Isospin prelude to nuclear forces

The nuclear forces are almost charge independent. If we assume they are, we can introduce a new quantum number which is conserved. For nucleons only, that is a proton and neutron, we can limit ourselves to two possible values which allow us to distinguish between the two particles. If we assign an isospin value of \( \tau = 1/2 \) for protons and neutrons (they belong to an isospin doublet, in the same way as we discuss the spin \( 1/2 \) multiplet), we can define the neutron to have isospin projection \( \tau_z = +1/2 \) and a proton to have \( \tau_z = -1/2 \). These assignments are the standard choices in low-energy nuclear physics. In particle physics, the opposite is the norm.

This leads to the introduction of an additional quantum number called isospin. We can define a single-nucleon state function in terms of the quantum numbers \( n, j, m_j, l, s, \tau \) and \( \tau_z \). Using our definitions in terms of an uncoupled basis, we can define a single-particle state with the state function

\[
\psi_{njm_jls\tau\tau_z} = \sum_{m_lm_s} \langle lm_s|jm_j \rangle \phi_{nlm_lsm_s} \xi_{\tau\tau_z},
\]

which we can now extend to

\[
\psi_{njm_jls\xi_{\tau\tau_z}} = \sum_{m_lm_s} \langle lm_s|jm_j \rangle \phi_{nlm_lsm_s} \xi_{\tau\tau_z},
\]

with the isospin spinors defined as

\[
\xi_{\tau=1/2\tau_z=+1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix},
\]

and

\[
\xi_{\tau=1/2\tau_z=-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.
\]
We can then define the proton state function as
\[ \psi^p(r) = \psi_{njm_1 s}(r) \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \]
and similarly for neutrons as
\[ \psi^n(r) = \psi_{njm_2 s}(r) \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \]

We can in turn define the isospin Pauli matrices (in the same as we define the spin matrices) as
\[ \hat{\tau}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \]
\[ \hat{\tau}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \]
and
\[ \hat{\tau}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \]

and operating with \( \hat{\tau}_z \) on the proton state function we have
\[ \hat{\tau}_z \psi^p(r) = -\frac{1}{2} \psi^p(r), \]
and for neutrons we have
\[ \hat{\tau}_z \psi^n(r) = \frac{1}{2} \psi^n(r). \]

We can now define the so-called charge operator as
\[ \hat{Q}_e = \frac{1}{2} (1 - \hat{\tau}_z) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \]
which results in
\[ \hat{Q}_e \psi^p(r) = \psi^p(r), \]
and
\[ \hat{Q}_e \psi^n(r) = 0, \]
as it should be.

The total isospin is defined as
\[ \hat{T} = \sum_{i=1}^{A} \hat{\tau}_i, \]
and its corresponding isospin projection as
\[ \hat{T}_z = \sum_{i=1}^{A} \hat{\tau}_z, \]
with eigenvalues $T(T + 1)$ for $\hat{T}$ and $1/2(N - Z)$ for $\hat{T}_z$, where $N$ is the number of neutrons and $Z$ the number of protons.

If charge is conserved, the Hamiltonian $\hat{H}$ commutes with $\hat{T}_z$ and all members of a given isospin multiplet (that is the same value of $T$) have the same energy and there is no $T_z$ dependence and we say that $\hat{H}$ is a scalar in isospin space.

**Phenomenology of nuclear forces: From Yukawa to Lattice QCD and Effective Field Theory**

- Chadwick (1932) discovers the neutron and Heisenberg (1932) proposes the first Phenomenology (Isospin).
- Yukawa (1935) and his Meson Hypothesis
- Discovery of the pion in cosmic ray (1947) and in the Berkeley Cyclotron Lab (1948).
- Multi-pion exchanges: Problems! Taketani, Machida, Onuma (1952):
  - *Pion Theories* Brueckner, Watson (1953).
- Many pions = multi-pion resonances: $\sigma(600)$, $\rho(770)$, $\omega(782)$ etc. One-Boson-Exchange Model.
- Refined Meson Theories
- Sophisticated models for two-pion exchange:

*Quark cluster models. Begin of effective field theory studies.*

- 1990’s
  - Advances in effective field theory: Weinberg (1990); Ordonez, Ray, van Kolck and many more.

- 3rd Millenium
Another "pion theory"; but now right: constrained by chiral symmetry. Three-body and higher-body forces appear naturally at a given order of the chiral expansion.

Phenomenology of nuclear forces: Features of the Nucleon-Nucleon (NN) Force. The aim is to give you an overview over central features of the nucleon-nucleon interaction and how it is constructed, with both technical and theoretical approaches.

- The existence of the deuteron with \( J^\pi = 1^+ \) indicates that the force between protons and neutrons is attractive at least for the \(^3S_1\) partial wave. Interference between Coulomb and nuclear scattering for the proton-proton partial wave \(^1S_0\) shows that the NN force is attractive at least for the \(^1S_0\) partial wave.
- It has a short range and strong intermediate attraction.
- Spin dependent, scattering lengths for triplet and singlet states are different.
- Spin-orbit force. Observation of large polarizations of scattered nucleons perpendicular to the plane of scattering.
- Strongly repulsive core. The s-wave phase shift becomes negative at \( \approx 250 \) MeV implying that the singlet \( S \) has a hard core with range \( 0.4 - 0.5 \) fm.
- Charge independence (almost). Two nucleons in a given two-body state always (almost) experience the same force. Modern interactions break charge and isospin symmetry lightly. That means that the pp, neutron-neutron and pn parts of the interaction will be different for the same quantum numbers.
- Non-central. There is a tensor force. First indications from the quadrupole moment of the deuteron pointing to an admixture in the ground state of both \( l = 2 \) \(^3D_1\) and \( l = 0 \) \(^3S_1\) orbital momenta.

Comparison of the binding energies of \(^2\)H (deuteron), \(^3\)H (triton), \(^4\)He (alpha-particle) show that the nuclear force is of finite range (1 – 2 fm) and very strong within that range.

For nuclei with \( A > 4 \), the energy saturates: Volume and binding energies of nuclei are proportional to the mass number \( A \).

Nuclei are also bound. The average distance between nucleons in nuclei is about 2 fm which must roughly correspond to the range of the attractive part.
Phenomenology of nuclear forces: Charge Dependence.

- After correcting for the electromagnetic interaction, the forces between nucleons (pp, nn, or np) in the same state are almost the same.
- Almost the same: Charge-independence is slightly broken.
- Equality between the pp and nn forces: Charge symmetry.
- Equality between pp/nn force and np force: Charge independence.
- Better notation: Isospin symmetry, invariance under rotations in isospin.

Phenomenology of nuclear forces: Charge Dependence, $^1S_0$ Scattering Lengths. Charge-symmetry breaking (CSB), after electromagnetic effects have been removed:

- $a_{pp} = -17.3 \pm 0.4$ fm
- $a_{nn} = -18.8 \pm 0.5$ fm. Note however discrepancy from nd breakup reactions resulting in $a_{nn} = -18.72 \pm 0.13 \pm 0.65$ fm and $\pi^- + d \rightarrow \gamma + 2n$ reactions giving $a_{nn} = -18.93 \pm 0.27 \pm 0.3$ fm.

Charge-independence breaking (CIB)

- $a_{pn} = -23.74 \pm 0.02$ fm

Symmetries of the Nucleon-Nucleon (NN) Force.

- Translation invariance
- Galilean invariance
- Rotation invariance in space
- Space reflection invariance
- Time reversal invariance
- Invariance under the interchange of particle 1 and 2
- Almost isospin symmetry
A typical form of the nuclear force. Here we display a typical way to parametrize (non-relativistic expression) the nuclear two-body force in terms of some operators, the central part, the spin-spin part and the central force.

\[ V(r) = \left\{ C_c + C_\sigma \sigma_1 \cdot \sigma_2 + C_T \left( 1 + \frac{3}{m_\alpha r} + \frac{3}{(m_\alpha r)^2} \right) S_{12}(\hat{r}) \right\} 
+ \left\{ C_{SL} \left( \frac{1}{m_\alpha r} + \frac{1}{(m_\alpha r)^2} \right) L \cdot S \right\} \frac{e^{-m_\alpha r}}{m_\alpha r} \]

How do we derive such terms? (Note: no isospin dependence and that the above is an approximation)

To derive the above famous form of the nuclear force using field theoretical concepts, we will need some elements from relativistic quantum mechanics. These derivations will be given below. The material here gives some background to this.

