, \vec{p}_i|$,

$$\langle \vec{q} | Z | \vec{q}' \rangle = \tag{5.57}$$

$$\int d\vec{q}_1 \, d\vec{q}_2' \, d\vec{p}_1 \, d\vec{p}_2' \; \frac{\langle \vec{q} | \langle \chi_1 | \vec{q}_1, \vec{p}_1 \rangle \langle \vec{q}_1, \vec{p}_1 | \vec{q}_2', \vec{p}_2' \rangle \langle \vec{q}_2', \vec{p}_2' | \chi_2 \rangle | \vec{q}' \rangle}{E + i\epsilon - \frac{q_1^2}{2M} - \frac{p_1^2}{2\mu}} \quad ,$$

where,

$$\langle \vec{q} | \langle \chi_i | \vec{p}_i, \vec{q}_i \rangle = \delta(\vec{q} - \vec{q}_i) \chi_i^*(\vec{p}_i) \quad . \tag{5.58}$$

From now on, we can drop the channel index at form factors because all form factors are the same. The fact that they act in different subsystems is already taken into account by the choice of coordinates.

The overlap $\langle \vec{q}_1, \vec{p}_1 | \vec{q}_2', \vec{p}_2' \rangle$ becomes

$$\langle \vec{q}_1, \vec{p}_1 | \vec{q}_2', \vec{p}_2' \rangle = \delta(\vec{q}_1 - \vec{q}_1'(\vec{q}_2', \vec{p}_2')) \, \delta(\vec{p}_1 - \vec{p}_1'(\vec{q}_2', \vec{p}_2')) \qquad (5.59)$$

$$= \delta(\vec{q}_1 + \vec{p}_2' + \tfrac{1}{2}\vec{q}_2') \, \delta(\vec{p}_1 + \tfrac{1}{2}\vec{p}_2' - \tfrac{3}{4}\vec{q}_2') \; .$$

The coordinate transformation needed here can easily be derived from the transformations (2.72). In Eq. (5.57), the integration can be carried out because of the δ-functions, and the "potential" becomes

$$\langle \vec{q} | Z(E+i\epsilon) | \vec{q}' \rangle = \frac{\chi^*(\vec{q}' + \frac{1}{2}\vec{q}) \, \chi(-\frac{1}{2}\vec{q}' - \vec{q})}{E + i\epsilon - \frac{q^2}{2m} - \frac{(\vec{q}+\vec{q}')^2}{2m} - \frac{q'^2}{2m}} \; . \qquad (5.60)$$

It is helpful to illustrate the calculation of expressions like (5.56) by a graphical representation [23] as in Fig. 15. There, a line represents a momentum eigenstate of a particle, a double line represents a momentum eigenstate of the center-of-mass motion of a bound subsystem, and a half-circle represents a form factor; the intermediate state, which consists of three free particles, is multiplied by the free propagator g_o . With a little experience, the result (5.60) can be read off directly from the graph.

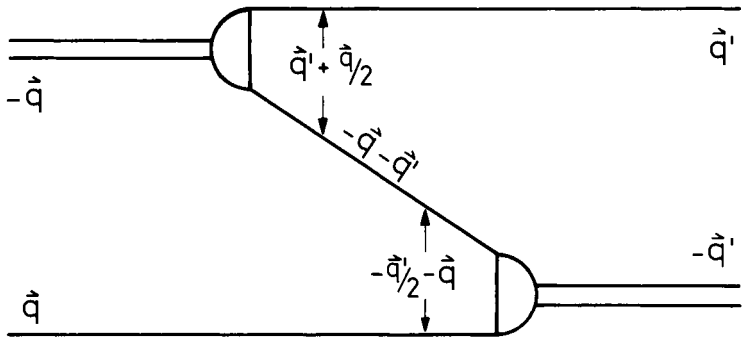

Fig. 15. Graphical representation of the "potential" in Eq. (5.54)

The unknown amplitude depends on seven variables, namely on $\vec{q}$, $\vec{q}\,'$, and E. The variable $\vec{q}$ is an integration variable while $\vec{q}\,'$ and E enter only as parameters into the integral equation. For the S-matrix, the amplitude $\langle \vec{q} | X(E+i0) | \vec{q}\,' \rangle$ is only needed on-shell for rearrangement and elastic scattering (see Eq. (5.33)), or half off-shell for breakup (see Eq. (5.45)). We can, therefore, put $\vec{q}\,'$ equal to the relative momentum of the initial state and have

$$E = \frac{3q'^2}{4m} + E^B \quad . \tag{5.61}$$

In spherical coordinates q, ϑ, φ which are chosen in such a way that $\vartheta = 0$ coincides with the direction of $\vec{q}\,'$, the integral equation becomes two-dimensional since φ does not appear. By partial wave decomposition, we get one-dimensional equations,

$$\begin{aligned} X_L(q,q',E+i\epsilon) &= Z_L(q,q',E+i\epsilon) \\ &+ \int_0^\infty dq''\, K_L(q,q'',E+i\epsilon)\, X_L(q'',q',E+i\epsilon) \quad , \end{aligned} \tag{5.62}$$

with

$$K_L(q,q'',E+i\epsilon) = 8\pi q''^2 Z_L(q,q'',E+i\epsilon)\, \tau\left(E+i\epsilon - \frac{3q''^2}{4m}\right) .$$

The quantum number L denotes the total angular momentum of the three-particle system. Because of angular momentum conservation, equations with different values of L are uncoupled.

The partial wave projections of X and Z are

$$Z_L(q,q',E+i\epsilon) = \frac{1}{2}\int_{-1}^{1} d\cos\vartheta\, P_L(\cos\vartheta)\, Z(\vec{q},\vec{q}\,',E+i\epsilon) \quad , \tag{5.63a}$$

$$X_L(q,q',E+i\epsilon) = \frac{1}{2}\int_{-1}^{1} d\cos\vartheta\, P_L(\cos\vartheta)\, X(\vec{q},\vec{q}\,',E+i\epsilon) \quad . \tag{5.63b}$$

The functions $P_L(\cos\vartheta)$ are the Legendre polynomials.

From the solutions X_L of Eq. (5.62), the solutions X of (5.54) are obtained by

$$X(\vec{q},\vec{q}',E+i\epsilon)=\sum_{L=0}^{\infty}(2L+1)P_L(\cos\vartheta)X_L(q,q',E+i\epsilon) \quad (5.64)$$

In Eq. (5.62), we now have to perform the ε-limit which, as we know, contains the boundary condition. As will be seen in the next section, there are poles which approach the real axis when ε goes to zero. The influence of these poles is given by the symbolic formula

$$\lim_{\epsilon\to 0}\frac{1}{x\pm i\epsilon}=P\frac{1}{x}\mp i\pi\delta(x) . \quad (5.65)$$

The formula replaces the integral over a pole by a principle value integral, to which half of the residuum of the pole is added (subtracted). The sign in front of the residuum is determined by the boundary condition.

2.4. Numerial Solution of the Faddeev Equations for Separable Potential

We are ready now to solve the Faddeev equation (5.62) by method (f) of Chapter 4, section 2. We have to be careful, however, since the kernel can have singularities. They can arise from the two-particle propagator τ , as well as from the "potential" Z.

a) Singularities of the Propagator τ

According to Eq. (5.42), we have

$$\tau(E+i\epsilon-\tfrac{3}{4}\tfrac{q''^2}{m})\sim(E+i\epsilon-\tfrac{3}{4}\tfrac{q''^2}{m}-E^B)^{-1} , \quad (5.66)$$

where $E^B < 0$ is the energy of the two-particle bound state. For $E > E^B$ and $\varepsilon \to 0$, we get a pole at

$$q''^2=\tfrac{4}{3}m(E-E^B) . \quad (5.67)$$

The pole will be there for any scattering since $E=3q'^2/4m+E^B\geq E^B$ (compare with Eq. (5.61)). Only for a bound-state calculation can we have $E < E^B$, and the pole will be missing.

b) Singularities of the "Potential" Z

The free resolvent g_0 , which appears in the "potential" Z, becomes singular above the three-particle breakup threshold because the free motion of all three particles becomes possible. The function Z, therefore, has poles for certain values of the momenta q, q' in the limit $\varepsilon \to 0$,

$$Z(\vec{q},\vec{q}',E+i\epsilon) \sim \left(E+i\epsilon - \frac{q^2}{m} - \frac{q'^2}{m} - \frac{qq'}{m}\cos\vartheta\right)^{-1} \qquad (5.68)$$

$$= \frac{m}{qq'}\left(y+i\epsilon-\cos\vartheta\right)^{-1} ,$$

with

$$y = \frac{mE-q^2-q'^2}{qq'} .$$

Partial wave projection leads to the expression

$$Z_L(q,q',E+i\epsilon) \sim \frac{1}{2}\int_{-1}^{1} \frac{P_L(x)\,dx}{y+i\epsilon-x} , \qquad (5.69)$$

where $x = \cos\vartheta$. Using Eq. (5.65), we get

$$Z_L(q,q',E+i0) \sim \frac{1}{2}\left[P\int_{-1}^{1}\frac{P_L(x)\,dx}{y-x} - i\pi\int_{-1}^{1}\delta(y-x)P_L(x)\,dx\right]$$

$$\equiv Q_L(y) . \qquad (5.70)$$

By the principle value integration, the pole becomes a logarithmic singularity, which appears at $y = \pm 1$; for these values of y, the pole coincides with the end of the integration region. The Legendre function of second kind $Q_L(y)$ has a cut for $-1<y<+1$ which is related to the boundary condition. Meeting the boundary condition implies choosing the appropriate values of the function $Q_L(y)$ (defined by Eq. (5.70)) at the cut.

As has been said, the logarithmic singularities appear at $y = \pm 1$. For the variables q, q' this means

$$mE - \left(q \pm \tfrac{1}{2}q'\right)^2 - \tfrac{3}{4}q'^2 = 0 . \qquad (5.71)$$

The function $Z_L(q,q',E+i\sigma)$ is present in the kernel of Eq.(5.62) and as inhomogeneity. In the inhomogeneity, the variable q is off-shell, but q' is on-shell (compare with Eq. (5.61)). The condition (5.71) cannot be fulfilled because, with Eq. (5.61), the left side of condition (5.71) becomes

$$m E - (q + \tfrac{1}{2} q')^2 - m E + m E^B \qquad (5.72)$$

$$= - (q + \tfrac{1}{2} q')^2 + m E^B < 0 \quad ,$$

which is always smaller than zero since the energy E^B is negative. Consequently, the singularity cannot appear.

Things are different for the kernel. Here, both q and q" are off-shell because q" is an integration variable. Condition (5.71) is fulfilled for

$$q = \pm \left(\tfrac{1}{2} q'' \pm \sqrt{m E - \tfrac{3}{4} q''^2} \right) \quad . \qquad (5.73)$$

The logarithmic singularities are located on the curves q(q") which are given by Eq. (5.73). Figure 16 gives an illustration of this.

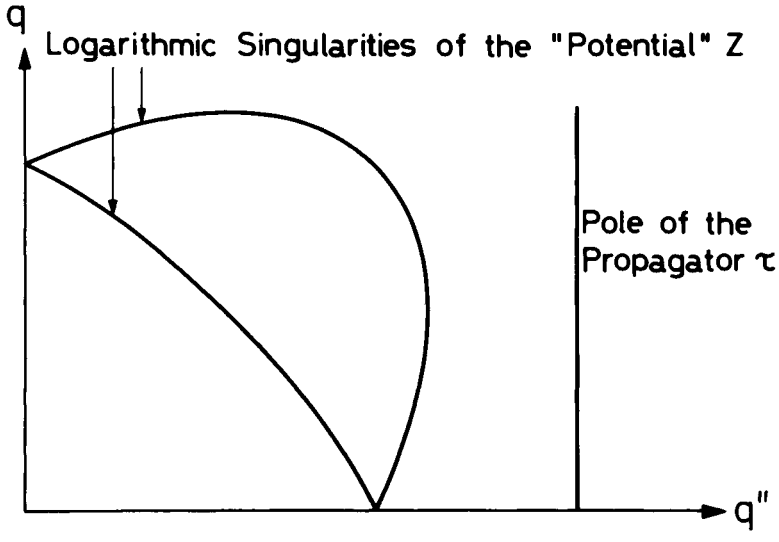

Fig. 16. Position of singularities in the kernel of Eq. (5.62)

Between the two elliptic arcs, the function Z_L is complex. This is the region where the δ-function of Eq. (5.70) contributes. Figure 16 also shows the position of the pole which comes from the two-particle propagator τ and has been discussed in a).

We thus see that the three-particle problem becomes more and more complicated as we go from the bound-state problem to the rearrangement scattering problem and to the breakup problem because the number of singularities increases. The situation is similar when the Schrödinger equation is to be solved in configuration space. In this case, difficulties increase because the boundary condition becomes more and more complicated. The following table gives a schematical survey:

		Faddeev equations in momentum space	Schrödinger equation in configuration space
Bound states	$E<E^B$	No singularities	$\psi(\infty) \to 0$
Pure elastic scattering	$E^B<E<0$	Pole of the effective two-particle propagator	$\psi(\infty) \sim e^{ikz}+f(\vartheta)e^{ikr}/r$
Scattering with breakup	$0<E$	Additional poles of the three-particle propagator	?

The question mark indicates the particular difficulty of a breakup boundary condition; such a condition cannot be written down in a concise way (compare with Chapter 8, section 3).

Let us now return to the integration of the Faddeev equation. Can we find an integration mesh which allows an accurate numerical integration despite the singularities shown in Fig. 16 ? The pole of the effective two-particle propagator doesn't make trouble because its position is fixed. It can be eliminated by a transformation [44], or it can simply be integrated

over [45,46]. Difficulties arise, however, from the poles of the function Z_L since these poles change their position in relation to the variable q.

In principle, the integration could be performed by choosing a new integration mesh for every value of q. There are integration meshes which allow for singularities [47], but we cannot use them because method (f) demands that we get along with one single mesh. Otherwise we would not get a system of N equations for N unknown values of the function X_L ; there would be more unknowns than equations.

There are two ways out: Firstly, we can mix numerical and analytical integration and, thereby, make use of our knowledge on the analytical behavior of the integrand [48-52]. Secondly, we can use Cauchy's theorem and shift the path of integration into the complex plane.

Let us first look at the second method. It has been introduced by Hetherington and Schick [53] and was used later by Amado [54] and by Cahill and Sloan [55]. Interesting variants have been given by Ebenhöh [56] and by Avishai [57]. The method consists of three steps.

a) An analytic continuation of the integral equation for complex momenta is made.

b) The integral equation is solved for complex momenta which are reasonably far away from singularities.

c) The solution for real momenta is obtained by a single iteration of Eq. (5.62), starting with the solution for complex momenta.

Let us discuss these three steps in more detail.

a) When we put $q = \varrho e^{-i\varphi}$ in our integral equation (5.62), solutions also are defined for complex momenta (we drop the dependence on q' and E in our notation),

$$X_L(\varrho e^{-i\varphi}) = 2 Z_L(\varrho e^{-i\varphi}) + \int_0^\infty dq'' K_L(\varrho e^{-i\varphi}, q'') X_L(q'') \quad . \qquad (5.74)$$

The path of integration in Eq. (5.74) is still the positive real axis of q". In order to get an integral equation which determines the function $X_L(\varrho e^{-i\varphi})$ without a knowledge of $X_L(q")$ along the positive real axis, we shift the path of integration, according to Fig. 17, from C to C'. That is, we integrate along $\varrho" e^{-i\varphi}$ from zero to infinity with a fixed value of φ . According to Cauchy's theorem, this is possible when the arc B does not contribute to the integral and when the integrand is analytic in the plane CC'B . The two conditions are fulfilled. The kernel has no singularities in the region CC'B , as can be seen from Eq. (5.73), and Brayshaw [58] could show that the solution $X_L(\varrho e^{-i\varphi})$ is analytic for

$$\varphi < \text{arc tan} \sqrt{-3E^B/(E-E^B)} \quad .$$

We thus have the integral equation

$$X_L(\varrho e^{-i\varphi}) = 2Z_L(\varrho e^{-i\varphi}) + e^{-i\varphi} \int_0^\infty d\varrho" K_L(\varrho e^{-i\varphi}, \varrho" e^{-i\varphi}) X_L(\varrho" e^{-i\varphi}) \quad . \tag{5.75}$$

b) The numerical solution of the integral equation (5.75) does not pose any problem since all functions are well behaved along the path C'.

c) Cauchy's theorem is used now for a second time to derive a relation between the solution for complex momenta and the solution for real momenta. In Eq. (5.62), we choose the variable q to be real and examine whether we can shift the path of integration from C to C' (along C' we know the solution). Let us look at the singularities and cuts in the complex q"-plane before the ε-limit is carried out. The cuts are given by $-1 < y < +1$ (see Eq. (5.71)). In the variables q,q", that means

$$q^2 + q"^2 + qq"y - mE - i\epsilon = 0 \quad , \tag{5.76}$$

with $|y| < 1$.

There are three different cases:

α) $o \leq q \leq \sqrt{mE}$ (see Fig. 18)

The path C passes below the singularities and below the cut. There is nothing which prevents us from shifting the path of integration into the lower complex half-plane (path C'). We therefore have

$$X_L(q) = 2Z_L(q) + e^{-i\varphi}\int_0^\infty d\varrho'' K_L(q, \varrho'' e^{-i\varphi})\, X_L(\varrho'' e^{-i\varphi}) \quad . \tag{5.77}$$

The next case is a bit more difficult.

β) $\sqrt{mE} \leq q \leq \sqrt{4mE/3}$ (see Fig. 19)

A singularity, which has been located in the 1st quadrant in case (α), has moved into the 4th quadrant and prevents us from shifting the path of integration into C' directly. We first have to integrate along the old path C, go around the singularity at P, and then back to Q. Near P, we pass through the cut (see figure) down into the second Riemann sheet. From Q on, we follow the path C', entering the first Riemann sheet again at R. By our excursion into the second sheet, we achieve that the integrand is analytic between C and C'. At the cut, only the discontinuity contributes to the integral from O to Q; the singularity at P is eliminated. We thus have, in the present case,

$$\begin{aligned} X_L(q) = 2Z_L(q) &+ \int_{O\to P\to Q} dq'' K_L(q, q'') X_L(q'') \\ &+ e^{-i\varphi}\int_0^\infty d\varrho'' K_L(q, \varrho'' e^{-i\varphi})\, X_L(\varrho'' e^{-i\varphi}) \quad . \end{aligned} \tag{5.78}$$

The amplitude $X_L(q)$ between O and P is given by Eq. (5.77) since $|\overrightarrow{OP}| \leq \sqrt{mE/3}$.

In the last case,

γ) $\sqrt{4mE/3} < q$,

the path of integration can again be shifted directly from C to C' since the singularities of the function Z_L have moved away from the real axis into the complex plane. Equation (5.77) is valid again.

From the solution of our integral equation for complex values of the momentum q, which is rather easily obtainable, we can thus get the solution for all real values of q.

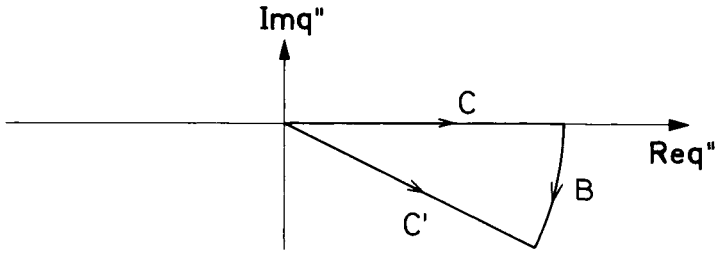

Fig. 17. Path of integration in Eqs. (5.74) and (5.75)

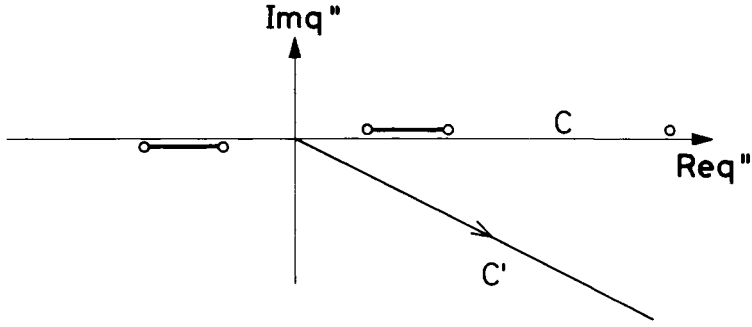

Fig. 18. Path of integration in Eq. (5.77). The singularities are indicated by circles, the cuts by thick lines (R.T. Cahill and I.H. Sloan [55]).

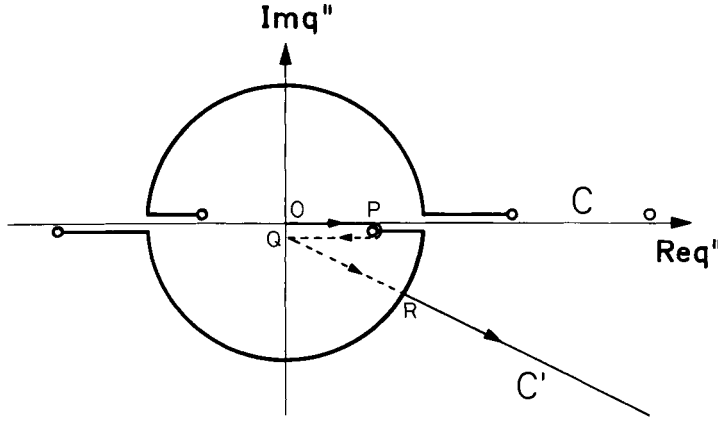

Fig. 19. Path of integration in Eq. (5.78). The dashed line indicates the path of integration in the second sheet. The singularities are indicated by circles, the cuts by thick lines (R.T. Cahill and I.H. Sloan [55]).

A certain disadvantage of the present method lies in the fact that the analytic behavior of kernel and solution in the momentum plane has to be known. For the present integral equation, this is no problem. But there are more complicated equations (those of Alt, Grassberger, and Sandhas, for instance, see Chapter 6) where this additional information can hardly be obtained.

For such equations, another method [48] is more adequate. In this method, the integration is carried out along the real q-axis. The important fact is that the solution $X_L(q)$ is continuous and can be approximated by an interpolation polynomial,

$$X_L(q) \approx \sum_{i=1}^{N} X_L(q_i)\, H_i(q) \quad , \tag{5.79}$$

where H_i is the polynomial,

$$H_i(q) = \frac{\prod_{j \neq i}^{N} (q - q_j)}{\prod_{j \neq i}^{N} (q_i - q_j)} \quad , \tag{5.80}$$

$$H_i(q_j) = \delta_{ij} \quad .$$

Inserted into the integral equation (5.62), we get for $q = q_i$,

$$X_L(q_i) = 2 Z_L(q_i) + \sum_{j=1}^{N} X_L(q_j) \int_0^\infty dq''\, K_L(q_i, q'')\, H_j(q'') \quad . \tag{5.81}$$

Instead of solving a singular integral equation, we only have to calculate the singular integrals

$$I_{ij} = \int_0^\infty dq''\, K_L(q_i, q'')\, H_j(q'') \quad , \tag{5.82}$$

(which is much simpler) and we get the matrix equation

$$X_L(q_i) = 2 Z_L(q_i) + \sum_{j=1}^{N} I_{ij}\, X_L(q_j) \quad . \tag{5.83}$$

2.5. Results for Three Identical Particles

2.5.1. Bound States

According to Faddeev (see page 48), all solutions of the homogeneous Faddeev equation correspond to bound states. We want to show that these solutions satisfy the Schrödinger equation, although this is obvious. We start from the homogeneous version of the Faddeev equation (3.35)

$$|\psi\rangle_i = \sum_{j\neq i} g_0(z)\, t_i(z)\, |\psi\rangle_j \quad . \tag{5.84}$$

Using Eq. (2.57a) (in three-particle space!), we get

$$|\psi\rangle_i = g_i(z) V_i \sum_{j\neq i} |\psi\rangle_j \tag{5.85}$$

or

$$g_i^{-1}(z)\,|\psi\rangle_i = (z - h_0 - V_i)\,|\psi\rangle_i = V_i \sum_{j\neq i} |\psi\rangle_j \quad . \tag{5.86}$$

Taking a sum over i and bearing in mind that $|\psi\rangle = \sum_{i=1}^{3} |\psi\rangle_i$, we get the Schrödinger equation

$$(z - h_0 - \sum_{i=1}^{3} V_i)\,|\psi\rangle = 0 \quad . \tag{5.87}$$

For separable potential and identical particles, the homogeneous version of Eq. (3.35) corresponds to the homogeneous version of Eq. (5.62). We get the bound states if we can find energies for which the homogeneous equation has a solution. When the integral equation is approximated by a matrix equation (as, for instance, Eq. (4.37) or Eq. (5.83)), we have to search for zeros of the determinant. Results of such a calculation [59] are plotted in Fig. 20. A three-boson system with a separable Yamaguchi potential is studied in this calculation in relation to the range parameter β . The coupling constant λ has been chosen in such a way that the two-particle binding energy is always $|E^B| = 1.5$ (in units where $\hbar = 2m = 1$). Since a three-particle bound state is rather densely packed, as compared to a two-particle bound state, its binding energy is sensitive to the range of the potential. This is true especially

for the ground state. Other than the three-nucleon system, the three-boson system, which is considered here, also has an excited state. For fermions and more realistic spin-dependent potentials (section 5.2.7), this state disappears.

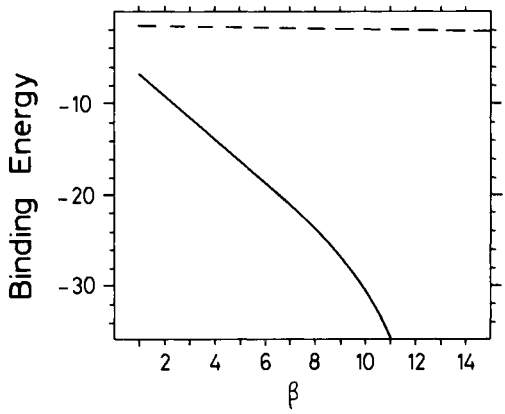

Fig. 20. Three-particle binding energy (——ground state, --- excited state) as a function of the range parameter β (R.D. Amado et al. [59])

2.5.2. Scattering States

Scattering calculations for the three-boson system have been performed with both methods of section 2.4. Figure 21 shows the result of a numerical solution of Eq. (5.83) above breakup threshold and the difference between this solution and the solution obtained by the contour deformation method. The agreement is rather good (1-2%).

