1. One-Boson-Exchange Potentials and Nucleon–Nucleon Scattering

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1.1 The Meson Theory of Nuclear Forces

The nuclear force has been the heart of nuclear physics ever since the field was born in 1932 with the discovery of the neutron by Chadwick [1.1]. In fact, during the first few decades of nuclear physics, the term nuclear force was often used as synonymous for nuclear physics as a whole. There are fundamental reasons why the nuclear force plays such an outstanding role.

The nucleon–nucleon (NN) interaction has been investigated by a huge army of physicists all over the world for the past 60 years. It is the empirically best-known strong interaction; in fact, for no other strong interaction has a comparable amount of experimental data been accumulated. Attempts to understand the nature of this force have spawned the sister discipline of particle physics.

The interaction between two nucleons is the basis for all of nuclear physics. Indeed, the traditional goal of nuclear physics is to understand the properties of atomic nuclei in terms of the "basic" interaction between pairs of nucleons. With the onset of quantumchromodynamics (QCD), it became clear that this interaction is not fundamental. However, even today as a first approach towards any nuclear-structure problem, one assumes the nucleons to be elementary particles. The failure or success of this approach may then teach us something about the relevance of subnuclear degrees of freedom for the nuclear-structure problem under consideration.

Historically, it turned out to be a terrible task to describe the nuclear force just phenomenologically. Nowadays, an acceptable nuclear potential should be derived from theoretical concepts. Ideally, these concepts should be based on QCD. Unfortunately, on the QCD scale, nuclear physics deals with low-energy processes for which QCD is highly non-perturbative. This implies horrific mathematical problems that are far from being solved.

The oldest attempt to explain the nature of the nuclear force is due to Yukawa [1.2]. According to his theory, massive bosons (mesons) mediate the interaction between two nucleons. Although, in the light of QCD, this is not a theory in the true sense of the word, the meson exchange concept is even today the only one capable of yielding a quantitative nucleon–nucleon potential. This fact is not as puzzling as it may appear at first glance: at low energies, the confinement of quarks into (colorless) hadrons, mesons, and baryons is one of the most fundamental predictions of QCD. Of course, the couplings between hadrons are not fundamental. However, they cannot be arbitrary, since effective hadron–hadron couplings also have to satisfy the symmetries of strong interactions.

K. Langanke et al. (eds.), *Computational Nuclear Physics 2*

There are essentially two ways to derive the nuclear force from meson theory: dispersion relations and field theory. The Stony Brook [1.3] and Paris [1.4] groups pursued the former concept. Dispersion relations determine the on-shell NN T-matrix from empirical information on π–N scattering. Since an on-shell T-matrix is not a potential, certain *ad hoc* prescriptions have to be introduced to define the potential. Furthermore, dispersion relations present formidable mathematical complexity. Therefore, the Paris potential [1.5] was eventually parametrized in terms of simple Yukawa functions of multiples of the pion mass. To fit the NN data correctly, a very large phenomenological short-range potential also had to be introduced. Our approach, on the other hand, is field-theoretic. This has the advantage that the potential is *a priori* well-defined on- and off-the-energy-shell.

A truly consistent field-theoretic meson model for the nuclear force is the Bonn full model [1.6]. Besides the one-meson-exchange contributions, it contains a comprehensive model for the two-pion exchange including virtual isobar excitation. Moreover, the important irreducible diagrams of π *and* ρ meson exchange are also taken into account. Finally, classes of 3π and 4π exchanges are considered. Among the multi-meson-exchange contributions, large cancellations occur suggesting some kind of convergence of the diagrammatic expansion. An even more important observation from the Bonn full model is that the sum of all two-pion and higher-order diagrams can, to a very good approximation, be replaced by the exchange of a scalar-isoscalar boson with a mass of about 550 MeV.

The development of the Bonn full model was necessary to assess systematically the range of validity of the meson-exchange concept for the nuclear force. Thus, the Bonn model provides a benchmark against which QCD-inspired work on the NN interaction can be tested. Furthermore, this model provides a basis for a comprehensive discussion of relativistic effects, medium effects, and many-body forces to be expected in the nuclear many-body problem. The medium effects on the nuclear force when inserted into nuclear matter have been calculated thoroughly. They have turned out to be repulsive, the largest effect coming from intermediate isobars. On the other hand, isobars also give rise to many-body forces that are attractive. Thus, there are large cancellations between these two classes of many-body forces/effects, and the net contribution is very small [1.7]. Relativistic effects, however, may play a non-negligible role in the nuclear many-body problem [1.7, 1.8].

In view of these results, the relativistic one-boson-exchange (OBE) model for the NN force is sufficient for many problems of nuclear-structure physics. This model takes into account only single exchanges of bosons with masses below 1 GeV. The model, which we will present below in more detail, consists of six bosons of which the following four play the major role:

- The pseudo-scalar pion with a mass of about 138 MeV. It is the lightest meson and provides the long-range part of the potential and most of the tensor force.
- The ρ meson, a 2π P-wave resonance of about 770 MeV. Its major effect is to cut down the tensor force provided by the pion at short range.
- The ω meson, a 3π resonance of 783 MeV and spin 1. It creates a strong repulsive central force of short range ("repulsive core") and the nuclear spin–orbit force.
- The (fictitious) σ boson of about 550 MeV. It provides the intermediate-range attraction necessary for nuclear binding and can be understood as a simulation of the correlated S-wave 2π-exchange.

The features of the various one-boson exchanges listed can be derived analytically in the non-relativistic approximation to the Feynman amplitudes for these processes [1.7]. However, these non-relativistic simplifications should be seen basically as a pedagogical matter: they yield a local potential that is easy to visualize. It has turned out that for a quantitative description of the NN scattering data the subtleties of the full-field-theoretic Feynman amplitude are important. In other words, non-localities play a subtle, but important, role. The local, non-relativistic expressions do not allow for a very quantitative description of the NN data unless additional phenomenological terms are introduced. This, however, increases substantially the number of parameters and thus destroys the beauty and self-consistency of the model.

The relativistic OBE model is able to describe the NN data with the parameters of just six mesons. The χ^2 for the fit of all NN data below 300 MeV laboratory energy is as good as the one of semiphenomenological models that use in the order of 200 parameters, such as the Paris potential [1.5].

The relativistic OBE potentials are suitable for application in relativistic as well as non-relativistic nuclear-structure physics (see the discussion of the appropriate equations below).

In the following sections, we will be mainly concerned with the mathematical and numerical aspects of NN scattering and one-boson-exchange forces. A broad introduction to the physics of the field is given in [1.7]. Ultimately, we present a computer code for one-boson-exchange potentials and one for the computation of phase shifts of NN scattering. All calculations are performed in momentum space. The advantage of working in momentum space is that local and non-local potentials can be handled mathematically in the same way. Thus, the calculations with non-local potentials are as easy as those with local ones. Moreover, the scattering equation in momentum space is an integral equation, which is easy to solve numerically. In coordinate space, the scattering equation is a differential equation, the numerical analysis of which is always more involved.

1.2 Relativistic Two-Nucleon Scattering

1.2.1 Covariant Equations

Two-nucleon scattering is described covariantly by the Bethe–Salpeter (BS) equation [1.9]. In operator notation, it may be written as

$$\mathcal{T} = \mathcal{V} + \mathcal{V}\mathcal{G}\mathcal{T}, \tag{1.1}$$

with $\mathcal{T}$ the invariant amplitude for the two-nucleon scattering process, $\mathcal{V}$ the sum of all connected two-particle irreducible diagrams, and $\mathcal{G}$ the relativistic two-nucleon propagator. As this four-dimensional integral equation is very difficult to solve, so-called three-dimensional reductions have been proposed, which are more amenable to numerical solution. Furthermore, it has been shown by Gross [1.10] that the full BS equation in ladder approximation (that is, the kernel $\mathcal{V}$ is restricted to the exchange of single particles, as, for example, in the OBE model) does not have the correct one-body limit (that is, when one of the particles becomes very massive), while a large family of three-dimensional quasi-potential equations does. These approximations to the BS equation are also covariant and satisfy relativistic elastic unitarity. However, the three-dimensional reduction is not unique, and in principle, infinitely many choices exist. Typically they are derived by replacing (1.1) with two coupled equations [1.11]:

$$\mathcal{T} = \mathcal{W} + \mathcal{W}g\mathcal{T} \tag{1.2}$$

and

$$\mathcal{W} = \mathcal{V} + \mathcal{V}(\mathcal{G} - g)\mathcal{W}, \tag{1.3}$$

where g is a covariant three-dimensional propagator with the same elastic unitarity cut as $\mathcal{G}$ in the physical region. In general, the second term on the right-hand side of (1.3) is dropped to obtain a true simplification of the problem.

More explicitly, the BS equation for an arbitrary frame reads (notation and conventions as in [1.12])

$$\mathcal{T}(q';q|P) = \mathcal{V}(q';q|P) + \int \mathrm{d}^4k\, \mathcal{V}(q';k|P)\, \mathcal{G}(k|P)\, \mathcal{T}(k;q|P), \tag{1.4}$$

with

$$\mathcal{G}(k|P) = \frac{\mathrm{i}}{2\pi} \frac{1}{(\frac{1}{2}\not{P} + \not{k} - M + \mathrm{i}\epsilon)^{(1)}} \frac{1}{(\frac{1}{2}\not{P} - \not{k} - M + \mathrm{i}\epsilon)^{(2)}} \tag{1.5}$$

$$= \frac{\mathrm{i}}{2\pi} \left[\frac{\frac{1}{2}\not{P} + \not{k} + M}{(\frac{1}{2}P + k)^2 - M^2 + \mathrm{i}\epsilon}\right]^{(1)} \left[\frac{\frac{1}{2}\not{P} - \not{k} + M}{(\frac{1}{2}P - k)^2 - M^2 + \mathrm{i}\epsilon}\right]^{(2)}, \tag{1.6}$$

where q, k, and q' are the initial, intermediate, and final relative four-momenta, respectively, and $P = (P_0, \boldsymbol{P})$ is the total four-momentum. For

example, in the initial state we have $q = \frac{1}{2}(p_1 - p_2)$, $P = p_1 + p_2$, and $p_{1/2} = \frac{1}{2}P \pm q$, with p_1 and p_2 the individual four-momenta of particles 1 and 2. In the center-of-mass (c.m.) frame, we will have $P = (\sqrt{s}, \mathbf{0})$, with $\sqrt{s}$ the total energy. For all four-momenta, our notation is $k = (k_0, \boldsymbol{k})$, $\not{k} \equiv \gamma^\mu k_\mu$. M denotes the nucleon mass. The superscripts in (1.6) refer to particles (1) and (2). At this stage, $\mathcal{M}, \mathcal{V}$, and $\mathcal{G}$ are operators in spinor space, that is, they are 16×16 matrices that, when sandwiched between Dirac spinors, yield the corresponding matrix elements.

It is common to the derivation of all three-dimensional reductions that the time component of the relative momentum is fixed in some covariant way, so that it no longer appears as an independent variable in the propagator.