<table>
<thead>
<tr>
<th>Baryons</th>
<th>Mass (MeV)</th>
<th>Mesons</th>
<th>Mass (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>p, n</td>
<td>938.926</td>
<td>π</td>
<td>138.03</td>
</tr>
<tr>
<td>Λ</td>
<td>1116.0</td>
<td>η</td>
<td>548.8</td>
</tr>
<tr>
<td>Σ</td>
<td>1197.3</td>
<td>σ</td>
<td>550.0</td>
</tr>
<tr>
<td>Δ</td>
<td>1232.0</td>
<td>ρ</td>
<td>770</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ω</td>
<td>782.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td>δ</td>
<td>983.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>K</td>
<td>495.8</td>
</tr>
<tr>
<td></td>
<td></td>
<td>K*</td>
<td>895.0</td>
</tr>
</tbody>
</table>

But before we proceed, we will look into specific quantum numbers of the relative system and study expectation values of the various terms of

\[ V(r) = \left\{ C_c + C_\sigma \sigma_1 \cdot \sigma_2 + C_T \left( 1 + \frac{3}{m_\alpha r} + \frac{3}{(m_\alpha r)^2} \right) S_{12}(\hat{r}) \right\} 
+ \left\{ C_{SL} \left( \frac{1}{m_\alpha r} + \frac{1}{(m_\alpha r)^2} \right) L \cdot S \right\} \frac{e^{-m_\alpha r}}{m_\alpha r} \]

When solving the scattering equation or solving the two-nucleon problem, it is convenient to rewrite the Schroedinger equation, due to the spherical symmetry of the Hamiltonian, in relative and center-of-mass coordinates. This will also define the quantum numbers of the relative and center-of-mass system and will aid us later in solving the so-called Lippman-Schwinger equation for the scattering problem.

We define the center-of-mass (CoM) momentum as

\[ K = \sum_{i=1}^{A} k_i, \]
with $\hbar = c = 1$ the wave number $k_i = p_i$, with $p_i$ the pertinent momentum of a single-particle state. We have also the relative momentum

$$k_{ij} = \frac{1}{2}(k_i - k_j).$$

We will below skip the indices $ij$ and simply write $k$

In a similar fashion we can define the CoM coordinate

$$R = \frac{1}{A} \sum_{i=1}^{A} r_i,$$

and the relative distance

$$r_{ij} = (r_i - r_j).$$

With the definitions

$$K = \sum_{i=1}^{A} k_i,$$

and

$$k_{ij} = \frac{1}{2}(k_i - k_j).$$

we can rewrite the two-particle kinetic energy (note that we use $\hbar = c = 1$ as

$$\frac{k_1^2}{2m_n} + \frac{k_2^2}{2m_n} = \frac{k^2}{m_n} + \frac{K^2}{4m_n},$$

where $m_n$ is the average of the proton and the neutron masses.

Since the two-nucleon interaction depends only on the relative distance, this means that we can separate Schroedinger’s equation in an equation for the center-of-mass motion and one for the relative motion.

With an equation for the relative motion only and a separate one for the center-of-mass motion we need to redefine the two-body quantum numbers.

Previously we had a two-body state vector defined as $| (j_1 j_2)JM_J \rangle$ in a coupled basis. We will now define the quantum numbers for the relative motion. Here we need to define new orbital momenta (since these are the quantum numbers which change). We define

$$\hat{l}_1 + \hat{l}_2 = \hat{\lambda} = \hat{l} + \hat{L},$$

where $\hat{l}$ is the orbital momentum associated with the relative motion and $\hat{L}$ the corresponding one linked with the CoM. The total spin $S$ is unchanged since it acts in a different space. We have thus that

$$\hat{J} = \hat{l} + \hat{L} + \hat{S},$$

which allows us to define the angular momentum of the relative motion

$$\mathcal{J} = \hat{l} + \hat{S},$$

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where $J$ is the total angular momentum of the relative motion.

The total two-nucleon state function has to be anti-symmetric. The total function contains a spatial part, a spin part and an isospin part. If isospin is conserved, this leads to in case we have an $s$-wave with spin $S = 0$ to an isospin two-body state with $T = 1$ since the spatial part is symmetric and the spin part is anti-symmetric.

Since the projections for $T$ are $T_z = -1, 0, 1$, we can have a $pp$, an $nn$ and a $pn$ state.

For $l = 0$ and $S = 1$, a so-called triplet state, $^3S_1$, we must have $T = 0$, meaning that we have only one state, a $pn$ state. For other partial waves, the following table lists states up to $f$ waves. We can systemize this in a table as follows, recalling that $|1 - S| \leq |J| \leq |1 + S|$.

| $^{2S+1}L_J$ | $J$ | $l$ | $S$ | $T$ | $|pp\rangle$ | $|pn\rangle$ | $|nn\rangle$ |
|-------------|-----|-----|-----|-----|------------|------------|------------|
| $^4S_0$     | 0   | 0   | 0   | 1   | yes        | yes        | yes        |
| $^3S_1$     | 1   | 0   | 1   | 0   | no         | yes        | no         |
| $^3P_0$     | 0   | 1   | 1   | 1   | yes        | yes        | yes        |
| $^1P_1$     | 1   | 1   | 0   | 0   | no         | yes        | no         |
| $^3P_1$     | 1   | 1   | 1   | 1   | yes        | yes        | yes        |
| $^3P_2$     | 2   | 1   | 1   | 1   | yes        | yes        | yes        |
| $^3D_1$     | 1   | 2   | 1   | 0   | no         | yes        | no         |
| $^3F_2$     | 2   | 3   | 1   | 1   | yes        | yes        | yes        |

The tensor force is given by

$$S_{12}(\hat{r}) = \frac{3}{r^2} (\sigma_1 \cdot \mathbf{r}) (\sigma_2 \cdot \mathbf{r}) - \sigma_1 \cdot \sigma_2$$

where the Pauli matrices are defined as

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$
$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$
$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

with the properties $\sigma = 2S$ (the spin of the system, being 1/2 for nucleons), $\sigma_2^2 = \sigma_y^2 = \sigma_z = 1$ and obeying the commutation and anti-commutation relations $[\sigma_x, \sigma_y] = 0, [\sigma_x, \sigma_y] = i\sigma_z$ etc.

When we look at the expectation value of $\langle \sigma_1 \cdot \sigma_2 \rangle$, we can rewrite this expression in terms of the spin $S = s_1 + s_2$, resulting in

$$\langle \sigma_1 \cdot \sigma_2 \rangle = 2(S^2 - s_1^2 - s_2^2) = 2S(S + 1) - 3,$$

where we $s_1 = s_2 = 1/2$ leading to

$$\begin{cases} 
\langle \sigma_1 \cdot \sigma_2 \rangle = 1 & \text{if } S = 1 \\
\langle \sigma_1 \cdot \sigma_2 \rangle = -3 & \text{if } S = 0
\end{cases}$$
Similarly, the expectation value of the spin-orbit term is
\[ \langle lS \rangle = \frac{1}{2} (J(J+1) - l(l+1) - S(S+1)), \]
which means that for s-waves with either \( S = 0 \) and thereby \( J = 0 \) or \( S = 1 \) and \( J = 1 \), the expectation value for the spin-orbit force is zero. With the above phenomenological model, the only contributions to the expectation value of the potential energy for s-waves stem from the central and the spin-spin components since the expectation value of the tensor force is also zero.

For \( s = 1/2 \) spin values only for two nucleons, the expectation value of the tensor force operator is
\[
\begin{array}{ccc|ccc}
   l & J+1 & J & J-1 & l & J+1 & J \\
   J+1 & -2J(J+2) & 0 & \frac{6\sqrt{J(J+1)}}{2J+1} & \frac{6\sqrt{J(J+1)}}{2J+1} \\
   J & 0 & 2 & 0 & 0 & 2(J+1) & 2J+1 \\
   J-1 & \frac{6\sqrt{J(J+1)}}{2J+1} & 0 & -\frac{2(2J+1)}{2J+1} & \end{array}
\]

If we now add isospin to our simple \( V_4 \) interaction model, we end up with 8 operators, popularly dubbed \( V_8 \) interaction model. The explicit form reads
\[
V(r) = \left\{ C_c + C_\sigma \sigma_1 \cdot \sigma_2 + C_T \left( 1 + \frac{3}{m_\alpha r} + \frac{3}{(m_\alpha r)^2} \right) S_{12}(\hat{r}) \right. \\
+ C_{SL} \left( \frac{1}{m_\alpha r} + \frac{1}{(m_\alpha r)^2} \right) L \cdot S e^{-\frac{m_\alpha r}{m_\alpha r}} \\
+ \left\{ C_{cT} + C_{\sigma T} \sigma_1 \cdot \sigma_2 + C_{TT} \left( 1 + \frac{3}{m_\alpha r} + \frac{3}{(m_\alpha r)^2} \right) S_{12}(\hat{r}) \\
+ C_{SLLT} \left( \frac{1}{m_\alpha r} + \frac{1}{(m_\alpha r)^2} \right) \tau_1 \cdot \tau_2 e^{-\frac{m_\alpha r}{m_\alpha r}} \right\}
\]

References for Various Phenomenological Interactions. From 1950 till approximately 2000: One-Boson-Exchange (OBE) models dominate. These are models which typically include several low-mass mesons, that is with masses below 1 GeV. Potentials which are based upon the standard non-relativistic operator structure are called 'Phenomenological Potentials.' Some historically important examples are

- Gammel-Thaler potential (Phys. Rev. 107, 291, 1339 (1957) and the
• Hamada-Johnston potential, Nucl. Phys. 34, 382 (1962), both with a hard core.