Another test on the accuracy of such calculations is furnished by the optical theorem, Eq. (3.92). Since the total angular momentum is conserved, the difference between the total cross section and the elastic cross section must be equal to the breakup cross section for each partial wave, separately. The breakup cross section is given by the six-dimensional integral on the right-hand side of Eq. (3.91). While two integrations are trivial, four of them must be carried out numerically [60]. The three-dimensional integral of the elastic cross section is trivial in angular momentum decomposition. The results of such a test are presented in the following table for E = 5 :

L	$\sigma^L_{tot.} - \sigma^L_{el.}$	$\sigma^L_{breakup}$
0	0.2090	0.2082
1	0.0172	0.0199
2	0.4014	0.4023
3	0.1428	0.1427
4	0.0324	0.0318
5	0.00648	0.00642
6	0.001409	0.001409
7	0.000295	0.000294

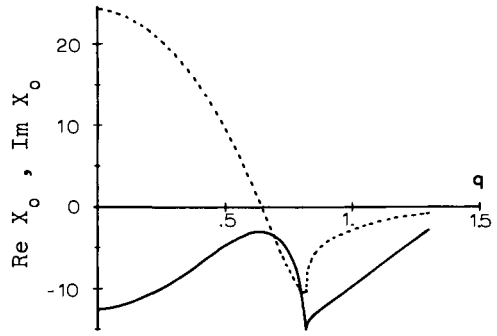

Fig. 21a. Solution $X_0(q,q',E)$ of Eq. (5.62) for zero total angular momentum; $E = 3q'^2/4m + E^B = 1$ with units: $\hbar=2m=1$, $E^B=-1.5$. Full line represents real part of X_0 , broken line represents imaginary part (F. Sohre and H. Ziegelmann [48]).

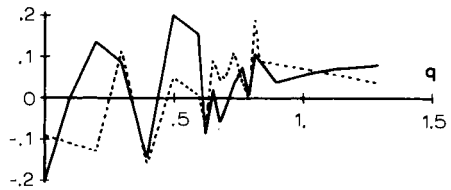

Fig. 21b. Differences of solutions calculated with and without contour deformation method. Full line represents real part, broken line imaginary part. Vertical scale 50 times larger than that of Fig. 21a.

Figure 22 shows the real part of the phase shifts in the elastic channel. They are related to the on-shell amplitude $X_L(q',q',E)$ by the formula

$$X_L \equiv X_L(q',q',E) = -\frac{3\pi}{m}\,\frac{e^{2i\delta_L}-1}{2iq'} \qquad (5.88)$$

Solved for $\tan(\mathrm{Re}\,\delta_L)$, we get [1]

$$\tan(\mathrm{Re}\,\delta_L) = \frac{\mathrm{Im}\,X_L}{\mathrm{Re}\,X_L} - \frac{\sqrt{1+\frac{4m^2q'^2}{9\pi^2}|X_L|^2+\frac{4mq'}{3\pi}\,\mathrm{Im}\,X_L}-1}{\frac{2mq'}{3\pi}\,\mathrm{Re}\,X_L} \qquad (5.89)$$

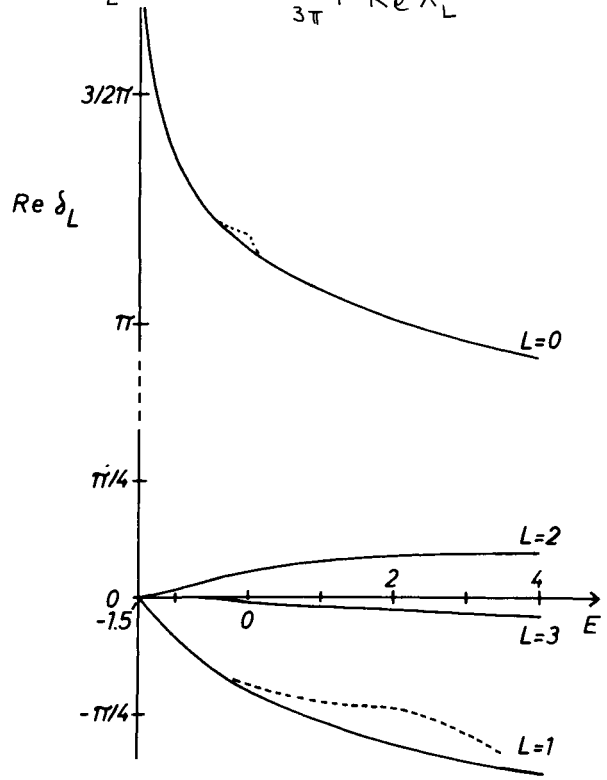

Fig. 22. Real part of the phase shifts versus total energy in the center-of-mass system (units: $\hbar$=2m=1, E^B=-1.5) for different total angular momenta (R.D. Amado et al. [59], F. Sohre and H. Ziegelmann [63])

---

[1] Below the breakup threshold, phases are real and Eq. (5.89) reduces to $\tan(\delta_L) = \mathrm{Im}X_L/\mathrm{Re}X_L$.

It is surprising that phases are positive for even values of L and negative for odd values of L. As has been shown by Amado [61], this comes from the fact that, in the three-particle system, the separable interaction is equivalent to an exchange mechanism.

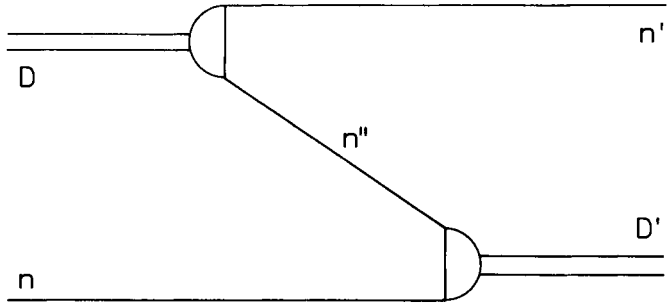

Fig. 23. Exchange mechanism in separable potential model

Assume two particles (see Fig. 23), n and D [1], where particle D can be broken up into two particles of type n,

$$D \rightleftharpoons n + n \quad .$$

The reaction,

$$n + D \rightarrow n' + D' \quad ,$$

can then be described by an exchange of a particle n" (compare also with Fig. 15; the line with momentum $-\vec{q}-\vec{q}'$ corresponds to the exchanged particle). Under the assumption of such a mechanism, Amado [61] derived the integral equation (5.53b) by field theoretical methods [62], without using the Faddeev equations. The effective potential Z_L in Eq. (5.62) becomes, as an exchange potential, necessarily attractive for even values of L and repulsive for odd L. This explains the sign of the phases. The dotted lines in Fig. 22 are older results of Amado [59]. In the meantime, more accurate calculations have shown that the δ_o-curve does not have a cusp at the breakup threshold [63]. This is in agreement with a prediction of Delves [64]

---

1) The names should remind us of "neutron" and "deuteron", although we are dealing here with spinless bosons.

which says that the small phase space, available for breakup at $E = o$, allows only a discontinuity in the second derivative.

It is also interesting to note that the $L = o$ phase starts at 2π and tends to zero for $E \to \infty$. The three-particle system we are dealing with has two bound states (compare with Fig. 20). The δ_o-curve, therefore, is in agreement with the Levinson theorem [65] which states that the number n_L of bound states (for given angular momentum L) is

$$n_L = \frac{\delta_L(o) - \delta_L(\infty)}{\pi} \qquad (5.90)$$

2.6. The Watson Model

For the experimentalist, the challenge of the three-particle problem lies in the fact that some two-nucleon data are accessible rather easily in a three-particle experiment, while it is hard or impossible to measure them in a two-particle experiment. Particles of very low energy, for instance, are difficult to handle and, therefore, the measurement of a scattering length in the two-particle system is afflicted with the uncertainty of an extrapolation. Or, since there are no neutron targets, the n-n data cannot be measured directly.

In a three-particle experiment, such things are no problem. When three particles leave the reaction volume they can have, for instance, a momentum distribution like the one shown in Fig. 24.

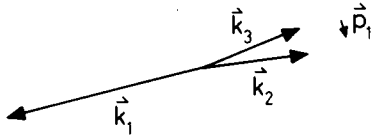

Fig. 24. Momentum configuration with small relative momentum in one subsystem

Particles 2 and 3 move almost parallel at the same velocity and have a relative momentum

$$\vec{p}_1 = \frac{1}{2} (\vec{k}_2 - \vec{k}_3) ,$$

which is close to zero. Nevertheless, the two particles are easy to detect since their momenta are reasonably large. Also, both particles may be neutrons. We thus have access to data at very low energy and to neutron-neutron data.

The difficulty in the present case lies in the theoretical interpretation of the experiment, that is, in the extraction of the desired data from the measured differential cross section.

Before the Faddeev equations and their solutions for breakup scattering were available, people were using the Watson model [66], which deals especially with states of low relative momentum $\vec{p}$. According to this model, a final state of three free particles is formed in two steps (Fig. 25).

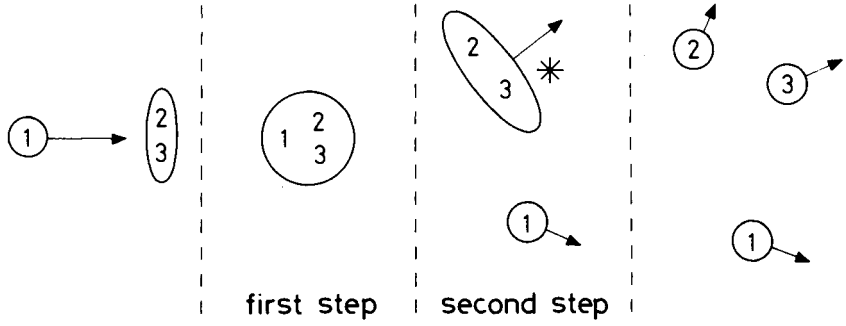

Fig. 25. Two-step breakup mechanism

In the first step, a three-particle compound state is formed (production process). In the second step, the particles leave the reaction volume, but two particles still interact for a rather long time because of their (assumed) small relative momentum. This interaction is called final state interaction. In this second step, the strong momentum dependence of the two-particle amplitude is superimposed on the three-particle amplitude. The momentum dependence of the latter is considered as comparatively small or negligible. The breakup amplitude is written as

$$U_{0\alpha} = \text{const} \cdot t_{\gamma} \quad , \tag{5.91}$$

where γ denotes the pair which undergoes a final state interaction ($p_{\gamma} \approx 0$). By Faddeev's theory, which can give an exact

expression for this amplitude (compare with Eq. (3.64)),

$$U_{0\alpha} = q_0^{-1} + \sum_{\gamma=1}^{3} t_\gamma q_0 U_{\gamma\alpha} \,, \tag{5.92}$$

the Watson model has been called in question. Firstly, there are three amplitudes adding up coherently in the exact expression, which could distort the t_γ-dependence and, secondly, the production amplitude $U_{\gamma\alpha}$ (or $X_{\gamma\alpha}$ in the separable case) shows a momentum dependence which is so strong (see Fig. 21a) that the approximation (5.91) becomes hard to believe. However, in the realistic nucleon-nucleon case, it turned out that the two effects act in opposite directions (see section 2.7 and reference [56]) and that the Watson model is not quite so bad for analyzing experiments. It also helps that in the two-nucleon singlet state the T-matrix has a pole extremely close to threshold which produces a very rapid momentum dependence for small relative momenta.

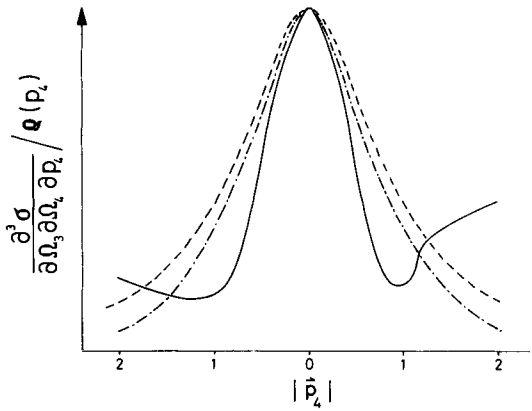

Fig. 26. Three-particle breakup cross section divided by the phase space factor for three identical bosons. Energy and angles in laboratory system, $E^{Lab}=79.5$, $\theta_3=15^\circ$, $\theta_4=23^\circ$ (the notation is as in Fig. 2 when the two-boson bound state is used as projectile; units: $\hbar=2m=1$, $E^B=-1.5$). Dashed line: Watson model; dot-dashed line: exact calculation, but only the leading term of the sum (5.92) is taken into account; full line: exact calculation, all terms of the sum (5.92) taken into account. The peaks are normalized to the same height (F. Sohre and H. Ziegelmann [63]).

Figure 26 shows a comparison of the Watson model with Faddeev theory for three identical bosons [63]. The differential cross section is plotted versus the relative momentum of the final state pair (as parameter of the kinematical curve; compare with Fig. 3). The dashed line shows the result of the Watson model (approximation (5.91)), the dot-dashed line is calculated with the leading term of the sum (5.92) alone, and the full line shows the Faddeev result (5.92). The discrepancy between the Watson and Faddeev theories is rather large in the present case.

2.7. Results for the Three-Nucleon System

The spin-dependence of nuclear forces is described, in lowest approximation, by a Yamaguchi potential of two terms,

$$V = \sum_{i=0}^{1} \lambda_i |\chi_i\rangle \langle\chi_i| \quad , \tag{5.93}$$

which yields a two-term separable T-matrix,

$$t = \sum_{i=0}^{1} |\chi_i\rangle \tau_i \langle\chi_i| \quad . \tag{5.94}$$

The form factors χ_i also act on the spin states to assure that the first term is effective only in the singlet state (i=o) and the second term only in the triplet state (i=1). The charge dependence of nuclear forces could be taken into account by introduction of a third term in the sum [55]. The form factors would then act also on the isospin states. With the T-matrix (5.94), the Faddeev equations (3.62) have a form similar to Eq. (5.39) and become, after antisymmetrization,

$$X^S_{i1} = Z^S_{i1} + \sum_{j=0}^{1} \eta^S_{ij} Z^S_{ij} X^S_{j1} \quad . \tag{5.95}$$

The superscript S denotes one of two possible values of total spin, $S = \frac{1}{2}$ or $S = \frac{3}{2}$, and the subscript i,j indicates transitions between different spin states of the subsystems.

In the doublet case ($S = \frac{1}{2}$), there are two coupled equations since three nucleon spins can be coupled in two different ways to form an $S = \frac{1}{2}$ state. In the quartet case ($S = \frac{3}{2}$), there is only one equation since $S = \frac{3}{2}$ can only be formed in one way

(all three spins parallel). The coupling is expressed by the spin factor η^S. This factor is [8,54,55]

$$\eta^{1/2} = \begin{pmatrix} 1/2 & -3/2 \\ -3/2 & 1/2 \end{pmatrix} , \qquad \eta^{3/2} = -1 . \qquad (5.96)$$

For the doublet scattering length $a^{1/2}$ of n-d scattering and for the triton binding energy E^T, it is difficult to obtain agreement between the results of Eq. (5.95) and experimental values. Figure 27 shows the present situation.

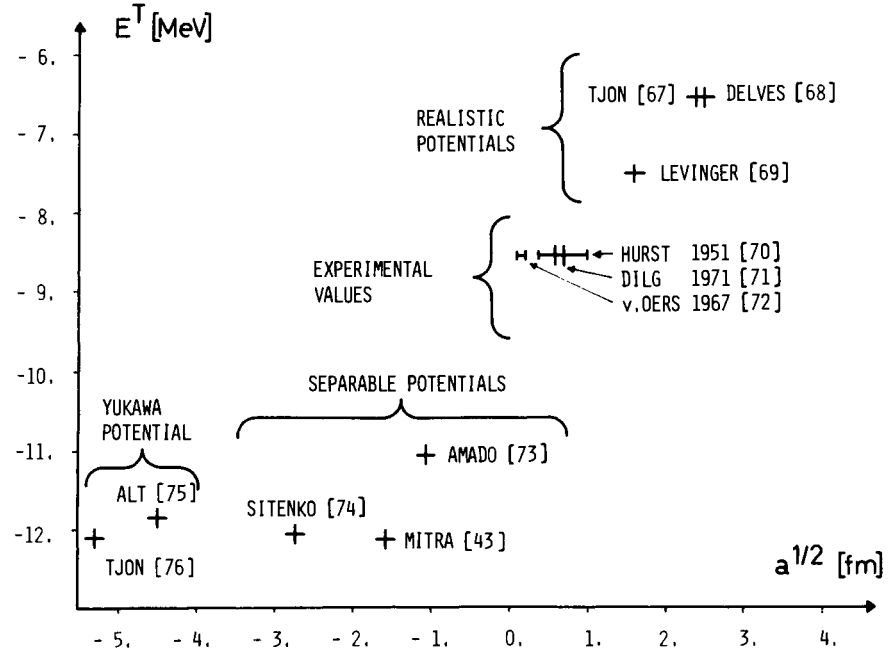

Fig. 27. Experimental and theoretical results of the triton binding energy plotted versus doublet scattering length ("Phillips' plot")

The triton is too tightly bound due to missing tensor and repulsive forces (the second bound state, mentioned in section 2.5, has disappeared, though). Calculations with local potentials seem to suffer even more from the missing repulsion. This may come from the fact that the high energy l = o phases are

reproduced considerably better by the separable potentials than by the local potentials, although all potential parameters have been fitted by low energy data, only. Potentials which are more realistic with respect to two-nucleon data give better three-particle results but, also here, the agreement is not perfect.

The quartet scattering length $a^{3/2}$ of n-d scattering, on the other hand, is in good agreement with experiment. In the quartet case (all spins parallel), the Pauli principle prevents the particles from coming close to each other and, thus, the details of the potential are less important. From Eq. (5.95), one obtains with a two-term Yamaguchi potential [73] $a^{3/2}$ = 6.32 fm. The experimental value [71] is $a^{3/2}$ = (6.35 ± 0.02)fm.

In view of the unsatisfactory results in the doublet case, it is astonishing to see how good the agreement between theory and experiment becomes for three-particle breakup, even with a simple ansatz (5.93). This may be partly due to the dominance of the antibound state pole in the singlet two-particle T-matrix at E = -0.067 MeV, which even causes the Watson model to yield good results.

In this context, it is interesting to note that Amado [77] has found a transformation of the Faddeev equations which supports the Watson model, Eq. (5.91). The breakup amplitude is, as we know,

$$U_{0\alpha} = \sum_{\gamma=1}^{3} t_\gamma g_0 U_{\gamma\alpha} + z - h_0 \quad . \tag{5.97}$$

As mentioned previously, it has been suspected that the coherent superposition of three amplitudes could destroy the typical Watson behavior of one single amplitude. However, subtracting from Eq. (5.97) the equation (3.61a) for rearrangement amplitudes,

$$U_{\beta\alpha} = \sum_{\gamma\neq\beta} t_\gamma g_0 U_{\gamma\alpha} + (1-\delta_{\beta\alpha})(z-h_0) , \tag{5.98}$$

one gets,

$$U_{0\alpha} - U_{\beta\alpha} = t_\beta g_0 U_{\beta\alpha} + \delta_{\beta\alpha}(z-h_0) ,$$

or,

$$U_{0\alpha} = (1 + t_\beta g_0) U_{\beta\alpha} + \delta_{\beta\alpha}(z - h_0) \quad . \tag{5.99}$$

According to Eq. (2.84b), we have

$$t_\beta = (1 + t_\beta g_0) v_\beta \ ,$$

or,

$$1 + t_\beta g_0 = t_\beta v_\beta^{-1} \quad . \tag{5.100}$$

Inserting this equation into Eq. (5.99), we get

$$U_{0\alpha} = t_\beta v_\beta^{-1} U_{\beta\alpha} + \delta_{\beta\alpha}(z - h_0) \quad . \tag{5.101}$$

This is an equation which is very similar to the Watson model, Eq. (5.91). The breakup amplitude $U_{0\alpha}$ is directly proportional to the two-particle T-matrix without any additional terms as in Eq. (5.97); the term $\delta_{\beta\alpha}(z-h_0)$ vanishes on the energy shell. In all configurations which have been explored experimentally and theoretically, the production amplitude $v_\beta^{-1} U_{\beta\alpha}$ of Eq. (5.101) seems to be weakly momentum dependent compared to t_β and, therefore, the approximation

$$U_{0\alpha} = \text{const} \cdot t_\beta \tag{5.102}$$

seems to be justified. This has been shown rather clearly for the solution of Eq. (5.95) by Ebenhöh [56]. He used a neutron-neutron potential which corresponds to an n-n scattering length of -16 fm. He analyzed his exact theoretical results by the Watson model, Eq. (5.91), as if they were experimental data. Under various kinematical conditions, he found values for the n-n scattering length between 15.4 fm and 16.4 fm. This means that by analyzing experimental data by the Watson model, one gets an error of less than ±0.5 fm, which is less than the experimental error. Nevertheless, breakup experiments are analyzed now by exact three-body calculations. Zeitnitz et al. [78]

have determined in this way the n-n scattering length to be [79]

$$a_{nn} = (-16.1 \pm 0.9)\ \text{fm} \quad . \tag{5.103}$$

This quantity is of interest in the theory of nuclear forces. The value given by Zeitnitz et al. supports the assumption of charge symmetry. According to this assumption, the forces in the n-n system and in the p-p system should be the same, except for Coulomb effects. Indeed, the difference between the p-p scattering length,

$$a_{pp} = -7.76\ \text{fm} \quad , \tag{5.104}$$

and the n-n scattering length (5.103) can be explained almost fully by Coulomb effects. Model calculations in which the Coulomb force has been "switched off" yield a chargeless scattering length [80] of

$$a = -17.2\ \text{fm} \quad . \tag{5.105}$$

The breakup reaction p + d → 2p + n is also described by Eq. (5.95) in kinematical regions where the Coulomb interaction, which is not present in the potential (5.93), plays only a minor role. In Fig. 28, the experimental results of Brückmann et al. [1] are shown together with a theoretical curve by Ebenhöh [56]. The differential cross section is plotted against the curve parameter S of the kinematical curve (see Fig. 3). The agreement is very good [1]. It is seen that the theory describes the experiment also for high relative momenta, where the Watson model fails.

One reason for the good agreement between theory and experiment is the fact that the quartet amplitude, which is

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[1] It should be noted, however, that the agreement is not always so good. Especially the absolute magnitude of the peaks sometimes [81,82] shows discrepancies up to 50%.

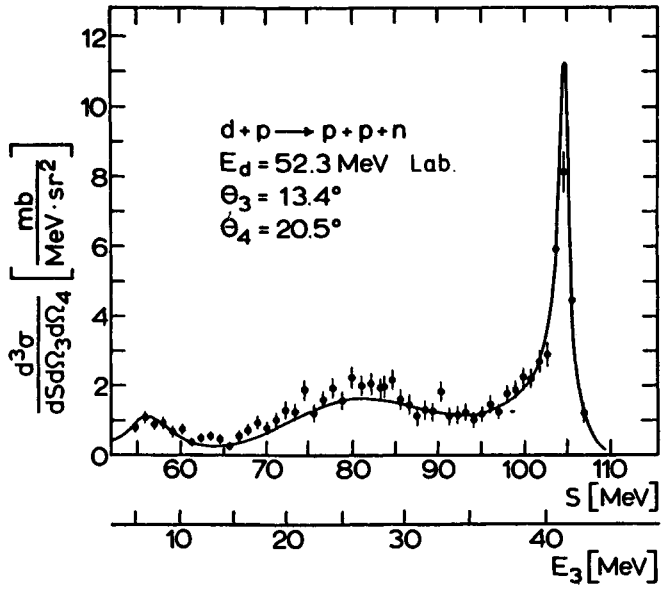

Fig. 28. Three-particle breakup cross section plotted versus curve parameter S, see Fig. 2 and 3 (W. Ebenhöh [56])

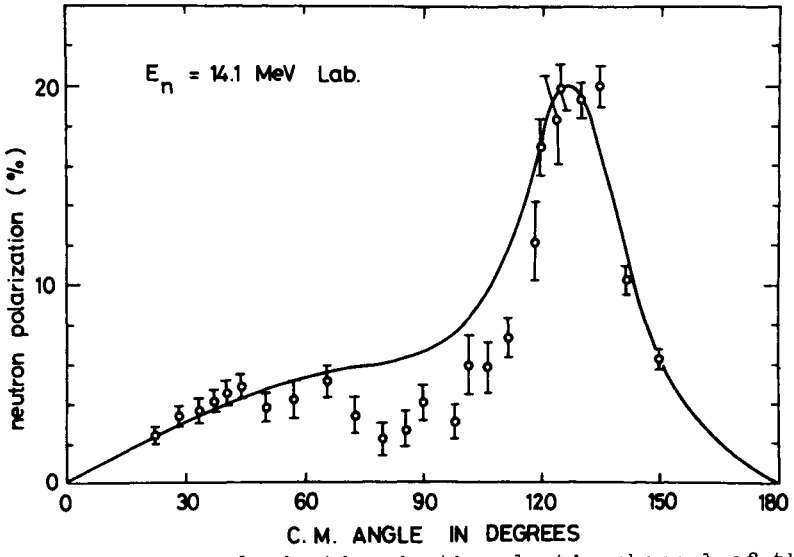

Fig. 29. Neutron polarization in the elastic channel of the n-d reaction (P. Doleschall [83], experimental values from J.C. Faivre et al.)

insensitive to details of the potential and which enters with higher weight, overrides the doublet amplitude. As soon as the two amplitudes are separated, it becomes more difficult to get good agreement, and more details of the nucleon-nucleon potential have to be included in order to get reliable results. In Fig. 29, the results of a polarization experiment are compared to the solution of Eq. (5.95). The theoretical curve [83] has been calculated with a separable potential which is a little more complicated than the potential (5.93). In addition to the S-state interaction, a $^3S_1$ - $^3D_1$ coupling and a P-state interaction have been included.

6. Solution of the Faddeev Equations for Local Potential

1. Direct Solution of the Faddeev Equations for Local Potential

The Faddeev equations have been solved for a local potential by a direct application of method (f) (p. 79) only once [84] and then only for the three-boson bound state under simplifying assumptions. It has been assumed that the local potential

$$V(\vec{p}-\vec{p}') = \sum_{\ell=0}^{\infty} (2\ell+1) P_\ell(\hat{p}\cdot\hat{p}') V_\ell(p,p') \tag{6.1}$$

is effective only in s-waves, i.e., all terms but the first one in the sum are neglected,

$$V(\vec{p}-\vec{p}') \approx V_0(p,p') \ . \tag{6.2}$$

If we would further assume that v_0 factorizes,

$$V_0(p,p') \approx \lambda \chi(p) \chi(p') \ , \tag{6.3}$$

we would be back at the separable approximation of the preceding chapter. It can be seen from the calculations of Osborn [84] that the "little difference" between the potentials (6.2) and (6.3) leads to unpleasant complications of the practical calculation. The way of directly solving the Faddeev equations for a local potential has, therefore, not been attempted for scattering states.

As has been mentioned previously, the Faddeev equations for local potential are, after angular momentum decomposition, an infinite set of coupled two-dimensional integral equations. For identical particles, they become decoupled by the assumption (6.2). Osborn obtained the bound state wave function by solving the (homogeneous) integral equation

$$F_0(q,Q) = \int_0^\infty dq' \int_{q^2+q'^2-qq'}^{q^2+q'^2+qq'} dQ' \, K_0(q,Q;q',Q') F_0(q',Q') \ , \tag{6.4}$$

with the kernel

$$K_0(q,Q;q',Q') = \frac{2q'}{\pi q} \frac{\hat{t}_0\left(\sqrt{Q^2-\frac{3}{4}q^2}, \sqrt{Q'^2-\frac{3}{4}q^2}, z-\frac{3}{4m}q^2\right)}{mz-Q'^2} .$$

It is rather time-consuming to approximate the two-dimensional integral by a sum. A second problem comes from the variable limits of the Q'-integration, which is caused by the δ-functions in Eq. (4.8). Figure 30 shows the two-dimensional integration region, together with a two-dimensional integration mesh [1].