Following Blankenbecler and Sugar (BbS) [1.13], one possible choice for g is (stated in manifestly covariant form for an arbitrary frame)

$$\begin{aligned} g_{\mathrm{BbS}}(k,s) = -\int_{4M^2}^{\infty} \frac{\mathrm{d}s'}{s'-s-\mathrm{i}\epsilon}\, \delta^{(+)}[(\tfrac{1}{2}P'+k)^2 - M^2] \\ \times \delta^{(+)}[(\tfrac{1}{2}P'-k)^2 - M^2] \\ \times (\tfrac{1}{2}\not{P}' + \not{k} + M)^{(1)} (\tfrac{1}{2}\not{P}' - \not{k} + M)^{(2)}, \end{aligned} \tag{1.7}$$

with $\delta^{(+)}$ indicating that only the positive energy root of the argument of the δ-function is to be included; $P^2 = s$ and $P' \equiv \frac{\sqrt{s'}}{\sqrt{s}} P$. By construction, the propagator g_{BbS} has the same imaginary part as $\mathcal{G}$ and therefore preserves the unitarity relation satisfied by $\mathcal{T}$. In the c.m. frame, integration yields

$$g_{\mathrm{BbS}}(k,s) = \delta(k_0)\, \bar{g}_{\mathrm{BbS}}(\boldsymbol{k}, s) \tag{1.8}$$

with

$$\bar{g}_{\mathrm{BbS}}(\boldsymbol{k}, s) = \frac{M^2}{E_k} \frac{\Lambda_+^{(1)}(\boldsymbol{k})\, \Lambda_+^{(2)}(-\boldsymbol{k})}{\frac{1}{4}s - E_k^2 + \mathrm{i}\epsilon}, \tag{1.9}$$

where

$$\Lambda_+^{(i)}(\boldsymbol{k}) = \left(\frac{\gamma^0 E_k - \boldsymbol{\gamma}\cdot\boldsymbol{k} + M}{2M} \right)^{(i)} \tag{1.10}$$

$$= \sum_{\lambda_i} |u(\boldsymbol{k}, \lambda_i)\rangle \langle \bar{u}(\boldsymbol{k}, \lambda_i)| \tag{1.11}$$

represents the positive-energy projection operator for nucleon i with $u(\boldsymbol{k})$ a positive-energy Dirac spinor of momentum $\boldsymbol{k}$, $\bar{u} \equiv u^\dagger \gamma^0$. λ_i denotes either the helicity or the spin projection of the respective nucleon, and $E_k = \sqrt{M^2 + \boldsymbol{k}^2}$. The projection operators imply that virtual anti-nucleon contributions are suppressed. These contributions have been shown to be small if the pseudovector coupling is used for the pion [1.14].

Using the approximation $\mathcal{W} = \mathcal{V}$, we obtain the explicit form of (1.2) replacing $\mathcal{G}$ by g_{BbS} in (1.4). This yields, in the c.m. frame,

$$\begin{aligned} &\mathcal{T}(0, \boldsymbol{q}'; 0, \boldsymbol{q} | \sqrt{s}) \\ &= \mathcal{V}(0, \boldsymbol{q}'; 0, \boldsymbol{q}) + \int \mathrm{d}^3k\, \mathcal{V}(0, \boldsymbol{q}'; 0, \boldsymbol{k})\, \bar{g}_{\mathrm{BbS}}(\boldsymbol{k}, s)\, \mathcal{T}(0, \boldsymbol{k}; 0, \boldsymbol{q} | \sqrt{s}). \end{aligned} \tag{1.12}$$

Note that four-momentum is conserved at each vertex, and that in the initial state the nucleons are on their mass-shell, therefore $q = (0, \boldsymbol{q})$. The total c.m. energy is

$$\sqrt{s} = 2E_q = 2\sqrt{M^2 + \boldsymbol{q}^2}. \tag{1.13}$$

With this we obtain, simplifying our notation,

$$\mathcal{T}(\boldsymbol{q}', \boldsymbol{q}) = \mathcal{V}(\boldsymbol{q}', \boldsymbol{q}) + \int \mathrm{d}^3k\, \mathcal{V}(\boldsymbol{q}', \boldsymbol{k}) \frac{M^2}{E_k} \frac{\Lambda_+^{(1)}(\boldsymbol{k})\, \Lambda_+^{(2)}(-\boldsymbol{k})}{\boldsymbol{q}^2 - \boldsymbol{k}^2 + \mathrm{i}\epsilon} \mathcal{T}(\boldsymbol{k}, \boldsymbol{q}). \tag{1.14}$$

Taking matrix elements between positive-energy spinors (see Sect. 1.3.1 where this is done explicitly for $\mathcal{V}$) yields an equation for the scattering amplitude

$$T(\boldsymbol{q}', \boldsymbol{q}) = V(\boldsymbol{q}', \boldsymbol{q}) + \int \mathrm{d}^3k\, V(\boldsymbol{q}', \boldsymbol{k}) \frac{M^2}{E_k} \frac{1}{\boldsymbol{q}^2 - \boldsymbol{k}^2 + \mathrm{i}\epsilon} T(\boldsymbol{k}, \boldsymbol{q}), \tag{1.15}$$

where, for the moment, spin (or helicity) and isospin indices are suppressed (these details will be discussed in Sect. 1.2.2).

Defining

$$\hat{T}(\boldsymbol{q}', \boldsymbol{q}) = \sqrt{\frac{M}{E_{q'}}}\, T(\boldsymbol{q}', \boldsymbol{q}) \sqrt{\frac{M}{E_q}} \tag{1.16}$$

and

$$\hat{V}(\boldsymbol{q}', \boldsymbol{q}) = \sqrt{\frac{M}{E_{q'}}}\, V(\boldsymbol{q}', \boldsymbol{q}) \sqrt{\frac{M}{E_q}}, \tag{1.17}$$

which have become known as "minimal relativity" [1.15], we can rewrite (1.15) as

$$\hat{T}(\boldsymbol{q}', \boldsymbol{q}) = \hat{V}(\boldsymbol{q}', \boldsymbol{q}) + \int \mathrm{d}^3k\, \hat{V}(\boldsymbol{q}', \boldsymbol{k}) \frac{M}{\boldsymbol{q}^2 - \boldsymbol{k}^2 + \mathrm{i}\epsilon} \hat{T}(\boldsymbol{k}, \boldsymbol{q}), \tag{1.18}$$

which has the form of the non-relativistic Lippmann–Schwinger equation. A potential defined within an equation that is formally identical to the (non-relativistic) Lippmann–Schwinger equation can then be applied in conventional (non-relativistic) nuclear-structure physics. This is the practical relevance of (1.16)–(1.18). On the other hand, for relativistic nuclear-structure physics, (1.15) is the starting point.

The BbS propagator is the most widely used approximation. Another choice that has been frequently applied is the version suggested by Thompson [1.16], which reads, in manifestly covariant form for an arbitrary frame,

$$\begin{aligned} g_{\mathrm{Th}}(k, s) = -\int_{2M}^{\infty} \frac{\mathrm{d}\sqrt{s'}}{\sqrt{s'} - \sqrt{s} - \mathrm{i}\epsilon}\, & \delta^{(+)}[(\tfrac{1}{2}P' + k)^2 - M^2] \\ & \times \delta^{(+)}[(\tfrac{1}{2}P' - k)^2 - M^2] \\ & \times (\tfrac{1}{2}\not{P}' + \not{k} + M)^{(1)} (\tfrac{1}{2}\not{P}' - \not{k} + M)^{(2)}. \end{aligned} \tag{1.19}$$

In the c.m. frame, integration yields

$$g_{\mathrm{Th}}(k,s) = \delta(k_0)\,\frac{M^2}{2E_k^2}\,\frac{\Lambda_+^{(1)}(\boldsymbol{k})\,\Lambda_+^{(2)}(-\boldsymbol{k})}{\frac{1}{2}\sqrt{s} - E_k + \mathrm{i}\epsilon}\,. \tag{1.20}$$

The corresponding T-matrix equation is

$$T(\boldsymbol{q}',\boldsymbol{q}) = V(\boldsymbol{q}',\boldsymbol{q}) + \int \mathrm{d}^3k\, V(\boldsymbol{q}',\boldsymbol{k})\,\frac{M^2}{2E_k^2}\,\frac{1}{E_q - E_k + \mathrm{i}\epsilon}\,T(\boldsymbol{k},\boldsymbol{q}). \tag{1.21}$$

Again, we may introduce some special definitions. In the case of the Thompson equation, it is convenient to define

$$\check{T}(\boldsymbol{q}',\boldsymbol{q}) = \frac{M}{E_{q'}}\,T(\boldsymbol{q}',\boldsymbol{q})\,\frac{M}{E_q} \tag{1.22}$$

and

$$\check{V}(\boldsymbol{q}',\boldsymbol{q}) = \frac{M}{E_{q'}}\,V(\boldsymbol{q}',\boldsymbol{q})\,\frac{M}{E_q}\,. \tag{1.23}$$

With this, we can rewrite (1.21) as

$$\check{T}(\boldsymbol{q}',\boldsymbol{q}) = \check{V}(\boldsymbol{q}',\boldsymbol{q}) + \int \mathrm{d}^3k\, \check{V}(\boldsymbol{q}',\boldsymbol{k})\frac{1}{2E_q - 2E_k + \mathrm{i}\epsilon}\check{T}(\boldsymbol{k},\boldsymbol{q}), \tag{1.24}$$

which looks like a Lippmann–Schwinger with relativistic energies in the propagator.

Notice that the quantity T in (1.15) and (1.21) is invariant, while $\hat{T}$ of (1.18) and $\check{T}$ of (1.22) are not. $\hat{T}$ is equivalent to the familiar non-relativistic T-matrix.

The relationship of the invariant T to the S-matrix is

$$\langle p_1' p_2' | S | p_1 p_2 \rangle = \langle p_1' p_2' | p_1 p_2 \rangle - 2\pi\mathrm{i}\delta^{(4)}(p_1' + p_2' - p_1 - p_2)\frac{M^2}{E_q^2}T(\boldsymbol{q}',\boldsymbol{q}) \tag{1.25}$$

with p_i the initial and p_i' $(i = 1, 2)$ the final four-momenta of the two interacting nucleons. The normalization is $\langle p'|p\rangle = \delta^{(3)}(\boldsymbol{p}' - \boldsymbol{p})$.

1.2.2 The R-Matrix Equation and Helicity State Basis

On a computer, real analysis is much faster than complex analysis. It is therefore desirable to deal with real quantities whenever possible. The scattering amplitude below particle production threshold can be expressed in terms of the real R-matrix (better known as the "K-matrix") which is defined by

$$T = R - \mathrm{i}\pi R\delta(E - H_0)T. \tag{1.26}$$

The equation for the real $\hat{R}$-matrix corresponding to the complex $\hat{T}$-matrix of (1.18) is

$$\hat{R}(\boldsymbol{q}', \boldsymbol{q}) = \hat{V}(\boldsymbol{q}', \boldsymbol{q}) + \mathcal{P} \int \mathrm{d}^3k \, \hat{V}(\boldsymbol{q}', \boldsymbol{k}) \, \frac{M}{\boldsymbol{q}^2 - \boldsymbol{k}^2} \, \hat{R}(\boldsymbol{k}, \boldsymbol{q}), \tag{1.27}$$

where $\mathcal{P}$ denotes the principal value.

Now, we also need to consider the spin of the nucleons explicitly. The easiest way to treat the spin projections of spin-$\frac{1}{2}$ particles in a covariant way is to use the helicity representation. In our further developments, we will therefore use a helicity state basis. Our presentation will be relatively brief, emphasizing the formulas used in the computer codes. A more detailed derivation is given in Appendix C of [1.6], which is based upon [1.17,18].

The helicity λ_i of particle i (with $i = 1$ or 2) is the eigenvalue of the helicity operator $\frac{1}{2}\boldsymbol{\sigma}_i \cdot \boldsymbol{p}_i/|\boldsymbol{p}_i|$, that is, $\pm\frac{1}{2}$.