Now: models based on chiral perturbation theory. These are effective models with nucleons and pions as degrees of freedom only. The other mesons which appeared in standard one-boson model appear as multi-pion resonances.

The total two-nucleon state function has to be anti-symmetric. The total function contains a spatial part, a spin part and an isospin part. If isospin is conserved, this leads to in case we have an s-wave with spin \( S = 0 \) to an isospin two-body state with \( T = 1 \) since the spatial part is symmetric and the spin part is anti-symmetric.

Since the projections for \( T \) are \( T_z = -1, 0, 1 \), we can have a \( pp \), an \( nn \) and a \( pn \) state.

For \( l = 0 \) and \( S = 1 \), a so-called triplet state, \( ^3S_1 \), we must have \( T = 0 \), meaning that we have only one state, a \( pn \) state. For other partial waves, see exercises below.

The one-pion exchange contribution (see derivation below), can be written as

\[
V_\pi(r) = -\frac{f_\pi^2}{4\pi m_\pi^2} \tau_1 \cdot \tau_2 \frac{1}{3} \{ \sigma_1 \cdot \sigma_2 + \left( 1 + \frac{3}{m_\pi r} + \frac{3}{(m_\pi r)^2} \right) S_{12}(\hat{r}) \} e^{-\frac{m_\pi r}{m_\pi r}}.
\]

Here the constant \( f_\pi^2/4\pi \approx 0.08 \) and the mass of the pion is \( m_\pi \approx 140 \text{ MeV}/c^2 \).

Let us look closer at specific partial waves for which one-pion exchange is applicable. If we have \( S = 0 \) and \( T = 0 \), the orbital momentum has to be an odd number in order for the total anti-symmetry to be obeyed. For \( S = 0 \), the tensor force component is zero, meaning that the only contribution is

\[
V_\pi(r) = \frac{3f_\pi^2}{4\pi m_\pi^2} e^{-\frac{m_\pi r}{m_\pi r}},
\]

since \( \langle \sigma_1 \cdot \sigma_2 \rangle = -3 \), that is we obtain a repulsive contribution to partial waves like \( ^1P_0 \).

Since \( S = 0 \) yields always a zero tensor force contribution, for the combination of \( T = 1 \) and then even \( l \) values, we get an attractive contribution

\[
V_\pi(r) = -\frac{f_\pi^2}{4\pi m_\pi^2} e^{-\frac{m_\pi r}{m_\pi r}}.
\]
With $S = 1$ and $T = 0$, $l$ can only take even values in order to obey the anti-symmetry requirements and we get

$$V_\pi(r) = -\frac{f_\pi^2}{4\pi m_\pi^2} \left( 1 + (1 + \frac{3}{m_\pi r} + \frac{3}{(m_\pi r)^2})S_{12}(\hat{r}) \right) e^{-m_\pi r},$$

while for $S = 1$ and $T = 1$, $l$ can only take odd values, resulting in a repulsive contribution

$$V_\pi(r) = \frac{1}{3} \frac{f_\pi^2}{4\pi m_\pi^2} \left( 1 + (1 + \frac{3}{m_\pi r} + \frac{3}{(m_\pi r)^2})S_{12}(\hat{r}) \right) e^{-m_\pi r}.$$

The central part of one-pion exchange interaction, arising from the spin-spin term, is thus attractive for $s$-waves and all even $l$ values. For $p$-waves and all other odd values it is repulsive. However, its overall strength is weak. This is discussed further in one of exercises below.

**Models for nuclear forces and derivation of non-relativistic expressions**

To describe the interaction between the various baryons and mesons of the previous table we choose the following phenomenological lagrangians for spin $1/2$ baryons

$$\mathcal{L}_{ps} = g^{ps} \bar{\Psi} \gamma^5 \Psi \phi^{(ps)},$$

$$\mathcal{L}_s = g^s \bar{\Psi} \Psi \phi^{(s)},$$

and

$$\mathcal{L}_v = g^v \bar{\Psi} \gamma^\mu \Psi \phi^{(v)} + g^t \bar{\Psi} \sigma^{\mu\nu} \Psi \left( \partial_\mu \phi^{(v)} - \partial_\nu \phi^{(v)} \right),$$

for pseudoscalar ($ps$), scalar ($s$) and vector ($v$) coupling, respectively. The factors $g^s$ and $g^v$ are the vector and tensor coupling constants, respectively.

For spin $1/2$ baryons, the fields $\Psi$ are expanded in terms of the Dirac spinors (positive energy solution shown here with $\pi u = 1$)

$$u(k\sigma) = \sqrt{\frac{E(k) + m}{2m}} \begin{pmatrix} \chi \\ \sigma_k \chi \end{pmatrix},$$

with $\chi$ the familiar Pauli spinor and $E(k) = \sqrt{m^2 + |\mathbf{k}|^2}$. The positive energy part of the field $\Psi$ reads

$$\Psi(x) = \frac{1}{(2\pi)^{3/2}} \sum_{k\sigma} u(k\sigma) \exp(-ikx) a_{k\sigma},$$

with $a$ being a fermion annihilation operator.

Expanding the free Dirac spinors in terms of $1/m$ ($m$ is here the mass of the relevant baryon) results, to lowest order, in the familiar non-relativistic
expressions for baryon-baryon potentials. The configuration space version of the interaction can be approximated as

\[
V(r) = \left\{ C_C^0 + C_C^1 + C_\sigma \sigma_1 \cdot \sigma_2 + C_T \left( 1 + \frac{3}{m_\alpha r} + \frac{3}{(m_\alpha r)^2} \right) S_{12}(\hat{r}) \right. \\
+ C_{SL} \left( \frac{1}{m_\alpha r} + \frac{1}{(m_\alpha r)^2} \right) L \cdot S \exp(-m_\alpha r) \right\},
\]

where \( m_\alpha \) is the mass of the relevant meson and \( S_{12} \) is the familiar tensor term.

We derive now the non-relativistic one-pion exchange interaction.

Here \( p_1, p'_1, p_2, p'_2 \) and \( k = p_1 - p'_1 \) denote four-momenta. The vertices are given by the pseudovector Lagrangian

\[
\mathcal{L}_{\pi\nu} = \frac{f_\pi}{m_\pi} \bar{\psi} \gamma_5 \gamma_\mu \psi \partial^\mu \phi_\pi.
\]

From the Feynman diagram rules we can write the two-body interaction as

\[
V^{\pi\nu} = \frac{f_\pi^2}{m_\pi^2} \frac{\bar{\pi}(p'_1) \gamma_5 \gamma_\mu (p_1 - p'_1) \gamma_\nu u(p_1) \bar{\pi}(p'_2) \gamma_5 \gamma_\nu (p'_2 - p_2) \gamma_\mu u(p_2)}{(p_1 - p'_1)^2 - m_\pi^2}.
\]

The factors \( p_1 - p'_1 = p'_2 - p_2 \) are both the four-momentum of the exchanged meson and come from the derivative of the meson field in the interaction Lagrangian. The Dirac spinors obey

\[
\gamma_\mu p^\mu u(p) = m u(p) \quad \bar{\pi}(p) \gamma_\mu p^\mu = m \bar{\pi}(p).
\]

Using these relations, together with \( \{ \gamma_5, \gamma_\mu \} = 0 \), we find

\[
\bar{\pi}(p'_1) \gamma_5 \gamma_\mu (p_1 - p'_1) \gamma_\nu u(p_1) = m \bar{\pi}(p'_1) \gamma_5 \gamma_\nu u(p_1) + \bar{\pi}(p'_1) \gamma_\mu p'^\mu_1 \gamma_5 u(p_1) = 2m \bar{\pi}(p'_1) \gamma_5 u(p_1)
\]

and

\[
\bar{\pi}(p'_2) \gamma_5 \gamma_\mu (p'_2 - p_2) \gamma_\mu u(p_1) = -2m \bar{\pi}(p'_2) \gamma_5 u(p_1).
\]

We get

\[
V^{\pi\nu} = -\frac{f_\pi^2}{m_\pi^2} \frac{4m^2}{4m^2} \frac{\bar{\pi}(p'_1) \gamma_5 u(p_1) \bar{\pi}(p'_2) \gamma_5 u(p_2)}{(p_1 - p'_1)^2 - m_\pi^2}.
\]