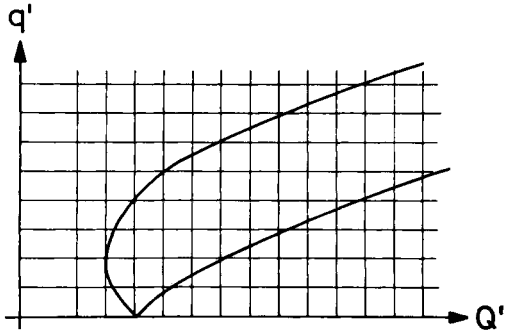

Fig. 30. Range of integration in Eq. (6.4) and integration mesh

Because of the particular shape of the integration region, only a fraction of the mesh points, which have been introduced for the Q'-integration, becomes effective. The approximation, therefore, is rather poor. Osborn solved this problem by approximating the integrand by an interpolation polynomial (in Q'-direction) which is built on a l l mesh points. The polynomial is then integrated analytically for every value of q'.

The integral equation is thus approximated rather accurately by a matrix equation for the values of the wave function at the mesh points. Osborn used 7 points in q'-direction and 15 points in Q'-direction which gives a 105 x 105 matrix. The energies for which the determinant of the matrix equation vanishes are three-particle binding energies, provided that they are lower than the two-particle binding energy. The wave functions can be

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[1] The infinite integration region does not pose a problem because it can be transformed into a finite one.

calculated from the corresponding eigenvectors. Figure 31 shows the results for the Yukawa potential $V(r) = g \exp(-0.633r)/r$.

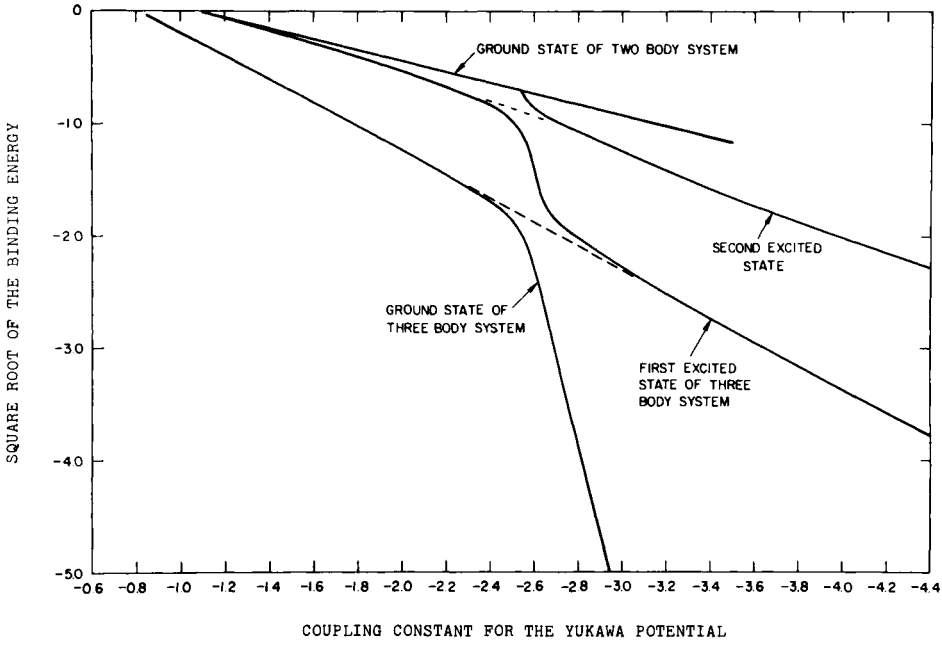

Fig. 31. Square root of the three-boson binding energy (units: $\hbar$=m=1) plotted versus Yukawa coupling constant (T.A. Osborn [84])

There is a three-particle bound state already for coupling constants $-0.8 \geq g \geq -1.1$ which are too weak to bind the two-particle system. As soon as two-particle binding occurs ($g \leq -1.1$), a second three-particle bound state appears. At $g = -2.5$, according to Osborn's interpretation, a third three-particle bound state appears. At the same time, something rather strange happens. Ground state and first excited state become very sensitive to small changes of the coupling constant. As has been seen in later calculations [85-87], this behavior arises from an instability of the matrix approximation and is caused by integration errors. Delves [88] has studied such matrix approximations and found out that, at the first instability, the lowest eigenvalue becomes meaningless and the second one takes over its role.

When the equation

$$A\vec{x}_i = \lambda_i \vec{x}_i \tag{6.5}$$

defines the exact eigenvalues λ_i , and the equation

$$\tilde{A}\tilde{\vec{x}}_i = \tilde{\lambda}_i \tilde{\vec{x}}_i \tag{6.6}$$

yields eigenvalues $\tilde{\lambda}_i$ which are afflicted with integration errors, then, before an instability occurs, the eigenvalues $\tilde{\lambda}_i$ are more or less good approximations to the exact eigenvalues in their natural order,

$$\lambda_i \approx \tilde{\lambda}_i \quad , \qquad i = 0,1,2,\cdots . \tag{6.7}$$

After the first instability has occurred, the lowest eigenvalue $\tilde{\lambda}_0$ has nothing more to do with the exact spectrum. Its existence is based solely on integration errors. But, ignoring $\tilde{\lambda}_0$ and making the assignment

$$\lambda_i \approx \tilde{\lambda}_{i+1} \quad , \qquad i = 0,1,2,\cdots . \tag{6.8}$$

the spectrum of Eq. (6.6) can still be a reasonable approximation.

The same effect can be seen in Fig. 31. As the results of more accurate calculations (broken lines) show, the first excited state takes over the role of the ground state and the second excited state becomes the first excited state. This interpretation is also supported by the behavior of the wave function. In Osborn's calculation, the wave function of the first excited state has two nodes for g > -2.5 and only one node for g < -2.5.

We see that it is difficult to solve the Faddeev equations directly, even for the three-boson bound-state problem under simplifying assumptions. Nevertheless, Kim et al. [85] succeeded in solving the Faddeev equations for the bound-state problem with realistic potentials by using a new integration technique.

Another possibility for solving the Faddeev equations for a local potential is the expansion method [89-91] of the previous chapter (see Eq. (5.27)). It leads to a coupled system of one-dimensional integral equations. In general, there will be N integral equations for an expansion of the local potential into

N independent, separable terms. Using an integration rule of n mesh points, the computer has to invert matrices of dimension (n x N). Also here, the limit in computer capacity is reached very quickly.

From this point of view, the dissection process of Erhard Schmidt (see Chapter 4, section 2) becomes interesting. Its application leads to a small number of coupled integral equations, which contain the finer details of the potential in the form of a fast converging Neumann series.

2. The Schmidt Method (Weinberg's Quasiparticle Method)

The dissection method of Schmidt [36] has first been used by Weinberg [34] in 1963 for scattering problems. Since Weinberg, this method is usually called the quasiparticle method because Weinberg called all two-particle bound states and resonances, which spoil the convergence of the Neumann series (see Chapter 4, section 2a), quasiparticles. We will assume in the following that there is only one quasiparticle, namely the two-particle bound state. A generalization to many quasiparticles is possible and not difficult, according to Chapter 4, section 2d.

We consider the equation for the two-particle T-matrix and study its solution by expansion into a Neumann series. According to Eqs. (4.17a,b), the Neumann series converges when all eigenvalues of the kernel have an absolute value smaller than 1. For the left eigenfunctions [1] of the kernel, we have

$$\langle\varphi_\nu(z)|K(z) = \langle\varphi_\nu(z)|V g_0(z) \qquad (6.9)$$

$$= \eta_\nu(z)\langle\varphi_\nu(z)| \ .$$

---

[1] Left eigenfunctions, $\langle\varphi_\nu|K = \eta_\nu\langle\varphi_\nu|$, and right eigenfunctions, $K|\bar{\varphi}_\nu\rangle = \eta_\nu|\bar{\varphi}_\nu\rangle$, are different for an unsymmetrical kernel K. The eigenvalues η_ν , however, are the same. We prefer left eigenfunctions because they are easier to relate to the Schrödinger equation.

Eigenfunctions and eigenvalues depend on the energy z, which is complex, in general. With respect to practical applications, we restrict the range of z to

$$z = E \quad \text{for} \quad E < o \tag{6.10a}$$

and

$$z = E+i\varepsilon \quad \text{for} \quad E \geq o \ , \tag{6.10b}$$

where E is the energy of the two-particle system. With the energy z taken from the range (6.10) the eigenfunctions will be normalizable. This is no longer true in the limit $\varepsilon \to o$, but everything that will be said about the eigenvalues also remains valid in this limit.

The physical meaning of the eigenvalues η_ν is easily understood. We multiply Eq. (6.9) by $[\eta_\nu(z)g_o(z)]^{-1}$ from the right and get

$$\langle\varphi_\nu(z)|\, V\, \eta_\nu^{-1}(z) = \langle\varphi_\nu(z)|\,(z-h_o) \ ,$$

or,

$$\langle\varphi_\nu(z)|(h_o + V\,\eta_\nu^{-1}(z)) = z\,\langle\varphi_\nu(z)| \ . \tag{6.11}$$

As we see, the eigenfunctions $\langle\varphi_\nu|$ of Eq. (6.9) are solutions of the adjoint Schrödinger equation (6.11) with energy z and potential $v\eta_\nu^{-1}(z)$; both energy and potential can be real or complex. The quantity $\eta_\nu^{-1}(z)$ plays the role of a coupling constant which causes the Schrödinger equation to have a normalizable solution for (real or complex) energy z.

In Fig. 32, the behavior of the first four eigenvalues $\eta_\nu(z)$ for s-wave functions and the Hulthén potential,

$$V(r) = \frac{2}{e^r - 1} \ , \tag{6.12}$$

is depicted. The argument z is given by Eqs. (6.10a,b) and by $-\infty < E < +\infty$. The arrows at the curves point in the direction of increasing energy. The transformation of Eq. (6.9) into Eq. (6.11) allows a qualitative interpretation of the curves. When the energy E becomes equal to the energy E^B of the bound state, the first eigenvalue η_1 becomes equal to one, and Eq. (6.11) becomes the Schrödinger equation for the bound state with an unmodified potential.

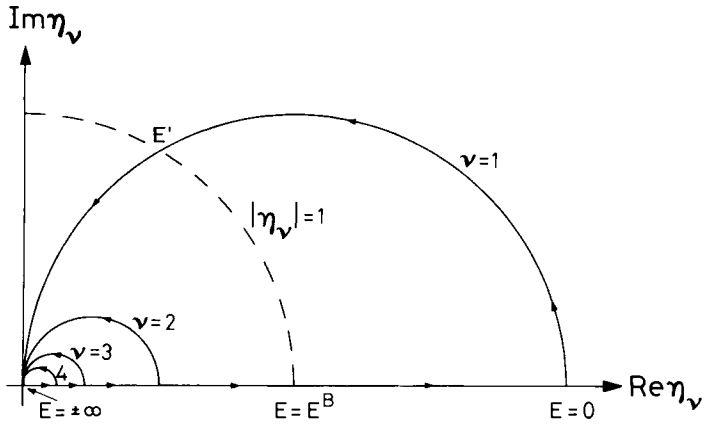

Fig. 32. The first four l = o eigenvalues $\eta_\nu(E+io)$ for the Hulthén potential, Eq. (6.12)

For $E < E^B$, the eigenvalue η_1 must be smaller than one because, in order to produce a bound state of energy $E < E^B$, the modified potential $v\eta_1^{-1}$ must become stronger. For $E \to -\infty$, all eigenvalues become zero because an infinite binding energy means infinitely strong coupling.

On the other hand, we get $\eta_1 > 1$ for $E^B < E < o$; since we ask for a smaller binding energy, the coupling becomes weaker. Our potential (6.12) has only one bound state and, therefore, the higher eigenvalues do not reach $\eta = 1$. For $E > o$, the eigenvalues can no longer be real because the kernel becomes complex. The curves $\eta_\nu(z)$, therefore, leave the real axis. For $E \to +\infty$, they all must come back to the origin.

In the present case, the Neumann series does not converge in the energy range

$$E^B \leq E \leq E' ,$$

because, here, $|\eta_1(E+i\varepsilon)| \geq 1$. In order to achieve convergence, we want to split off a separable kernel in such a way that all eigenvalues of the residual kernel lie within the unit circle. We can do this by subtracting the separable potential

$$V^S(z) = |\bar{\varphi}_1(z)\rangle\langle\bar{\varphi}_1(z^*)| \qquad (6.13)$$

from the original one, as can be seen immediately from Eq.(5.27). This dissection eliminates the eigenvalue η_1 , while all other eigenvalues remain unchanged. Splitting off potential (6.13) is, of course, not the only possibility. Any subtraction of a separable potential,

$$V' = V - V^S = V - \lambda |\chi\rangle\langle\chi| \quad , \tag{6.14}$$

leads to a converging Neumann series for the residual kernel,

$$K'(z) = V' g_0(z) = (V - V^S) g_0(z) = V g_0(z) - \lambda |\chi\rangle\langle\chi| g_0(z) \quad , \tag{6.15}$$

if all eigenvalues η'_ν of this kernel have absulute values smaller than 1 ,

$$\langle \varphi'_\nu(z)| K'(z) = \eta'_\nu(z) \langle \varphi'_\nu(z)| \quad , \qquad |\eta'_\nu(z)| < 1 \quad . \tag{6.16}$$

In general, though, it is not as easy to check whether condition (6.16) is fulfilled, as in case of the "ideal choice" (6.13).

We assume now that condition (6.16) is fulfilled for the splitting (6.14), and we solve Eq. (2.56a) for the two-body T-matrix [1],

$$t = V' + \lambda |\chi\rangle\langle\chi| (1 + g_0 t) + V' g_0 t \quad . \tag{6.17}$$

Bringing the last term on the right-hand side to the left-hand side, and multiplying by $(1-v'g_0)^{-1} = 1+t'g_0$ (compare with Eq. (2.59b)) from the left, we get

$$t = t' + (1 + t' g_0) |\chi\rangle \lambda \langle\chi| (1 + g_0 t) \quad . \tag{6.18}$$

---

[1] For simplicity, we assume that the potential v has only one bound state, and we also assume that the form factors χ do not depend on the energy z. Such a dependence could be included without difficulty.

We have introduced here the T-matrix of the residual interaction v' ,

$$t' = (1 - v' g_0)^{-1} v' \quad . \tag{6.19}$$

Assuming t' to be known, we can solve Eq. (6.18). We multiply the equation by $\langle\chi| g_0$ from the left and add $\langle\chi|$ on both sides,

$$\langle\chi|(1+g_0 t) = \langle\chi|(1+g_0 t') \tag{6.20}$$
$$+ \langle\chi| g_0 (1+t' g_0)|\chi\rangle \lambda \langle\chi|(1+g_0 t) \quad .$$

This gives us the unknown state $\langle\chi|(1+g_0 t)$,

$$\langle\chi|(1+g_0 t) = \frac{\langle\chi|(1+g_0 t')}{1 - \lambda \langle\chi| g_0 (1+t' g_0)|\chi\rangle} \quad . \tag{6.21}$$

Inserting this expression into Eq. (6.18), we finally get

$$t(z) = t'(z) + |\tilde{\chi}(z)\rangle \tau(z) \langle\tilde{\chi}(z^*)| \quad , \tag{6.22}$$

with

$$|\tilde{\chi}(z)\rangle = (1 + t'(z) g_0(z))|\chi\rangle \quad , \tag{6.23}$$

and

$$\tau(z) = \left(\lambda^{-1} - \langle\chi| g_0(z)\left[1 + t'(z) g_0(z)\right]|\chi\rangle\right)^{-1} \tag{6.24}$$
$$= \left(\lambda^{-1} - \langle\chi| g_0(z)|\tilde{\chi}(z)\rangle\right)^{-1} \quad .$$

The T-matrix can thus be written as a sum of a separable T-matrix and a non-separable rest. Note the similarity between this result and the result (5.9) for purely separable potential. For $v = v^s$, i.e., $v' = o$, we have $t' = o$, and Eq. (6.22) goes over into Eq. (5.9).

We have assumed the matrix $t'(z)$ to be known. It can be obtained by its Neumann series,

$$t'(z) = \sum_{\nu=0}^{\infty} (v' g_0(z))^{\nu} v' \quad , \tag{6.25}$$

since, according to our assumption, all eigenvalues of the kernel $v'g_0$ have an absolute value smaller than 1.

From our result (6.22), we can derive a necessary condition for the separable potential. We know that the T-matrix has a pole at the energy of the bound state (we have assumed one bound state in the present case). This pole must be fully contained in the separable part $|\tilde{\chi}>\tau<\tilde{\chi}|$ of the T-matrix because the Neumann series for t' does not converge when there is a pole in t'. For this reason, we have to postulate that the denominator of the function $\tau(z)$ vanishes at $z = E^B$. We thus obtain a relation for the coupling parameter λ (in analogy to Eqs. (5.16a,b),

$$\lambda^{-1} = \langle \chi | g_0(E^B) (1 + t'(E^B) g_0(E^B)) | \chi \rangle \quad . \tag{6.26}$$

This relation becomes clearer when we calculate the bound state of our potential by the quasiparticle method. As has been discussed earlier (compare with Eq. (5.11)), the wave function of the bound state satisfies the equation

$$\langle \psi | = \langle \psi | v g_0(E^B) \quad . \tag{6.27}$$

With the splitting (6.14), this becomes

$$\langle \psi | = \lambda \langle \psi | \chi \rangle \langle \chi | g_0(E^B) + \langle \psi | v' g_0(E^B) \quad .$$

Bringing the second term on the right-hand side to the left-hand side and multiplying by $(1-v'g_0)^{-1} = 1+t'g_0$ (see Eq. (2.59b)) from the right, we get

$$\langle \psi | = \lambda \langle \psi | \chi \rangle \langle \chi | g_0(E^B) (1 + t'(E^B) g_0(E^B)) \quad . \tag{6.28}$$

Up to a normalization constant N, the bound state wave function is

$$\langle \psi | = N \langle \chi | g_0(E^B) (1 + t'(E^B) g_0(E^B)) = N \langle \tilde{\chi} | g_0(E^B) \quad . \tag{6.29}$$

The quasiparticle method fails unless

$$\langle\psi|\chi\rangle \neq 0 \quad , \tag{6.30}$$

otherwise $\langle\psi|(1-v'g_0(E^B))$ would be zero, and the operator $(1-v'g_0(E^B))^{-1}$ would not exist.

Condition (6.26) for the coupling constant λ can be written, by help of Eq. (6.29), as

$$\lambda^{-1} = \langle\psi|\chi\rangle \quad , \tag{6.31}$$

when the form factor χ is normalized in such a way that the normalization constant N is equal to one. In practical calculations, only a small number of terms of the Neumann series (6.25) can be taken into account. As a zero order approximation, $t' \approx 0$, we get, as mentioned before, the separable approximation, Eq. (5.9). In the first approximation, we get from Eqs. (6.22-6.25)

$$t(z) = v' + \frac{(1+v'g_0(z))|\chi\rangle\langle\chi|(g_0(z^*)v'+1)}{\lambda^{-1} - \langle\chi|g_0(z)(1+v'g_0(z))|\chi\rangle} \quad . \tag{6.32}$$

Scadron and Weinberg [92] have used the various approximations to find out for which value of the coupling constant g in a Yukawa potential,

$$V(r) = g\frac{e^{-r}}{r} \quad , \tag{6.33}$$

the scattering length becomes infinite (at this value the two-particle system has a bound state of zero energy).

If one used the so-called Born approximation,

$$t(z) \approx v \quad , \tag{6.34}$$

despite the fact that the Neumann series does not converge, one would get

$$g = \infty \quad . \tag{6.35}$$

The zero order approximation of Eqs. (6.22-6.25), $t' \approx o$ yields, for the form factor used by Scadron and Weinberg,

$$g = -2. \tag{6.36}$$

In first order, Eq. (6.32), with the same form factor, the constant g becomes

$$g = -1.765\ldots, \tag{6.37}$$

while the exact value is

$$g = -1.6798\ldots . \tag{6.38}$$

As we see, the first order approximation (sometimes called quasi-Born approximation) gives a rather good result in a case where the Born approximation fails completely.

3. The Quasiparticle Method in the Three-Particle Problem

3.1. The Alt-Grassberger-Sandhas Equations

The simplification of the Faddeev equations which we get for a separable potential in Chapter 5 had essentially two reasons. Firstly, the T-matrix,

$$t_\gamma = |\chi_\gamma\rangle \tau_\gamma \langle\chi_\gamma| , \tag{6.39}$$

became a projection operator, and we could derive simple equations for the operator $g_o U_{\beta\alpha} g_o$ sandwiched between projection states,

$$X_{\beta\alpha} = \langle\chi_\beta| g_o U_{\beta\alpha} g_o |\chi_\alpha\rangle , \tag{6.40}$$

and secondly, the operators $X_{\beta\alpha}$ already contained enough information to determine the S-matrix.

In the same way, we should try now not to calculate "too much" when we apply the quasiparticle method to the Faddeev equations. In this method, we have a T-matrix which is similar

to the T-matrix (6.39), even though we have a local potential [1],

$$t_\gamma(z) = |\tilde{\chi}_\gamma(z)\rangle \tau_\gamma(z) \langle \tilde{\chi}_\gamma(z^*)| + t'_\gamma(z) = t^s_\gamma(z) + t'_\gamma(z) \quad . \tag{6.41}$$

We do not insist, now, on calculating the full operators $U_{\beta\alpha}$, but settle for a calculation of the operators

$$\langle \vec{q}'_\beta | X_{\beta\alpha}(E_\alpha + i0) | \vec{q}_\alpha \rangle = \langle \phi_\beta | U_{\beta\alpha}(E_\alpha + i0) | \phi_\alpha \rangle \quad , \alpha, \beta = 1,2,3 \quad , \tag{6.42}$$

which are the only relevant ones for the S-matrix. For the channel functions ϕ_α, ϕ_β, $\alpha,\beta = 1,2,3$, we can write, by generalizing Eq. (6.29) to three-particle space,

$$|\phi_\alpha\rangle = g_0(E_\alpha)\left(1 + t'_\alpha(E_\alpha) g_0(E_\alpha)\right)|\chi_\alpha\rangle|\vec{q}_\alpha\rangle = g_0(E_\alpha)|\tilde{\chi}_\alpha(E_\alpha)\rangle|\vec{q}_\alpha\rangle \quad . \tag{6.43}$$

The operators $X_{\beta\alpha}$ thus get a form analogous to Eq. (5.36),

$$X_{\beta\alpha}(z) = \langle \tilde{\chi}_\beta(z^*)| g_0(z) U_{\beta\alpha}(z) g_0(z) |\tilde{\chi}_\alpha(z)\rangle \quad , \alpha, \beta = 1,2,3 \quad , \tag{6.44}$$

also in the present case of a local potential. Again, we have represented the important transition operators $X_{\beta\alpha}$ as matrix elements of the operators $g_o U_{\beta\alpha} g_o$ between the states which are the projection states of the T-matrix.

In deriving an integral equation for the operators $X_{\beta\alpha}$, we now have to take care of the quantities t'_γ which express the fact that we are dealing with a non-separable potential.

We use the analogy (as mentioned on page 63) of the equation for the two-particle T-matrix and the Faddeev equations for the operators $U_{\beta\alpha}$.

---

[1] This is our result (6.22) in three-particle space. For the separable part of the T-matrix, we get in momentum representation

$$\langle \vec{p}_\gamma, \vec{q}_\gamma | t^s_\gamma(z) | \vec{p}'_\gamma, \vec{q}'_\gamma \rangle =$$

$$\delta(\vec{q}_\gamma - \vec{q}'_\gamma)\tilde{\chi}_\gamma(\vec{p}_\gamma; z - q_\gamma^2/2M_\gamma)\tau_\gamma(z - q_\gamma^2/2M_\gamma)\tilde{\chi}_\gamma(\vec{p}'_\gamma; z - q_\gamma^2/2M_\gamma) \quad .$$

By the definition (α, β = 1,2,3)

$$(G_0^s)_{\beta\alpha} = \delta_{\beta\alpha} g_0 t_\beta^s g_0 \quad , \quad (G_0')_{\beta\alpha} = \delta_{\beta\alpha} g_0 t_\beta' g_0 \quad , \tag{6.45}$$

we introduce the dissection (6.41) into the Faddeev equations (3.70),

$$T = V + VG_0^s T + VG_0' T \quad .$$

We bring the last term on the right-hand side to the left-hand side and multiply by $(1 - VG_0')^{-1}$. With the definition,

$$T' = (1 - VG_0')^{-1} V \quad , \tag{6.46}$$

we get

$$T = T' + T' G_0^s T \quad . \tag{6.47}$$

Returning to our explicit notation with partition indices, we have for α, β = 1,2,3

$$U_{\beta\alpha} = U'_{\beta\alpha} + \sum_{\gamma=1}^{3} U'_{\beta\gamma} g_0 |\tilde{\chi}_\gamma\rangle \tau_\gamma \langle\tilde{\chi}_\gamma| g_0 U_{\gamma\alpha} \quad , \tag{6.48}$$

where $U'_{\beta\alpha}$ is defined by

$$U'_{\beta\alpha} = (T')_{\beta\alpha} \quad .$$

Equation (6.48) corresponds to the Faddeev equations for separable potential, except for the appearance of an operator $U'_{\beta\alpha}$ which contains the non-separable part of the potential. We only have to take matrix elements of Eq. (6.48) between the states $\langle\tilde{\chi}_\beta(z^*)| g_0(z)$ and $g_0(z)|\tilde{\chi}_\alpha(z)\rangle$ to get an equation for the relevant operators (6.44),

$$X_{\beta\alpha}(z) = X'_{\beta\alpha}(z) + \sum_{\gamma=1}^{3} X'_{\beta\gamma}(z) \tau_\gamma(z) X_{\gamma\alpha}(z) \quad , \tag{6.49}$$

with

$$X'_{\beta\alpha}(z) = \langle\tilde{\chi}_\beta(z^*)| g_0(z) U'_{\beta\alpha}(z) g_0(z) |\tilde{\chi}_\alpha(z)\rangle \quad , \quad \alpha,\beta = 1,2,3 \quad .$$

The set of equations (6.49) are the AGS-equations (Alt, Grassberger, Sandhas [23]) for the transition operators. The Faddeev equations have thus been reduced to a set of simpler

equations, just as in the case of a separable potential. The problem is now to calculate the operators $X'_{\beta\alpha}$ or $U'_{\beta\alpha} = (T')_{\beta\alpha}$. From the definition (6.46), we get by multiplying with $(1-VG'_0)$ from the left

$$T' = V + VG'_0T' \quad . \tag{6.50a}$$

This is a Faddeev equation,

$$U'_{\beta\alpha} = (1-\delta_{\beta\alpha})\,g_0^{-1} + \sum_{\gamma=1}^{3}(1-\delta_{\beta\gamma})\,t'_\gamma\,g_0\,U'_{\gamma\alpha} \quad , \tag{6.50b}$$

which would be as hard to solve as the original one, Eq. (3.62). But we do not have to solve it ! It is the essence of the quasiparticle method to get along with an iteration approximation for the operators which represent the non-separable rest of the potential,

$$U'_{\beta\alpha} = (1-\delta_{\beta\alpha})\,g_0^{-1} + \sum_{\gamma\neq\alpha,\beta} t'_\gamma + \ldots \quad . \tag{6.51}$$

The breakup operators are obtained in a similar way as in the case of a purely separable potential. Eq. (3.70) is also valid for α, $\beta = 0,1,2,3$; it then represents Eq. (3.61a) instead of Eq. (3.62). The same is true for Eq. (6.48). Taking matrix elements of this equation between the states $\langle\vec{p}_\alpha|$ and $g_0(z)|\tilde{\chi}_\alpha(z)\rangle$ and putting $\beta = 0$, we get the analogue of Eq. (3.64) which relates the breakup operators $X_{0\alpha}$ to the rearrangement operators $X_{\beta\alpha}$.