Using helicity states, the $\hat{R}$-matrix equation reads, after partial wave decomposition,

$$\begin{aligned}\langle \lambda_1' \lambda_2' | \hat{R}^J(q', q) | \lambda_1 \lambda_2 \rangle = {} & \langle \lambda_1' \lambda_2' | \hat{V}^J(q', q) | \lambda_1 \lambda_2 \rangle \\ & + \sum_{h_1, h_2} \mathcal{P} \int_0^\infty \mathrm{d}k \, k^2 \frac{M}{q^2 - k^2} \langle \lambda_1' \lambda_2' | \hat{V}^J(q', k) | h_1 h_2 \rangle \\ & \times \langle h_1 h_2 | \hat{R}^J(k, q) | \lambda_1 \lambda_2 \rangle, \end{aligned} \tag{1.28}$$

where J denotes the total angular momentum of the two nucleons. Here and throughout the rest of this chapter, momenta denoted by non-bold letters are absolute three-momenta, so that $q \equiv |\boldsymbol{q}|$, $k \equiv |\boldsymbol{k}|$, etc.; h_1 and h_2 are the helicities in intermediate states for nucleons 1 and 2, respectively. Equation (1.28) is a system of coupled integral equations that needs to be solved to obtain the desired matrix elements of $\hat{R}^J$.

Ignoring antiparticles, there are $4 \times 4 = 16$ helicity amplitudes for $\hat{R}^J$. However, time-reversal invariance, parity conservation, and the fact that we are dealing with two identical fermions imply that only six amplitudes are independent. For these six amplitudes, we choose the following set:

$$\begin{aligned} \hat{R}_1^J(q', q) &\equiv \langle ++ | \hat{R}^J(q', q) | ++ \rangle, \\ \hat{R}_2^J(q', q) &\equiv \langle ++ | \hat{R}^J(q', q) | -- \rangle, \\ \hat{R}_3^J(q', q) &\equiv \langle +- | \hat{R}^J(q', q) | +- \rangle, \\ \hat{R}_4^J(q', q) &\equiv \langle +- | \hat{R}^J(q', q) | -+ \rangle, \\ \hat{R}_5^J(q', q) &\equiv \langle ++ | \hat{R}^J(q', q) | +- \rangle, \\ \hat{R}_6^J(q', q) &\equiv \langle +- | \hat{R}^J(q', q) | ++ \rangle, \end{aligned} \tag{1.29}$$

where $\pm$ stands for $\pm\frac{1}{2}$. Notice that

$$\hat{R}_5^J(q', q) = \hat{R}_6^J(q, q'). \tag{1.30}$$

We now have six coupled equations. To partially decouple this system, it is useful to introduce the following linear combinations of helicity amplitudes:

$${}^0\hat{R}^J \equiv \hat{R}_1^J - \hat{R}_2^J,$$

$$
\begin{aligned}
{}^{1}\hat{R}^J &\equiv \hat{R}^J_3 - \hat{R}^J_4, \\
{}^{12}\hat{R}^J &\equiv \hat{R}^J_1 + \hat{R}^J_2, \\
{}^{34}\hat{R}^J &\equiv \hat{R}^J_3 + \hat{R}^J_4, \\
{}^{55}\hat{R}^J &\equiv 2\hat{R}^J_5, \\
{}^{66}\hat{R}^J &\equiv 2\hat{R}^J_6.
\end{aligned} \tag{1.31}
$$

We also introduce corresponding definitions for $\hat{V}^J$. (Of course, analogous definitions exist for $R, \check{R}, V$, and $\check{V}$.) Using these definitions, (1.28) decouples into the following three subsystems of integral equations:
Spin singlet

$$
{}^{0}\hat{R}^J(q',q) = {}^{0}\hat{V}^J(q',q) + \mathcal{P}\int_0^\infty \mathrm{d}k\, k^2 \frac{M}{q^2-k^2}\, {}^{0}\hat{V}^J(q',k)\, {}^{0}\hat{R}^J(k,q); \tag{1.32}
$$

Uncoupled spin triplet

$$
{}^{1}\hat{R}^J(q',q) = {}^{1}\hat{V}^J(q',q) + \mathcal{P}\int_0^\infty \mathrm{d}k\, k^2 \frac{M}{q^2-k^2}\, {}^{1}\hat{V}^J(q',k)\, {}^{1}\hat{R}^J(k,q); \tag{1.33}
$$

Coupled triplet states

$$
\begin{aligned}
{}^{12}\hat{R}^J(q',q) &= {}^{12}\hat{V}^J(q',q) + \mathcal{P}\int_0^\infty \mathrm{d}k\, k^2 \frac{M}{q^2-k^2}[\, {}^{12}\hat{V}^J(q',k)\, {}^{12}\hat{R}^J(k,q) \\
&\quad + {}^{55}\hat{V}^J(q',k)\, {}^{66}\hat{R}^J(k,q)], \\
{}^{34}\hat{R}^J(q',q) &= {}^{34}\hat{V}^J(q',q) + \mathcal{P}\int_0^\infty \mathrm{d}k\, k^2 \frac{M}{q^2-k^2}[\, {}^{34}\hat{V}^J(q',k)\, {}^{34}\hat{R}^J(k,q) \\
&\quad + {}^{66}\hat{V}^J(q',k)\, {}^{55}\hat{R}^J(k,q)], \\
{}^{55}\hat{R}^J(q',q) &= {}^{55}\hat{V}^J(q',q) + \mathcal{P}\int_0^\infty \mathrm{d}k\, k^2 \frac{M}{q^2-k^2}[\, {}^{12}\hat{V}^J(q',k)\, {}^{55}\hat{R}^J(k,q) \\
&\quad + {}^{55}\hat{V}^J(q',k)\, {}^{34}\hat{R}^J(k,q)], \\
{}^{66}\hat{R}^J(q',q) &= {}^{66}\hat{V}^J(q',q) + \mathcal{P}\int_0^\infty \mathrm{d}k\, k^2 \frac{M}{q^2-k^2}[\, {}^{34}\hat{V}^J(q',k)\, {}^{66}\hat{R}^J(k,q) \\
&\quad + {}^{66}\hat{V}^J(q',k)\, {}^{12}\hat{R}^J(k,q)].
\end{aligned} \tag{1.34}
$$

More common in nuclear physics is the representation of two-nucleon states in terms of an $|LSJM\rangle$ basis, where S denotes the total spin, L the total orbital angular momentum, and J the total angular momentum with projection M. In this basis, we will denote the $\hat{R}$ matrix elements by $\hat{R}^{JS}_{L',L} \equiv \langle L'SJM|\hat{R}|LSJM\rangle$. These are obtained from the helicity state matrix elements by the following unitary transformations:
Spin singlet

$$
\hat{R}^{J0}_{J,J} = {}^{0}\hat{R}^J; \tag{1.35}
$$

Uncoupled spin triplet

$$\hat{R}^{J1}_{J,J} = {}^1\hat{R}^J; \tag{1.36}$$

Coupled triplet states

$$\begin{aligned}
\hat{R}^{J1}_{J-1,J-1} &= \frac{1}{2J+1} \\
&\times \left[J\,{}^{12}\hat{R}^J + (J+1)\,{}^{34}\hat{R}^J + \sqrt{J(J+1)}({}^{55}\hat{R}^J + {}^{66}\hat{R}^J) \right], \\
\hat{R}^{J1}_{J+1,J+1} &= \frac{1}{2J+1} \\
&\times \left[(J+1)\,{}^{12}\hat{R}^J + J\,{}^{34}\hat{R}^J - \sqrt{J(J+1)}({}^{55}\hat{R}^J + {}^{66}\hat{R}^J) \right], \\
\hat{R}^{J1}_{J-1,J+1} &= \frac{1}{2J+1} \\
&\times \left[\sqrt{J(J+1)}({}^{12}\hat{R}^J - {}^{34}\hat{R}^J) - J\,{}^{55}\hat{R}^J + (J+1)\,{}^{66}\hat{R}^J \right], \\
\hat{R}^{J1}_{J+1,J-1} &= \frac{1}{2J+1} \\
&\times \left[\sqrt{J(J+1)}({}^{12}\hat{R}^J - {}^{34}\hat{R}^J) + (J+1)\,{}^{55}\hat{R}^J - J\,{}^{66}\hat{R}^J \right].
\end{aligned} \tag{1.37}$$

Analogous transformations exist for $\hat{V}, R, \check{R}, V$, and $\check{V}$. Notice that the transformation matrix is symmetric, which implies that the inverse transformation has the same matrix.

Instead of solving the coupled system in the form of (1.34), one can also first apply the transformation (1.37) to $\hat{V}$ and $\hat{R}$ in (1.34), yielding a system of four coupled integral equations for $\hat{R}$ in LSJ representation:

$$\begin{aligned}
\hat{R}^{J1}_{++}(q',q) &= \hat{V}^{J1}_{++}(q',q) + \mathcal{P}\int_0^\infty \mathrm{d}k\, k^2\, \frac{M}{q^2-k^2}[\, \hat{V}^{J1}_{++}(q',k)\, \hat{R}^{J1}_{++}(k,q) \\
&\quad + \hat{V}^{J1}_{+-}(q',k)\, \hat{R}^{J1}_{-+}(k,q)], \\
\hat{R}^{J1}_{--}(q',q) &= \hat{V}^{J1}_{--}(q',q) + \mathcal{P}\int_0^\infty \mathrm{d}k\, k^2\, \frac{M}{q^2-k^2}[\, \hat{V}^{J1}_{--}(q',k)\, \hat{R}^{J1}_{--}(k,q) \\
&\quad + \hat{V}^{J1}_{-+}(q',k)\, \hat{R}^{J1}_{+-}(k,q)], \\
\hat{R}^{J1}_{+-}(q',q) &= \hat{V}^{J1}_{+-}(q',q) + \mathcal{P}\int_0^\infty \mathrm{d}k\, k^2\, \frac{M}{q^2-k^2}[\, \hat{V}^{J1}_{++}(q',k)\, \hat{R}^{J1}_{+-}(k,q) \\
&\quad + \hat{V}^{J1}_{+-}(q',k)\, \hat{R}^{J1}_{--}(k,q)], \\
\hat{R}^{J1}_{-+}(q',q) &= \hat{V}^{J1}_{-+}(q',q) + \mathcal{P}\int_0^\infty \mathrm{d}k\, k^2\, \frac{M}{q^2-k^2}[\, \hat{V}^{J1}_{--}(q',k)\, \hat{R}^{J1}_{-+}(k,q) \\
&\quad + \hat{V}^{J1}_{-+}(q',k)\, \hat{R}^{J1}_{++}(k,q)],
\end{aligned} \tag{1.38}$$

where we have introduced the abbreviations $\hat{R}^{J1}_{++} \equiv \hat{R}^{J1}_{J+1,J+1}$, $\hat{R}^{J1}_{--} \equiv \hat{R}^{J1}_{J-1,J-1}$, $\hat{R}^{J1}_{+-} \equiv \hat{R}^{J1}_{J+1,J-1}$, $\hat{R}^{J1}_{-+} \equiv \hat{R}^{J1}_{J-1,J+1}$. Conventionally, the coupled

triplet channels in NN scattering are considered in this form, which can also be obtained by decomposing (1.27) directly into LSJ states. In a non-relativistic consideration, it is the tensor force that couples triplet states with $L = J \pm 1$.

So far, we have never mentioned the total isospin of the two-nucleon system, T (which is either 0 or 1). The reason for this is simply that T is not an independent quantum number. That is, owing to the antisymmetry of the two-fermion state, the quantum numbers L, S, and T have to fulfill the condition

$$(-1)^{L+S+T} = -1\,. \tag{1.39}$$

Thus, for given L and S, T is fixed.