By inserting expressions for the Dirac spinors, we find

\[
\bar{u}(p'_1) \gamma_5 u(p_1) = \sqrt{(E'_1 + m)(E'_1 + m)} \left( \begin{array}{c} \chi^\dagger - \frac{\sigma_1 \cdot P_1}{E'_1 + m} \chi^\dagger \\ 0 \\ 1 \end{array} \right) \left( \begin{array}{c} 0 \\ 1 \\ 0 \end{array} \right)
\]

\[
\times \left( \sigma_1 \cdot \chi_{E'_1 + m} \right)
\]

\[
= \sqrt{(E'_1 + m)(E'_1 + m)} \left( \begin{array}{c} \sigma_1 \cdot P_1 \\ E'_1 + m \end{array} \right) \left( \begin{array}{c} \sigma_1 \cdot P_1 \\ E'_1 + m \end{array} \right)
\]

\[
= \sqrt{(E'_1 + m)(E'_1 + m)} \left( \begin{array}{c} \sigma_1 \cdot P_1 \\ E'_1 + m \end{array} \right) \left( \begin{array}{c} \sigma_1 \cdot P_1 \\ E'_1 + m \end{array} \right)
\]

\[
= \sqrt{(E'_1 + m)(E'_1 + m)} \left( \begin{array}{c} \sigma_1 \cdot P_1 \\ E'_1 + m \end{array} \right) \left( \begin{array}{c} \sigma_1 \cdot P_1 \\ E'_1 + m \end{array} \right)
\]

\[
= \sqrt{(E'_1 + m)(E'_1 + m)} \left( \begin{array}{c} \sigma_1 \cdot P_1 \\ E'_1 + m \end{array} \right) \left( \begin{array}{c} \sigma_1 \cdot P_1 \\ E'_1 + m \end{array} \right)
\]

\[
= \sqrt{(E'_1 + m)(E'_1 + m)} \left( \begin{array}{c} \sigma_1 \cdot P_1 \\ E'_1 + m \end{array} \right) \left( \begin{array}{c} \sigma_1 \cdot P_1 \\ E'_1 + m \end{array} \right)
\]
Similarly
\[ \pi(p_2')\gamma_5 u(p_2) = \sqrt{(E_2' + m)(E_2 + m)} \left( \frac{\sigma_2 \cdot p_2}{E_2 + m} - \frac{\sigma_2 \cdot p_2'}{E_2' + m} \right). \]

In the CM system we have \( p_2 = -p_1 \), \( p_2' = -p_1' \) and so \( E_2 = E_1, E_2' = E_1' \). We can then write down the relativistic contribution to the NN potential in the CM system:

\[ V^{pv} = -f^2 \pi m^2 \left( \frac{1}{(p_1 - p_1')^2 - m^2} \frac{(E_1 + m)(E_1' + m)}{4m^2} \right) \times \left( \frac{\sigma_1 \cdot p_1}{E_1 + m} - \frac{\sigma_1 \cdot p_1'}{E_1' + m} \right) \left( \frac{\sigma_2 \cdot p_1}{E_1 + m} - \frac{\sigma_2 \cdot p_1'}{E_1' + m} \right). \]

In the non-relativistic limit we have to lowest order
\[ E_1 = \sqrt{p_1^2 + m^2} \approx m \approx E_1' \]
and then \( (p_1 - p_1')^2 = -k^2 \), so we get for the contribution to the NN potential

\[ V^{pv} = -f^2 \pi m^2 \frac{2m \cdot (p_1 - p_1')}{2m \cdot (p_1 - p_1')} \frac{(\sigma_2 \cdot p_1)(\sigma_2 \cdot p_1')}{k^2 + m^2}. \]

We have omitted exchange terms and the isospin term \( \tau_1 \cdot \tau_2 \).

We have
\[ V^{pv}(k) = -f^2 \pi \frac{(\sigma_1 \cdot k)(\sigma_2 \cdot k)}{k^2 + m^2}. \]

In coordinate space we have
\[ V^{pv}(r) = \int \frac{d^3k}{(2\pi)^3} e^{ikr} V^{pv}(k) \]
resulting in
\[ V^{pv}(r) = -f^2 \pi \frac{\sigma_2}{m^2} \sigma_1 \cdot \nabla \sigma_2 \cdot \nabla \int \frac{d^3k}{(2\pi)^3} e^{ikr} \frac{1}{k^2 + m^2}. \]

We obtain
\[ V^{pv}(r) = -f^2 \pi \frac{\sigma_2}{m^2} \sigma_1 \cdot \nabla \sigma_2 \cdot \nabla \frac{e^{-m_\pi r}}{r}. \]

Carrying out the differentiation of
\[ V^{pv}(r) = -f^2 \pi \frac{\sigma_2}{m^2} \sigma_1 \cdot \nabla \sigma_2 \cdot \nabla \frac{e^{-m_\pi r}}{r}. \]
we arrive at the famous one-pion exchange potential with central and tensor parts

\[ V(r) = -\frac{f_\pi^2}{m_\pi^2} \left\{ C_\sigma \sigma_1 \cdot \sigma_2 + C_T \left( 1 + \frac{3}{m_\pi r} + \frac{3}{(m_\pi r)^2} \right) S_{12}(\hat{r}) \right\} \exp\left( -\frac{m_\pi r}{m_\pi r} \right). \]

For the full potential add the exchange part and the \( \tau_1 \cdot \tau_2 \) term as well. (Subtle point: there is a divergence which gets cancelled by using cutoffs) This leads to coefficients \( C_\sigma \) and \( C_T \) which are fitted to data.

When we perform similar non-relativistic expansions for scalar and vector mesons we obtain for the \( \sigma \) meson

\[ V^\sigma = g_{\sigma NN}^2 \frac{1}{k^2 + m_\sigma^2} \left( -1 + \frac{\mathbf{q}^2}{2M_N^2} - \frac{k^2}{8M_N^2} - \frac{\mathbf{LS}}{2M_N^2} \right). \]

We note an attractive central force and spin-orbit force. This term has an intermediate range. We have defined \( 1/2(p_1 + p'_1) = \mathbf{q} \). For the full potential add the exchange part and the isospin dependence as well.

We obtain for the \( \omega \) meson

\[ V^\omega = g_{\omega NN}^2 \frac{1}{k^2 + m_\omega^2} \left( 1 - 3 \frac{\mathbf{LS}}{2M_N^2} \right). \]

We note a repulsive central force and an attractive spin-orbit force. This term has short range. For the full potential add the exchange part and the isospin dependence as well.

Finally for the \( \rho \) meson

\[ V^\rho = g_{\rho NN}^2 \frac{k^2}{k^2 + m_\rho^2} \left( -2\sigma_1 \sigma_2 + S_{12}(\hat{k}) \right) \tau_1 \tau_2. \]

We note a tensor force with sign opposite to that of the pion. This term has short range. For the full potential add the exchange part and the isospin dependence as well.

We have seen that:

- Can use a one-boson exchange picture to construct a nucleon-nucleon interaction a la QED
- Non-relativistic approximation yields amongst other things a spin-orbit force which is much stronger than in atoms.
- At large intermediate distances pion exchange dominates while pion resonances (other mesons) dominate at intermediate and short range
  - Potentials are parameterized to fit selected two-nucleon data, binding energies and scattering phase shifts.
- Nowadays, chiral perturbation theory gives an effective theory that allows a systematic expansion in terms of controllable parameters. Good basis for many-body physics
The Lippman-Schwinger equation for two-nucleon scattering

What follows now is a more technical discussion on how we can solve the two-nucleon problem. This will lead us to the so-called Lippman-Schwinger equation for the scattering problem and a rewrite of Schroedinger’s equation in relative and center-of-mass coordinates.

Before we break down the Schroedinger equation into a partial wave decomposition, we derive now the so-called Lippman-Schwinger equation. We will do this in an operator form first. Thereafter, we rewrite it in terms of various quantum numbers such as relative momenta, orbital momenta etc. The Schroedinger equation in abstract vector representation is

\[
(\hat{H}_0 + \hat{V}) |\psi_n\rangle = E_n |\psi_n\rangle.
\]

In our case for the two-body problem $\hat{H}_0$ is just the kinetic energy. We rewrite it as

\[
(\hat{H}_0 - E_n) |\psi_n\rangle = -\hat{V} |\psi_n\rangle.
\]

We assume that the invers of $(\hat{H}_0 - E_n)$ exists and rewrite this equation as

\[
|\psi_n\rangle = \frac{1}{(E_n - \hat{H}_0)} \hat{V} |\psi_n\rangle.
\]

The equation

\[
|\psi_n\rangle = \frac{1}{(E_n - \hat{H}_0)} \hat{V} |\psi_n\rangle,
\]

is normally solved in an iterative fashion. We assume first that

\[
|\psi_n\rangle = |\phi_n\rangle,
\]

where $|\phi_n\rangle$ are the eigenfunctions of

\[
\hat{H}_0 |\phi_n\rangle = \omega_n |\phi_n\rangle
\]

the so-called unperturbed problem. In our case, these will simply be the kinetic energies of the relative motion.