3.2. Application of the Quasiparticle Method to the Three-Particle Resolvent Equation

The effective two-particle equations, which have been derived in the last section from the Faddeev equations by means of the quasiparticle method, can be obtained also without using Faddeev's theory [93]. In the derivation, we did not have to use the compactness property of the Faddeev kernel, since the Faddeev equations (6.50a,b) have been solved by iteration. It becomes intelligible, therefore, that the quasiparticle method can also be used for integral equations (like the resolvent equation, for instance) which do not have a compact kernel.

It has become clear in the last section that the complexity of the Faddeev equation comes mainly from the fact that this equation yields the full set of transition operators $U_{\beta\alpha}$. Since only matrix elements of these operators between two-particle bound states are needed for the S-matrix, it has been possible to get simpler equations. If we now start to derive quasiparticle equations for the resolvent, we should also first find out which matrix elements are really needed.

According to Eq. (2.99), the resolvent yields the scattering states in the form of an ε-limit. From the scattering state, we get the S-matrix by a time limit, Eqs. (3.40a,b,c). Combining the two equations, we get

$$S_{\beta\alpha}(\vec{q}'_\beta,\vec{q}_\alpha)=\lim_{t\to\infty}\lim_{\epsilon\to 0} e^{i(E_\beta-E_\alpha)t}\, i\epsilon\,\langle\vec{q}'_\beta|\langle\psi_\beta|G(E_\alpha+i\epsilon)|\psi_\alpha\rangle|\vec{q}_\alpha\rangle. \quad (6.52)$$

In the following, it will be important that Eq. (6.52) remains valid when the two-particle bound states ψ_γ are replaced by the states $\lambda_\gamma|\chi_\gamma\rangle$ [93], provided that

$$\lambda_\gamma^{-1}=\langle\psi_\gamma|\chi_\gamma\rangle\ . \quad (6.53)$$

The state $\lambda_\gamma|\chi_\gamma\rangle$ will then contain the bound state $|\psi_\gamma\rangle$ with amplitude 1 plus a component $|\varphi_\gamma\rangle$ of the two-particle continuum (as previously, we assume that there is only one bound state in each subsystem),

$$\lambda_\gamma|\chi_\gamma\rangle=|\psi_\gamma\rangle+|\varphi_\gamma\rangle\ . \quad (6.54)$$

The bound state wave function does not have to be known. Only the overlap (6.53) enters into the S-matrix,

$$S_{\beta\alpha}(\vec{q}'_\beta,\vec{q}_\alpha)= \quad (6.55)$$

$$\lim_{t\to\infty}\lim_{\epsilon\to 0} e^{i(E_\beta-E_\alpha)t}\, i\epsilon\,\lambda_\beta\langle\vec{q}'_\beta|\langle\chi_\beta|G(E+i\epsilon)|\chi_\alpha\rangle|\vec{q}_\alpha\rangle\lambda_\alpha\ .$$

For breakup, we similarly get

$$S_{0\alpha}(\vec{q}'_\alpha, \vec{p}'_\alpha; \vec{q}_\alpha) = \lim_{t\to\infty}\lim_{\epsilon\to 0} e^{i\left(\frac{q'^2_\alpha}{2M_\alpha} + \frac{p'^2_\alpha}{2\mu_\alpha} - E_\alpha\right)t} \; i\epsilon \langle \vec{q}'_\alpha, \vec{p}'_\alpha | G(E_\alpha + i\epsilon) | \chi_\alpha \rangle | \vec{q}_\alpha \rangle \lambda_\alpha . \tag{6.56}$$

The reason for this simplification lies in the fact that the continuum component $|\varphi_\gamma\rangle$ of the state $\lambda_\gamma|\chi_\gamma\rangle$ does not "survive" the limit process in Eqs. (6.55 and 6.56). The component $|\varphi_\gamma\rangle$ does not lead to a pole which would be needed in order to get a contribution to the S-matrix (compare with Eqs. (2.48-2.50)). We now will show that application of the quasiparticle method to the resolvent equation (2.101a) yields exactly the matrix elements

$$\langle \chi_\beta | G(z) | \chi_\alpha \rangle , \tag{6.57}$$

which are needed in Eq. (6.55). We split the given two-particle potential v_γ into a separable part v^s_γ and a non-separable rest v'_γ ,

$$v_\gamma = v^s_\gamma + v'_\gamma = \lambda_\gamma |\chi_\gamma\rangle\langle\chi_\gamma| + v'_\gamma . \tag{6.58}$$

The separable potential has to fulfill condition (6.53), and the rest v'_γ has to be weak enough to be taken into account by a perturbation approximation. What is meant exactly by "weak enough" will be seen during the following calculation. For three particles, we have the potential

$$V = \sum_{\gamma=1}^{3} v_\gamma = \sum_{\gamma=1}^{3} v^s_\gamma + \sum_{\gamma=1}^{3} v'_\gamma = V^s + V' , \tag{6.59}$$

which we insert now into the resolvent equation (2.101a),

$$G(z) = g_0(z) + g_0(z) V^s G(z) + g_0(z) V' G(z) , \tag{6.60}$$

or,

$$(1 - g_0(z) V') G(z) = g_0(z) + g_0(z) V^s G(z) . \tag{6.61}$$

We assume that the inverse of $(1-g_0V')$ can be calculated by its Neumann series,

$$(1-g_0(z)V')^{-1} = \sum_{i=0}^{\infty} (g_0(z)V')^i . \qquad (6.62)$$

We then get from Eq. (6.61) by multiplication with $(1-g_0V')^{-1}$ from the left

$$G(z) = G'(z) + G'(z)V^S G(z) , \qquad (6.63)$$

with

$$G'(z) = (1-g_0(z)V')^{-1} g_0(z) . \qquad (6.64a)$$

For the rest resolvent G', we get by algebraic manipulation

$$(z-h_0-V')^{-1} = G'(z) = g_0(z) + g_0(z)V'G'(z) , \qquad (6.64b)$$

or,

$$G'(z) = g'_\beta(z) + g'_\beta(z)\bar{V}'_\beta G'(z) , \qquad (6.64c)$$

with

$$g'_\beta(z) = (z-h_0-v'_\beta)^{-1} . \qquad (6.64d)$$

We also have

$$G'(z) = \sum_{i=0}^{\infty} g_0(z)(V'g_0(z))^i , \qquad (6.64e)$$

and

$$g'_\beta(z) = \sum_{i=0}^{\infty} g_0(z)(v'_\beta g_0(z))^i . \qquad (6.64f)$$

In the kernel of Eq. (6.63), only the separable potential V^S appears explicitly, in contrast to the original resolvent equation. The rest potential V' is contained in the resolvent G'. We now take matrix elements of Eq. (6.63) between the states $\langle x_\beta|$ and $|x_\alpha\rangle$,

$$\langle\chi_\beta|G|\chi_\alpha\rangle=\langle\chi_\beta|G'|\chi_\alpha\rangle+\sum_{\gamma=1}^{3}\langle\chi_\beta|G'|\chi_\gamma\rangle\lambda_\gamma\langle\chi_\gamma|G|\chi_\alpha\rangle \quad . \tag{6.65}$$

The matrix elements $\langle\chi_\beta|G|\chi_\alpha\rangle$ are still operators with respect to the states $\langle\vec{q}'_\beta|$ and $|\vec{q}_\alpha\rangle$.

The kernel of Eq. (6.65) is not compact because of the δ-functions which are contained in the operator $\langle\chi_\beta|G'|\chi_\alpha\rangle$. This can be seen from the Neumann series of Eq. (6.64c),

$$G'=g'_\beta+\sum_{i=1}^{\infty}g'_\beta\left[(V'-v'_\beta)g'_\beta\right]^i \quad . \tag{6.66}$$

Taking matrix elements between the states $\langle\vec{q}_\beta,\chi_\beta|$ and $|\chi_\beta,\vec{q}'_\beta\rangle$, this equation becomes

$$\begin{aligned}\langle\vec{q}_\beta,\chi_\beta|G'(z)|\chi_\beta,\vec{q}'_\beta\rangle&=\langle\vec{q}_\beta,\chi_\beta|g'_\beta(z)|\chi_\beta,\vec{q}'_\beta\rangle\\&+\sum_{i=1}^{\infty}\langle\vec{q}_\beta,\chi_\beta|g'_\beta(z)\left[(V'-v'_\beta)g'_\beta(z)\right]^i|\chi_\beta,\vec{q}'_\beta\rangle \quad .\end{aligned} \tag{6.67}$$

The operator $g'_\beta(z)$ affects only the subsystem β (see Eq.(6.64d)) and, therefore, we get

$$\begin{aligned}\langle\vec{q}_\beta,\chi_\beta|G'(z)|\chi_\beta,\vec{q}'_\beta\rangle&=\delta(\vec{q}_\beta-\vec{q}'_\beta)\langle\chi_\beta|\hat{g}'_\beta(z-\tfrac{q_\beta^2}{2m_\beta})|\chi_\beta\rangle\\&+\sum_{i=1}^{\infty}\langle\vec{q}_\beta,\chi_\beta|g'_\beta(z)\left[(V'-v'_\beta)g'_\beta(z)\right]^i|\chi_\beta,\vec{q}'_\beta\rangle \quad .\end{aligned} \tag{6.68}$$

There are no δ-functions in the infinite sum which could compensate the δ-function in the first term on the right-hand side, since the operator $(V'-v'_\beta)$ acts in the part of the three-particle space which is not affected by g'_β .

Despite this difficulty, we can get from Eq. (6.65) an integral equation with a compact kernel. We only have to move the term which contains the δ-function to the left-hand side of the equation (compare with the manipulation which led us to Eq. (3.7)!),

$$(\lambda_\beta^{-1} - \langle\chi_\beta|q_\beta'|\chi_\beta\rangle)\,\lambda_\beta\langle\chi_\beta|G|\chi_\alpha\rangle = \langle\chi_\beta|G'|\chi_\alpha\rangle + \sum_{\gamma=1}^{3}\langle\chi_\beta|G'-\delta_{\beta\gamma}q_\gamma'|\chi_\gamma\rangle\lambda_\gamma\langle\chi_\gamma|G|\chi_\alpha\rangle \quad . \tag{6.69}$$

This procedure is successful for two reasons. Firstly, the inverse of

$$\lambda_\beta^{-1} - \langle\chi_\beta|q_\beta'(z)|\chi_\beta\rangle \equiv \Delta_\beta^{-1}(z) \tag{6.70}$$

is easy to calculate:

$$\langle\vec{q}_\beta|\Delta(z)|\vec{q}_\beta'\rangle = \frac{\delta(\vec{q}_\beta - \vec{q}_\beta')}{\lambda_\beta^{-1} - \langle\chi_\beta|\hat{q}_\beta'(z-\frac{q_\beta^2}{2M_\beta})|\chi_\beta\rangle} \quad . \tag{6.71}$$

Secondly, the application of this non-compact operator on the compact kernel of Eq. (6.69) leads again to a compact kernel. Multiplying Eq. (6.69) by $\Delta_\beta\lambda_\alpha$, we get

$$\lambda_\beta\langle\chi_\beta|G|\chi_\alpha\rangle\lambda_\alpha = \Delta_\beta\langle\chi_\beta|G'|\chi_\alpha\rangle\lambda_\alpha + \sum_{\gamma=1}^{3}\Delta_\beta\langle\chi_\beta|G'-\delta_{\beta\gamma}q_\beta'|\chi_\gamma\rangle\lambda_\gamma\langle\chi_\gamma|G|\chi_\alpha\rangle\lambda_\alpha \quad . \tag{6.72}$$

This equation with its compact kernel allows the calculation of the matrix elements $\lambda_\beta\langle\vec{q}_\beta', \chi_\beta|G|\chi_\alpha, \vec{q}_\alpha\rangle\lambda_\alpha$ which we are looking for. There is a close relationship between this equation and the two-particle resolvent equation (2.22a) which becomes apparent when we go over to an equation for the quantity .

$$\lambda_\beta\langle\chi_\beta|G|\chi_\alpha\rangle\lambda_\alpha + \delta_{\beta\alpha}\lambda_\alpha \quad . \tag{6.73}$$

The S-matrix for rearrangement scattering can be calculated equally well from this quantity because the constant term vanishes when the limits are carried out in Eq. (6.55). Adding $\delta_{\beta\alpha}\lambda_\alpha$ on both sides of Eq. (6.72), we get, after a short calculation,

$$\lambda_\beta \langle \chi_\beta | G(z) | \chi_\alpha \rangle \lambda_\alpha + \delta_{\beta\alpha}\lambda_\alpha = \delta_{\beta\alpha}\Delta_\beta(z) \tag{6.74}$$

$$+\sum_{\gamma=1}^{3} \Delta_\beta(z) \langle \chi_\beta | G'(z) - \delta_{\beta\gamma} q'_\beta(z) | \chi_\gamma \rangle \left\{ \lambda_\gamma \langle \chi_\gamma | G(z) | \chi_\alpha \rangle \lambda_\alpha + \delta_{\gamma\alpha}\lambda_\alpha \right\}.$$

With the definitions [1]

$$\begin{aligned} \big(\mathbf{G}(z)\big)_{\beta\alpha} &= \lambda_\beta \langle \chi_\beta | G(z) | \chi_\alpha \rangle \lambda_\alpha + \delta_{\beta\alpha}\lambda_\alpha \,, \\ \big(\mathbf{G}_0(z)\big)_{\beta\alpha} &= \delta_{\beta\alpha}\Delta_\beta(z) \,, \\ \big(\mathbf{V}(z)\big)_{\beta\alpha} &= \langle \chi_\beta | G'(z) - \delta_{\beta\alpha} q'_\beta(z) | \chi_\alpha \rangle \,, \end{aligned} \tag{6.75}$$

$(\alpha,\beta = 1,2,3)$

we get

$$\mathbf{G}(z) = \mathbf{G}_0(z) + \mathbf{G}_0(z)\mathbf{V}(z)\mathbf{G}(z) \,. \tag{6.76}$$

This is the AGS equation for the resolvent [93], which is an effective two-body equation. Not only do all its operators act in two-particle space (which has important consequences for its numerical solution!), it also has the same mathematical form as Eq. (2.22a). The latter is of great heuristic value because we can simply take over the manipulations of Chapter 2, section 1.5 which allowed us to carry out the limits in the S-matrix. In analogy to Eq. (2.46), we define a T-operator,

$$\mathbf{T}(z) = \mathbf{V}(z) + \mathbf{V}(z)\mathbf{G}(z)\mathbf{V}(z) \,, \tag{6.77}$$

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[1] The notation should remind us of the "resolvent" $(\mathbf{G})_{\beta\alpha}$ of Eq. (3.73).

and get, by help of Eq. (6.76),

$$\mathbf{G}(z) = \mathbf{G}_0(z) + \mathbf{G}_0(z)\mathbf{T}(z)\mathbf{G}_0(z) \quad . \tag{6.78}$$

Since, as mentioned before, the constant term of expression (6.73) does not contribute to the S-matrix, we can write

$$S_{\beta\alpha}(\vec{q}'_\beta, \vec{q}_\alpha) = \lim_{t\to\infty}\lim_{\epsilon\to 0} e^{i(E_\beta - E_\alpha)t}\, i\epsilon \langle \vec{q}'_\beta | \left(\mathbf{G}(E_\alpha + i\epsilon)\right)_{\beta\alpha} | \vec{q}_\alpha \rangle \quad , \tag{6.79}$$

or, with Eq. (6.78),

$$S_{\beta\alpha}(\vec{q}'_\beta, \vec{q}_\alpha) = \lim_{t\to\infty}\lim_{\epsilon\to 0} e^{i(E_\beta - E_\alpha)t}\, i\epsilon \langle \vec{q}'_\beta | \left(\mathbf{G}_0(E_\alpha + i\epsilon)\right)_{\beta\alpha} | \vec{q}_\alpha \rangle \tag{6.80}$$

$$+ \lim_{t\to\infty}\lim_{\epsilon\to 0} e^{i(E_\beta - E_\alpha)t}\, i\epsilon \langle \vec{q}'_\beta | \left(\mathbf{G}_0 \mathbf{T} \mathbf{G}_0\right)_{\beta\alpha} | \vec{q}_\alpha \rangle \quad .$$

To carry out the limits, we have to study the pole behavior of $\mathbf{G}_0(z)$. Analogy leads us to expect a pole at

$$z - \frac{q'^2_\beta}{2M_\beta} = E^B_\beta \quad . \tag{6.81}$$

From Eq. (6.75) and Eq. (6.71), we have

$$\langle \vec{q}'_\beta | \left(\mathbf{G}_0(z)\right)_{\beta\alpha} | \vec{q}_\alpha \rangle \tag{6.82}$$

$$= \delta_{\beta\alpha}\, \delta(\vec{q}'_\beta - \vec{q}_\alpha) \left\{ \lambda_\beta^{-1} - \langle \chi_\beta | \hat{q}'^{\,2}_\beta \left(z - \frac{q'^2_\beta}{2M_\beta}\right) | \chi_\beta \rangle \right\}^{-1} .$$

Using Eq. (6.53) and the expression (6.29)

$$\langle \psi_\beta | = \langle \chi_\beta | \hat{q}'^{\,2}_\beta (E^B_\beta) \quad ,$$

for the two-particle bound state, which has been derived in the last section by the quasiparticle method, we get

$$\langle \vec{q}'_\beta | (\mathbf{G}_0(z))_{\beta\alpha} | \vec{q}_\alpha \rangle = \tag{6.83}$$

$$\delta_{\beta\alpha}\,\delta(\vec{q}'_\beta - \vec{q}_\alpha)\left\{\langle \chi_\beta | \hat{q}'_\beta (E^B_\beta) - \hat{q}'_\beta (z - \frac{q'^2_\beta}{2M_\beta}) | \chi_\beta \rangle\right\}^{-1} ,$$

and, with Eq. (2.20a),

$$\langle \vec{q}'_\beta | (\mathbf{G}_0(z))_{\beta\alpha} | \vec{q}_\alpha \rangle = \tag{6.84}$$

$$\delta_{\beta\alpha}\,\delta(\vec{q}'_\beta - \vec{q}_\alpha)\left\{(z - \frac{q'^2_\beta}{2M_\beta} - E^B_\beta)\langle \chi_\beta | \hat{q}'_\beta (E^B_\beta)\, \hat{q}'_\beta (z - \frac{q'^2_\beta}{2M_\beta}) | \chi_\beta \rangle\right\}^{-1} .$$

As expected, there is a pole at $z = E^B_\beta + q'^2_\beta/2M_\beta$. We can now use Eq. (2.50) to carry out the limits in Eq. (6.80) and get

$$\mathcal{S}_{\beta\alpha}(\vec{q}'_\beta, \vec{q}_\alpha) = \tag{6.85}$$

$$\delta_{\beta\alpha}\,\delta(\vec{q}'_\beta - \vec{q}_\alpha) - 2\pi i\,\delta(E_\beta - E_\alpha)\langle \vec{q}'_\beta | \left(\mathbf{T}(E_\alpha + i0)\right)_{\beta\alpha} | \vec{q}_\alpha \rangle .$$

Since the S-matrix is given directly by the matrix elements of $\mathbf{T}$, it is unnecessary to calculate first the matrix $\mathbf{G}$ by Eq. (6.76) and then go over to $\mathbf{T}$ by Eq. (6.77). One can get the matrix $\mathbf{T}$ directly. From Eqs. (6.76) and (6.77), we get, in analogy to the derivation of Eq. (2.56a),

$$\mathbf{T}(z) = \mathbf{V}(z) + \mathbf{V}(z)\mathbf{G}_0(z)\mathbf{T}(z) . \tag{6.86}$$

The question now is whether we can also get the breakup amplitudes in this way. For the S-matrix (6.56), we need the operator $G|\chi_\alpha\rangle$, while Eq. (6.76) can only yield the operator matrix $\langle \chi_\beta | G | \chi_\alpha \rangle$. This matrix, however, contains enough information also to determine the operator $G|\chi_\alpha\rangle$. To this end, we use Eq. (6.63) which can be written as

$$G = \sum_{\gamma=1}^{3} G'(|\chi_\gamma\rangle \lambda_\gamma \langle \chi_\gamma | G + \delta_{\gamma\alpha}) . \tag{6.87}$$

Multiplying by $|\chi_\alpha\rangle\lambda_\alpha$ from the right, we get [1]

$$G|\chi_\alpha\rangle\lambda_\alpha = \sum_{\gamma=1}^{3} G'|\chi_\gamma\rangle\left(\lambda_\gamma\langle\chi_\gamma|G|\chi_\alpha\rangle\lambda_\alpha + \delta_{\gamma\alpha}\lambda_\alpha\right) \tag{6.88}$$

$$= \sum_{\gamma=1}^{3} G'|\chi_\gamma\rangle(\mathbf{G})_{\gamma\alpha} \quad .$$

We want to keep to our shorthand notation of operator matrices and define the vectors (α = 1,2,3)

$$\left(\mathbf{q}_{(z)}\right)_\alpha \equiv q_0^{-1}(z)\, G(z)|\chi_\alpha\rangle\lambda_\alpha \quad , \tag{6.89a}$$

and,

$$\left(\mathbf{U}_{(z)}\right)_\alpha \equiv q_0^{-1}(z)\, G'(z)|\chi_\alpha\rangle \quad . \tag{6.89b}$$

Equation (6.88) then becomes

$$q_0\,\mathbf{q} = q_0\,\mathbf{U}\,\mathbf{G} \quad . \tag{6.90}$$

The factor g_0 has been extracted in view of the limit which has to be carried out in Eq. (6.56). Using Eq. (6.78), we can write

$$q_0\,\mathbf{q} = q_0\,\mathbf{U}\{1+\mathbf{G}_0\mathbf{T}\}\mathbf{G}_0 = q_0\,\boldsymbol{\Upsilon}\,\mathbf{G}_0 \quad , \tag{6.91}$$

with the definition

$$\boldsymbol{\Upsilon}_{(z)} \equiv \mathbf{U}_{(z)} + \mathbf{U}_{(z)}\mathbf{G}_{0(z)}\mathbf{T}_{(z)} \quad .$$

In this expression, the operator $\mathbf{T}$ enters off-shell; the product $\mathbf{U}\mathbf{G}_0\mathbf{T}$ is evaluated by introducing intermediate states $|\vec{q}_\gamma\rangle\langle\vec{q}_\gamma|$ and integrating over all momenta $\vec{q}_\gamma$. When expression (6.91) is inserted into Eq. (6.56), the pole behavior of g_0

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[1] In the same way we can get, of course, the operator $\lambda_\gamma\langle\chi_\gamma|G$ and, by use of Eq. (6.63), the full resolvent G which would be needed to describe transitions from three-particle continuum to three-particle continuum.

and G_0 allows one to carry out the limits, and we get for the S-matrix

$$S_{0\alpha}(\vec{q}'_\beta, \vec{p}'_\beta; \vec{q}_\alpha) = -2\pi i\, \delta\left(\frac{p'^2_\beta}{2\mu_\beta} + \frac{q'^2_\beta}{2M_\beta} - E_\alpha\right) \langle \vec{q}'_\beta, \vec{p}'_\beta | \left(T(E_\alpha + i0)\right)_\alpha | \vec{q}_\alpha \rangle \,. \tag{6.92}$$

It has thus become possible to reduce the general three-particle-problem to an effective two-body problem (Eq. (6.86)). The effective potential $V(z)$, which is determined by the given two-particle potentials (Eq. (6.64a-f) and (6.75)), describes the interaction between a particle and a quasiparticle (the latter being a pair of particles in a certain state which is given by an adopted form factor). The "propagator" $G_0(z)$ describes the free relative motion of particle and quasiparticle, and the on-shell T-matrix $T(z)$ describes the scattering (elastic or rearrangement) of these two "particles". So far, our result is not amazing since we have, indeed, a two-body scattering problem, although one of the bodies is a composite particle. But it is interesting that also the breakup reaction, which is a genuine three-particle problem, can be treated as an effective two-body problem. To make this a little more transparent, we introduce a graphical representation of our operators [23]. Let us resume the argument of Fig. 15 on page 96.

The motion of a free particle in a momentum state is represented by a single line ———, the c.m. motion of a bound state by a double line ═══. A form factor becomes a half-circle, $|\chi\rangle \to D$ ($\langle\chi| \to D$), and the rest potential v' is represented by a wavy line ≷. The incoming state stands on the right, as in the equations. We thus get for the effective potential (Eq. (6.75)) with $\beta \neq \alpha$ the graphical representation which is depicted in Fig. 33. When G' is calculated by its Neumann series, we get Fig. 34. The first graph on the right-hand side of Fig. 34 illustrates the exchange process of the separable model (Fig. 15), while the following graphs are corrections which have to be added to take into account the non-separable rest v' of our potential.

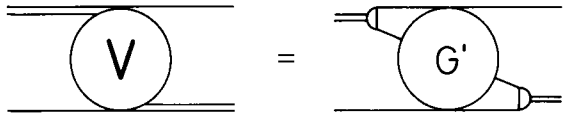

Fig. 33. Graphical representation of the effective potential in Eq. (6.75)

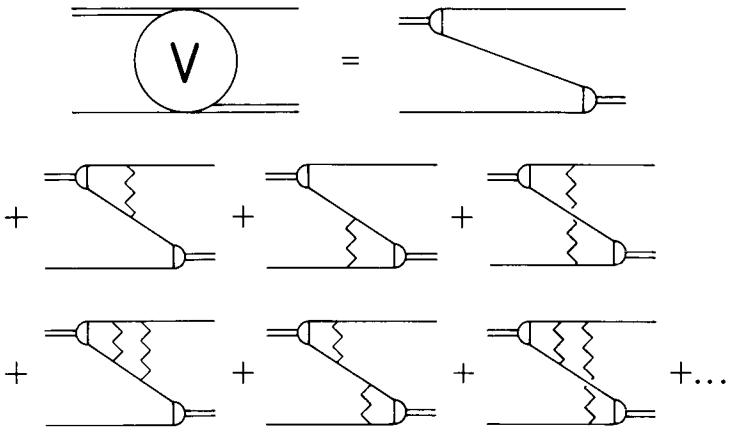

Fig. 34. Graphical representation of the effective potential in Eq. (6.75) with operator G' expanded into its Neumann series, Eq. (6.64e)

The operator $\mathcal{T}$ which yields the breakup elements of the S-matrix is represented in Fig. 35 where $\mathcal{U}$, according to Eqs. (6.89b) and (6.64e), is shown in Fig. 36. The first graph of the effective interaction $\mathcal{U}$ must be zero on-shell since it describes breakup without an interaction. Therefore, we get the graphical representation of $\mathcal{T}$ shown in Fig. 37.