1.2.3 The On-Shell R-Matrix and Phase Shifts

Phase shifts are a parametrization of the unitary S-matrix, which for uncoupled cases is given by

$$S_J = \mathrm{e}^{2\mathrm{i}\delta_J}. \tag{1.40}$$

Using the above and (1.25) and (1.26) in partial-wave decomposition, one can relate the on-energy-shell R-matrix to the phase shifts as follows:
Spin singlet

$$\tan\,{}^0\delta^J(E_{\mathrm{lab}}) = -\frac{\pi}{2} qM\,{}^0\hat{R}^J(q,q); \tag{1.41}$$

Uncoupled spin triplet

$$\tan\,{}^1\delta^J(E_{\mathrm{lab}}) = -\frac{\pi}{2} qM\,{}^1\hat{R}^J(q,q). \tag{1.42}$$

For the *coupled states*, a unitary transformation is needed to diagonalize the two-by-two coupled R-matrix. This requires an additional parameter, known as the "mixing parameter" ϵ_J. Using the convention introduced by Blatt and Biedenharn [1.19], the eigenphases for the coupled channels are, in terms of the on-shell $\hat{R}$-matrix,

$$\tan\,\delta^J_{\mp}(E_{\mathrm{lab}}) = -\frac{\pi}{4} qM \left(\hat{R}^J_{J-1,J-1} + \hat{R}^J_{J+1,J+1} \pm \frac{\hat{R}^J_{J-1,J-1} - \hat{R}^J_{J+1,J+1}}{\cos 2\epsilon_J} \right),$$

$$\tan 2\epsilon_J(E_{\mathrm{lab}}) = \frac{2\hat{R}^J_{J+1,J-1}}{\hat{R}^J_{J-1,J-1} - \hat{R}^J_{J+1,J+1}}\,. \tag{1.43}$$

All $\hat{R}$-matrix elements in these formulas carry the arguments (q,q) where q denotes the c.m. on-energy-shell momentum that is related to the energy in the laboratory system, E_{lab}, by

$$E_{\mathrm{lab}} = 2q^2/M. \tag{1.44}$$

An alternative convention for the phase parameters has been used by Stapp et al. [1.20], known as "bar" phase shifts. These are related to the Blatt–Biedenharn parameters by

$$\begin{aligned} \bar{\delta}^J_+ + \bar{\delta}^J_- &= \delta^J_+ + \delta^J_-, \\ \sin(\bar{\delta}^J_- - \bar{\delta}^J_+) &= \tan 2\bar{\epsilon}_J / \tan 2\epsilon_J, \\ \sin(\delta^J_- - \delta^J_+) &= \sin 2\bar{\epsilon}_J / \sin 2\epsilon_J. \end{aligned} \tag{1.45}$$

Phase-shift output from our codes is stated in terms of the "bar" conventions.

Using the transformation (1.37), the phase parameters for the coupled case can also be expressed directly in terms of the helicity-state $\hat{R}$-matrix elements; one obtains

$$\begin{aligned} \tan \delta^J_\mp(E_{\rm lab}) &= -\frac{\pi}{4} qM \\ &\quad \times \left[{}^{12}\hat{R}^J + {}^{34}\hat{R}^J \mp \frac{{}^{12}\hat{R}^J - {}^{34}\hat{R}^J - 4\sqrt{J(J+1)}\,{}^{55}\hat{R}^J}{(2J+1)\cos 2\epsilon_J} \right], \\ \tan 2\epsilon_J(E_{\rm lab}) &= -2\frac{\sqrt{J(J+1)}({}^{12}\hat{R}^J - {}^{34}\hat{R}^J) + {}^{55}\hat{R}^J}{{}^{12}\hat{R}^J - {}^{34}\hat{R}^J - 4\sqrt{J(J+1)}\,{}^{55}\hat{R}^J}. \end{aligned} \tag{1.46}$$

1.2.4 Effective Range Parameters

For low-energy S-wave scattering, $q \cot \delta$ can be expanded as a function of q:

$$\frac{q}{\tan \delta} = q \cot \delta \approx -\frac{1}{a} + \frac{1}{2} r q^2, \tag{1.47}$$

where a is called the scattering length and r the effective range.

Rewriting this equation for two different (small) on-shell momenta q_1 and q_2 (with $E^{(i)}_{\rm lab} = 2q_i^2/M$ and phase shifts δ_i, $i = 1, 2$), we can determine the two unknown constants a and r:

$$r = \frac{4}{M} \frac{\frac{q_1}{\tan \delta_1} - \frac{q_2}{\tan \delta_2}}{E^{(1)}_{\rm lab} - E^{(2)}_{\rm lab}} \tag{1.48}$$

and

$$\frac{1}{a} = \frac{M}{4} r\, E^{(i)}_{\rm lab} - \frac{q_i}{\tan \delta_i}, \tag{1.49}$$

with $i = 1$ or 2.

1.2.5 Using Thompson's Equation

The Thompson equation (1.21) is solved most conveniently in "check" notation (1.22–24). The corresponding equations for the $\check{R}$-matrix are obtained from (1.32–34) by replacing

$$\frac{M}{q^2-k^2} \longmapsto \frac{1}{2E_q-2E_k} = \frac{\frac{1}{2}(E_q+E_k)}{q^2-k^2} \tag{1.50}$$

and

$$\hat{R} \longmapsto \check{R}. \tag{1.51}$$

This is easily understood by comparing (1.18) with (1.24). $\check{R}$ is defined in analogy to (1.22). The phase-shift relation is

$$\tan {}^0\delta^J(E_{\rm lab}) = -\frac{\pi}{2} q E_q \, {}^0\check{R}^J(q,q) \tag{1.52}$$

and similarly for the other channels.

1.3 One-Boson-Exchange Potentials

1.3.1 Interaction Lagrangians and OBE Amplitudes

We use the following Lagrangians for meson–nucleon coupling:

$$\mathcal{L}_{\rm ps} = -g_{\rm ps}\bar{\psi}{\rm i}\gamma^5\psi\varphi^{\rm (ps)}, \tag{1.53}$$

$$\mathcal{L}_{\rm pv} = -\frac{f_{\rm ps}}{m_{\rm ps}}\bar{\psi}\gamma^5\gamma^\mu\psi\partial_\mu\varphi^{\rm (ps)}, \tag{1.54}$$

$$\mathcal{L}_{\rm s} = +g_{\rm s}\bar{\psi}\psi\varphi^{\rm (s)}, \tag{1.55}$$

$$\mathcal{L}_{\rm v} = -g_{\rm v}\bar{\psi}\gamma^\mu\psi\varphi_\mu^{\rm (v)} - \frac{f_{\rm v}}{4M}\bar{\psi}\sigma^{\mu\nu}\psi(\partial_\mu\varphi_\nu^{\rm (v)} - \partial_\nu\varphi_\mu^{\rm (v)}), \tag{1.56}$$

with ψ the nucleon and $\varphi_{(\mu)}^{(\alpha)}$ the meson fields (notation and conventions as in [1.12]). For isospin 1 mesons, $\varphi^{(\alpha)}$ is to be replaced by $\boldsymbol{\tau}\cdot\boldsymbol{\varphi}^{(\alpha)}$ with τ^l ($l=1,2,3$) the usual Pauli matrices. ps, pv, s, and v denote pseudo-scalar, pseudo-vector, scalar, and vector coupling/fields, respectively.

The one-boson-exchange potential (OBEP) is defined as a sum of one-particle-exchange amplitudes of certain bosons with given mass and coupling. We use the six non-strange bosons with masses below 1 GeV/c^2. Thus,

$$V_{\rm OBEP} = \sum_{\alpha=\pi,\eta,\rho,\omega,\delta,\sigma} V_\alpha^{\rm OBE}, \tag{1.57}$$

with π and η pseudo-scalar, σ and δ scalar, and ρ and ω vector particles. The contributions from the iso-vector bosons π,δ, and ρ contain a factor $\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2$.

The above Lagrangians imply the following OBE amplitudes:[1]

[1]Strictly speaking, we give here the potential defined as i times the Feynman amplitude; furthermore, there is a factor of i for each vertex and propagator; since $\mathrm{i}^4=1$, we simply ignore these factors of i.

$$\langle \boldsymbol{q}'\lambda_1'\lambda_2'|V_{\rm ps}^{\rm OBE}|\boldsymbol{q}\lambda_1\lambda_2\rangle$$
$$= -\frac{g_{\rm ps}^2}{(2\pi)^3}\bar{u}(\boldsymbol{q}',\lambda_1')\mathrm{i}\gamma^5 u(\boldsymbol{q},\lambda_1)\bar{u}(-\boldsymbol{q}',\lambda_2')\mathrm{i}\gamma^5 u(-\boldsymbol{q},\lambda_2)$$
$$/[(\boldsymbol{q}'-\boldsymbol{q})^2+m_{\rm ps}^2]; \tag{1.58}$$

$$\langle \boldsymbol{q}'\lambda_1'\lambda_2'|V_{\rm pv}^{\rm OBE}|\boldsymbol{q}\lambda_1\lambda_2\rangle$$
$$= \frac{1}{(2\pi)^3}\frac{f_{\rm ps}^2}{m_{\rm ps}^2}\bar{u}(\boldsymbol{q}',\lambda_1')\gamma^5\cdot$$
$$\gamma^\mu \mathrm{i}(q'-q)_\mu u(\boldsymbol{q},\lambda_1)\bar{u}(-\boldsymbol{q}',\lambda_2')\gamma^5\gamma^\mu \mathrm{i}(q'-q)_\mu u(-\boldsymbol{q},\lambda_2)$$
$$/[(\boldsymbol{q}'-\boldsymbol{q})^2+m_{\rm ps}^2]$$
$$= \frac{f_{\rm ps}^2}{(2\pi)^3}\frac{4M^2}{m_{\rm ps}^2}\{\bar{u}(\boldsymbol{q}',\lambda_1')\gamma^5 u(\boldsymbol{q},\lambda_1)\bar{u}(-\boldsymbol{q}',\lambda_2')\gamma^5 u(-\boldsymbol{q},\lambda_2)$$
$$+[(E'-E)/(2M)]^2\bar{u}(\boldsymbol{q}',\lambda_1')\gamma^5\gamma^0 u(\boldsymbol{q},\lambda_1)\bar{u}(-\boldsymbol{q}',\lambda_2')\gamma^5\gamma^0 u(-\boldsymbol{q},\lambda_2)$$
$$+[(E'-E)/(2M)][\bar{u}(\boldsymbol{q}',\lambda_1')\gamma^5 u(\boldsymbol{q},\lambda_1)\bar{u}(-\boldsymbol{q}',\lambda_2')\gamma^5\gamma^0 u(-\boldsymbol{q},\lambda_2)$$
$$+\bar{u}(\boldsymbol{q}',\lambda_1')\gamma^5\gamma^0 u(\boldsymbol{q},\lambda_1)\bar{u}(-\boldsymbol{q}',\lambda_2')\gamma^5 u(-\boldsymbol{q},\lambda_2)]\}$$
$$/[(\boldsymbol{q}'-\boldsymbol{q})^2+m_{\rm ps}^2]; \tag{1.59}$$