Inserting $|\phi_n\rangle$ on the right-hand side of

\[
|\psi_n\rangle = \frac{1}{(E_n - \hat{H}_0)} \hat{V} |\psi_n\rangle,
\]

yields

\[
|\psi_n\rangle = |\phi_n\rangle + \frac{1}{(E_n - \hat{H}_0)} \hat{V} |\phi_n\rangle,
\]

\[15\]
as our first iteration. Reinserting again gives

$$|\psi_n\rangle = |\phi_n\rangle + \frac{1}{(E_n - \hat{H}_0)} \hat{V} |\phi_n\rangle + \frac{1}{(E_n - \hat{H}_0)} \hat{V} \frac{1}{(E_n - \hat{H}_0)} \hat{V} |\phi_n\rangle,$$

and continuing we obtain

$$|\psi_n\rangle = \sum_{i=0}^{\infty} \left[ \frac{1}{(E_n - \hat{H}_0)} \hat{V} \right]^i |\phi_n\rangle.$$

It is easy to see that

$$|\psi_n\rangle = \sum_{i=0}^{\infty} \left[ \frac{1}{(E_n - \hat{H}_0)} \hat{V} \right]^i |\phi_n\rangle,$$

can be rewritten as

$$|\psi_n\rangle = |\phi_n\rangle + \frac{1}{(E_n - \hat{H}_0)} \hat{V} \left( 1 + \frac{1}{(E_n - \hat{H}_0)} \hat{V} + \frac{1}{(E_n - \hat{H}_0)} \hat{V} \frac{1}{(E_n - \hat{H}_0)} \hat{V} \hat{V} + \ldots \right) |\phi_n\rangle,$$

which we rewrite as

$$|\psi_n\rangle = |\phi_n\rangle + \frac{1}{(E_n - \hat{H}_0)} \hat{V} |\psi_n\rangle.$$

In operator form we have thus

$$|\psi_n\rangle = |\phi_n\rangle + \frac{1}{(E_n - \hat{H}_0)} \hat{V} |\psi_n\rangle.$$

We multiply from the left with \(\hat{V}\) and \(\langle \phi_m |\) and obtain

$$\langle \phi_m | \hat{V} |\psi_n\rangle = \langle \phi_m | \hat{V} |\phi_n\rangle + \langle \phi_m | \hat{V} \frac{1}{(E_n - \hat{H}_0)} \hat{V} |\psi_n\rangle.$$

We define thereafter the so-called \(T\)-matrix as

$$\langle \phi_m | \hat{T} |\phi_n\rangle = \langle \phi_m | \hat{V} |\psi_n\rangle.$$

We can rewrite our equation as

$$\langle \phi_m | \hat{T} |\phi_n\rangle = \langle \phi_m | \hat{V} |\phi_n\rangle + \langle \phi_m | \hat{V} \frac{1}{(E_n - \hat{H}_0)} \hat{T} |\phi_n\rangle.$$

The equation

$$\langle \phi_m | \hat{T} |\phi_n\rangle = \langle \phi_m | \hat{V} |\phi_n\rangle + \langle \phi_m | \hat{V} \frac{1}{(E_n - \hat{H}_0)} \hat{T} |\phi_n\rangle,$$
is called the Lippman-Schwinger equation. Inserting the completeness relation
\[ 1 = \sum_n |\phi_n\rangle\langle\phi_n|, \quad \langle\phi_n|\phi_{n'}\rangle = \delta_{n,n'} \]
we have
\[ \langle\phi_m|\hat{T}|\phi_n\rangle = \langle\phi_m|\hat{V}|\phi_n\rangle + \sum_k \langle\phi_m|\hat{V}|\phi_k\rangle \frac{1}{(E_n - \omega_k)} \langle\phi_k|\hat{T}|\phi_n\rangle, \]
which is (when we specify the state \( |\phi_n\rangle \)) an integral equation that can actually be solved by matrix inversion easily! The unknown quantity is the \( T \)-matrix.

Now we wish to introduce a partial wave decomposition in order to solve the Lippman-Schwinger equation. With a partial wave decomposition we can reduce a three-dimensional integral equation to a one-dimensional one.

Let us continue with our Schroedinger equation in the abstract vector representation
\[ (T + V)|\psi_n\rangle = E_n|\psi_n\rangle \]
Here \( T \) is the kinetic energy operator and \( V \) is the potential operator. The eigenstates form a complete orthonormal set according to
\[ 1 = \sum_n |\psi_n\rangle\langle\psi_n|, \quad \langle\psi_n|\psi_{n'}\rangle = \delta_{n,n'} \]

The most commonly used representations are the coordinate and the momentum space representations. They define the completeness relations
\[ 1 = \int dr \, |r\rangle\langle r|, \quad \langle r|r'\rangle = \delta(r - r') \]
\[ 1 = \int dk \, |k\rangle\langle k|, \quad \langle k|k'\rangle = \delta(k - k') \]
Here the basis states in both r- and k-space are dirac-delta function normalized. From this it follows that the plane-wave states are given by,
\[ \langle r|k\rangle = \left(\frac{1}{2\pi}\right)^{3/2} \exp(i k \cdot r) \]
which is a transformation function defining the mapping from the abstract \( |k\rangle \) to the abstract \( |r\rangle \) space.

That the r-space basis states are delta-function normalized follows from
\[ \delta(r - r') = \langle r|r'\rangle = \langle r|1|r'\rangle = \int dke^{i(k \cdot r')} = \left(\frac{1}{2\pi}\right)^{3} \int dke^{i(k \cdot r')} \]
and the same for the momentum space basis states,
\[ \delta(k - k') = \langle k|k'\rangle = \langle k|1|k'\rangle = \int dr e^{i(k \cdot r)} \langle r|k'\rangle = \left(\frac{1}{2\pi}\right)^{3} \int dr e^{i(k \cdot r')} \]
Projecting on momentum states, we obtain the momentum space Schroedinger equation as

$$\frac{\hbar^2}{2\mu}k^2\psi_n(k) + \int dk' V(k, k')\psi_n(k') = E_n \psi_n(k)$$  \hspace{1cm} (1)

Here the notation \(\psi_n(k) = \langle k | \psi_n \rangle\) and \(\langle k | V | k' \rangle = V(k, k')\) has been introduced. The potential in momentum space is given by a double Fourier-transform of the potential in coordinate space, i.e.

$$V(k, k') = \left(\frac{1}{2\pi}\right)^3 \int dr \int dr' \exp(-ikr) V(r, r') \exp(ik'r')$$

Here it is assumed that the potential interaction does not contain any spin dependence. Instead of a differential equation in coordinate space, the Schroedinger equation becomes an integral equation in momentum space. This has many tractable features. Firstly, most realistic nucleon-nucleon interactions derived from field-theory are given explicitly in momentum space. Secondly, the boundary conditions imposed on the differential equation in coordinate space are automatically built into the integral equation. And last, but not least, integral equations are easy to numerically implement, and convergence is obtained by just increasing the number of integration points. Instead of solving the three-dimensional integral equation, an infinite set of 1-dimensional equations can be obtained via a partial wave expansion.

The wave function \(\psi_n(k)\) can be expanded in a complete set of spherical harmonics, that is

$$\psi_n(k) = \sum_{lm} \psi_{nml}(k) Y_{lm}(\hat{k})$$  \hspace{1cm} (2)

By inserting equation (2) in equation (1), and projecting from the left \(Y_{lm}(\hat{k})\), the three-dimensional Schroedinger Eq. (1) is reduced to an infinite set of 1-dimensional angular momentum coupled integral equations,

$$\left(\frac{\hbar^2}{2\mu}k^2 - E_{nml} \right) \psi_{nml}(k) = -\sum_{l'm'} \int_0^{\infty} dk' k'^2 V_{lm,l'm'}(k, k') \psi_{nml'}(k')$$  \hspace{1cm} (3)

where the angular momentum projected potential takes the form,

$$V_{lm,l'm'}(k, k') = \int d\hat{k} \int d\hat{k}' Y_{lm}^*(\hat{k}) V(k\hat{k}) Y_{l'm'}(\hat{k}')$$  \hspace{1cm} (4)

Here \(d\hat{k} = d\theta \sin(\theta) d\phi\). Note that we discuss only the orbital momentum, we will include angular momentum and spin later.