The graphical representation suggests the following interpretation. In the separable model (graph a), we have at first the production of a two-particle state with positive energy (indicated by a star) which will then decay. This mechanism makes it clear that breakup can, indeed, be treated as an effective two-body process. We only need the off-shell effective T-matrix $\mathcal{T}$ of Eq. (6.86). The quasiparticle model brings about the corrections b, c, d, etc..

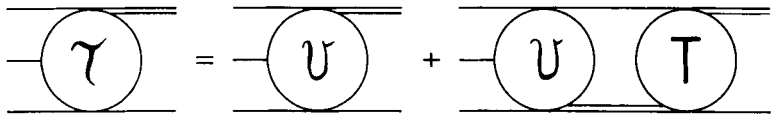

Fig. 35. Graphical representation of the breakup operator, Eq. (6.91)

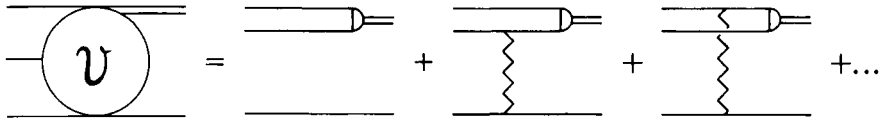

Fig. 36. Graphical representation of the "potential" $\mathcal{U}$, Eq. (6.89b)

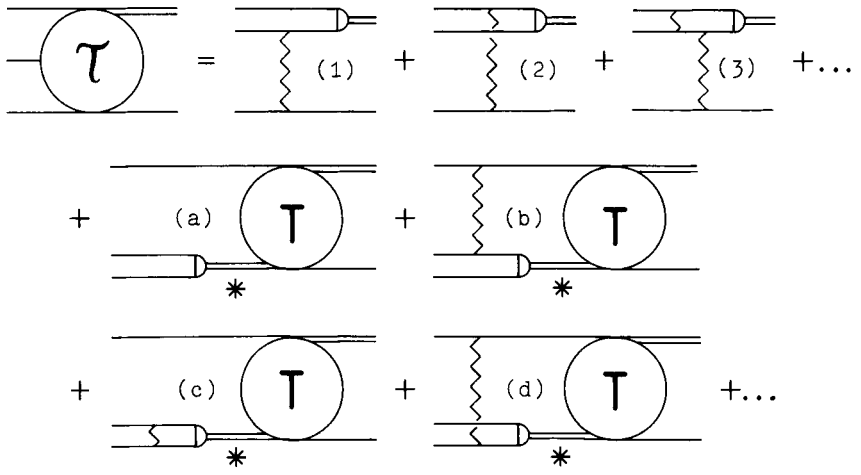

Fig. 37. Graphical representation of the breakup operator, Eq. (6.91), as obtained by combining Figs. 35 and 36

In addition, there is a completely different process (graph 1, 2, etc.) in which one of the bound particles does not even interact, except with its bound-state partner. Breakup is induced by the residual interaction of the incoming free particle with one of the particles from the bound state. This process is related to the "spectator model" which has been used for many years to describe breakup at high energies. In the present description, the spectator model follows from

an exact theory and competes with the final-state-interaction model (graph a, b, c, etc.).

It remains to be shown under what conditions the rest resolvents G' and g'_β can be calculated by a fast-converging series. There is no other way to calculate them since a rigorous solution of the defining integral equations (6.64b,c) would be as difficult as a rigorous solution of the original resolvent-equation for G ; in both cases the kernels are not compact.

The rest resolvent G' can be calculated by iteration when the operator norm of the kernel of Eq. (6.64b) is smaller than 1,

$$\| g_0(z) V' \| < 1 \quad . \tag{6.93}$$

Weinberg [7] has estimated this norm to be

$$\| g_0(z) V' \| < \sum_{\gamma=1}^{3} \sigma_\gamma(z) \quad , \tag{6.94}$$

where the function $\sigma_\gamma(z)$ is an upper bound of the Schmidt norm (2.28) of the operator $\hat{g}_0 v'_\gamma$,

$$\| \hat{g}_0(z-E) v'_\gamma \|_S \leq \sigma_\gamma(z) \quad , \tag{6.95a}$$

for all $E \geq 0$.

The norm (6.94) cannot be related to the Schmidt norm of the subsystem kernels at one single energy. At a given three-particle energy z interaction takes place in the subsystem at all energies E_γ with $-\infty < E_\gamma \leq \mathrm{Re}\ z$. For real $z \geq 0$, the Schmidt norm of Eq. (6.95a) does not exist (compare with Eq. (2.30)). Equation (6.95a) can then be replaced by

$$| \eta'_\gamma(z-E) | \leq \sigma_\gamma(z) \quad . \tag{6.95b}$$

Here, η'_γ is the greatest eigenvalue of the rest kernel $\hat{g}_0(z-E)v'_\gamma$ (compare with Eq. (6.16)).

According to the estimate (6.94), the Neumann series for G' does not necessarily converge when the Neumann series for g'_γ converges. In order to fulfill condition (6.93), it may become necessary to split off more than one separable term

in Eq. (6.58), even when there is only one two-particle bound state. In case of several bound states per subsystem, we obviously have to use several separable terms.

The general form of the equations is not altered by the introduction of more separable potential terms. There will only be more matrix elements,

$$\lambda_{\beta i} \langle \chi_{\beta i} | G(z) | \chi_{\gamma j} \rangle \lambda_{\gamma j} \ , \tag{6.96}$$

and, accordingly, more coupled equations. The condition (6.53) becomes

$$\delta_{ij} \lambda_{\gamma i}^{-1} = \langle \psi_{\gamma i} | \chi_{\gamma j} \rangle \ . \tag{6.97}$$

It means that all form factors which do not have a corresponding bound state must be orthogonal to the bound states. Matrix elements (6.96) which contain such form factors do not contribute directly to the rearrangement part of the S-matrix, just as the continuum components $|\psi_\gamma\rangle$ of Eq. (6.54) do not contribute directly. However, they influence those matrix elements which do contribute by their coupling over the integral equation. In the breakup part of the S-matrix, matrix elements (6.96) with a continuum form factor do contribute directly. Under condition (6.97), we can generalize Eqs. (6.76-6.93) to become valid for an arbitrary number of form factors. The indices β will be replaced by an index pair (β,i) where i stands for the i^{th} form factor of subsystem β . This generalization contains the separable expansion method because we can introduce as many form factors as are needed to have

$$\| q_0 V' \| \ll 1 \ . \tag{6.98}$$

The rest potential V' can then be neglected. In practice, however, one wants to keep the number of separable terms small, because of computer capacity, and to take into account the details of the potential by the first terms of the Neumann series.

3.3. Practical Calculations with the Quasiparticle Method

In the following, we will study an application of the quasiparticle method to the system of three identical bosons. As interaction, we take the Yukawa potential,

$$V(r) = g \frac{e^{-\mu r}}{r} \quad ,$$

or,

$$V(\vec{p}, \vec{p}') = \frac{g}{2\pi^2 \left[(\vec{p} - \vec{p}')^2 + \mu^2 \right]} \quad . \tag{6.99}$$

Next, we need a separable potential which leads to a rest potential v' (Eq. (6.58)) which is weak enough to be taken into account in good approximation by the first terms of the Neumann series (6.64e). Alt, Grassberger and Sandhas [94] have chosen, for this purpose, a Yamaguchi potential (5.31). The parameters of the Yamaguchi potential have been fitted to the two-particle binding energy and scattering length of the Yukawa potential (6.99) with $\mu = 1$. In the effective potential $\mathbf{V}$ (Eq. (6.75)), all terms of the Neumann series for G' which are of higher than first order in v' have been neglected. This approximation is called "first quasi-Born approximation" (1.QBA). Numerically, it would be very difficult to take into account terms of higher order in v' because the operator products $g_0 (v' g_0)^i$ become integrals of high dimension.

For identical particles, the effective potential becomes, according to Chapter 5, section 2.3 and Eq. (6.75),

$$\mathbf{V} = \mathbf{V}_{\alpha\alpha} + 2\mathbf{V}_{\beta \neq \alpha} = \langle \chi_1 | G' - g_1' | \chi_1 \rangle + 2 \langle \chi_2 | G' | \chi_1 \rangle \quad . \tag{6.100}$$

The rest resolvents are in 1.QBA (Eqs. (6.64e,f))

$$G' \approx g_0 + g_0 \sum_{\gamma=1}^{3} v_\gamma' g_0 \tag{6.101a}$$

and

$$g_\beta' \approx g_0 + g_0 v_\beta' g_0 \quad . \tag{6.101b}$$

Inserting this into Eq. (6.100), we get

$$V = 2\{\langle\chi_2|g_0|\chi_1\rangle + \langle\chi_2|g_0 v_2' g_0|\chi_1\rangle + \langle\chi_2|g_0 v_1' g_0|\chi_1\rangle + \langle\chi_2|g_0 v_3' g_0|\chi_1\rangle + \langle\chi_1|g_0 v_2' g_0|\chi_1\rangle\} \quad . \qquad (6.102)$$

The first term represents the purely separable interaction ($v' = o$) ; we call it the zeroth quasi-Born approximation (O.QBA). The relevance of the non-separable part of the potential can thus be tested by comparing the results obtained by the zeroth and first quasi-Born approximation. Such a comparison is shown in Fig. 38 for the three-particle binding energies.

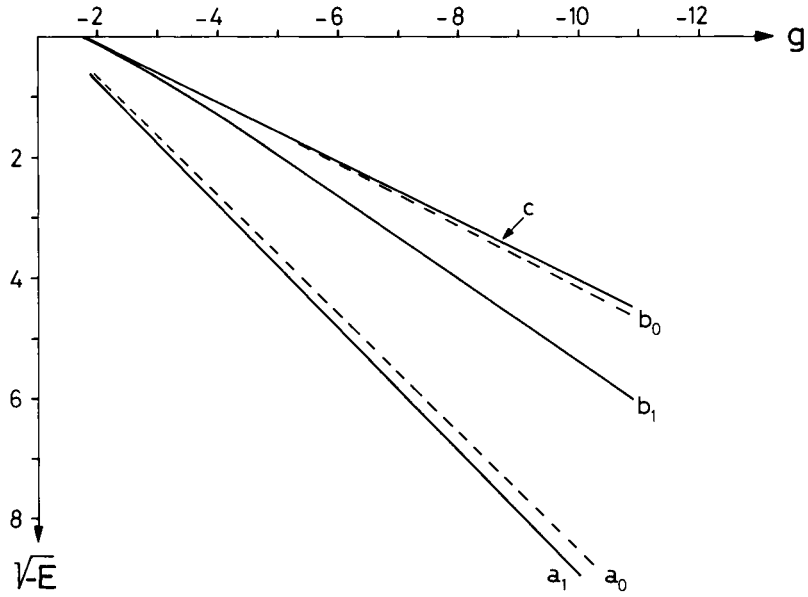

Fig. 38. Square root of the three-boson binding energy (units: $\hbar$=m=1) plotted versus Yukawa coupling constant. Broken line: 0^{th} quasi-Born approximation, full line: 1^{st} quasi-Born approximation; the label a refers to the ground state, the label b to the first excited state, the full line c indicates the two-particle ground state (E.O. Alt et al. [94]).

The difference between the two approximations is not very large for the ground state. The situation is different in case of the excited state and in case of elastic scattering (Fig. 39). As we can see in Fig. 39 the difference between 0.QBA and 1.QBA is very large, and only the 1.QBA is in agreement with the solution of the Faddeev equations by Tjon [95]. The latter has been obtained by the Padé approximation which will be discussed later in Chapter 7.

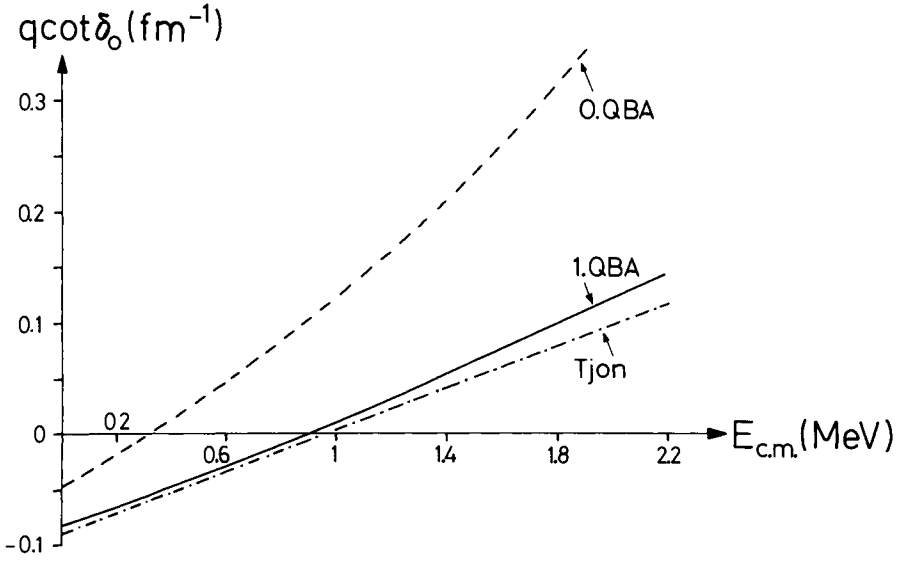

Fig. 39. Plot of q cot δ_0 versus center-of-mass energy for Yukawa coupling constant g = -2.373 in 0^{th} and 1^{st} quasi-Born approximation compared with the result of Tjon (E.O. Alt et al. [94])

The difference between the differential cross sections in 0.QBA and 1.QBA (Fig. 40) is quite conceivable. Since the separable approximation corresponds to an exchange process (see p. 111), the 0.QBA shows a pronounced maximum mainly in the backward direction, while the 1.QBA has also a strong maximum in the forward direction.

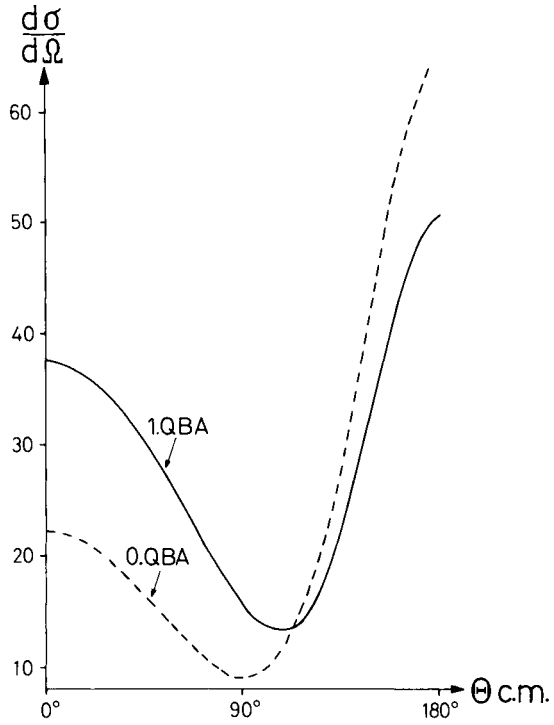

Fig. 40. Differential cross section for elastic scattering at $q^2 = 0.06$ (units: $\hbar=m=1$) for Yukawa coupling constant $g = -2.373$ in 0^{th} and 1^{st} quasi-Born approximation (E.O. Alt et al. [94])

Above the breakup threshold, some extra complications arise in 1.QBA, compared to O.QBA, by the appearance of the singular operator $v'g_o$ [96]. Also, the results show a rather large difference between 1.QBA and O.QBA (see Figs. 41 and 42).

Differential breakup cross sections have not yet been calculated. One expects here some information on the competing processes of final-state interaction and spectator model.

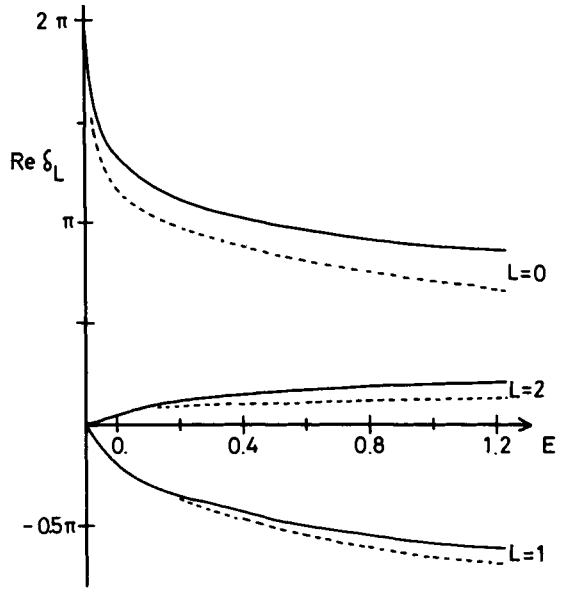

Fig. 41. Real part of the phase shift δ_L plotted versus total energy E (units: $\hbar$=m=1). Broken line: 0^{th} quasi-Born approximation, full line: 1^{st} quasi-Born approximation (H. Ziegelmann [96]).

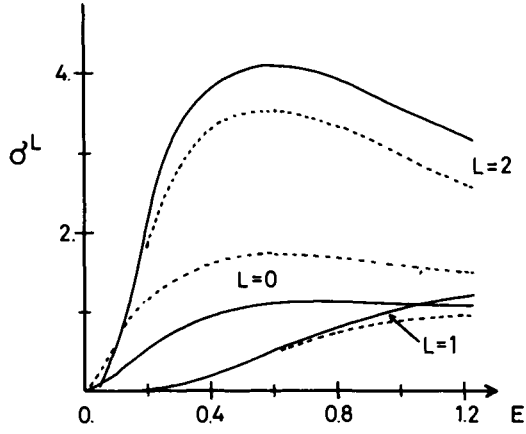

Fig. 42. Energy dependence of the total breakup cross section σ^L (units: $\hbar$=m=1). Broken line: 0^{th} quasi-Born approximation, full line: 1^{st} quasi-Born approximation (H. Ziegelmann [96]).

7. Solution of the Faddeev Equations by Padé Approximation

1. The Technique of Padé Approximation

We consider a function f(z) which is analytic in the vicinity of z = o . The Taylor series,

$$f(z) = \sum_{\nu=o}^{\infty} z^{\nu} f_{\nu} \quad , \tag{7.1}$$

converges within a circle around z = o which passes through the singularity of f(z) which is located closest to the origin.

Outside of the circle, the function f(z) cannot be calculated by its Taylor series, although it is uniquely determined by the coefficients f_{ν} .

The Padé approximation allows the approximate continuation of the function f(z) into the region outside of the circle of convergence by using the information which is contained in a finite number of coefficients f_{ν} .

The function f(z) is approximated by a rational function,

$$f(z) \approx f^{[N,M]}(z) = \frac{P_M(z)}{Q_N(z)} = \frac{\sum_{\nu=o}^{M} P_{M,\nu} z^{\nu}}{\sum_{\nu=o}^{N} Q_{N,\nu} z^{\nu}} \quad , \tag{7.2}$$

in such a way that the lowest N + M derivatives of f(z) and of the [N,M] approximant coincide at z = o . This condition defines a set of linear equations for the coefficients $P_{M,\nu}$, $Q_{N,\nu}$. Its solution by Kramer's rule gives the Padé approximants in terms of determinants (see Eq. (7.3) where $f_{\nu} \equiv o$ for $\nu < o$).

The [N,M] approximant makes use of the information which is contained in the coefficients of the Taylor series up to order N + M . The advantage of the ansatz lies in the fact that it allows one to approximate singularities and cuts of the function f(z) by the zeros of $Q_N(z)$.

$$f^{[N,M]}(z) = \frac{\begin{vmatrix} f_{M-N+1} & f_{M-N+2} & \cdots & f_{M+1} \\ \vdots & \vdots & & \vdots \\ f_M & f_{M+1} & \cdots & f_{M+N} \\ \sum_{j=N}^{M} f_{j-N} z^j & \sum_{j=N-1}^{M} f_{j-N+1} z^j & \cdots & \sum_{j=0}^{M} f_j z^j \end{vmatrix}}{\begin{vmatrix} f_{M-N+1} & f_{M-N+2} & \cdots & f_{M+1} \\ \vdots & \vdots & & \vdots \\ f_M & f_{M+1} & \cdots & f_{M+N} \\ z^N & z^{N-1} & \cdots & 1 \end{vmatrix}} \qquad (7.3)$$

For $N = M = 1$, we get

$$f^{[1,1]}(z) = \frac{\begin{vmatrix} f_1 & f_2 \\ f_0 z & f_0 + f_1 z \end{vmatrix}}{\begin{vmatrix} f_1 & f_2 \\ z & 1 \end{vmatrix}} = \frac{f_0 f_1 + f_1^2 z - f_0 f_2 z}{f_1 - f_2 z} \quad . \qquad (7.4)$$

The [1,1] approximant of

$$f(z) = \sum_{\nu=0}^{\infty} z^\nu \quad \rightsquigarrow \quad f_\nu = 1 \quad ,$$

is, for example,

$$f^{[1,1]}(z) = (1-z)^{-1} \quad .$$

In this simple case, the first Padé approximant reproduces the Taylor series exactly. For

$$f(z) = \log(1+z) = -\sum_{\nu=1}^{\infty} (-1)^\nu \frac{z^\nu}{\nu}$$

we have,

$$f_0 = 0 \ , \quad f_1 = 1 \ , \quad f_2 = -\frac{1}{2}$$

and

$$f^{[1,1]}(z) = \frac{z}{1 + \frac{z}{2}} \ .$$

The first Padé approximant yields a better approximation than the first three terms of the Taylor series within the circle of convergence, $|z| < 1$, and is still a rather good approximation outside of the circle, as can be seen from the following table.

z	Taylor series up to $\nu = 2$	Padé approximation $f^{[1,1]}(z)$	Exact $\log(1+z)$
1	0.5	0.67	0.69
2	0	1.00	1.10

2. Padé Approximation and Integral Equations

We now want to use the technique of the Padé approximation to solve integral equations by extracting information from their Neumann series (4.16), even though the series do not converge. To accomplish this, we have to relate the solution of our integral equation (4.14),

$$f = h + Kf \ , \tag{7.5}$$

to an analytic function. We get such a function by introducing a complex parameter λ ,

$$f(\lambda) = h + \lambda K f(\lambda) \ . \tag{7.6}$$

The solution f depends now on the complex variable λ (we suppress the dependence on the integration variables in our notation). According to the theory of integral equations [7,22,35, 97], it is a meromorphic function in λ . Singularities can have

a limit point only at infinity, as long as the kernel is compact. In the vicinity of the origin $\lambda = 0$, the function $f(\lambda)$ is analytic and can be calculated by its Taylor series,

$$f(\lambda) = \sum_{\nu=0}^{\infty} \lambda^{\nu} K^{\nu} h \quad . \tag{7.7}$$

For $\lambda = 1$, the Taylor series becomes identical to the Neumann series of Eq. (7.5), and we see that the Neumann series does not converge when $f(\lambda)$ has a singularity within the unit circle $|\lambda| \leq 1$.

The singularities of $f(\lambda)$ are related to the eigenvalues (4.17a) of the kernel by

$$\lambda_{\nu} = \eta_{\nu}^{-1} \quad . \tag{7.8}$$

In the two-particle case, the quantities λ_{ν} are the coupling constants which produce normalizable solutions of the Schrödinger equation at prescribed energies (see p. 127). The Neumann series does not converge at energies in which we are interested, namely, in the vicinity of bound states, antibound states, and resonances (compare with Eq. (5.28)). For such energies, however, we can use the Padé approximation to get a solution of our integral equation. In the special case of a degenerate kernel of rank N, the [N,N] approximant represents the exact solution since the solution is a rational function of order N. The convergence of the Padé approximation thus becomes believable since every compact kernel can be approximated by a series of degenerate kernels. Nevertheless, many questions of convergence are still unanswered. It has not yet been possible, for instance, to prove that the convergence is uniform since the limit positions of the poles of the approximants are unknown; an [N,M] approximant has N poles by its denominator Q_N, and not all of them must be related to poles of the true solution.

3. Padé Approximation and the Faddeev Equations

We write the Faddeev equations (3.10) as

$$\mathcal{T}(\lambda) = 1 + \lambda K_I \mathcal{T}(\lambda) \quad , \tag{7.9}$$

where we have introduced a complex parameter λ , according to the previous section 2. The solution $\mathcal{T}(\lambda)$ is a meromorphic function of λ (see p. 48) and, therefore, the analytic continuation to $\lambda = 1$ can be done by Padé approximation.

The difficulty of the method lies in the calculation of matrix elements of the operators $t_i g_o t_j \ldots g_o t_n$. These matrix elements are integrals of high dimension, and the integrands can become singular by the poles of g_o and t_i (see p. 47). The calculations, nevertheless, are much simpler than a direct solution of the singular, multidimensional Faddeev equations. Moreover, the Padé approximants converge very rapidly, as can be seen in Fig. 43.

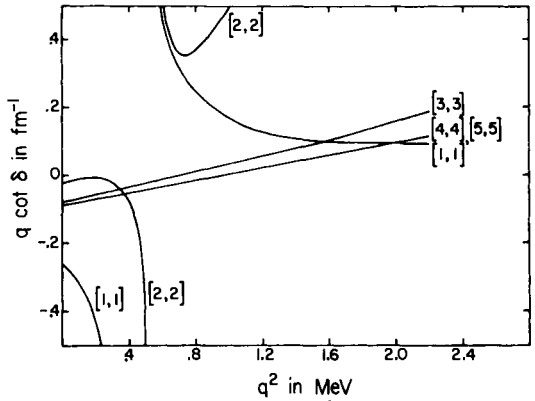

Fig. 43. q cot δ_o in different Padé approximants (J.A. Tjon [95])

In this example, the elastic scattering of a particle from a two-particle bound state has been calculated [95]; see also Fig. 39. The approximants [4,4] and [5,5] give almost identical results.
The approximants [1,1] and [2,2] show false resonances which arise from the above-mentioned singularities and have nothing to do with the true solution. In most calculations of this kind, the two-body interaction has been restricted to $l = o$ in order to save computation time. Only in one calculation has the $l = 2$ interaction also been taken into account.

Figure 44 shows the differential cross section of neutron-deuteron scattering at 14.1 MeV (Lab).

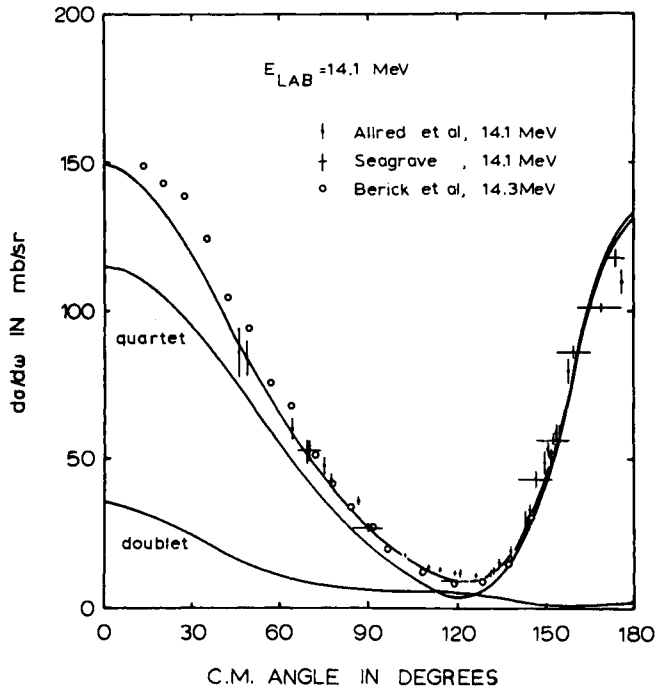

Fig. 44. Experimental and theoretical elastic differential cross section for neutron-deuteron scattering (W.M. Kloet and J.A. Tjon [98])

The calculation has been done with a spin-dependent local potential which also describes repulsion [98]. The agreement with experiment is very good. Especially the agreement in forward direction is remarkable. In this region, calculations with a separable potential yield a differential cross section which is 25% too low. In Fig. 44, one can also see the high quartet contribution which has been mentioned on page 119.