$$\langle \boldsymbol{q}'\lambda_1'\lambda_2'|V_{\rm s}^{\rm OBE}|\boldsymbol{q}\lambda_1\lambda_2\rangle$$
$$= -\frac{g_{\rm s}^2}{(2\pi)^3}\bar{u}(\boldsymbol{q}',\lambda_1')u(\boldsymbol{q},\lambda_1)\bar{u}(-\boldsymbol{q}',\lambda_2')u(-\boldsymbol{q},\lambda_2)/[(\boldsymbol{q}'-\boldsymbol{q})^2+m_{\rm s}^2]; \tag{1.60}$$

$$\langle \boldsymbol{q}'\lambda_1'\lambda_2'|V_{\rm v}^{\rm OBE}|\boldsymbol{q}\lambda_1\lambda_2\rangle$$
$$= \frac{1}{(2\pi)^3}\Big[g_{\rm v}\bar{u}(\boldsymbol{q}',\lambda_1')\gamma_\mu u(\boldsymbol{q},\lambda_1)$$
$$+\frac{f_{\rm v}}{2M}\bar{u}(\boldsymbol{q}',\lambda_1')\sigma_{\mu\nu}\mathrm{i}(q'-q)^\nu u(\boldsymbol{q},\lambda_1)\Big]$$
$$\times\Big[g_{\rm v}\bar{u}(-\boldsymbol{q}',\lambda_2')\gamma^\mu u(-\boldsymbol{q},\lambda_2)$$
$$-\frac{f_{\rm v}}{2M}\bar{u}(-\boldsymbol{q}',\lambda_2')\sigma^{\mu\nu}\mathrm{i}(q'-q)_\nu u(-\boldsymbol{q},\lambda_2)\Big]$$
$$/[(\boldsymbol{q}'-\boldsymbol{q})^2+m_{\rm v}^2]$$
$$= \frac{1}{(2\pi)^3}\{(g_{\rm v}+f_{\rm v})\bar{u}(\boldsymbol{q}',\lambda_1')\gamma_\mu u(\boldsymbol{q},\lambda_1)$$
$$-\frac{f_{\rm v}}{2M}\bar{u}(\boldsymbol{q}',\lambda_1')[(q'+q)_\mu+(E'-E)(g_\mu^0-\gamma_\mu\gamma^0)]u(\boldsymbol{q},\lambda_1)\}$$
$$\times\{(g_{\rm v}+f_{\rm v})\bar{u}(-\boldsymbol{q}',\lambda_2')\gamma^\mu u(-\boldsymbol{q},\lambda_2)$$
$$-\frac{f_{\rm v}}{2M}\bar{u}(-\boldsymbol{q}',\lambda_2')[(q'+q)_\mu+(E'-E)(g^{\mu 0}-\gamma^\mu\gamma^0)]u(-\boldsymbol{q},\lambda_2)\}$$
$$/[(\boldsymbol{q}'-\boldsymbol{q})^2+m_{\rm v}^2]. \tag{1.61}$$

Working in the two-nucleon center-of-mass frame, the momenta of the two incoming (outgoing) nucleons are $\boldsymbol{q}$ and $-\boldsymbol{q}$ ($\boldsymbol{q}'$ and $-\boldsymbol{q}'$). $E \equiv \sqrt{M^2+\boldsymbol{q}^2}$ and $E' \equiv \sqrt{M^2+\boldsymbol{q}'^2}$. Using the BbS or Thompson equation, the four-momentum transfer between the two nucleons is $(q'-q) = (0, \boldsymbol{q}' - \boldsymbol{q})$. The Dirac equation is applied repeatedly in the evaluations for the pv-coupling, and the Gordon identity [1.12] is used in the case of the v-coupling. [Note that in (1.61), second line from the bottom, the term $(q'+q)_\mu$ carries μ as a *sub*script to ensure the correct sign of the space component of that term.] The propagator for vector bosons is

$$\mathrm{i}\frac{-g_{\mu\nu} + (q'-q)_\mu (q'-q)_\nu / m_{\mathrm{v}}^2}{-(\boldsymbol{q}'-\boldsymbol{q})^2 - m_{\mathrm{v}}^2}, \tag{1.62}$$

where we drop the $(q'-q)_\mu (q'-q)_\nu$-term, which vanishes on-shell, anyhow, since the nucleon current is conserved. The off-shell effect of this term was examined in [1.21] and was found to be unimportant.

The Dirac spinors in helicity representation are given by

$$u(\boldsymbol{q},\lambda_1) = \sqrt{\frac{E+M}{2M}} \begin{pmatrix} 1 \\ \frac{2\lambda_1 q}{E+M} \end{pmatrix} |\lambda_1\rangle, \tag{1.63}$$

$$u(-\boldsymbol{q},\lambda_2) = \sqrt{\frac{E+M}{2M}} \begin{pmatrix} 1 \\ \frac{2\lambda_2 q}{E+M} \end{pmatrix} |\lambda_2\rangle. \tag{1.64}$$

They are normalized covariantly, that is,

$$\bar{u}(\boldsymbol{q},\lambda) u(\boldsymbol{q},\lambda) = 1 \tag{1.65}$$

with $\bar{u} = u^\dagger \gamma^0$.

At each meson–nucleon vertex, a form factor is applied that has the analytical form

$$\mathcal{F}_\alpha[(\boldsymbol{q}'-\boldsymbol{q})^2] = \left[\frac{\Lambda_\alpha^2 - m_\alpha^2}{\Lambda_\alpha^2 + (\boldsymbol{q}'-\boldsymbol{q})^2}\right]^{n_\alpha}, \tag{1.66}$$

with m_α the mass of the meson involved, Λ_α the so-called cutoff mass, and n_α an exponent. Thus, the OBE amplitudes (1.58–61) are multiplied by $\mathcal{F}_\alpha^2$.

In practice, it is desirable to have the potential represented in partial waves, since scattering phase shifts are defined in such a representation and nuclear-structure calculations are conventionally performed in an LSJ basis. We will turn to this in the next subsection.

1.3.2 Partial-Wave Decomposition

The OBE amplitudes are decomposed into partial waves according to

$$\begin{aligned}&\langle \lambda_1' \lambda_2' | V^J(q',q) | \lambda_1 \lambda_2 \rangle \\ &\quad = 2\pi \int_{-1}^{+1} \mathrm{d}(\cos\theta)\, d^J_{\lambda_1-\lambda_2,\lambda_1'-\lambda_2'}(\theta) \langle \boldsymbol{q}' \lambda_1' \lambda_2' | V | \boldsymbol{q} \lambda_1 \lambda_2 \rangle,\end{aligned} \tag{1.67}$$

where θ is the angle between $\boldsymbol{q}$ and $\boldsymbol{q}'$, and $d^J_{m,m'}(\theta)$ is the conventional reduced rotation matrix.

In the present code, the integration over $\cos\theta$ is performed numerically. The $d^J_{m,m'}(\theta)$ is expressed in terms of Legendre polynominals, $P_J(\cos\theta)$. The following types of integrals will occur repeatedly:

$$
\begin{aligned}
I_J^{(0)} &\equiv \int_{-1}^{+1} \mathrm{d}t \, \frac{P_J(t)}{(\boldsymbol{q}'-\boldsymbol{q})^2+m_\alpha^2} \, \mathcal{F}_\alpha^2[(\boldsymbol{q}'-\boldsymbol{q})^2], \\
I_J^{(1)} &\equiv \int_{-1}^{+1} \mathrm{d}t \, \frac{tP_J(t)}{(\boldsymbol{q}'-\boldsymbol{q})^2+m_\alpha^2} \, \mathcal{F}_\alpha^2[(\boldsymbol{q}'-\boldsymbol{q})^2], \\
I_J^{(2)} &\equiv \frac{1}{J+1} \int_{-1}^{+1} \mathrm{d}t \, \frac{JtP_J(t)+P_{J-1}(t)}{(\boldsymbol{q}'-\boldsymbol{q})^2+m_\alpha^2} \, \mathcal{F}_\alpha^2[(\boldsymbol{q}'-\boldsymbol{q})^2], \\
I_J^{(3)} &\equiv \sqrt{\frac{J}{J+1}} \int_{-1}^{+1} \mathrm{d}t \, \frac{tP_J(t)-P_{J-1}(t)}{(\boldsymbol{q}'-\boldsymbol{q})^2+m_\alpha^2} \, \mathcal{F}_\alpha^2[(\boldsymbol{q}'-\boldsymbol{q})^2], \\
I_J^{(4)} &\equiv \int_{-1}^{+1} \mathrm{d}t \, \frac{t^2P_J(t)}{(\boldsymbol{q}'-\boldsymbol{q})^2+m_\alpha^2} \, \mathcal{F}_\alpha^2[(\boldsymbol{q}'-\boldsymbol{q})^2], \\
I_J^{(5)} &\equiv \frac{1}{J+1} \int_{-1}^{+1} \mathrm{d}t \, \frac{Jt^2P_J(t)+tP_{J-1}(t)}{(\boldsymbol{q}'-\boldsymbol{q})^2+m_\alpha^2} \, \mathcal{F}_\alpha^2[(\boldsymbol{q}'-\boldsymbol{q})^2], \\
I_J^{(6)} &\equiv \sqrt{\frac{J}{J+1}} \int_{-1}^{+1} \mathrm{d}t \, \frac{t^2P_J(t)-tP_{J-1}(t)}{(\boldsymbol{q}'-\boldsymbol{q})^2+m_\alpha^2} \, \mathcal{F}_\alpha^2[(\boldsymbol{q}'-\boldsymbol{q})^2],
\end{aligned}
\tag{1.68}
$$

where $t \equiv \cos\theta$. Notice that these integrals are functions of q', q, m_α, Λ_α, and n_α.

We state the final expressions for the partial-wave OBE amplitudes in terms of the combinations of helicity amplitudes defined in (1.31). More details concerning their derivation are to be found in Appendix E of [1.6].

Pseudo-scalar bosons (η and π meson; for π apply an additional factor of $\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$):
Pseudo-scalar coupling (ps)

$$
\begin{aligned}
{}^0V_{\rm ps}^J &= C_{\rm ps}\,(F_{\rm ps}^{(0)}\, I_J^{(0)} + F_{\rm ps}^{(1)}\, I_J^{(1)}), \\
{}^1V_{\rm ps}^J &= C_{\rm ps}\,(-F_{\rm ps}^{(0)}\, I_J^{(0)} - F_{\rm ps}^{(1)}\, I_J^{(2)}), \\
{}^{12}V_{\rm ps}^J &= C_{\rm ps}\,(F_{\rm ps}^{(1)}\, I_J^{(0)} + F_{\rm ps}^{(0)}\, I_J^{(1)}), \\
{}^{34}V_{\rm ps}^J &= C_{\rm ps}\,(-F_{\rm ps}^{(1)}\, I_J^{(0)} - F_{\rm ps}^{(0)}\, I_J^{(2)}), \\
{}^{55}V_{\rm ps}^J &= C_{\rm ps}\, F_{\rm ps}^{(2)}\, I_J^{(3)}, \\
{}^{66}V_{\rm ps}^J &= -C_{\rm ps}\, F_{\rm ps}^{(2)}\, I_J^{(3)},
\end{aligned}
\tag{1.69}
$$

with

$$C_{\rm ps} = \frac{g_{\rm ps}^2}{4\pi}\,\frac{1}{2\pi M^2} \tag{1.70}$$

and

$$\begin{aligned} F_{\rm ps}^{(0)} &= E'E - M^2, \\ F_{\rm ps}^{(1)} &= -q'q, \\ F_{\rm ps}^{(2)} &= -M(E'-E). \end{aligned} \tag{1.71}$$

Alternatively, the pseudo-vector (pv) coupling can be used for pseudo-scalar mesons. The basic scheme is the same as above; just replace the subscript ps by pv and use

$$\begin{aligned} F_{\rm pv}^{(0)} &= E'E - M^2 + (E'-E)^2(E'E+3M^2)/(4M^2), \\ F_{\rm pv}^{(1)} &= -q'q + q'q(E'-E)^2/(4M^2), \\ F_{\rm pv}^{(2)} &= -(E'-E)[\tfrac{1}{4}(E'-E)^2 + E'E]/M, \end{aligned} \tag{1.72}$$

and

$$C_{\rm pv} = \frac{f_{\rm ps}^2}{4\pi}\,\frac{4M^2}{m_\alpha^2}\,\frac{1}{2\pi M^2}\,. \tag{1.73}$$

Defining

$$g_{\rm ps} = f_{\rm ps}\,\frac{2M}{m_{\rm ps}}\,, \tag{1.74}$$

we see that $C_{\rm pv} = C_{\rm ps}$.