The potential is often given in position space. It is then convenient to establish the connection between \(V_{lm,l'm'}(k, k')\) and \(V_{lm,l'm'}(r, r')\). Inserting the completeness relation for the position quantum numbers in equation (4) results in

$$V = \int dr \int dr' \left\{ \int d\hat{k} Y_{lm}^*(\hat{k}) \langle k | r \rangle \right\} \langle r | V | r' \rangle \left\{ \int d\hat{k}' Y_{lm}(\hat{k}') \langle r' | k' \rangle \right\}$$  \hspace{1cm} (5)
Since the plane waves depend only on the absolute values of position and momentum, $|k|$ and $|r|$, and the angle between them, $\theta_{kr}$, they may be expanded in terms of bipolar harmonics of zero rank, i.e.

$$\exp(ik \cdot r) = 4\pi \sum_{l=0}^{\infty} i^l j_l(kr) \left( Y_l(\hat{k}) \cdot Y_l(\hat{r}) \right) = \sum_{l=0}^{\infty} (2l + 1) i^l j_l(kr) P_l(\cos \theta_{kr})$$

where the addition theorem for spherical harmonics has been used in order to write the expansion in terms of Legendre polynomials. The spherical Bessel functions, $j_l(z)$, are given in terms of Bessel functions of the first kind with half integer orders,

$$j_l(z) = \sqrt{\frac{\pi}{2z^2}} J_{l+1/2}(z).$$

Inserting the plane-wave expansion into the brackets of Eq. (5) yields,

$$\int d\hat{k} Y^*_lm(\hat{k}|r) \langle k| r \rangle = \left( \frac{1}{2\pi} \right)^{3/2} 4\pi i^{-l} j_l(kr) Y^*lm(\hat{r}),$$

$$\int d\hat{k}' Y^*lm(\hat{k}'|r') \langle r'| k' \rangle = \left( \frac{1}{2\pi} \right)^{3/2} 4\pi i^{l'} j_{l'}(k'r') Y^*lm'(\hat{r}).$$

The connection between the momentum- and position space angular momentum projected potentials are then given,

$$V_{lm,l'm'}(k, k') = \frac{2}{\pi} i^{l'-l} \int_0^{\infty} dr r^2 \int_0^{\infty} dr' r'^2 j_l(kr) V_{lm,l'm'}(r, r') j_{l'}(k'r'),$$

which is known as a double Fourier-Bessel transform. The position space angular momentum projected potential is given by

$$V_{lm,l'm'}(r, r') = \int d\hat{r} \int d\hat{r}' Y^*lm(\hat{r}) V(r, r') Y_{lm'}(\hat{r}).$$

No assumptions of locality/non-locality and deformation of the interaction has so far been made, and the result in Eq. (6) is general. In position space the Schroedinger equation takes form of an integro-differential equation in case of a non-local interaction, in momentum space the Schroedinger equation is an ordinary integral equation of the Fredholm type, see Eq. (3). This is a further advantage of the momentum space approach as compared to the standard position space approach. If we assume that the interaction is of local character, i.e.

$$\langle r| V| r' \rangle = V(r) \delta(r - r') = V(r) \frac{\delta(r - r')}{r^2} \delta(\cos \theta - \cos \theta') \delta(\varphi - \varphi'),$$

then Eq. (6) reduces to

$$V_{lm,l'm'}(r, r') = \frac{\delta(r - r')}{r^2} \int d\hat{r} Y^*_lm(\hat{r}) V(r) Y_{lm'}(\hat{r}), \quad (6)$$
and Eq. (1) reduces to

\[ V_{lm,l'm'}(k,k') = \frac{2}{\pi} \int_0^\infty dr r^2 j_l(kr)V_{lm,l'm'}(r)j_{l'}(kr) \]  \hspace{1cm} (7)

where

\[ V_{lm,l'm'}(r) = \int d\hat{r} Y_{lm}^*(\hat{r}) V(r) Y_{l'm'}(\hat{r}), \]  \hspace{1cm} (8)

In the case that the interaction is central, \( V(r) = V(r) \), then

\[ V_{lm,l'm'}(r) = V(r) \int d\hat{r} Y_{lm}^*(\hat{r}) Y_{l'm'}(\hat{r}) = V(r) \delta_{l'l'} \delta_{m'm'}, \]  \hspace{1cm} (9)

and

\[ V_{lm,l'm'}(k,k') = \frac{2}{\pi} \int_0^\infty dr r^2 j_l(kr)V(r)j_{l'}(k'r)\delta_{m,m'} = V_l(k,k') \delta_{l'l'} \delta_{m,m'}, \]  \hspace{1cm} (10)

where the momentum space representation of the interaction finally reads,

\[ V_l(k,k') = \frac{2}{\pi} \int_0^\infty dr r^2 j_l(kr)V(r)j_l(k'r). \]  \hspace{1cm} (11)

For a local and spherical symmetric potential, the coupled momentum space Schrödinger equations given in Eq. (3) decouples in angular momentum, giving

\[ \frac{\hbar^2}{2\mu} k^2 \psi_{nl}(k) + \int_0^\infty dk' k'^2 V_l(k,k')\psi_{nl}(k') = E_{nl} \psi_{nl}(k) \]  \hspace{1cm} (12)

Where we have written \( \psi_{nl}(k) = \psi_{nl'm}(k) \), since the equation becomes independent of the projection \( m \) for spherical symmetric interactions. The momentum space wave functions \( \psi_{nl}(k) \) defines a complete orthogonal set of functions, which spans the space of functions with a positive finite Euclidean norm (also called \( l^2 \)-norm), \( \sqrt{\langle \psi_n | \psi_n \rangle} \), which is a Hilbert space. The corresponding normalized wave function in coordinate space is given by the Fourier-Bessel transform

\[ \phi_{nl}(r) = \sqrt{\frac{2}{\pi}} \int dk k^2 j_l(kr)\psi_{nl}(k) \]

We will thus assume that the interaction is spherically symmetric and use the partial wave expansion of the plane waves in terms of spherical harmonics. This means that we can separate the radial part of the wave function from its angular dependence. The wave function of the relative motion is described in terms of plane waves as

\[ \exp (i kr) = \langle r | k \rangle = 4\pi \sum_{lm} j_l(kr) Y_{lm}(\hat{k}) Y_{lm}(\hat{r}), \]

where \( j_l \) is a spherical Bessel function and \( Y_{lm} \) the spherical harmonics.
In terms of the relative and center-of-mass momenta \( \mathbf{k} \) and \( \mathbf{K} \), the potential in momentum space is related to the nonlocal operator \( V(\mathbf{r}, \mathbf{r}') \) by

\[
(k'K'|V|kK) = \int d\mathbf{r}d\mathbf{r}' \exp(-i(k'\cdot \mathbf{r}'))V(\mathbf{r}', \mathbf{r})\exp(i\mathbf{k}\mathbf{r}\delta(\mathbf{K}, \mathbf{K}')).
\]

We will assume that the interaction is spherically symmetric. Can separate the radial part of the wave function from its angular dependence. The wave function of the relative motion is described in terms of plane waves as

\[
\exp(i\mathbf{k}\cdot \mathbf{r}) = \langle \mathbf{r}|\mathbf{k} \rangle = 4\pi \sum_{lm}^l j_l(kr)Y_{lm}^*(\hat{\mathbf{k}})Y_{lm}(\hat{\mathbf{r}}),
\]

where \( j_l \) is a spherical Bessel function and \( Y_{lm} \) the spherical harmonic.

This partial wave basis is useful for defining the operator for the nucleon-nucleon interaction, which is symmetric with respect to rotations, parity and isospin transformations. These symmetries imply that the interaction is diagonal with respect to the quantum numbers of total relative angular momentum \( \mathcal{J} \), spin \( S \) and isospin \( T \) (we skip isospin for the moment). Using the above plane wave expansion, and coupling to final \( \mathcal{J} \) and \( S \) and \( T \) we get

\[
\langle k'|V|k \rangle = (4\pi)^2 \sum_{STl'lm'l}\; l'^+l\; Y_{lm}^*(\hat{k})Y_{l'm'}(\hat{k}')
\]

where we have defined

\[
\langle k'l'S\mathcal{J}M|V|klS\mathcal{J}M \rangle = \int j_{l'}(kr')\langle k'l'S\mathcal{J}M|V(\mathbf{r'}, \mathbf{r})|klS\mathcal{J}M \rangle j_l(kr)kr'dr'dr.
\]

We have omitted the momentum of the center-of-mass motion \( \mathbf{K} \) and the corresponding orbital momentum \( L \), since the interaction is diagonal in these variables.

We wrote the Lippman-Schwinger equation as

\[
\langle \phi_m|\hat{T}|\phi_n \rangle = \langle \phi_m|\hat{V}|\phi_n \rangle + \sum_{k} \langle \phi_m|\hat{V}|\phi_k \rangle \frac{1}{E_n - \omega_k} \langle \phi_k|\hat{T}|\phi_n \rangle.
\]

How do we rewrite it in a partial wave expansion with momenta \( k' \)?

The general structure of the \( T \)-matrix in partial waves is

\[
T_{ll'}^{00}(kk'K\omega) = V_{ll'}^{00}(kk')
\]

\[
+ \frac{2}{\pi} \sum_{l''m''M_S} \int_0^\infty d\omega (\langle l''m''S|\mathcal{J}M \rangle)^2 \frac{Y_{l''m''}^*(\hat{q})Y_{l'm'}(\hat{q})V_{ll'}^{00}(kq)T_{ll'}^{00}(qk'K\omega)}{\omega - H_0},
\]

The shorthand notation

\[
T_{ll'}^{00}(kk'K\omega) = \langle kl\mathcal{J}S|T(\omega)|k'l\mathcal{J}S \rangle,
\]
denotes the $T$-matrix with momenta $k$ and $k'$ and orbital momenta $l$ and $l'$ of the relative motion, and $K$ is the corresponding momentum of the center-of-mass motion. Further, $L$, $J$, $S$ and $T$ are the orbital momentum of the center-of-mass motion, the total angular momentum, spin and isospin, respectively. Due to the nuclear tensor force, the interaction is not diagonal in $ll'$.