The differential breakup cross section has been calculated with the same potential [82]. The difference between this result and the result by Cahill et al. [81] with separable potential is small. The experimental cross section is reproduced rather well in shape, see Fig. 45. In absolute value, however, the theoretical curves are about 50% too high.

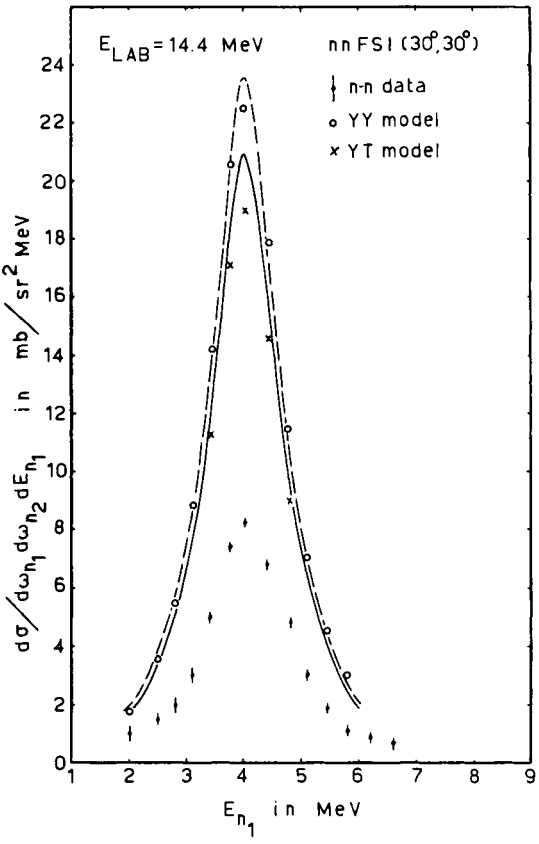

Fig. 45. Experimental and theoretical differential breakup cross section of the reaction n + d → 2n + p' , experimental setup as in Fig. 2 (W.M. Kloet and J.A. Tjon [82]). The full line gives the result for the local potential (I-III) and the dashed line for the local potential (I-IV) of Ref. [76]. The experimental values as well as the results for different separable models are from Ref. [81].

8. Variational Methods

An approximate solution of the Schrödinger equation can be obtained also by variational methods. For bound states, such methods seem to be superior to integral equations, since rather accurate results on the triton binding energy for realistic potentials have been known for a long time. Variational methods have also been successfully applied to elastic scattering and to multichannel scattering. For three-particle breakup, however, variational methods have been suggested, but, to date, not too many impressive results have come out. Judging from success, one could suppose that integral equations are unseemingly complicated for problems with a simple boundary condition, such as bound state problems, while for breakup reactions the variational methods run into trouble because of the complicated boundary condition.

We shall discuss in this chapter variational methods for bound states, for elastic and rearrangement scattering, and for the breakup reaction. Finally, we shall present a promising variational method for solving the Faddeev equations.

1. Variational Methods for Bound States

There are mainly two methods: the Rayleigh-Ritz variational principle for the ground state and the Hylleraas principle for the discrete spectrum.

The boundary condition for a bound state problem is very simple. It only demands that the wave function be normalizable, which means that it must vanish fast enough for large particle distances.

The Ritz variational principle states that the expectation value of the Hamilton operator H with an arbitrary normalized wave function $|\psi\rangle$ is an upper bound E_o to the ground-state energy E_o ,

$$E_o \leq \bar{E}_o = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \quad . \tag{8.1}$$

This statement can be verified easily by expanding $|\psi\rangle$ into

normalized eigenstates of H ,

$$|\psi\rangle = \sum_{(\nu)} \!\!\!\!\!\!\int\; a_\nu |\varphi_\nu\rangle \,. \tag{8.2}$$

The normalization condition is expressed by

$$\sum_{(\nu)} \!\!\!\!\!\!\int\; |a_\nu|^2 = 1 \,, \tag{8.3}$$

and the expectation value of the Hamiltonian becomes

$$\langle\psi|H|\psi\rangle = \sum_{(\nu)} \!\!\!\!\!\!\int\; |a_\nu|^2 E_\nu \geq \sum_{(\nu)} \!\!\!\!\!\!\int\; |a_\nu|^2 E_0 = E_0 \,. \tag{8.4}$$

The Ritz principle is especially suited for a variation of non-linear parameters. Using intuition and physical insight, a trial function is chosen which contains a small number of effective, non-linear parameters, such as width and asymptotic descent of two-particle correlation functions. The expectation value of the Hamiltonian is calculated with this trial function and the parameters are varied, either by hand or by a search programm, until the lowest value in parameter space is reached. For the triton binding energy with a spin-dependent exponential potential, for instance, one needs 6 parameters to get within the binding energy of about 7.9 MeV by less than 0.2 MeV [99].

As can be seen from Eq. (8.4), the Ritz principle can also be applied to excited states when it is possible to construct trial functions which are orthogonal to all eigenfunctions of lower states. In practice, this is only feasible when the excited state differs from all lower levels by good quantum numbers.

A lower bound $\underline{E}_0$ of E_0 can be calculated by the formula of Temple [100]. This formula contains, in addition to the expectation value of the Hamiltonian, the expectation value of the square of the Hamiltonian and the energy E_1 of the first excited state. It reads in shorthand notation (leaving away the normalized trial function ψ),

$$E_0 \geq \underline{E}_0 = \frac{\langle H^2\rangle - E_1\langle H\rangle}{\langle H\rangle - E_1} \,. \tag{8.5}$$

Also this formula is verified easily by inserting the expansion (8.2) and using condition (8.3).

The energy E_1 of the first excited state (with the same quantum numbers as the ground state!) is usually as little known as the energy of the ground state. The inequality (8.5), however, remains valid when an estimate of E_1 is used, instead of E_1, which is smaller than E_1 but larger than $\langle H \rangle$. When the continuum starts at E_1, as in the case of the triton, we do not need such an estimate since the deuteron binding energy which determines the elastic threshold is relatively easy to calculate.

The Temple formula yields the best lower bound that can be obtained from $\langle H \rangle$, $\langle H^2 \rangle$, and E_1. This can be seen in the following way.

Assume that we have, for a given Hamiltonian H and a certain trial function ψ,

$$\underline{E}_0 < E_0 < \langle H \rangle < E_1 .$$

Suppose that there is a formula,

$$q = q(E_1, \langle H \rangle, \langle H^2 \rangle) ,$$

which yields a better lower bound than the Temple formula, i.e.,

$$\underline{E}_0 < q \leq E_0 .$$

The new formula must yield lower bounds for the ground states of all Hamilton operators U and all trial functions v. Let us construct now an operator U which has the energies $\underline{E}_0$ and E_1 as eigenvalues of its ground state and first excited state. The corresponding normalized eigenstates are u_0 and u_1. We choose as trial function

$$v = \sqrt{1 - c^2}\, u_0 + c\, u_1 ,$$

with

$$c^2 = \frac{\langle H \rangle - \underline{E}_0}{E_1 - \underline{E}_0} .$$

It can be shown for this trial function that

$$\langle v|U|v\rangle = \langle\psi|H|\psi\rangle ,$$

and

$$\langle v|U^2|v\rangle = \langle\psi|H^2|\psi\rangle ,$$

which means that

$$g\left(E_1, \langle\psi|H|\psi\rangle, \langle\psi|H^2|\psi\rangle\right) = g\left(E_1, \langle v|U|v\rangle, \langle v|U^2|v\rangle\right) .$$

For the ground state energy of U , we get the same lower bound g as for the ground state energy of H , although the ground state energy of U is identical with Temple's lower bound $\underline{E}_0$. This contradicts our assumption of a "better" lower bound g .

Nevertheless, the lower bound by Temple is usually a very bad bound, compared to the Rayleigh-Ritz upper bound. A ratio of 100 : 1 for the distances from bounds to eigenvalue is rather common in practice, especially when the potentials have a hard core. Delves and Hennell [68], who have performed the most accurate calculations on the triton binding energy known today, do not bother with lower bounds for this reason. Instead, they study the convergence behavior of the upper bound and extrapolate to an infinite number of parameters.

A systematic variation of parameters is most simple when the trial function depends linearly on the parameters. We can then use the method of Hylleraas which is identical to a diagonalization of the Hamiltonian in a restricted Hilbert space.

We choose a test function space,

$$\mathcal{H}_t \equiv \{\psi_n\} , \quad n = 0, 1, \ldots N ,$$

of normalizable, linearly independent functions ψ_n . For a system of fermions, for instance, one could use Slater determinants of oscillator functions. The trial function is written as

$$|\psi\rangle = \sum_{n=0}^{N} c_n |\psi_n\rangle . \qquad (8.6)$$

The quantities c_n are the linear variational parameters.

They are determined by the eigenvalue equation

$$\sum_{n=0}^{N} (H - \Lambda B)_{mn} c_n = 0 , \qquad (8.7)$$

$m = 0,1, \ldots N$,

where H_{mn} is the matrix $\langle\psi_m|H|\psi_n\rangle$ and B_{mn} is the matrix $\langle\psi_m|\psi_n\rangle$. From Eq. (8.7), we see that the Hylleraas method is just the diagonalization of the Hamiltonian in the function space $\mathcal{H}_t$. We get eigenvalues Λ_i and eigenvectors $c_i \equiv \{c_{i0}, \ldots c_{iN}\}$. The lowest eigenvalue Λ_0 is identical to the upper bound $\bar{E}_0$ which would follow from the Ritz principle with the trial function (8.6),

$$\Lambda_0 = \bar{E}_0 . \qquad (8.8a)$$

The state

$$|\Psi_0\rangle = \sum_{n=0}^{N} c_{0n} |\psi_n\rangle , \qquad (8.8b)$$

is the optimal ground state in the sense of the Ritz principle.

In the Hylleraas principle, it can be shown that we have, quite generally,

$$\Lambda_i \geq E_i , \qquad (8.9)$$

which means that all eigenvalues of Eq. (8.7) are upper bounds to the corresponding eigenvalues of the Hamiltonian; in this respect, the Hylleraas principle is superior to the Ritz principle. The states

$$|\Psi_i\rangle = \sum_{n=0}^{N} c_{in} |\psi_n\rangle \qquad (8.10)$$

are, in a certain sense, approximations to the eigenfunctions of the Schrödinger equation. A measure of the quality of the approximation is the overlap of the states (8.10) with the true eigenstates. In the discrete part of the spectrum of H , the overlap converges to one when the test function space is allowed to become the complete Hilbert space.

In the continuous part of the spectrum, the eigenvalues Λ_i and eigenstates $|\Psi_i\rangle$ have no relevance; Eq. (8.9) remains valid in the sense that all such eigenvalues are upper bounds to the elastic threshold, and the states $|\Psi_i\rangle$ are just an orthogonal set of wave packets with increasing energy expectation value.

Non-linear parameters can, of course, be used also in the Hylleraas principle by letting each test function $|\psi_n\rangle$ in the expansion (8.6) depend on such parameters. The eigenvalue problem (8.7) is then solved for every set of non-linear parameters to find the lowest upper bounds.

Delves and Hennell [68] have used this method to calculate the triton binding energy for very complicated realistic potentials, like the Hamada-Johnston potential. Such potentials contain a spin-dependent central potential with a core, a tensor potential, a spin-orbit potential, and a quadratic spin-orbit potential. The authors use up to 70 linear parameters and extrapolate to the true binding energy which becomes, for the Hamada-Johnston potential, (6.5 ± 0.2)MeV . The use of such complicated potentials is still unthinkable in a calculation like the one by Osborn (see Chapter 6). It is the advantage of a variational calculation that one has to essentially calculate only matrix elements $\langle\psi_m|H-E|\psi_n\rangle$. The integrations can be performed by very accurate integration rules [88] which yield a six to eight digit accuracy already with an integration mesh of 12 mesh points per dimension. The numerical solution of the eigenvalue equation does not pose any problem (except for numerical stability, see Chapter 6, section 1).

2. Variational Methods for Elastic Scattering and for Multichannel Scattering

Variational methods for scattering states are also characterized by a restriction of the function space which is used to construct an approximate solution of the Schrödinger equation. We shall call our function spaces (restricted) "Hilbert" spaces, even when "improper Hilbert states",.i.e., non-normalizable functions, are present; although this is not quite correct, it is customary in the literature. Scattering states always have asymptotically non-vanishing components which describe the

system before and after scattering. We assume them to be known up to a complex factor.

For the scattering wave function, we make an ansatz of the following form

$$\psi = \sum_i S(\varphi_i \chi_i) + \sum_j a_j h_j \,. \tag{8.11}$$

The first sum runs over all open channels in which the system is described by a bound pair and a particle which move relative to each other. The bound state wave function φ_i is assumed to be known, and the relative motion function χ_i is freely varied. The operator S denotes symmetrization for bosons and antisymmetrization for fermions. The second sum runs over a set of square integrable wave functions h_j of the three-particle system, which already have the right symmetry. They are called distortions and are used to correct the first sum, which satisfies the Schrödinger equation only asymptotically. The parameters a_j are varied. There are only channels with two-body fragmentation taken into account by our ansatz, which means that we are either below the breakup threshold or that we neglect the breakup channel.

We want to introduce a partial wave decomposition right at the beginning; therefore, we have to formulate the ansatz (8.11) a little more carefully. The channel functions are specified by a set of quantum numbers

$$c = \{\alpha, l, m, \mu_1, \mu_2, \tau_1, \tau_2\} \,. \tag{8.12}$$

The index α stands for all internal quantum numbers of the two reaction partners in channel c , including their spins and isospins; l and m are the orbital angular momentum of the relative motion and its z-component; μ_1 and μ_2 are the z-components of the two spins, and τ_1 , τ_2 are the third components of the two isospins. Channel functions with these indices form a basic set from which we can go over to channel functions with given channel spin (isospin) and given total angular momentum by superposition with Clebsch-Gordan coefficients. In this way, an irreducible representation of the final variational equations

is obtained, which means that the equations are decoupled as much as possible. Here, however, we want to pay no attention to the decoupling and stay with the basis given by the quantum numbers (8.12).

A channel function ψ_c , that is a single term of the first sum of Eq. (8.12), is written as

$$\psi_c = S\left\{\lambda_c \chi_c(\eta_c)\right\} , \tag{8.13}$$

where the relative motion function $\chi(\eta_c)$ now is a radial function. The function λ_c is called surface function and has the form

$$\lambda_c = Y_\ell^m(\theta_c, \phi_c)\, \eta_c^{-1}\, \varphi_{1,\alpha\mu_1\tau_1}\, \varphi_{2,\alpha\mu_2\tau_2} . \tag{8.14}$$

The functions φ_1, φ_2 describe the internal motion of the reaction partners, including spin and isospin; one of the φ-s , say φ_2 , describes only spin and isospin since one of the partners is a single nucleon. The coordinates η_c , θ_c , ϕ_c are polar coordinates of the relative distance of the reaction partners in channel c .

Channel functions have to be asymptotically orthogonal, which is expressed by the condition

$$\int S\left\{\lambda_c^*\right\} S\left\{\lambda_{c'}\right\} d\vec{r} = \delta_{cc'} . \tag{8.15}$$

The integral, which includes a sum over spin and isospin components, extends over all coordinates except η_c or $\eta_{c'}$, for which a fixed large value is assumed. We can also say: the range of integration is a large surface, which passes through all channels.

For each channel c , the Hamiltonian can be decomposed into an internal part $H_{i,c}$ and a relative part $H_{r,c}$,

$$H = H_{i,c} + H_{r,c} . \tag{8.16}$$

The internal motion function $\varphi_{1,\alpha\mu_1\tau_1}$ is an eigenfunction of

the Hamiltonian $H_{i,c}$ with an eigenvalue $E_{i,c}$,

$$(H_{i,c} - E_{i,c})\,\varphi_{1,\alpha\mu_1\tau_1} = 0 \,.$$

As mentioned above, the function $\varphi_{2,\alpha\mu_2\tau_2}$ is just a spin and isospin state. The total energy E of the system is

$$E = E_{i,c} + \epsilon_c \,, \tag{8.17}$$

where ϵ_c is the asymptotic value of the kinetic energy in channel c and is called channel energy.

For large distances η_c , we can write down the Schrödinger equation for the relative motion function $\chi_c(\eta_c)$,

$$\left[-\frac{1}{2M_c}\left(\frac{d^2}{d\eta_c^2} - \frac{\ell(\ell+1)}{\eta_c^2}\right) + V_{coul}\right] \chi_c(\eta_c) = \epsilon_c \chi_c(\eta_c) \,. \tag{8.18}$$

We have assumed, here, that a Coulomb potential v_{coul} is present. When there is no Coulomb potential, we get some well-known simplifications. The quantities c and l are related to each other by Eq. (8.12), M_c is the reduced mass of the reaction partners.

Solutions of Eq. (8.18) are the regular and irregular Coulomb functions f_l , g_l or incoming and outgoing Coulomb waves. The Coulomb functions have the asymptotic form

$$f_\ell \to \sqrt{\frac{M_c}{q_c}} \sin\left(q_c\eta_c - \tfrac{1}{2}\ell\pi + \zeta_\ell - \beta \log 2 q_c \eta_c\right) \,, \tag{8.19a}$$

$$g_\ell \to \sqrt{\frac{M_c}{q_c}} \cos\left(q_c\eta_c - \tfrac{1}{2}\ell\pi + \zeta_\ell - \beta \log 2 q_c \eta_c\right) \,, \tag{8.19b}$$

with

$$q_c = \sqrt{2 M_c \epsilon_c} \,, \tag{8.20}$$

$$\zeta_\ell = \arg\Gamma(\ell + 1 + i\beta) \,, \tag{8.21}$$

$$\beta = \frac{Z_c Z_c' e^2 M_c}{q_c} \,, \tag{8.22}$$

where $Z_c e$ and $Z'_c e$ are the electric charges of the reaction partners in channel c .

The incoming and outgoing waves are, asymptotically,

$$g_\ell^- - i f_\ell^- \to \sqrt{\frac{M_c}{q_c}} \exp i\left(-q_c r_c + \tfrac{1}{2}\ell\pi - \zeta_\ell + \beta \log 2 q_c r_c\right), \quad (8.23a)$$

$$g_\ell^+ + i f_\ell^+ \to \sqrt{\frac{M_c}{q_c}} \exp i\left(+q_c r_c - \tfrac{1}{2}\ell\pi + \zeta_\ell - \beta \log 2 q_c r_c\right). \quad (8.23b)$$

We have discussed here the most general case of a two-body channel function with three elementary particles. As an example, we want to mention now the simplifications which we get for the neutron-deuteron system. There is only one two-particle bound state, namely the one of the deuteron with spin 1 and isospin 0. The neutron has spin 1/2 and isospin 1/2 . In an irreducible representation there are, first of all, two sorts of channels: the doublet channels, where the spin of the free neutron is antiparallel to the spin of the deuteron, and the quartet channels, where the spin of the free neutron is parallel to the spin of the deuteron. The multiplicity of channels in each case is given by the possible values of angular momenta and channel spin directions.

We now can rewrite our ansatz (8.11) with exact definitions and get

$$\psi = \sum_c S\left\{\lambda_c \chi_c(r_c)\right\} + \sum_j a_j h_j \,. \quad (8.24)$$

Continuous variation of the relative motion function χ_c and variation of the linear parameters a_j leads, in a variational principle to be described later, to a set of integrodifferential equations which is coupled to a set of linear equations. Such a set of equations is solved in practice either by iteration or by approximating the integrodifferential equations by linear equations. In any case, the continuous variation parameter $\chi_c(r_c)$ is replaced by a finite set of discrete function values. We can just as well go over to discrete parameters right at the beginning by expanding the function $\chi_c(r_c)$ into the asymptotic solutions $f_l(r_c)$ and $g_l(r_c)$ together with a set of square

integrable functions of η_c . The square integrable terms of the expansion can be added to the second sum of Eq. (8.24) after multiplication by the surface function λ_c and (anti-) symmetrization. The boundary condition has to be chosen, and we want to choose it in such a way so that we may avoid complex functions as much as possible.

Asymptotically, the scattering solution is a superposition of channel functions. The amplitudes are determined by the properties of the system in the reaction volume and by boundary conditions. For n channels, we can postulate n different boundary conditions, since, in principle, the incoming flux can be prescribed freely in n different channels. It would be physically meaningful to demand that the incoming flux be equal to unity in one channel and zero in all other channels. But such a boundary condition implies complex relative motion functions. It is easier to calculate a set of linearly independent solutions with real relative motion functions and get the physical solution by superposition. Real relative motion functions are obtained by the condition that, in the i^{th} channel, the regular Coulomb function has an amplitude equal to one and all other regular Coulomb functions have an amplitude equal to zero. For n channels, we get n different boundary conditions of this type by letting i run from 1 to n .

For the i^{th} boundary condition, we thus have the following ansatz

$$\Psi_i(E,\vec{r}) = F_i(\epsilon_i,\vec{r}) + \sum_{j=1}^{n} a_{ij} G_j(\epsilon_j,\vec{r}) + \sum_{j=n+1}^{N} a_{ij} h_{j-n}(\vec{r}) , \quad (8.25)$$

with

$$F_i(\epsilon_i,\vec{r}) = S\{\lambda_i f_\ell(q_i\eta_i)\} , \quad (8.26a)$$

$$G_j(\epsilon_j,\vec{r}) = S\{\lambda_j [1+(q_j\eta_j)^{-\ell-1}]^{-1} g_\ell(q_j\eta_j)\} . \quad (8.26b)$$

The indices i , j , and l are again correlated by Eq. (8.12), where i and j stand for the channel index c . The function G_j

would be singular at $n_j = o$ without a cutoff factor. We have, therefore, introduced the factor $(1+(q_j n_j)^{-l-1})^{-1}$ with the understanding that it can be replaced in practice by any similar function. The second sum in Eq. (8.25) contains distortions as well as square integrable channel structures, that is, functions which are an (anti-) symmetrized product of a surface function and a square integrable relative motion function.

We have mentioned at the beginning of this section that variational methods for scattering states are characterized by a restriction of the function space which is used to construct an approximate solution of the Schrödinger equation. We can see clearly now what our restricted function space is. First of all, we have the finite space of square integrable functions,

$$\mathcal{H}^{(1)} = \{ h_\mu^{(1)} \} . \tag{8.27}$$

In addition, we have the non-normalizable asymptotic solutions G_j which are multiplied by variational parameters while the functions F_i have fixed parameters and do not take part in the variation. The variation is thus restricted to the space

$$\mathcal{H}^{(2)} = \{ h_\nu^{(2)} \} \equiv \{ G_j, h_\mu^{(1)} \} . \tag{8.28}$$

We have introduced here the new symbols $h_\nu^{(2)}$ which allow us to write down the variational equations in a closer form. In the new notation, the ansatz (8.25) is just

$$\Psi_i(E,\vec{r}) = F_i(\epsilon_i,\vec{r}) + \sum_{\nu=1}^{N} a_{i\nu} h_\nu^{(2)}(\vec{r}) . \tag{8.29}$$

Having an ansatz, we now come to the question of how to determine the parameters. We want to use the freedom furnished by the linear parameters $a_{i\nu}$ to get an approximation to a true Schrödinger solution in the "best" way.

The idea of solving the Schrödinger equation in a restricted space instead of a full space suggests that the vector $(H-E)|\Psi_i\rangle$ has zero components in the space $\mathcal{H}^{(2)}$. We thus obtain a linear set of equations which is part of the Hulthén-Kohn variational

principle [101,102],

$$\sum_{\nu=1}^{N} \langle h_\mu^{(2)} | H-E | h_\nu^{(2)} \rangle \, a_{i\nu} = - \langle h_\mu^{(2)} | H-E | \bar{F}_i \rangle \; . \qquad (8.30)$$

This equation, however, leads to false resonances [103-105]. There are two types of them. The first type arises from the channel structures in the space (8.27). They are the typical false Kohn-resonances. The second type arises from the distortion functions. They appear above the threshold of the first channel, which has not been taken into account in our ansatz (like the breakup channel, for instance), and they would even be there if we had stayed with the integrodifferential equations approach [106,107].

Formally, false resonances arise from the zeros of the determinant of the coefficient matrix. A closer look shows that they are produced by the peculiar defect minimization which has been chosen in Eq. (8.30). With a restricted ansatz, the Schrödinger equation $(H-E)|\Psi_i\rangle = 0$ cannot be satisfied exactly. Instead of a zero on the right-hand side, there will be a defect δ which has to be minimized in some way. We have demanded that the defect have zero components in the space $\mathcal{H}^{(2)}$, and we did not take into account any components outside of $\mathcal{H}^{(2)}$. It turns out that the false resonances are caused just by these latter components. So we have to change the defect minimization if we do not want to run into false resonances.

We want to give some consideration to the components of $(H-E)|\Psi_i\rangle$ outside of the space $\mathcal{H}^{(2)}$, and introduce a space which is a little larger than $\mathcal{H}^{(2)}$,

$$\mathcal{H}^{(3)} = \{ h_\nu^{(3)} \} \equiv \{ G_j, h_\mu^{(A)}, \omega_\varrho \} \; .$$

The additional functions ω_ρ may be normalizable or non-normalizable. Their special behavior is unimportant as long as they are linearly independent of the functions h_ν and non-vanishing in the region of configuration space where the functions h_μ fall off to zero. We want to leave the ansatz (8.29) unchanged but carry out the defect minimization in $\mathcal{H}^{(3)}$ instead of $\mathcal{H}^{(2)}$. We can no longer demand to have zero components in $\mathcal{H}^{(3)}$ because

this would mean having more conditions than degrees of freedom. But we can demand that the sum of squared components of $(H-E)|\Psi_i\rangle$ in $\mathcal{H}^{(3)}$ becomes a minimum. Such a least-squares condition leads to the equation

$$A^+ A\, a = A^+ b \quad , \tag{8.31}$$

where A is the rectangular matrix $\langle h_\mu^{(3)}|H-E|h_\nu^{(2)}\rangle$, a is the column vector $a_{i\nu}$ with ν as vector index, b is the column vector $-\langle h_\mu^{(3)}|H-E|F_i\rangle$ with μ as vector index, and A^+ is the Hermitian conjugate of A . When the choice of the functions ω_ρ is not too unreasonable, Eq. (8.31) no longer leads to false resonances. As has been previously stated, the choice of these functions it not critical. In a one-channel test calculation [103], one single function $\omega_1 \equiv F_1$ is good enough to suppress false resonances of the first kind. In a three-boson system, false resonances of the second type are suppressed rather well by choosing ω equal to a constant or equal to an overall gaussian function of wide range [107].