Scalar coupling (s) (σ and δ boson; for δ apply an additional factor of $\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2$):

$$\begin{aligned} {}^0V_{\rm s}^J &= C_{\rm s}\,(F_{\rm s}^{(0)}\,I_J^{(0)} + F_{\rm s}^{(1)}\,I_J^{(1)}), \\ {}^1V_{\rm s}^J &= C_{\rm s}\,(F_{\rm s}^{(0)}\,I_J^{(0)} + F_{\rm s}^{(1)}\,I_J^{(2)}), \\ {}^{12}V_{\rm s}^J &= C_{\rm s}\,(F_{\rm s}^{(1)}\,I_J^{(0)} + F_{\rm s}^{(0)}\,I_J^{(1)}), \\ {}^{34}V_{\rm s}^J &= C_{\rm s}\,(F_{\rm s}^{(1)}\,I_J^{(0)} + F_{\rm s}^{(0)}\,I_J^{(2)}), \\ {}^{55}V_{\rm s}^J &= C_{\rm s}\,F_{\rm s}^{(2)}\,I_J^{(3)}, \\ {}^{66}V_{\rm s}^J &= C_{\rm s}\,F_{\rm s}^{(2)}\,I_J^{(3)}, \end{aligned} \tag{1.75}$$

with

$$C_{\rm s} = \frac{g_{\rm s}^2}{4\pi}\,\frac{1}{2\pi M^2} \tag{1.76}$$

and

$$
\begin{aligned}
F_{\rm s}^{(0)} &= -(E'E + M^2), \\
F_{\rm s}^{(1)} &= q'q, \\
F_{\rm s}^{(2)} &= M(E' + E).
\end{aligned} \tag{1.77}
$$

Vector bosons (v) (ω and ρ meson; for ρ apply an additional factor of $\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$):
Vector–vector coupling

$$
\begin{aligned}
{}^0V_{\rm vv}^J &= C_{\rm vv}\,(2E'E - M^2)\,I_J^{(0)}, \\
{}^1V_{\rm vv}^J &= C_{\rm vv}\,(E'E\,I_J^{(0)} + q'q\,I_J^{(2)}), \\
{}^{12}V_{\rm vv}^J &= C_{\rm vv}\,(2q'q\,I_J^{(0)} + M^2\,I_J^{(1)}), \\
{}^{34}V_{\rm vv}^J &= C_{\rm vv}\,(q'q\,I_J^{(0)} + E'E\,I_J^{(2)}), \\
{}^{55}V_{\rm vv}^J &= -C_{\rm vv}\,ME\,I_J^{(3)}, \\
{}^{66}V_{\rm vv}^J &= -C_{\rm vv}\,ME'\,I_J^{(3)},
\end{aligned} \tag{1.78}
$$

with

$$
C_{\rm vv} = \frac{g_{\rm v}^2}{4\pi}\,\frac{1}{\pi M^2}\,. \tag{1.79}
$$

Tensor–tensor coupling

$$
\begin{aligned}
{}^0V_{\rm tt}^J &= C_{\rm tt}\,\{(q'^2 + q^2)(3E'E + M^2)\,I_J^{(0)} \\
&\quad +[q'^2 + q^2 - 2(3E'E + M^2)]q'q\,I_J^{(1)} - 2q'^2q^2\,I_J^{(4)}\}, \\
{}^1V_{\rm tt}^J &= C_{\rm tt}\,\{[4q'^2q^2 + (q'^2 + q^2)(E'E - M^2)]\,I_J^{(0)} \\
&\quad +2(E'E + M^2)q'q\,I_J^{(1)} \\
&\quad -(q'^2 + q^2 + 4E'E)q'q\,I_J^{(2)} - 2q'^2q^2\,I_J^{(5)}\}, \\
{}^{12}V_{\rm tt}^J &= C_{\rm tt}\,\{[4M^2 - 3(q'^2 + q^2)]q'q\,I_J^{(0)} \\
&\quad +[6q'^2q^2 - (q'^2 + q^2)(E'E + 3M^2)]\,I_J^{(1)} + 2(E'E + M^2)q'q\,I_J^{(4)}\}, \\
{}^{34}V_{\rm tt}^J &= C_{\rm tt}\,\{-(q'^2 + q^2 + 4E'E)q'q\,I_J^{(0)} - 2q'^2q^2\,I_J^{(1)} \\
&\quad +[4q'^2q^2 + (q'^2 + q^2)(E'E - M^2)]\,I_J^{(2)} + 2(E'E + M^2)q'q\,I_J^{(5)}\}, \\
{}^{55}V_{\rm tt}^J &= C_{\rm tt}\,M\{[E'(q'^2 + q^2) + E(3q'^2 - q^2)]\,I_J^{(3)} - 2(E' + E)q'q\,I_J^{(6)}\}, \\
{}^{66}V_{\rm tt}^J &= C_{\rm tt}\,M\{[E(q'^2 + q^2) + E'(3q^2 - q'^2)]\,I_J^{(3)} - 2(E' + E)q'q\,I_J^{(6)}\},
\end{aligned} \tag{1.80}
$$

with

$$
C_{\rm tt} = \frac{f_{\rm v}^2}{4\pi}\,\frac{1}{8\pi M^4}. \tag{1.81}
$$

Vector–tensor coupling

$$
{}^0V_{\rm vt}^J = C_{\rm vt}\,M[(q'^2 + q^2)\,I_J^{(0)} - 2q'q\,I_J^{(1)}],
$$

$$
\begin{aligned}
{}^{1}V_{\rm vt}^{J} &= C_{\rm vt}\, M[-(q'^2+q^2)\, I_J^{(0)} + 2q'q\, I_J^{(2)}],\\
{}^{12}V_{\rm vt}^{J} &= C_{\rm vt}\, M[6q'q\, I_J^{(0)} - 3(q'^2+q^2)\, I_J^{(1)}],\\
{}^{34}V_{\rm vt}^{J} &= C_{\rm vt}\, M[2q'q\, I_J^{(0)} - (q'^2+q^2)\, I_J^{(2)}],\\
{}^{55}V_{\rm vt}^{J} &= C_{\rm vt}\, (E'q^2+3Eq'^2)\, I_J^{(3)},\\
{}^{66}V_{\rm vt}^{J} &= C_{\rm vt}\, (Eq'^2+3E'q^2)\, I_J^{(3)},
\end{aligned}
\tag{1.82}
$$

with

$$
C_{\rm vt} = \frac{g_{\rm v} f_{\rm v}}{4\pi}\,\frac{1}{2\pi M^3}. \tag{1.83}
$$

We use units such that $\hbar = c = 1$. Energies, masses, and momenta are in MeV. The potential is in units of MeV^{-2}. The conversion factor is $\hbar c = 197.3286$ MeV fm. If the user wants to relate our units and conventions to those used in the work of other researchers, he/she should compare our (1.32) and our phase-shift relation (1.41) with the corresponding equations in other works.

1.3.3 Meson Parameters and Two-Nucleon Predictions

As an example of a relativistic momentum-space OBEP, we give here the potential presented in Section 4 of [1.7], which has become known as the Bonn B potential.[2] Its description of the NN data is excellent. This potential uses the pseudo-scalar coupling for π and η and is constructed within the framework of the BbS equation (1.15). The $\hat{V}$ version of this potential (1.17) is appropriate for application in non-relativistic nuclear-structure physics, since it satisfies (1.18).

In Table 1.1 we give the meson parameters. The predictions for the deuteron and low-energy scattering parameters are displayed in Table 1.2 together with the experimental values. Some phase shifts for neutron–proton scattering are listed in Table 1.3. Plots of the phase shifts predicted by Bonn B are shown in Fig. 5.10 of [1.7] together with the predictions by other NN models and results from phase-shift analyses.

1.4 Numerics and Codes

Two computer codes are supplied. The first (named `SPRING1` on the disk) computes the momentum-space OBEP described in Sect. 1.3. The second (file `SPRING2`) calculates the R-matrix by solving (1.32–34).

[2] It is customary to denote the OBE parametrizations of the Bonn full model [1.6] by the first letters of the alphabet, A, B, or C. See, for example, Appendix A of [1.7].

Table 1.1. Parameters for the Bonn B potential

Meson	J^P	I^G	$g_\alpha^2/4\pi$	f_α/g_α	m_α(MeV)	Λ_α(GeV)	$2n_\alpha$
π	0^-	1^-	14.4		138.03	1.7	2
η	0^-	0^+	3		548.8	1.5	2
ρ	1^-	1^+	0.9	6.1	769	1.85	4
ω	1^-	0^-	24.5	0	782.6	1.85	4
δ	0^+	1^-	2.488		983	2.0	2
σ^a	0^+	0^+	8.9437		550	1.9	2
			(18.3773)		(720)	(2.0)	(2)

J, P, I, and G denote spin, parity, isospin, and G-parity of the meson, respectively. Λ_α and n_α are the parameters for the form factor (1.66).
[a] The σ parameters given in parentheses apply to the $T = 0$ NN potential.

1.4.1 Momentum-Space OBEP

The subroutine `BONN` computes the momentum-space OBEP in terms of partial-wave helicity matrix elements according to the formulas (1.69–83). Though the code uses several subroutines, the user needs to call only `BONN` without worrying about the other computer programs contained in the package.

Nevertheless, we will briefly explain the purpose of each of those subroutines. Equations (1.69, 75, 78, 80, 82) obviously show a common pattern. This common structure of the mathematical expressions for the six OBE amplitudes is calculated by the subroutine `OBSTR`. The factors $F_\alpha^{(i)}$ (with $i = 0, 1, 2, \ldots,$), which are functions of q' and q only, are calculated in the major subroutine `BONN` itself, while the integrals $I_J^{(i)}$ (with $i = 0, \ldots, 6$) are computed in `OBAI`. The transfer of the Fs and Is to `OBSTR` proceeds via the `COMMON /COB/`. They are stored in the arrays `F` and `AI` with `F(`$i+1$`)` $= F_\alpha^{(i)}$ and `AI(`$i+1$`,M)` $= I_J^{(i)}$, where the index `M` runs over mesons using the same coupling.

Almost all communication between `BONN` and its `OB`-subroutines is done by means of the `COMMON /COB/`, which consists of many variables and arrays. The dimensions of the arrays are chosen generously such that extensions of the code will in general not require any extensions of this basic `COMMON` block.

`OBAI` computes the integrals (1.68) numerically using a mesh of Gauss points provided by the subroutine `GSET`. Up to 96 Gauss points can be ordered from `GSET`. The number of Gauss points necessary to compute the integrals with sufficient numerical accuracy depends on q', q, and m_α and is calculated by `OBAI` before `GSET` is called. Via the input-parameter set for `BONN`, the user sets a lower and upper limit for the number of mesh points to be used (see below).