Using the orthogonality properties of the Clebsch-Gordan coefficients and the spherical harmonics, we obtain the well-known one-dimensional angle independent integral equation

$$T_{ll'}^{\omega}(kk'K) = V_{ll'}^{\omega}(kk') + \frac{2}{\pi} \sum_{l''} \int_0^\infty dq q^2 V_{ll''}^{\omega}(kq) \frac{1}{k^2 - q^2 + i\epsilon} T_{l''l'}^{\omega}(qk') \omega - H_0.$$ 

Inserting the denominator we arrive at

$$T_{ll'}^{\omega}(kk'K) = V_{ll'}^{\omega}(kk') + \frac{2}{\pi} \sum_{l''} \int_0^\infty dq q^2 V_{ll''}^{\omega}(kq) \frac{1}{k^2 - q^2 + i\epsilon} T_{l''l'}^{\omega}(qk') .$$

To parameterize the nucleon-nucleon interaction we solve the Lippman-Schwinger equation

$$T_{ll'}^{\omega}(kk'K) = V_{ll'}^{\omega}(kk') + \frac{2}{\pi} \sum_{l''} \int_0^\infty dq q^2 V_{ll''}^{\omega}(kq) \frac{1}{k^2 - q^2 + i\epsilon} T_{l''l'}^{\omega}(qk') .$$

The shorthand notation

$$T(V)_{ll'}^{\omega}(kk'K\omega) = \langle kKlLJ|T(\omega)|k'K'l'LJ\rangle ,$$

denotes the $T(V)$-matrix with momenta $k$ and $k'$ and orbital momenta $l$ and $l'$ of the relative motion, and $K$ is the corresponding momentum of the center-of-mass motion. Further, $L$, $J$, and $S$ are the orbital momentum of the center-of-mass motion, the total angular momentum and spin, respectively. We skip for the moment isospin.

For scattering states, the energy is positive, $E > 0$. The Lippman-Schwinger equation (a rewrite of the Schroedinger equation) is an integral equation where we have to deal with the amplitude $R(k, k')$ (reaction matrix, which is the real part of the full complex $T$-matrix) defined through the integral equation for one partial wave (no coupled-channels)

$$R_t(k, k') = V_t(k, k') + \frac{2}{\pi} P \int_0^\infty dq q^2 V_t(k, q) \frac{1}{E - q^2/m} R_t(q, k').$$

(14)

For negative energies (bound states) and intermediate states scattering states blocked by occupied states below the Fermi level.

The symbol $P$ in the previous slide indicates that Cauchy's principal-value prescription is used in order to avoid the singularity arising from the zero of the denominator.

The total kinetic energy of the two incoming particles in the center-of-mass system is

$$E = \frac{k_0^2}{m_n}.$$
The matrix $R_l(k, k')$ relates to the phase shifts through its diagonal elements as

$$ R_l(k_0, k_0) = -\frac{\tan \delta_l}{mk_0}. \quad (15) $$

From now on we will drop the subscript $l$ in all equations. In order to solve the Lippman-Schwinger equation in momentum space, we need first to write a function which sets up the mesh points. We need to do that since we are going to approximate an integral through

$$ \int_a^b f(x) dx \approx \sum_{i=1}^N w_i f(x_i), $$

where we have fixed $N$ lattice points through the corresponding weights $w_i$ and points $x_i$. Typically obtained via methods like Gaussian quadrature.

If you use Gauss-Legendre the points are determined for the interval $x_i \in [-1, 1]$ You map these points over to the limits in your integral. You can then use the following mapping

$$ k_i = \text{const} \times \tan \left\{ \frac{\pi}{4} (1 + x_i) \right\}, $$

and

$$ \omega_i = \text{const} \frac{\pi}{4} \frac{w_i}{\cos^2 \left( \frac{\pi}{4} (1 + x_i) \right)}. $$

If you choose units fm$^{-1}$ for $k$, set const = 1. If you choose to work with MeV, set $\text{const} \sim 200$ ($\hbar c = 197$ MeVfm).

The principal value integral is rather tricky to evaluate numerically, mainly since computers have limited precision. We will here use a subtraction trick often used when dealing with singular integrals in numerical calculations. We introduce first the calculus relation

$$ \int_{-\infty}^{\infty} \frac{dk}{k - k_0} = 0. $$

It means that the curve $1/(k - k_0)$ has equal and opposite areas on both sides of the singular point $k_0$. If we break the integral into one over positive $k$ and one over negative $k$, a change of variable $k \to -k$ allows us to rewrite the last equation as

$$ \int_0^{\infty} \frac{dk}{k^2 - k_0^2} = 0. $$

We can then express a principal values integral as

$$ P \int_0^{\infty} \frac{f(k) dk}{k^2 - k_0^2} = \int_0^{\infty} \frac{(f(k) - f(k_0)) dk}{k^2 - k_0^2}, \quad (16) $$

where the right-hand side is no longer singular at $k = k_0$, it is proportional to the derivative $df/dk$, and can be evaluated numerically as any other integral.
We can then use this trick to obtain

$$R(k, k') = V(k, k') + \frac{2}{\pi} \int_0^\infty dq \frac{q^2 V(k, q) R(q, k') - k_0^2 V(k, k_0) R(k_0, k')}{(k_0^2 - q^2)/m}. \quad (17)$$

This is the equation to solve numerically in order to calculate the phase shifts. We are interested in obtaining $R(k_0, k_0)$. How do we proceed?

Using the mesh points $k_j$ and the weights $\omega_j$, we reach

$$R(k, k') = V(k, k') + \frac{2}{\pi} \sum_{j=1}^N \omega_j k_j^2 V(k, k_j) R(k_j, k') - \frac{2}{\pi} k_0^2 V(k, k_0) R(k_0, k') \sum_{n=1}^N \frac{\omega_n}{(k_0^2 - k_n^2)/m}. \quad (18)$$

This equation contains now the unknowns $R(k_i, k_j)$ (with dimension $N \times N$) and $R(k_0, k_0)$. We can turn it into an equation with dimension $(N + 1) \times (N + 1)$ with a mesh which contains the original mesh points $k_j$ for $j = 1, N$ and the point which corresponds to the energy $k_0$. Consider the latter as the ‘observable’ point. The mesh points become then $k_j$ for $j = 1, n$ and $k_{N+1} = k_0$.

With these new mesh points we define the matrix

$$A_{i,j} = \delta_{i,j} - V(k_i, k_j)u_j, \quad (18)$$

where $\delta$ is the Kronecker $\delta$ and

$$u_j = \frac{2}{\pi} \frac{\omega_j k_j^2}{(k_0^2 - k_j^2)/m} \quad j = 1, N$$

and

$$u_{N+1} = -\frac{2}{\pi} \sum_{j=1}^N \frac{k_0^2 \omega_j}{(k_0^2 - k_j^2)/m}.$$

The first task is then to set up the matrix $A$ for a given $k_0$. This is an $(N + 1) \times (N + 1)$ matrix. It can be convenient to have an outer loop which runs over the chosen observable values for the energy $k_0^2/m$. Note that all mesh points $k_j$ for $j = 1, N$ must be different from $k_0$. Note also that $V(k_i, k_j)$ is an $(N + 1) \times (N + 1)$ matrix.

With the matrix $A$ we can rewrite the problem as a matrix problem of dimension $(N + 1) \times (N + 1)$. All matrices $R$, $A$ and $V$ have this dimension and we get

$$A_{i,1} R_{i,j} = V_{i,j},$$

or just

$$AR = V. \quad (19)$$

Since you already have defined $A$ and $V$ (these are stored as $(N + 1) \times (N + 1)$ matrices) The final equation involves only the unknown $R$. We obtain it by matrix inversion, i.e.,

$$R = A^{-1} V.$$
Thus, to obtain $R$, you will need to set up the matrices $A$ and $V$ and invert the matrix $A$. With the inverse $A^{-1}$, perform a matrix multiplication with $V$ results in $R$.

With $R$ you can then evaluate the phase shifts by noting that

$$R(k_{N+1}, k_{N+1}) = R(k_0, k_0) = -\frac{\tan \delta}{mk_0}$$

where $\delta$ are the phase shifts.