Phases calculated from Eq. (8.31) cannot pass through $\pi/2$ (modulo π) any more (since the Gauß-transform A^+A is positive (semi-) definite). Before reaching the value $\pi/2$, they will make a sharp turn and continue shifted by π . If we were to choose a boundary condition which fixes the amplitudes of the functions G_i instead of F_i , the same thing would not happen at $\pi/2$ but at zero (modulo π). The best way to avoid such a behavior is to let the amplitudes of both F_i and G_i be free, and solve an eigenvalue equation instead of the linear equation (8.31). In this case, the least squares condition is met by looking for the n eigensolutions with the smallest eigenvalues [104,105]. Since it is a little easier in practice to solve a linear equation instead of an eigenvalue equation, one will usually stay with Eq. (8.31) and ignore the strange behavior of the phases near $\pi/2$.

Equation (8.31) is a set of linear equations for every value of i from 1 to n . The solutions of all these equations form the matrix $a_{i\nu}$. The information on the scattering cross sections is contained in the square part a_{ij} (i,j = 1 ... n) of this matrix.

We can improve the matrix a_{ij} by the so-called Kato correction [109]. To this end we study the expression

$$\langle \Psi_i^t | H-E | \Psi_j \rangle - \langle \Psi_j | H-E | \Psi_i^t \rangle , \tag{8.32}$$

where Ψ_i^t is the true solution of the Schrödinger equation satisfying the i^{th} boundary condition, while Ψ_j is an approximate solution satisfying the j^{th} boundary condition. We insert for the approximate solution the expansion (8.25) with coefficients a_{ij} determined by Eq. (8.31). For the true solution Ψ_i^t, we also insert expansion (8.25) with true coefficients a_{ij}^t ($j = 1 \ldots n$, the second sum in Eq. (8.25) is irrelevant). With the following relations, which are easily verified by the definitions (8.26a,b),

$$\langle F_i | H-E | F_k \rangle - \langle F_k | H-E | F_i \rangle = 0 , \tag{8.33a}$$

$$\langle F_i | H-E | G_k \rangle - \langle G_k | H-E | F_i \rangle = \tfrac{1}{2} \delta_{ik} , \tag{8.33b}$$

$$\langle F_i | H-E | h_\nu^{(\lambda)} \rangle - \langle h_\nu^{(\lambda)} | H-E | F_i \rangle = 0 , \tag{8.33c}$$

$$\langle G_i | H-E | h_\nu^{(\lambda)} \rangle - \langle h_\nu^{(\lambda)} | H-E | G_i \rangle = 0 , \tag{8.33d}$$

we get

$$\langle \Psi_i^t | H-E | \Psi_j \rangle - \langle \Psi_j | H-E | \Psi_i^t \rangle = \tfrac{1}{2} (a_{ji} - a_{ij}^t) . \tag{8.34}$$

Introducing the difference W_i between true solution and approximate solution,

$$W_i = \Psi_i^t - \Psi_i ,$$

and bearing in mind that $(H-E)|\Psi_i^t\rangle = 0$, we get the Kato identity,

$$\tfrac{1}{2}(a_{ji} - a^{t}_{ij}) = \langle \Psi_i | H - E | \Psi_j \rangle - \langle W_i | H - E | W_j \rangle \,. \qquad (8.35)$$

The second term on the right-hand side is of second order in W_i , which is supposed to be small. If we leave this term out, we get an equation which defines new amplitudes a'_{ij} ,

$$a'_{ij} = a_{ji} - 2\langle \Psi_i | H - E | \Psi_j \rangle \,. \qquad (8.36)$$

This equation is referred to as the Kato-correction formula. The amplitudes a'_{ij} are usually much better approximations than the amplitudes a_{ij} . The Kato correction, however, cannot correct for missing distortions but only for missing channel structures in the second sum of Eq. (8.25).

We now have to carry out the transition from our boundary condition, which has been mathematically convenient, to the physical boundary condition. The solutions Ψ_i (with coefficients a'_{ij} instead of a_{ij}) are superimposed in such a way that the Coulomb functions (8.19a,b) become incoming and outgoing waves and the incoming waves have zero flux in all but one channel. This procedure yields the well-known formula which relates the S-matrix to the reactance matrix a'_{ij} ,

$$S = [1 + i(a'_{ij})][1 - i(a'_{ij})]^{-1} \,. \qquad (8.37)$$

For its derivation, we refer to textbooks on quantum mechanics [6].

We should mention here that difficulties arise when approximations are used for the two-particle bound states in the channel functions. In this case, there will be no convergence with respect to an increasing number of distortions [110]. The distortion functions will try to correct also the internal motion functions in the channels. Because of square integrability, they can only succeed in a finite region. A mismatch arises at the end of this region, and this mismatch can always be changed drastically by adding new distortion functions.

3. Variational Methods for Multichannel Scattering with Three-Particle Breakup

In order to include the breakup reaction, we have to extend the function space $\mathcal{H}^{(2)}$ by including functions which asymptotically describe three free particles and which obey certain boundary conditions.

At rather low energies, where the breakup cross section is small, it seems to be reasonable to neglect breakup altogether and use the method of the last section. False resonances of the second type, which arise from virtual states formed by the distortion functions in the region of the neglected breakup channel, are suppressed by the least-squares principle. This principle, however, cannot be a substitute for neglected channels. It can only cure unpleasant side effects such as false resonances. It has to be investigated, therefore, whether the neglection of the breakup channel has a large influence on the amplitudes of the other channel functions and how much loss of accuracy the neglection brings about.

Figure 46 shows a comparison of a variational result [108] with the solution of the AGS equation (Eq. (6.86)) [96]. In both cases, the elastic phase shifts have been calculated for the scattering of a boson from a bound pair of bosons. The bosons interact via Yukawa potentials. In the variational calculation, the breakup channel has been neglected while the AGS result contains the influence of the breakup reaction above $E = o$. The variational result and the first quasi-Born approximation differ by about 6 degrees (for $L = o$). But the difference is already there below the breakup threshold where the variational result is a lower bound to the true phase shift curve and is probably very close to the true one. The AGS result, therefore, does not contradict the variational result, and the comparison can rather serve as a check to the quality of the first quasi-Born approximation in this special example (Yamaguchi potential as zero-order approximation).

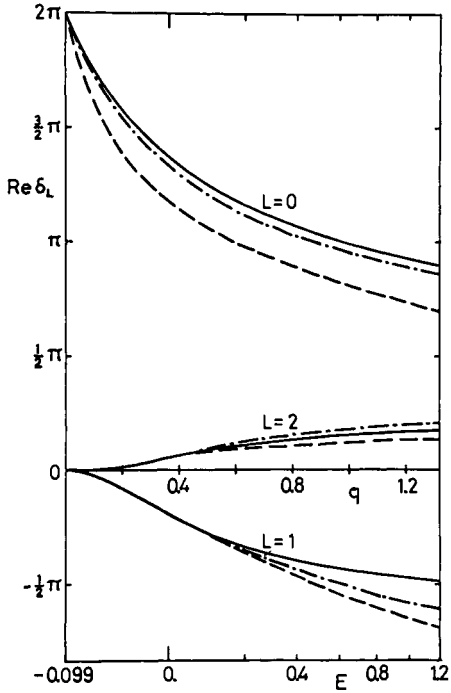

Fig. 46. Variational result (J. Schwager [108]) for the real part of the phase shifts δ_L for three identical bosons interacting by a Yukawa potential compared with quasi-particle calculations (H. Ziegelmann [96], see Fig. 41). The dashed lines represent the 0.QBA, the dashed-dotted lines the 1.QBA and the full lines the variational results.

Figure 47 shows once more the L = o phase of the three-boson system. In this case, however, a separable Yamaguchi potential has been used, and the broken line shows the exact Faddeev result [63]. The full line shows the variational result with neglected breakup [111]. It is seen that there is, indeed, a slight discrepency of the two curves above the breakup threshold, but the difference is smaller than 1.5 degrees up to 4.5 MeV (c.m.). It seems to be promising, therefore, to use the variational method of the last section for a calculation of elastic phases in the three-nucleon system, even above the breakup threshold.

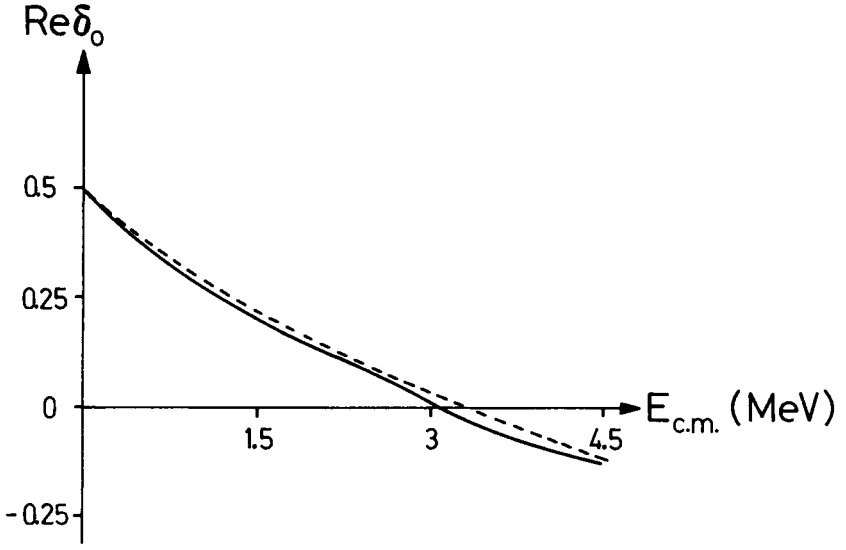

Fig. 47. Variational result (full line, F. Sohre and E.W. Schmid [111]) for the real part of the phase shift δ_o for three identical bosons interacting by a Yamaguchi potential compared with the exact Faddeev solution (broken line, F. Sohre and H. Ziegelmann [63]). The energy region starts at breakup threshold, the coupling constant is adjusted to a deuteron binding energy of 2.2 MeV .

We shall come back now to our problem of including the breakup reaction in the variational calculation.

The difficulties have already been mentioned in the introduction. The three particles which emerge from a breakup reaction are free, but correlated. As we have seen, the total energy can be distributed over the three particles in a continuous way. If, for instance, one particle gets four times as much kinetic energy as another particle, it will travel twice as fast and, after a few nanoseconds, be approximately twice as far away from the scattering center. Therefore, an approximate description of the free motion by plane waves is not possible. In a two-body decay, the outgoing spherical wave is approximately a plane wave in the region of a particle counter in an

experiment; the spherical structure of the wave is not detected by the counter. In a three-body decay, the particle correlation is an important measurable quantity. If plane waves were used to describe the free motion, the correlation would have to be described by a complicated superposition of waves.

A second difficulty, besides asymptotic correlation, is the infiniteness of the reaction volume. The two-particle interaction potential can become effective at an arbitrary distance from the scattering center because of the possibility of rescattering (see Fig. 8).

A third difficulty arises from the necessity of introducing a time-independent boundary condition. We can formulate such a condition if we succeed in writing down three-particle breakup states of purely outgoing character. To illustrate the difficulty, the question has been raised in the introduction whether a situation, where one particle approaches the common center-of-mass while two particles depart, has an outgoing or incoming character. The construction of purely outgoing states seems to be difficult, but possible. We can see that it is possible, in principle, by the following consideration. We introduce a coordinate ρ which describes the size of the triangle formed by the three particles. A wave function will have purely outgoing character when its waves move in the direction of increasing values of ρ . Since the shape of the triangle may change, it can happen that one particle approaches the common center-of-mass for a little while, that is, in a certain region of ρ . But for $\rho \to \infty$, all distances will increase beyond any limit and, therefore, we have an asymptotically outgoing state. We see that the correlation of free particles plays a decisive role also in the formulation of a boundary condition.

In the following, we shall discuss two possibilities of constructing outgoing three-particle states. The first possibility leads to hyperspherical functions, which are also called "hyperspherical harmonics" or "K-harmonics". The second possibility is the introduction of time-independent two-particle wave packets in which the position of the third particle replaces the time scale. The function system of K-harmonics is suited mainly for the description of the sudden decay, while

the wave packet description can also be used for breakup reactions with a strong final state interaction.

The system of variational equations is not changed by the inclusion of breakup. The system of breakup states is just added to the test function space $\mathcal{H}^{(2)}$. There are a few difficulties with the Kato correction, which are still under investigation (see also Lieber, Rosenberg, and Spruch [125]).

Before we discuss the two systems of functions which can be used to described breakup, we want to mention two other methods which avoid problems arising in the asymptotic region by introducing complex energies [112] or complex coordinates [113]. The methods have some similarity to the integration method of Hetherington and Schick which avoids singularities of the Faddeev equations by shifting the path of integration into the complex plane. There is, indeed, a relation between the singularities in the Faddeev equations and the complicated asymptotic behavior of the wave function above the breakup threshold, which can be attenuated by complex energies or complex coordinates.

For all approximation schemes, it is desirable to test them with known exact solutions. Curiously enough, in 1951 Wildermuth [114] has already presented a model which allows one to solve a breakup problem by solving the Schrödinger equation analytically. This model is not realistic in a physical sense, but it is helpful in the testing of approximation methods.

3.1. Hyperspherical Functions

As a first step, we have to introduce the so-called hyperspherical coordinates; one of them is the above-mentioned coordinate ρ . We redefine our Jacobi coordinates (without changing the notation) by

$$\vec{\xi} = \left(\frac{m_1 m_2}{m_1+m_2}\right)^{\frac{1}{2}} (\vec{r}_1 - \vec{r}_2) , \tag{8.38a}$$

and

$$\vec{\eta} = \left(\frac{m_3(m_1+m_2)}{m_1+m_2+m_3}\right)^{\frac{1}{2}} \left(\frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1+m_2} - \vec{r}_3\right) . \tag{8.38b}$$

Again, the coordinate ξ is essentially the distance between particles 1 and 2 , while η is essentially the distance between particle 3 and the center-of-mass of particles 1 and 2 . The only difference between the new Jacobi coordinates and the old ones is a mass factor, which is the square root of the corresponding reduced mass. This factor has the effect that, in the new coordinates, the expression for the kinetic energy is a sum of second derivatives multiplied by (-1/2) . In the old coordinates, the second derivatives were partly multiplied by (-1/2μ) and partly by (-1/2M) . The new Jacobi coordinates are called rationalized Jacobi coordinates. As in Eq. (2.71), there are three different sets of them, depending on which particle is chosen to be the third one. In a sudden breakup, no subsystem is preferred and, therefore, we need only one set of rationalized Jacobi coordinates.

The hyperspherical functions diagonalize the free three-particle Hamiltonian h_0 . In rationalized Jacobi coordinates, this operator has the simple form,

$$h_0 = -\frac{1}{2}\left(\Delta_\xi + \Delta_\eta\right) = -\frac{1}{2}\Delta \ , \tag{8.39}$$

where Δ is the six-dimensional Laplace operator.
The hyperspherical coordinates

$$\vec{\rho} = (\rho, \hat{\rho}) = (\rho, \alpha, \vartheta_\xi, \varphi_\xi, \vartheta_\eta, \varphi_\eta) \tag{8.40}$$

are now defined by the following transformations,

$$\xi_x = \rho \cos\alpha \sin\vartheta_\xi \cos\varphi_\xi \ ,$$

$$\xi_y = \rho \cos\alpha \sin\vartheta_\xi \sin\varphi_\xi \ ,$$

$$\xi_z = \rho \cos\alpha \cos\vartheta_\xi \ ,$$

$$\eta_x = \rho \sin\alpha \sin\vartheta_\eta \cos\varphi_\eta \,, \tag{8.41}$$

$$\eta_y = \rho \sin\alpha \sin\vartheta_\eta \sin\varphi_\eta \,,$$

$$\eta_z = \rho \sin\alpha \cos\vartheta_\eta \,,$$

$$d\vec{\rho} = \rho^5 d\rho\, d\hat{\rho} \,, \quad d\hat{\rho} = \sin^2\alpha \cos^2\alpha \, d\alpha \, d\hat{\xi} \, d\hat{\eta} \,,$$

$$0 \le \alpha \le \pi/2, \; 0 \le \vartheta_\xi \le \pi, \; 0 \le \varphi_\xi \le 2\pi, \; 0 \le \vartheta_\eta \le \pi, \; 0 \le \varphi_\eta \le 2\pi \,.$$

They are rather easy to comprehend. The coordinates ϑ_ξ and φ_ξ are identical to the second and third polar coordinate of

$$\vec{\xi} = (\xi, \vartheta_\xi, \varphi_\xi) \,, \tag{8.42}$$

and similar to ϑ_η and φ_η . For the two absolute values ξ and η , polar coordinates are introduced by

$$\xi = \rho \cos\alpha \,, \quad \eta = \rho \sin\alpha \,, \quad 0 \le \alpha \le \pi/2 \,, \tag{8.43}$$

with

$$\rho = \sqrt{\xi^2 + \eta^2} \tag{8.44}$$

With ρ as the length of the six-dimensional vector $(\vec{\xi},\vec{\eta})$, we have the important coordinate which measures the size of the triangle which is formed by the three particles. The other five coordinates determine the shape of the triangle and its orientation in space.

In hyperspherical coordinates, the free Hamiltonian becomes

$$h_o = -\frac{1}{2}\left(\frac{\partial^2}{\partial\rho^2} + \frac{5}{\rho}\frac{\partial}{\partial\rho} - \frac{\vec{K}^2}{\rho^2}\right) . \tag{8.45}$$

The operator $\vec{K}^2$ acts only on the five angular coordinates. The term $\vec{K}^2/\rho^2$ plays the same role as $\vec{L}^2/r^2$ in the three-dimensional angular momentum decomposition. Therefore, the operator $\vec{K}^2$ is sometimes referred to as the operator of "hyperangular momentum". It has the eigenvalues $K(K+4)$, in resemblance to the eigenvalues $L(L+1)$ of $\vec{L}^2$. But, instead of one magnetic quantum number M , we now have 4 "magnetic" quantum numbers. We denote them, in collected form, by the symbol q .

The eigenfunctions of the free Hamiltonian h_o factorize into a radial part $R_K(\rho)$ and an angular part $Y_K^q(\hat{\rho})$,

$$\psi(\vec{\rho}) = R_K(\rho)\, Y_K^q(\hat{\rho}) \quad . \tag{8.46}$$

The radial part has the asymptotic form

$$R_K(\rho) \to a\frac{e^{-ik\rho}}{\rho^{5/2}} + b\frac{e^{ik\rho}}{\rho^{5/2}} \quad , \tag{8.47}$$

which means that it consists of incoming and outgoing waves. Choosing $a = o$, we can obtain from Eq. (8.46) a basis of free three-particle states with purely outgoing character.

The shape of the function $R_K(\rho)$ for small values of ρ is unimportant in a variational calculation, since it is corrected anyway by the addition of square integrable functions. The angular functions Y_K^q have the somewhat complicated form [115]

$$Y_K^q(\hat{\rho}) \equiv Y_K^{\ell m \lambda \mu}(\hat{\rho}) = Y_\ell^m(\hat{\xi})\, Y_\lambda^\mu(\hat{\eta})\, H_K^{\ell\lambda}(\alpha) \quad , \tag{8.48}$$

with

$$H_K^{\ell\lambda}(\alpha) = N_K^{\ell\lambda} \cos^\ell\alpha \sin^\lambda\alpha\, P_\varkappa^{(\ell+1/2,\,\lambda+1/2)}(-\cos 2\alpha) \quad , \tag{8.49}$$

$$N_K^{\ell\lambda} = \left[\frac{2\varkappa!\, 4^{K+2}(K+2)(\ell+\lambda+\varkappa+1)!(\ell+\varkappa+1)!(\lambda+\varkappa+1)!}{\pi(2\ell+2\varkappa+2)!(2\lambda+2\varkappa+2)!}\right]^{1/2} \quad , \tag{8.50}$$

and

$$\varkappa = (K-\ell-\lambda)/2 \quad . \tag{8.51}$$

The functions Y_l^m are the ordinary spherical harmonics, and the functions $P_\varkappa^{(\mu,\nu)}$ are Jacobi polynomials. In a sudden breakup, the most important functions are those with $l = \lambda = o$ (and low values of K). In this case, we have

$$\mathcal{Y}_\varkappa^{0000}(\hat{\xi}) = \pi^{-3/2} C_{\varkappa/2}^{1}(-\cos 2\alpha) , \qquad (8.52)$$

where C_μ^ν is the Gegenbauer polynomial.

There is another, more systematic way of introducing the hyperspherical functions $\mathcal{Y}_K^q$ [126]. One chooses a certain algebra of operators which commute with the free Hamiltonian h_o and obtains the hyperspherical functions as an irreducible representation space of this algebra. The intuition, which is the essential part of choosing a testfunction space, enters by the choice of the algebra. The rest is automatic. When the generators of rotations in the six-dimensional coordinate space $(\vec{\xi},\vec{\eta})$ are chosen as an algebra, we get the hyperspherical functions as representation space, just as the spherical harmonics Y_l^m are obtained via the generators of rotations in three-dimensional space.

In order to get an irreducible form of the variational equations, we have to construct eigenstates of the total angular momentum and of the isospin. This is done by multiplying the functions $\mathcal{Y}_K^q$ with spin- and isospin vectors and adding them with suitable factors. We do not want to go into these details but would rather discuss the physical meaning of the hyperspherical function basis.

What is the meaning of the quantum number K ? We want to use the analogy to ordinary angular momentum to understand this quantity. When a particle is scattered from a potential $V(\vec{r})$, the angular momentum decomposition of the scattering solution $\psi(\vec{r})$ is an expansion into components of different impact parameters p . Classically, the impact parameter is the closest distance in which a particle of given angular momentum and given velocity v passes the scattering center. In quantum mechanics, the impact parameter has no sharp value. But we have still approximately

$$\rho \approx \frac{L\hbar}{v} \quad , \tag{8.53}$$

and, thus, an expansion into angular momentum quantum numbers L is an expansion into impact parameters. When the potential $V(\vec{r})$ is short-ranged and the velocity v is not too large, only the first few terms of the expansion will contribute to the scattering process.

The quantum number K has a quite similar meaning. We could call it a three-particle impact parameter. Thinking in terms of classical orbits, a large value of K means that the three particles cannot come close to each other at the same time. Either all three particles are far apart or, when two particles are close together, the third particle is far away. When K ist equal to zero, on the other hand, all three particles meet in the scattering center. The minimum value of ρ is related to K just as the minimum value of r is related to L . For $K = o$, the particles seem to come right out of the scattering center. For higher values of K , they seem to have left the scattering center in a more and more "crooked way". For the description of a sudden breakup (with little final state interaction), we should expect that only functions with low values of K are important.

Two advantages of the expansion into angular momentum eigenstates are not present in the hyperangular momentum expansion of a scattering wave function. Firstly, a sum of two-particle interaction potentials is not spherical symmetric in the six-dimensional coordinate space $(\vec{\xi},\vec{n})$. The operator K , therefore, does not commute with the Hamiltonian H , while L commutes with H for a spherical symmetrical potential V(r) . The various hyperspherical states are coupled by the interaction. Secondly, and this may be even more important, high-order terms of the expansion into hyperspherical functions become unimportant only in certain special cases (sudden breakup without rescattering). A sum of two-particle interaction potentials has an infinite range in ρ-space, that is, $V(\vec{\rho})$ does not tend to zero with $\rho \to \infty$. The integration volume of the "potential grooves" which run to infinity is small enough, though, that the matrix

elements $\langle h_\mu^{(2)} | H-E | h_\nu^{(2)} \rangle$ exist even when both $h_\mu^{(2)}$ and $h_\nu^{(2)}$ are hyperspherical functions [1]. The expansion, however, converges slowly, especially when two-particle excited states with a long lifetime are involved in the decay.

To illustrate the concept of "three-particle impact parameters", we now want to consider the scattering of three particles moving in one-dimensional space. The expansion into hyperspherical functions becomes rather simple, in this case, and its physical meaning can easily be understood.

As rationalized Jacobi coordinates, we have in this case, with $m = 1$,

$$\begin{aligned} \xi &= \frac{1}{\sqrt{2}} (x_1 - x_2) \quad , \\ \eta &= \sqrt{\frac{2}{3}} \left(\frac{x_1 + x_2}{2} - x_3 \right) \quad , \end{aligned} \tag{8.54}$$

where x_1 , x_2 , x_3 denote the positions of the three particles. Figure 48 shows the region of interaction in two-dimensional (ξ,η) space. In each of the shaded grooves, one of the two-particle interaction potentials is different from zero. In the center of the figure, two or three pairs of interactions are different from zero. The hyperspherical coordinates are simply polar coordinates (ρ,α) in the (ξ,η) plane. Contrary to Eq. (8.43), the angle α varies from o to 2π , since both ξ and η can assume negative values. The hyperspherical functions become angular momentum eigenstates in a plane, i.e., they have the form

$$Y_m(\alpha) = e^{im\alpha} \quad , \quad m = 0, \pm 1, \pm 2 \ldots \tag{8.55}$$

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[1] This is only true for three particles in three-dimensional space. Analogous functions can be constructed for three particles moving in one-dimensional space. In this case, however, the integration volume of the grooves is comparatively larger and the matrix elements diverge.

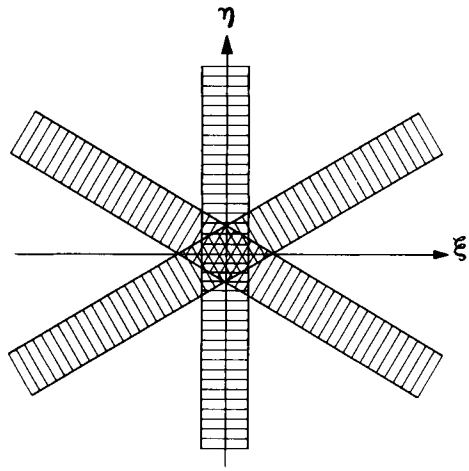

Fig. 48. The regions of interaction in the (ξ,η) plane

The radial function has the asymptotic form

$$R_m(\varrho) \longrightarrow a\frac{e^{-ik\varrho}}{\varrho^{1/2}} + b\frac{e^{ik\varrho}}{\varrho^{1/2}} \quad . \tag{8.56}$$

The Schrödinger equation of the three-particle system is

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}\right)+V(\xi,\eta)\right]\psi = E\psi \quad , \tag{8.57}$$

or,

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial\varrho^2}+\frac{1}{\varrho}\frac{\partial}{\partial\varrho}+\frac{1}{\varrho^2}\frac{\partial^2}{\partial\alpha^2}\right)+V(\varrho,\alpha)\right]\psi = E\psi \quad , \tag{8.58}$$

which means that the motion of the three-particle system in configuration space is the same as the motion of one particle in the (ξ,η) plane.

The hyperspherical "channel" functions,

$$\psi_m = R_m(\varrho)\,Y_m(\alpha) \quad , \tag{8.59}$$

satisfy the free Schrödinger equation ($V = o$) . The classical motion corresponding to these functions is depicted by arrows in Fig. 49a for $a = o$ and $m = o$, and in Fig. 49b for $a = o$ and $m = +1$.