The meson propagator and the form factor, which are both functions of $\cos\theta$, are calculated in the subroutine `OBAA` and transferred to `OBAI` in the

Table 1.2. Deuteron and low-energy scattering parameters as predicted by the Bonn B potential (Theory) and from empirical sources (Experiment)

	Theory	Experiment[a]
Deuteron:		
Binding energy (MeV)	2.2246	2.224575(9)
D-state probability (%)	4.99	
Quadrupole moment (fm^2)	0.278 [b]	0.2860(15)
Asymptotic D/S-state ratio	0.0264	0.0264(12)
Root-mean-square radius (fm)	1.9688	1.9635(45)
Neutron–proton low-energy scattering (scattering length a, effective range r):		
$^1S_0$: a_{np} (fm)	−23.75	−23.748(10)
r_{np} (fm)	2.71	2.75(5)
$^3S_1$: a_t (fm)	5.424	5.424(4)
$r_t = \rho(0,0)$ (fm)	1.761	1.759(5)

[a] The figures in parentheses after the experimental values give the one-standard-deviation uncertainties in the last digits. References to experiment can be found in [1.7].
[b] Without meson-exchange current contributions, which add 0.009(5) fm^2.

array AA. Subroutine LEGP provides the Legendre polynominals and is called by OBAI.

The helicity matrix elements for each boson exchange are calculated individually in OBSTR and stored separately in the array VJ of COMMON /COB/. These contributions from the individual mesons are finally added up at the end of the major subroutine BONN and stored in the array V of COMMON /CPOT/, which is used to transfer the potential values to the program that is calling BONN.

Input and output for the code system BONN are in units of MeV for momenta, masses, and cutoff masses, and in units of MeV^{-2} for the potential. However, *within* the code system BONN, all momenta, masses, and cutoff masses are in units of the nucleon mass M.

1.4.2 $\hat{R}$-Matrix and Phase Shifts

The $\hat{R}$-matrix is calculated by solving the integral equations (1.32–34). We apply the matrix-inversion method as introduced by Haftel and Tabakin [1.22].

To explain the method, let us consider an uncoupled case, for example, (1.32). First, we add to the right-hand side of this equation the term

$$-Mq^2\,{}^0\hat{V}^J(q',q)\,{}^0\hat{R}^J(q,q)\,\mathcal{P}\int_0^\infty \frac{\mathrm{d}k}{q^2-k^2}, \tag{1.84}$$

Table 1.3. Neutron–proton phase shifts (in degrees) in some low angular momentum partial waves for various laboratory energies (in MeV) as predicted by the Bonn B potential

State	25	50	100	200	300
$^1S_0$	50.72	39.98	25.19	5.66	−8.18
$^3P_0$	9.34	12.24	9.80	−1.02	11.48
$^1P_1$	−7.20	−11.15	−16.31	−23.47	−28.70
$^3P_1$	−5.33	−8.77	−13.47	−20.48	−26.38
$^3S_1$	80.32	62.16	41.99	19.03	4.07
$^3D_1$	−2.99	−6.86	−12.98	−20.29	−23.72
ϵ_1	1.76	2.00	2.24	3.03	4.03
$^1D_2$	0.68	1.58	3.34	6.21	7.49
$^3D_2$	3.88	9.29	17.67	24.94	25.36
$^3P_2$	2.62	6.14	11.74	16.65	17.40
$^3F_2$	0.11	0.34	0.77	1.10	0.52
ϵ_2	−0.86	−1.82	−2.84	−2.85	−2.02

which is equal to zero. This yields

$$
\begin{aligned}
{}^0\hat{R}^J(q',q) = {}^0\hat{V}^J(q',q) + \int_0^\infty \mathrm{d}k \, \frac{M}{q^2-k^2} [k^2 \, {}^0\hat{V}^J(q',k) \, {}^0\hat{R}^J(k,q) \\
- q^2 \, {}^0\hat{V}^J(q',q) \, {}^0\hat{R}^J(q,q)] \, ,
\end{aligned} \tag{1.85}
$$

where we replaced the principal-value integral by an ordinary integral, since the added term makes the integrand smooth; for $k \longrightarrow q$ the integrand is now finite.

The integral in (1.85) is computed by summing over N mesh points according to

$$
\int_0^\infty \mathrm{d}k \, f(k) = \sum_{i=1}^{N} f(k_i) s_i \, . \tag{1.86}
$$

We use Gaussian integration points and weights. Since the original Gauss points, x_i (with weights w_i), are in the interval $(-1,+1)$, we have to map them to the interval $(0,\infty)$, the range of our integration. For this purpose, we use the mapping

$$
k_i = C \, \tan[\pi(x_i+1)/4], \tag{1.87}
$$

with the new weights

$$
s_i = C \, \frac{\pi}{4} \, \frac{w_i}{\cos^2[\pi(x_i+1)/4]}, \tag{1.88}
$$

where C should be chosen in the order of 1000 MeV.

After rearranging (1.85),

$$
{}^0\hat{R}^J(q',q) - \int_0^\infty \mathrm{d}k \, \frac{M}{q^2-k^2}[k^2 \, {}^0\hat{V}^J(q',k) \, {}^0\hat{R}^J(k,q) - q^2 \, {}^0\hat{V}^J(q',q) \, {}^0\hat{R}^J(q,q)]
$$
$$
= {}^0\hat{V}^J(q',q) \,, \tag{1.89}
$$

we rewrite it in discrete form:

$$
\sum_{j=1}^{N+1} {}^0A_{ij}^J \, {}^0\hat{R}^J(k_j,k_{N+1}) = {}^0\hat{V}^J(k_i,k_{N+1}), \tag{1.90}
$$

with $i = 1,\ldots,N+1$ and $k_{N+1} \equiv q$, the on-shell momentum. ${}^0A_{ij}^J$ is defined by

$$
{}^0A_{ij}^J = \delta_{ij} + u_j \, {}^0\hat{V}^J(k_i,k_j), \tag{1.91}
$$

with

$$
u_j = Mk_j^2 \frac{s_j}{k_j^2-q^2} \qquad \text{for } 1 \le j \le N \tag{1.92}
$$

and

$$
u_{N+1} = -Mq^2 \sum_{j=1}^{N} \frac{s_j}{k_j^2-q^2}, \tag{1.93}
$$

where all grid points k_j have to be distinct from q. Notice that the "weight" u_{N+1} is just the added zero term that makes it possible to calculate the principal-value integral like an ordinary integral.

Defining ${}^0A^J \equiv ({}^0A_{ij}^J)$, which is an $(N+1)\times(N+1)$ matrix, (1.90) can be written in matrix notation

$$
{}^0A^J \, {}^0\hat{R}^J = {}^0\hat{V}^J, \tag{1.94}
$$

where ${}^0\hat{R}^J$ and ${}^0\hat{V}^J$ are vectors of dimension $N+1$. This is a system of $N+1$ linear equations with $N+1$ unknowns and has the familiar form

$$
AX = B, \tag{1.95}
$$

with $X \equiv {}^0\hat{R}^J$ the unknown vector. It is solved by standard methods.

For the computation of the phase shifts, δ_l, only the on-shell $\hat{R}$-matrix element

$$
{}^0\hat{R}^J(q,q) \equiv {}^0\hat{R}^j(k_{N+1},k_{N+1}) \tag{1.96}
$$

is needed. From this, δ_l is obtained by means of (1.42). As a by-product, the half-off-shell $\hat{R}$-matrix, ${}^0\hat{R}^J(q',q) \equiv {}^0\hat{R}^J(k_i,k_{N+1})$, with $i = 1,\ldots,N$, is also obtained.

It is easy also to calculate the fully off-shell $\hat{R}$ matrix. Just consider ${}^0\hat{R}^J$ and ${}^0\hat{V}^J$ in (1.94) as $(N+1)\times(N+1)$ matrices with matrix elements ${}^0\hat{V}^J(k_i,k_j)$ and ${}^0\hat{R}^J(k_i,k_j)$ $(i,j = 1,\ldots,N+1)$. ${}^0A^J$ is the same as before. This option is built into the code (see below).

The extension to coupled channels is straightforward. In matrix notation, we have for the coupled case [cf. (1.34)]

$$\begin{pmatrix} {}^{12}A^J & {}^{55}\dot{A}^J \\ {}^{66}\dot{A}^J & {}^{34}A^J \end{pmatrix} \begin{pmatrix} {}^{12}\hat{R}^J & {}^{55}\hat{R}^J \\ {}^{66}\hat{R}^J & {}^{34}\hat{R}^J \end{pmatrix} = \begin{pmatrix} {}^{12}\hat{V}^J & {}^{55}\hat{V}^J \\ {}^{66}\hat{V}^J & {}^{34}\hat{V}^J \end{pmatrix}, \tag{1.97}$$

where the ${}^aA^J$ $(a = 12, 34, \ldots,)$ are defined similarly to (1.91) and ${}^a\dot{A}^J \equiv {}^aA^J - \mathbf{1}$ with $\mathbf{1}$ the unit matrix. The matrix involving the As is a $(2N + 2) \times (2N + 2)$ matrix. If only the on-shell and half-off-shell $\hat{R}$ matrix is to be calculated, the matrices involving the $\hat{R}$s and $\hat{V}$s have two columns and $2N+2$ rows. If the fully off-shell $\hat{R}$ matrix is computed, all matrices in (1.97) are $(2N + 2) \times (2N + 2)$.

If $\hat{V}$ and $\hat{R}$ are considered in LSJ representation, the coupled system is [cf. (1.38)]

$$\begin{pmatrix} A^{J1}_{++} & \dot{A}^{J1}_{+-} \\ \dot{A}^{J1}_{-+} & A^{J1}_{--} \end{pmatrix} \begin{pmatrix} \hat{R}^{J1}_{++} & \hat{R}^{J1}_{+-} \\ \hat{R}^{J1}_{-+} & \hat{R}^{J1}_{--} \end{pmatrix} = \begin{pmatrix} \hat{V}^{J1}_{++} & \hat{V}^{J1}_{+-} \\ \hat{V}^{J1}_{-+} & \hat{V}^{J1}_{--} \end{pmatrix}. \tag{1.98}$$

For the coupled channels, our code offers both options, (1.97) and (1.98).

When building up the matrices in (1.97) or (1.98), our code takes advantage of the symmetries of $\hat{V}$: ${}^{12}\hat{V}^J$ and ${}^{34}\hat{V}^J$ are symmetric in q' and q, and ${}^{55}\hat{V}^J(q', q) = {}^{66}\hat{V}^J(q, q')$; in LSJ representation: $\hat{V}^{J1}_{++}$ and $\hat{V}^{J1}_{--}$ are symmetric in q' and q, and $\hat{V}^{J1}_{+-}(q', q) = \hat{V}^{J1}_{-+}(q, q')$.

For the coupled cases, the phase shifts are obtained from the on-shell $\hat{R}$-matrix elements by means of (1.43) or (1.46). Notice that for $\hat{R}^J_{--} \gg \hat{R}^J_{++}$ and ϵ_J small, the calculation of δ^J_+ may be inaccurate. This happens for the ${}^3S_1/{}^3D_1$ phase shifts around $E_{\text{lab}} \approx 16 - 18$ MeV, where $\delta^1_- \approx 90^0$. If more accuracy is needed for this particular case, an expansion of $\cos 2\epsilon_J$ should be used in (1.43).

The subroutine `PHASES` computes the $\hat{R}$ matrix and the phase shifts. Since it is a subroutine, there is a very small main program, `CPH`, that calls `PHASES` and, in addition, defines the potential subroutine to be applied and the dimensions of the various matrices and vectors needed in the computations of `PHASES`. For both vectors and matrices, vector arrays are used. Matrices are stored columnwise. The required dimensions depend on the number of Gauss points used and are specified in `CPH` by a parameter statement.

The notation used in `PHASES` is mostly identical to the one used in this section. Some differences in the notation are

$$\begin{aligned} \texttt{Q(}i\texttt{)} &= k_i, \\ \texttt{QO(K)} &= k_{N+1} = q, \\ \texttt{UQO} &= u_{N+1}, \end{aligned} \tag{1.99}$$

where `K` is an index that refers to the laboratory energy under consideration.

For the matrices and vectors involved in the system of linear equations, the notation of (1.95) is used in the code, where $B = \hat{V}^J$ *before* the solution, and $B = \hat{R}^J$ *after* the solution.

1.5 Using the Codes

A common feature of all codes is that most variables are transferred in common blocks. All routines that contain READ or WRITE statements have the COMMON /CRDWRT/ KREAD,KWRITE,.... The integer variable KREAD carries the number of the unit from which the input parameters are read. KWRITE is the corresponding unit number for output. The user should include the COMMON /CRDWRT/ KREAD,KWRITE,..., in his/her main program and define the input and output unit numbers. Input and output files carry names defined in open statements that appear in the beginning of the corresponding code.

1.5.1 OBEP Code BONN

BONN and all subroutines needed to run the code are contained in one file together with a short calling (main) program and a sample input and output file. To calculate the OBEP, only the subroutine BONN is called. At a single call, BONN computes six OBEP matrix elements for a given pair of momentum arguments (q', q) and a given total angular momentum J. When called for the first time, it also reads an input-parameter set from unit KREAD. As an example, the input-parameter set for the Bonn B potential (Sect. 1.3.3 and Table 1.1) is provided. The input is read in terms of fixed formats. Thus, if the user applies other meson parameter sets, he/she has to follow the formats of the sample set strictly. However, the number of mesons to be exchanged, their properties, the type of their coupling, and the cutoff parameters are variable.

The subroutine that does the reading and storing of the input parameters is OBPAR. It is called by BONN only once (the first time BONN is activated). We discuss now the meaning of the various records of the input file. The first record is a 70-character field which may be used to identify the potential. It is passed to the output file. All following records start with a 10-character field followed by either integer or real number(s). In the case of records 2 to 4, the 10-character field is used to name the parameter(s) for which values are given (on the record). The second record, starting with the identifier FACTOR TYP, provides in column 13 an integer parameter that can be 0, 1, or 2 and is stored in the array element IFT(1). It tells the code by which factors the invariant version of the potential V as given in (1.69–83) is to be multiplied. For IFT(1)=0, no additional factors are applied, that is, following our notation introduced in Sect. 1.2.1, the invariant potential V is computed. If IFT(1)=1, the square-root factors of (1.16) are applied, that is, $\hat{V}$ is calculated. Finally, if IFT(1)=2, the factors of (1.23) are applied, so $\check{V}$ is provided. The third input record, starting with NUM. INT., defines the minimum and maximum number of Gauss points to be used in the numerical angular integrations of (1.68). We recommend 4 48. For test purposes, these parameters can be increased up to 96 96. The fourth record, NUCL. MASS, gives the mass of the

nucleon, which we take to be 938.926 MeV, the average between proton and neutron masses, appropriate for neutron–proton scattering.

The following records define the various mesons to be exchanged, their parameters, and cutoff parameters. By comparing Table 1.1 with the sample input file, it is easy to see how this part of the input has to be arranged. The first four characters of each record indicate either meson or cutoff parameters. If the record starts with CUT, it contains the cutoff parameters for the meson of the previous record. The first numerical parameter on a cutoff record identifies the type of cutoff to be used with 2., denoting the cutoff (1.66). Meson parameter records always start with the type of coupling to be applied, where the following abbreviations are used:

$$\begin{aligned} &\texttt{0-} \quad = \text{pseudo-scalar}, \\ &\texttt{0-T} \quad = \text{pseudo-vector}, \\ &\texttt{0+} \quad = \text{scalar}, \\ &\texttt{1-T} \quad = \text{vector (including tensor)} \end{aligned} \tag{1.100}$$

(cf. Sect. 1.3.1).

In general, all meson parameters are, of course, the same for the T=1 and the T=0 NN potential. However, in some OBE models (such as Bonn B), the σ boson is different for the two NN isospin states. In this case, the σ parameters and its cutoff parameters to be used for the $T = 0$ potential must be the last two records (before END MESONS) and must be preceded by a record that consists of between 4 and 10 asterisks (**********) and nothing else. The σ-parameters to be used for the T=1 potential must be right above the asterisks record. The records for the other mesons have to appear before all σ-records; otherwise, their order is arbitrary.

The last input record has to start with END.[3]

The transfer of arguments and values between the calling program and the potential subroutine BONN proceeds via two common blocks:

```
COMMON /CPOT/    V(6),XMEV,YMEV
COMMON /CSTATE/ J,HEFORM,SING,TRIP,COUP,ENDEP,LABEL
```

The user may ignore the logical variable ENDEP and the integer variable LABEL. We recommend setting, once and forever, in the calling program the logical variables SING, TRIP, and COUP to .TRUE.. Thus, only four parameters and V are of relevance. The calling program has to define J, the total angular momentum, and the relative momenta XMEV and YMEV, which are q' and q, respectively, in units of MeV. Given these arguments, the subroutine BONN computes six potential matrix elements and stores them in the array V. If HEFORM=.TRUE., these six matrix elements are given in the helicity formalism;

[3] In the notation used in this chapter, quotations from the codes and their input/output are printed in upper case typewriter type style. Notice, however, that if the source codes are applied in lower case (as in the files provided), input control words like END or 1-T have to be in lower case, that is, end, 1-t, etc.

they are

$$\begin{aligned}
\texttt{V(1)} &= {}^0V^J(q',q),\\
\texttt{V(2)} &= {}^1V^J(q',q),\\
\texttt{V(3)} &= {}^{12}V^J(q',q),\\
\texttt{V(4)} &= {}^{34}V^J(q',q),\\
\texttt{V(5)} &= {}^{55}V^J(q',q),\\
\texttt{V(6)} &= {}^{66}V^J(q',q)\,.
\end{aligned} \tag{1.101}$$

If `HEFORM=.FALSE.`, the six matrix elements are given in the LSJ formalism; they are

$$\begin{aligned}
\texttt{V(1)} &= V^{J0}_{J,J}(q',q),\\
\texttt{V(2)} &= V^{J1}_{J,J}(q',q),\\
\texttt{V(3)} &= V^{J1}_{J+1,J+1}(q',q),\\
\texttt{V(4)} &= V^{J1}_{J-1,J-1}(q',q),\\
\texttt{V(5)} &= V^{J1}_{J+1,J-1}(q',q),\\
\texttt{V(6)} &= V^{J1}_{J-1,J+1}(q',q)\,.
\end{aligned} \tag{1.102}$$

(Similar formulas apply to $\hat{V}$ and $\check{V}$.) Thus, depending on what formalism is used in the application (LSJ or helicity), the logical parameter `HEFORM` should be set accordingly at the beginning of the user's application main program.

We provide a small main program that calls the subroutine `BONN` and writes the potential matrix elements to an output file that is also given.

1.5.2 Code PHASES

All routines needed to run `PHASES` are contained in the second file `SPRING2` provided, except for `GSET` and `BONN` (together with its subroutines `OBPAR`, `OBSTR`, `OBAI`, `OBAA`, and `LEGP`) that are contained in the potential package `SPRING1`. The input for `PHASES` is read from unit `KREAD`. A sample input and output file is provided. The input file consists of two parts. The second part is just the input for `BONN` (see above). The first part contains the parameters that control `PHASES`. The meaning of each input parameter is explained in the source code `PHASES` in comment line(s) preceeding the corresponding read statement. Therefore, there is no need to discuss them all here. Each input record starts with a 10-character field that is used to name the parameters for which values are provided. The information on the 10-character field has the relevance of a comment for the user and not of keywords for the code.

For the coupled channels, the code offers the option of solving the system of equations either in the helicity or the LSJ formalism (input parameter `IHEF`).

In a typical run, the phase shifts are written to unit KWRITE and there is no other output. If the first two values for $E_{\rm lab}$ are below 2 MeV, the low-energy scattering parameters in S-waves (cf. Sect. 1.2.4) are calculated and printed automatically.

In the sample run provided, the phase shifts of Table 1.3 and the low-energy scattering parameters in Table 1.2 are calculated.

If the $\hat{R}$ matrix is also to be written on a file, the integer input parameter IRMA must be non-zero (for example, 1). The $\hat{R}$ matrix is then written to the unit with unit number KPUNCH to be specified in the main program that calls PHASES (such a sample main program is included). If the fully off-shell $\hat{R}$ matrix is wanted, the parameter IQUA must also be non-zero. Note that the $\hat{R}$-matrix is always written in LSJ representation, no matter if the calculations were performed in the helicity or LSJ formalism. Because of the symmetries of $\hat{R}^{J1}_{L',L}(k_i, k_j)$, $i, j = 1, \ldots, N$, only the lower triangle of this matrix is written columnwise for each $\hat{R}^{J1}_{L',L}$.

We have discussed the formalism for the computation of the R matrix using the "hat" notation ($\hat{R}$), that is, we have considered the BbS equation in the form (1.18), which is identical to the non-relativistic Lippmann–Schwinger equation. We are, however, not restricted to this equation and $\hat{R}$. PHASES can also solve the Thompson equation. This is done in the "check" notation, as discussed in Sect. 1.2.5. The input parameters to be used for the two different scattering equations are the following:

		LS eq.[a]	Th. eq.[b]
in the input for BONN:	FACTOR TYP	1	2
in the input for PHASES:	IPROP	1	2
	IPHREL	1	2

[a] Lippmann–Schwinger equation (=BbS equation in "hat" notation), (1.18).

[b] Thompson equation in "check" notation (1.24).

1.6 What Else?

The nuclear-matter Brueckner G-matrix can be calculated in the same way as the $\hat{R}$-matrix of free-space scattering. The paper by Haftel and Tabakin [1.22] contains all details and all necessary formulas for nuclear-matter Brueckner calculations. The nuclear-matter results for the Bonn B potential are given in Section 9 of [1.7] (see also Chapter 2 of this book).

Potentials constructed in the framework of the Thompson equation are given in Appendix A, Table A.2, of [1.7]. These potentials use the pseudovector coupling for π and η. They are very appropriate for nuclear-matter calculations that include the (relativistic) medium effects on the Dirac spinors representing the nucleons in nuclear matter. This relativistic Dirac–Brueckner approach is sketched in Section 10.5 of [1.7] and discussed in detail in [1.8] where more results can be found.

Finally, we mention that the code PHASES can be used for the calculation of phase shifts and the $\hat{R}$-matrix applying any NN potential such as the Reid [1.23] or Paris [1.5] potential. However, the NN potential has to be given in momentum space (such codes exist for Reid and Paris). If a potential is represented in the LSJ formalism (which is usually the case), PHASES must be applied with the option IHEF=0. Furthermore, when applying non-relativistic potentials, the parameter settings IPROP=1 and IPHREL=1 must be used.

Acknowledgments

This work was supported in part by the U.S. National Science Foundation (NSF) through the Idaho-EPSCoR Program under Grant No. RII-8902065, by the NSF Physics Program under Grant No. PHY-8911040, and by the NSF-San Diego Supercomputer Center.

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