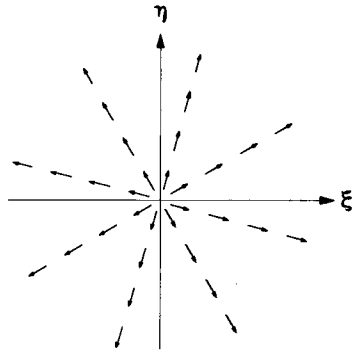

Fig. 49a. Classical motion corresponding to hyperspherical "channel" function, Eq. (8.59), with a = o , m = o

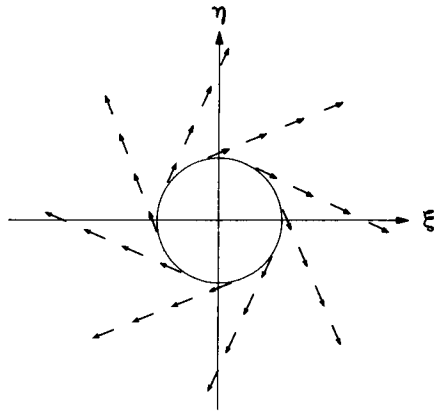

Fig. 49b. As above, but with a = o , m = 1 .

For m = o , the system emerges from the scattering center, where all three particles have the same position ($x_1 = x_2 = x_3$). For m = 1 , the system emerges from the periphery of a circle. The radius of this circle is the three-particle impact parameter. Going back to the coordinates x_1 , x_2 , x_3 , the meaning of this parameter can easily be visualized.

3.2. Sequential Decay States

The potential grooves of Fig. 48 and the corresponding grooves of the scattering problem in the three-dimensional space are not only responsible for the existence of the two-particle bound states inherent to elastic and rearrangement channels, but they also lead to the final state interaction of breakup states. When a compound state suddenly decays into three free particles, it is expected that the potential grooves have no great influence on the asymptotic state for most scattering angles and free particle energies. Few terms of the expansion into hyperspherical waves will suffice to describe breakup well. When, however, a pair of particles interacts over a rather long distance from the center - either by forming a long-lived two-particle excited state or by accidentally having small relative momentum - a good description would have to use very many hyperspherical waves. In this case, it is advantageous to introduce another kind of outgoing three-particle breakup states which can be termed as decaying wave packet states [103,116].

This second sort of states describes breakup as a sequential two-particle decay. An excited two-particle state together with a free third particle are formed in the first step. In the second step, then, the excited two-particle state decays into free particles. The two-particle states may be arbitrarily chosen in a variational calculation. They may be wave packets which describe a long-lived resonance state or wave packets which decay rather quickly. With the latter possibility, a sudden decay can also be described in terms of decaying wave packets.

There is an essential difference to the hyperspherical functions approach of the last section. The two-particle wave packets are written down in practice as a superposition of continuum states of the corresponding two-particle Hamiltonian. This means that one of the potential grooves is taken into account exactly, which leads to a faster convergence of the expansion into (discrete) breakup channels. In principle, one could use also continuum states of the free two-particle Hamiltonian but, then, the new approach would only mean a reordering of terms within a finite hyperspherical expansion. The third

alternative would be to have exact asymptotic solutions of the full three-particle Hamiltonian, as we had in the case of the elastic and rearrangement channels. This is not feasible, however, in the breakup case, since one would have to solve almost the full three-particle scattering problem in order to find these states. Recall that the potential grooves have to be regarded as "reaction volume", even in a region far away from the scattering center !

The decaying wave packet states are constructed in a similar way to the channel states of section 2. Again, a channel is characterized by an index c which contains information on the preferred subsystem and on the relative motion,

$$c = \{\alpha, \ell, m, \mu_1, \mu_2, \tau_1, \tau_2\} \quad . \tag{8.60}$$

The meaning of the quantum numbers l , m , μ_1 , μ_2 , τ_1 , τ_2 is the same as in Eq. (8.12). Only the meaning of the index α has changed. Formerly, this index contained information on which particles are bound in which bound state, and it also contained the quantum numbers of total spin S_1 , S_2 , and isospin T_1 , T_2 of the two reaction fragments. Now, we have a wave packet instead of a bound-state function $\varphi_{1,\alpha\mu_1\tau_1}$. The wave packet is described by a superposition amplitude $D(p_c, n_c)$. Since the wave packet decays, the amplitude D does not only depend on the relative momentum p_c of the subsystem, but also on the distance n_c of the third particle. The dependence on n_c will be discussed later. The wave packet is formed with $n_c = o$, and we call the function $D(p_c, o)$ simply $D(p_c)$. We then have for $n_c = o$, instead of a bound-state function, the wave packet

$$\varphi_{1,\alpha\mu_1\tau_1}(\vec{\xi}_c) = \int D(p_c)\,\varphi(S_1, \mu_1, T_1, \tau_1, p_c, \vec{\xi}_c)\, dp_c \quad , \tag{8.61}$$

where $\vec{\xi}_c$ is the relative coordinate of the subsystem. The internal properties of the wave packet are given by the function $D(p_c)$, besides spin and isospin. The index α , therefore, must contain this information,

$$\alpha = \{\ldots D \ldots\} \quad . \tag{8.62}$$

The function $\varphi(S_1,\mu_1,T_1,\tau_1,p_c,\vec{\xi}_c)$ is a regular solution of the Schrödinger equation of the subsystem with given total angular momentum S_1 , μ_1 , given isospin T_1 , τ_1 , and given energy $p_c^2/2\mu_c$. The sequential decay channel function can now be written down as

$$\Psi_c = \int S\{\lambda_c(\ldots p_c\ldots)\chi_c(q_c,\eta_c)\}\, d p_c \ , \tag{8.63}$$

with

$$\lambda_c = Y_\ell^m(\Theta_c,\Phi_c)\,\eta_c^{-1}\,D(p_c)\,\varphi(S_1,\mu_1,T_1,\tau_1,p_c,\vec{\xi}_c). \tag{8.64}$$

The analogy to Eqs. (8.13) and (8.14) is now only superficial. There is no longer o n e surface function since the wave packet decays. The decay is expressed by the dependence of the function $D(p_c,\eta_c)$ on η_c ; the distance η_c of the third particle somehow replaces the time scale of the decay process. We have to construct a surface function $\lambda_c(\ldots p_c\ldots)$ for every component $D(p_c)\varphi(S_1,\mu_1,T_1,\tau_1,p_c,\vec{\xi}_c)$. Everyone of these surface functions is multiplied by an appropriate relative motion function $\chi_c(q_c,\eta_c)$. By (anti-) symmetrization and integration over p_c , we get the discrete channel state of a decaying wave packet.

It is seen from Eqs. (8.63) and (8.64) that the η_c-dependent superposition amplitude $D(p_c,\eta_c)$, which contains the decay of the wave packet, has the form

$$D(p_c,\eta_c) = D(p_c)\,\chi(q_c,\eta_c) \ . \tag{8.65}$$

In order to have asymptotic orthogonality of the channel functions ψ_c , we demand orthogonality of different wave packets,

$$\int D_i^*(p)\, D_j(p)\, d p = \delta_{ij} \ . \tag{8.66}$$

The asymptotic correlation of the three particles follows from energy conservation. The relative motion function $\chi_c(q_c,\eta_c)$ is again a Coulomb function (or Bessel function), Eqs. (8.19) and (8.23), but, for every component of the wave packet, this function has another q_c-value. From asymptotic energy conservation,

we have the condition

$$\frac{p_c^2}{2\mu_c} + \frac{q_c^2}{2M_c} = E \quad , \tag{8.67}$$

i.e., the Coulomb function must have the wave number

$$q_c = \sqrt{2M_c\left(E - \frac{p_c^2}{2\mu_c}\right)} \quad . \tag{8.68}$$

This condition also ensures that the channel function ψ_c is an exact eigenfunction of the channel Hamiltonian. Depending on which kind of Coulomb function we choose, the channel function ψ_c has incoming or outgoing character or is a standing wave. The irregular Coulomb function must again be multiplied by a cutoff function. Note the close resemblance of Eq. (8.65) with the equation which describes the time development of a wave packet,

$$D(p,t) = D(p)\exp\left(-i\frac{p^2}{2\mu}t\right) \tag{8.69}$$

The distance η_c of the third particle can indeed be regarded as a substitute for the time scale; only the factors in front of t and η_c have a different p-dependence, which expresses the fact that the "arms of our clock" move with different velocity for different values of p . It should also be noted that the decaying wave packet states are wave packets only with respect to the internal motion of the subsystem. On the whole, they are non-normalizable channel states. Intuition is used in choosing the functions $D_c(p_c)$. Equation (8.67) determines the range of p_c . For larger values of p_c , we want to have $D(p_c)$ equal to zero [1]. When two-particle resonances play a role,

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[1] This condition is not a necessary one. According to Eq. (8.68), the wave number q_c becomes purely imaginary for $p_c^2/2\mu_c > E$. Choosing the positive sign of the square root, we get a square integrable contribution from Eq. (8.63). Only for convenience do we want to separate square integrable functions (distortions) and non-normalizable functions (channel states) in the variational ansatz for the scattering function.

we choose distributions $D_c(p_c)$ which are narrow, according to the expected life time of the virtual state. A very broad distribution $D_c(p_c)$, on the other hand, describes a sudden breakup process. The continuous manifold of breakup channels is thus reduced to a finite number of functions $D_c(p_c)$.

A variational calculation, which avoids complex functions as far as possible, can again be carried out by introducing the channel states

$$F_i = \int S\{\lambda_i(\dots p_i \dots) f_\ell(q_i r_i)\} dp_i \,, \qquad (8.70a)$$

$$G_j = \int S\{\lambda_j(\dots p_j \dots)[1+(q_j r_j)^{-\ell-1}]^{-1} g_\ell(q_j r_j)\} dp_j \qquad (8.70b)$$

(i,j = n + 1, n + 2, ... n') ,
where λ_i is given by Eq. (8.64) and the wave numbers p_i and q_i are related by Eq. (8.67). The states G_j are added to the test function space $\mathcal{H}^{(2)}$ of section 2, and we have again the variational ansatz (8.29) with standing wave boundary conditions,

$$\Psi_i = F_i + \sum_{\nu=1}^{N} a_{i\nu} h_\nu^{(2)} \,, \qquad (8.71)$$

where i now ranges from 1 to n' . The square integrable states of $\mathcal{H}^{(2)}$ now also have to correct the breakup states. Rescattering effects are taken into account only in the region which is covered by the square integrable corrections. Long-range rescattering is not described by the ansatz (8.71) since the square integrable functions have only finite range, and the set of channel states is far from being a complete set of functions. The space $\mathcal{H}^{(3)}$ contains, as before, all functions $h_\mu^{(2)}$ and, in addition, one or several functions ω_ρ . The least squares equation which determines the linear parameters $a_{i\nu}$ is again Eq. (8.31),

$$A^+ A\, a = A^+ b$$

with definitions analogous to section 2.

The wave packets move along the potential grooves while they decay. When they do not run into the other grooves during their decay, the channel functions are eigenstates of the total Hamiltonian, asymptotically, and the Kato correction formula (8.36) remains formally correct. But, since only a finite set of discrete breakup channels is taken into account, there are open channels present in the neglected "second-order term" of the Kato identity, and it becomes doubtful whether the Kato correction brings about a real improvement.

The S-matrix follows from the improved or unimproved reactance matrix according to Eq. (8.37). Because of condition (8.66), we have an orthogonal basis of outgoing (incoming) states also in the breakup part of the S-matrix.

3.3. The Method of Pieper, Schlessinger and Wright [128]

In conclusion, we want to discuss a method which combines the advantages of the Faddeev equations with those of variational methods. In the Kohn variational principle and its least-squares version, the trial function has to satisfy the Schrödinger equation, asymptotically, and obey a certain boundary condition. In multichannel scattering, these conditions do not pose a problem except that it may be hard to obtain exact internal motion functions. In breakup scattering, some effort was needed to introduce a boundary condition and, in connection with that, asymptotic particle correlations. In the hyperspherical approach, we even had to break the requirement of having asymptotic Schrödinger solutions, since K-harmonics satisfy only the free Schrödinger equation. This approach converges only because the potential grooves cover a very small fraction of the asymptotic region. To a lesser extent, the same argument is true in the wave packet approach, since decaying wave packet states are only eigenstates of a channel Hamiltonian and not of the total Hamiltonian.

It is of special interest, therefore, that variational methods for scattering processes can be constructed, in which the asymptotic behavior of the trial function is irrelevant. A method of this kind has first been presented by Schwinger [117] for the solution of the Lippmann-Schwinger equation.

Pieper, Schlessinger, and Wright [118] have adapted the Schwinger method to the Faddeev equations.

We want to discuss first the Schwinger variational principle and then the method of Pieper, Schlessinger, and Wright (PSW). Attention will be payed to the question of how the freedom in the asymptotic behavior of the trial function comes about and whether any sacrifices have to be made for this. In the variational methods of the previous sections, important information on the scattering problem as, for instance, the total energy and the boundary condition, has been contained in the asymptotic behavior of the trial function. In the present methods, this information must enter in some other way and we want to investigate how.

We follow in this section a presentation given by Grassberger, Alt, and Sandhas [119] in which several variational methods are derived in an efficient way from one fundamental equation. The fundamental equation is obtained in the following way. Assume that we are interested in an operator A (or in matrix elements of A) of which we know the inverse A^{-1}. Obviously, the equation

$$A = 2A - A A^{-1} A \tag{8.72}$$

is valid. This equation has the remarkable property that its left-hand side varies only by terms of the order $(\delta A)^2$ when A on the right-hand side (not A^{-1} !) is varied by δA . We, therefore, can write down as a variational principle,

$$[A] = 2A^t - A^t A^{-1} A^t , \tag{8.73}$$

where A^t is a trial operator and [A] is a variational approximation of A . By inserting $A^t = A + \delta A$, our statement can be verified. If we can find a trial operator A^t for which the left-hand side of Eq. (8.73) becomes stationary for all variations δA , then, we have $A^t = [A] = A$. In practice, "all variations" have to be replaced by a finite number of variations. In most cases, the trial operator will be a linear superposition of operators, and the coefficients are varied. Equation (8.73) will then be used in two steps. Firstly, a set of linear

equations is obtained by taking derivatives of $[A]$, with respect to the parameters, and making them equal to zero. This set of equations determines the parameters. Secondly, a correction is obtained, similar to the Kato correction, by again using Eq. (8.73). When A^t is inserted with parameter values determined by the linear equation of the first step, the operator $[A]$ will, in general, be a better approximation to A than A^t .

As an alternative to Eq. (8.73), we can also use the formula

$$\left[\langle A\rangle\right] = \frac{\langle A^t\rangle \langle A^t\rangle}{\langle A^t A^{-1} A^t\rangle} \quad . \tag{8.74}$$

The brackets indicate that matrix elements have to be inserted instead of the abstract operators. The variational principle (8.74) has the advantage that the normalization of A^t is canceled. In three-particle scattering, however, Eq. (8.74) has not yet been used.

In order to see how the principle (8.73) can be used, we first consider two-particle scattering or potential scattering. As operator A , we take the T-matrix t(z) which is defined by Eq. (2.56a). From Eq. (2.61), we can assume its inverse $t^{-1}(z)$ to be known, and Eq. (8.73) reads

$$[t] = 2t^t - t^t (v^{-1} - g_0) t^t \quad . \tag{8.75}$$

This is the Schwinger variational principle in the formulation of Schwartz [120]. For the S-matrix we need, according to Eq. (2.51), the matrix element $\langle \vec{p}' | t | \vec{p} \rangle$. Using the relations

$$\begin{aligned} t(E+i0)|\vec{p}\rangle &= v|\vec{p}\rangle^{(+)} \quad , \\ \langle \vec{p}'|t(E+i0) &= \langle \vec{p}'|^{(-)} v \quad , \end{aligned} \tag{8.76}$$

which follow from Eqs. (2.25) and (2.58), we get the Schwinger principle in its original formulation,

$$\left[\langle \vec{p}' | t | \vec{p} \rangle\right] = \langle \vec{p}' | v | \psi_t^{(+)} \rangle + \langle \psi_t^{(-)} | v | \vec{p} \rangle$$
$$- \langle \psi_t^{(-)} | v | \psi_t^{(+)} \rangle + \langle \psi_t^{(-)} | v g_0 v | \psi_t^{(+)} \rangle \quad . \tag{8.77}$$

Here, the functions $|\psi_t^{(+)}\rangle$ and $\langle\psi_t^{(-)}|$ are trial functions for the scattering solutions $|\vec{p}\rangle^{(+)}$ and $\langle\vec{p}'|^{(-)}$.
From Eq. (8.77), we see that the asymptotic behavior of the trial functions $\psi_t^{(\pm)}$ becomes irrelevant for a short-ranged potential v . Instead, the variational principle contains the Green's function $g_0(z)$. A representation of the free Green's function, however, contains the asymptotic solutions of the Schrödinger equation. The boundary condition is imposed by the prescription of how to let the complex argument of $g_0(z)$ approach the real axis.

In the present case of potential scattering, we realize the important difference between the Kohn variational principle, and its least-squares version, and the Schwinger principle. In Kohn's principle [1], the trial function is a superposition of exact asymptotic solutions containing the boundary condition and of square integrable functions. In the Schwinger principle, a superposition of square integrable functions alone is good enough as a trial function. The asymptotic solutions and the boundary condition enter by the free Green's function.

Schwartz [120] has shown by a numerical example that the Schwinger principle has no advantage over the Kohn principle in potential scattering. The numerical expenditure is about the same with both methods when the quantity $t^t v^{-1} t^t$ is evaluated in configuration space and $t^t g_0 t^t$ is evaluated in momentum space (to avoid double integration). In the chosen example, the Kohn method converged much faster, but it is unclear whether this experience may be generalized. Because of this

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[1] The Kohn principle can also be derived from Eq. (8.72), see reference [119]. In the derivation, an on-shell condition is used together with the condition that the trial function is an exact asymptotic solution of the Schrödinger equation.

negative result, it becomes interesting to see that a generalization of the Schwinger principle has an advantage over the Kohn principle in three-particle scattering with breakup.

The generalization of the Schwinger principle to three-particle scattering has first been presented by Pieper, Schlessinger, and Wright [118]. According to Grassberger, Alt, and Sandhas [119], we can derive the PSW variational principle rather easily from Eq. (8.73).

As operator A , we choose the operator $M_{\beta\alpha}$ from Eq. (3.75). The inverse of this operator can be derived by the formalism described on page 63 ff . Using Eqs. (3.73) - (3.75), one obtains

$$(M^{-1})_{\gamma\delta} = -(1-\delta_{\gamma\delta})\, q_0 + \delta_{\gamma\delta}\, t_\delta^{-1} \,. \tag{8.78}$$

Inserting this into the variational principle (8.73), we get,

$$[M_{\gamma\delta}] = 2M^t_{\gamma\delta} + \sum_{\varrho\neq\delta}\sum M^t_{\gamma\varrho}\, q_0\, M^t_{\varrho\delta} - \sum_{\varrho} M^t_{\gamma\varrho}\, t_\varrho^{-1} M^t_{\varrho\delta} \,. \tag{8.79}$$

The matrix elements needed in expression (3.50) for the S-matrix are given in the case of rearrangement scattering by

$$R^{(+)}_{\beta n,\alpha m} = (1-\delta_{\beta\alpha})\langle\phi_{\beta n}|v_\alpha|\phi_{\alpha m}\rangle + \sum_{\gamma\neq\beta}\sum_{\delta\neq\alpha}\langle\phi_{\beta n}|M_{\gamma\delta}|\phi_{\alpha m}\rangle \,, \tag{8.80}$$

where Eqs. (3.51a) and (3.75) have been used. In this equation, we insert the variational expression (8.79) for $M_{\gamma\delta}$ and get

$$\begin{aligned}[R^{(+)}_{\beta n,\alpha m}] &= (1-\delta_{\beta\alpha})\langle\phi_{\beta n}|v_\alpha|\phi_{\alpha m}\rangle \\ &+ \sum_{\delta\neq\alpha}\langle\chi_{\beta n,\delta}|\phi_{\alpha m}\rangle + \sum_{\gamma\neq\beta}\langle\phi_{\beta n}|\chi_{\gamma,\alpha m}\rangle \\ &+ \sum_{\varrho\neq\delta}\sum\langle\chi_{\beta n,\varrho}|q_0|\chi_{\delta,\alpha m}\rangle - \sum_{\varrho}\langle\chi_{\beta n,\varrho}|t_\varrho^{-1}|\chi_{\varrho,\alpha m}\rangle \,,\end{aligned} \tag{8.81}$$

with

$$\langle\chi_{\beta n,\varrho}| = \sum_{\gamma\neq\beta}\langle\phi_{\beta n}|M^t_{\gamma\varrho} \,, \tag{8.82a}$$

$$|\chi_{\delta,\alpha m}\rangle = \sum_{\delta \neq \alpha} M^{t}_{\delta\delta} |\phi_{\alpha m}\rangle \quad , \tag{8.82b}$$

as trial functions.

Equation (8.81) is the PSW variational principle [118]. The trial functions are varied. All summations run from 1 to 3 . Equation (8.81), however, is also valid for $\beta = 0$. In this case, the breakup matrix elements are obtained.

For $\beta = 0$, a δ-function arises in Eq. (8.82a) in the limit $M^{t} \to M$,

$$\begin{aligned} \langle \chi_{0,\delta}| &= \sum_{\gamma} \langle \phi_0 | M_{\gamma\delta} = \langle \phi_0 | (v_\delta + VGv_\delta) \\ &= \langle \phi_0 | (v_\delta + v_\delta g_0 v_\delta + \ldots) \quad . \end{aligned} \tag{8.83}$$

We, therefore, modify this trial function and write

$$\langle \tilde{\chi}_{0,\delta}| = \sum_{\gamma} \langle \phi_0 | M_{\gamma\delta} - \langle \phi_0 | t_\delta \quad . \tag{8.84}$$

Introduction of this modification in Eq. (8.81) for $\beta = 0$ yields the PSW variational principle for the breakup case [127].

Let us investigate the relation between the trial functions and the scattering wave function. From Eqs. (2.99), (2.101b), (2.104), and (3.75), we get for $M^{t}_{\sigma\delta} = M_{\sigma\delta}$,

$$|\chi_{\delta,\alpha m}\rangle = v_\delta (\psi^{(+)}_{\alpha m} - \delta_{\delta\alpha} |\phi_{\alpha m}\rangle) \quad . \tag{8.85}$$

The potential v_σ in Eq. (8.85) cuts off most of the asymptotic part of the scattering function $|\psi^{(+)}_{\alpha m}\rangle$. Only for $\sigma = \alpha$ we get a contribution in the asymptotic region,

$$\langle \vec{\xi}_\alpha, \vec{\eta}_\alpha | \chi_{\alpha,\alpha m} \rangle \underset{\eta_\alpha \to \infty}{\sim} v_\alpha(\xi_\alpha) \hat{\psi}_{\alpha m}(\xi_\alpha) \frac{e^{i q_\alpha \eta_\alpha}}{\eta_\alpha} \quad . \tag{8.86}$$

The rest is square integrable if the potentials are square integrable. The elastic and rearrangement channels are no problem in Kohn's principle, and they have to be taken into

account by introducing exact asymptotic solutions also in the PSW principle. The complicated part of $|\psi^{(+)}_{\alpha m}\rangle$, where all three particles are free, is attenuated in Eq. (8.85) by the potential v_σ . In the trial function $|\chi_{\sigma,\alpha m}\rangle$, this part can be approximated by a superposition of square integrable functions, provided that the potentials are short-ranged. Using Eq. (8.47) with a = o for the asymptotic behavior of three free particles, which have emerged from the breakup reaction, we can write for $\rho \to \infty$,

$$\langle \vec{\xi}_\delta, \vec{\eta}_\delta | \chi_{\delta,\alpha m}\rangle \sim V_\delta(\xi_\delta)\frac{e^{ikg}}{g^{5/2}} \quad , \tag{8.87}$$

and get (compare with Eq. (8.41))

$$\begin{aligned}\langle \chi_{\alpha m,\delta} | \chi_{\delta,\alpha m}\rangle &\sim \int d\vec{g}\ \frac{V_\delta^2(g\cos\alpha)}{g^5} \\ &= \int d\hat{\xi}_\delta\, d\hat{\eta}_\delta \int_0^{\pi/2} d\alpha\, \sin^2\alpha\cos^2\alpha \int_0^\infty dg\, V_\delta^2(g\cos\alpha) \\ &= \int d\hat{\xi}_\delta\, d\hat{\eta}_\delta \int_0^{\pi/2} d\alpha\, \sin^2\alpha\cos\alpha \int_0^\infty dx\, V^2(x) < \infty \quad ,\end{aligned} \tag{8.88}$$

i.e., the contribution arising from three particles in the continuum is square integrable. A similar statement can be made for the trial functions $\langle \chi_{\beta n,\rho}|$.

Asymptotic particle correlations and boundary conditions for breakup states are, therefore, no problem in the PSW principle. Since the principle is based on the Faddeev formalism, the physical boundary condition of three-particle scattering is taken care of automatically. The inclusion of the boundary condition in the formalism is the main difficulty and the merit of the Faddeev theory. The PSW principle, as a generalization of the Schwinger principle to the Faddeev equations, takes advantage of this and is, therefore, ahead of the Kohn principle. It reduces the breakup problem to a calculation of matrix elements. The only difficulty arises from the singular structure of the free Green's function in the matrix elements $\langle \chi | g_o | \chi \rangle$.

The elastic and rearrangement channel functions have been left in the formalism on purpose by PSW. This has the advantage

that the channel resolvents $g_\gamma(z)$ do not appear. Grassberger, Alt, and Sandhas have shown that the two-body channel functions could easily be eliminated by choosing

$$U_{\beta\alpha} = (1-\delta_{\beta\alpha})\, g_{0}^{-1} + \sum_{\gamma\neq\beta} t_\gamma\, g_0\, U_{\gamma\alpha} \qquad (8.89)$$

as operator A in the basic equation (8.73). But, as expected, the channel resolvents appear in this case.

Pieper, Schlessinger, and Wright have applied their method to the scattering of three distinguishable particles and to the scattering of three identical bosons [121]. In both cases, separable Yamaguchi potentials have been used, and only s-wave scattering has been considered. Fast convergence has been observed with respect to the number of parameters. In the example of distinguishable particles, 40 parameters were sufficient to obtain results of about 5-digit accuracy. In the example of identical particles, about one-third of the parameters were needed to get the same accuracy. The numerical expense was small enough to make the inclusion of spin, isospin, and more separable potential terms feasible. This has been done by Pieper [122] in a calculation of nucleon-deuteron polarization.

For local potentials, another integration would have to be carried out numerically, and the trial functions would have to be more flexible. Pieper, Schlessinger, and Wright believe that also such a calculation is possible on present computers. But here, the limit could soon be reached and, thus, the Kohn principle with wave packet states or hyperspherical functions seems to have a chance, too, especially for questions like final state interaction and resonances.

Finally, let us mention another interesting method which is similar to the PSW method. A generalization of Eq. (8.73) with two different trial operators t_1 , t_2 for the two-particle T-matrix,

$$[A] = A_1^t + A_2^t - A_2^t\, A^{-1}\, A_1^t \quad , \qquad (8.90a)$$

$$A_1^t = v + v g_0 t_1 \,, \tag{8.90b}$$

$$A_2^t = t_2 \,, \tag{8.90c}$$

has led Sloan and Brady [123] to the variational principle

$$[t] = v + v g_0 t_1 + t_2 g_0 v - t_2 g_0 t_1 + t_2 g_0 v g_0 t_1 \,. \tag{8.91}$$

They successfully applied this principle to the Lippmann-Schwinger equation of the two-body T-matrix [123] and to the Lippmann-Schwinger-type equation (5.39) of the three-particle problem with separable potential [124].

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