For elastic scattering, the scattering potential can only change the outgoing spherical wave function up to a phase. In the asymptotic limit, far away from the scattering potential, we get for the spherical bessel function

$$j_l(kr) \xrightarrow{r \gg 1} \frac{\sin(kr - l\pi/2)}{kr} = \frac{1}{2ik} \left( \frac{e^{i(kr-l\pi/2)}}{r} - \frac{e^{-i(kr-l\pi/2)}}{r} \right)$$

The outgoing wave will change by a phase shift $\delta_l$, from which we can define the S-matrix $S_l(k) = e^{2i\delta_l(k)}$. Thus, we have

$$\frac{e^{i(kr-l\pi/2)}}{r} \xrightarrow{\text{phase change}} S_l(k)\frac{e^{i(kr-l\pi/2)}}{r}$$

The solution to the Schrödinger equation for a spherically symmetric potential, will have the form

$$\psi_k(r) = e^{ikr} + f(\theta) \frac{e^{ikr}}{r}$$

where $f(\theta)$ is the scattering amplitude, and related to the differential cross section as

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

Using the expansion of a plane wave in spherical waves, we can relate the scattering amplitude $f(\theta)$ with the partial wave phase shifts $\delta_l$ by identifying the outgoing wave

$$\psi_k(r) = e^{ikr} + \left[ \frac{1}{2ik} \sum_l i^l (2l + 1)(S_l(k) - 1)P_l(\cos(\theta))e^{-il\pi/2} \right] \frac{e^{ikr}}{r}$$

which can be simplified further by cancelling $i^l$ with $e^{-il\pi/2}$

We have

$$\psi_k(r) = e^{ikr} + f(\theta) \frac{e^{ikr}}{r}$$

with

$$f(\theta) = \sum_l (2l + 1)f_l(\theta)P_l(\cos(\theta))$$

where the partial wave scattering amplitude is given by

$$f_l(\theta) = \frac{1}{k} \frac{(S_l(k) - 1)}{2i} = \frac{1}{k} \sin(\delta_l(k)e^{i\delta_l(k)}$$
With Euler’s formula for the cotangent, this can also be written as

$$f_l(\theta) = \frac{1}{k \cot \delta_l(k)} - i.$$

The integrated cross section is given by

$$\sigma = 2\pi \int_0^\pi |f(\theta)|^2 \sin \theta d\theta$$

$$= 2\pi \sum_l \left( \frac{2l+1}{k} \sin\delta_l \right)^2 \int_0^\pi (P_l(\cos(\theta)))^2 \sin(\theta) d\theta$$

$$= \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l(k) = 4\pi \sum_l (2l+1)|f_l(\theta)|^2,$$

where the orthogonality of the Legendre polynomials was used to evaluate the last integral

$$\int_0^\pi P_l(\cos \theta)^2 \sin \theta d\theta = \frac{2}{2l+1}.$$  

Thus, the total cross section is the sum of the partial-wave cross sections. Note that the differential cross section contains cross-terms from different partial waves. The integral over the full sphere enables the use of the Legendre orthogonality, and this kills the cross-terms.

At low energy, $k \to 0$, S-waves are most important. In this region we can define the scattering length $a$ and the effective range $r$. The S-wave scattering amplitude is given by

$$f_l(\theta) = \frac{1}{k \cot \delta_l(k)} - i.$$

Taking the limit $k \to 0$, gives us the expansion

$$k \cot \delta_0 = -\frac{1}{a} + \frac{1}{2} r_0 k^2 + \ldots$$

Thus the low energy cross section is given by

$$\sigma = 4\pi a^2.$$
If the system contains a bound state, the scattering length will become positive (neutron-proton in $^3S_1$). For the $^1S_0$ wave, the scattering length is negative and large. This indicates that the wave function of the system is at the verge of turning over to get a node, but cannot create a bound state in this wave.

It is important to realize that the phase shifts themselves are not observables. The measurable scattering quantity is the cross section, or the differential cross section. The partial wave phase shifts can be thought of as a parameterization of the (experimental) cross sections. The phase shifts provide insights into the physics of partial wave projected nuclear interactions, and are thus important quantities to know.

The nucleon-nucleon differential cross section have been measured at almost all energies up to the pion production threshold (290 MeV in the Lab frame), and this experimental data base is what provides us with the constraints on our nuclear interaction models. In order to pin down the unknown coupling constants of the theory, a statistical optimization with respect to cross sections need to be carried out. This is how we constrain the nucleon-nucleon interaction in practice!

The $pp$-data is more accurate than the $np$-data, and for $nn$ there is no data. The quality of a potential is gauged by the $\chi^2$/datum with respect to the scattering data base.

### The Lippman-Schwinger equation for two-nucleon scattering: Nijmegen multi-energy $pp$ PWA phase shifts.

<table>
<thead>
<tr>
<th>$T_{lab}$ bin (MeV)</th>
<th>N3LO$^1$</th>
<th>NNLO$^2$</th>
<th>NLO$^3$</th>
<th>AV18$^4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-100</td>
<td>1.05</td>
<td>1.7</td>
<td>4.5</td>
<td>0.95</td>
</tr>
<tr>
<td>100-190</td>
<td>1.08</td>
<td>22</td>
<td>100</td>
<td>1.10</td>
</tr>
<tr>
<td>190-290</td>
<td>1.15</td>
<td>47</td>
<td>180</td>
<td>1.11</td>
</tr>
<tr>
<td>0 – 290</td>
<td>1.10</td>
<td>20</td>
<td>86</td>
<td>1.04</td>
</tr>
</tbody>
</table>

The Lippman-Schwinger equation for two-nucleon scattering: An example: chiral twobody interactions.

\[ \mathcal{L}_{\text{eff}} = \mathcal{L}_{\pi\pi}(f_\pi, m_\pi) + \mathcal{L}_{\pi N}(f_\pi, M_N, g_A, c_i, d_i, \ldots) + \mathcal{L}_{NN}(C_i, \tilde{C}_i, D_i, \ldots) + \ldots \]


Note that the Nijm93 PWA phase shift becomes negative at \( T_{\text{lab}} > 250 \text{MeV} \). This indicates that the nucleon-nucleon potential is repulsive at short distances.

**Exercise 1:** List all partial waves up to a given orbital momentum

a) List all allowed according to the Pauli principle partial waves with isospin \( T \), their projection \( T_z \), spin \( S \), orbital angular momentum \( l \) and total spin \( J \) for \( J \leq 3 \). Use the standard spectroscopic notation \( 2S+1L_J \) to label different partial waves. A proton-proton state has \( T_z = -1 \), a proton-neutron state has \( T_z = 0 \) and a neutron-neutron state has \( T_z = 1 \).
Exercise 2: Expressions for various components

a) Find the closed form expression for the spin-orbit force. Show that the spin-orbit force $LS$ gives a zero contribution for $S$-waves (orbital angular momentum $l = 0$). What is the value of the spin-orbit force for spin-singlet states ($S = 0$)?

b) Find thereafter the expectation value of $\sigma_1 \cdot \sigma_2$, where $\sigma_i$ are so-called Pauli matrices.

c) Add thereafter isospin and find the expectation value of $\sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2$, where $\tau_i$ are also so-called Pauli matrices. List all the cases with $S = 0, 1$ and $T = 0, 1$. 
Exercise 3: Analysis of the open-pion exchange component of the force

A simple parametrization of the nucleon-nucleon force is given by what is called the $V_8$ potential model, where we have kept eight different operators. These operators contain a central force, a spin-orbit force, a spin-spin force and a tensor force. Several features of the nuclei can be explained in terms of these four components. Without the Pauli matrices for isospin the final form of such an interaction model results in the following form:

$$V(r) = \left\{ C_c + C_\sigma \sigma_1 \cdot \sigma_2 + C_T \left( 1 + \frac{3}{m_\alpha r} + \frac{3}{(m_\alpha r)^2} \right) S_{12}(\hat{r}) \right. + \left. C_{SL} \left( \frac{1}{m_\alpha r} + \frac{1}{(m_\alpha r)^2} \right) \mathbf{L} \cdot \mathbf{S} \right\} e^{-m_\pi r}$$

where $m_\alpha$ is the mass of the relevant meson and $S_{12}$ is the familiar tensor term. The various coefficients $C_i$ are normally fitted so that the potential reproduces experimental scattering cross sections. By adding terms which include the isospin Pauli matrices results in an interaction model with eight operators. The expectation value of the tensor operator is non-zero only for $S = 1$. We will show this in a forthcoming lecture, after that we have derived the Wigner-Eckart theorem. Here it suffices to know that the expectation value of the tensor force for different partial values is (with $l$ the orbital angular momentum and $J$ the total angular momentum in the relative and center-of-mass frame of motion)

$$\langle lJ S = 1 | S_{12} | l' J S = 1 \rangle = \begin{cases} -\frac{2(J+2)}{2J+1} & l = J + 1 \text{ and } l' = J + 1, \\ \frac{6\sqrt{J(J+1)}}{2J+1} & l = J + 1 \text{ and } l' = J - 1, \\ \frac{6\sqrt{J(J+1)}}{2J+1} & l = J - 1 \text{ and } l' = J + 1, \\ -\frac{2(J-1)}{2J+1} & l = J - 1 \text{ and } l' = J - 1, \\ 2 & l = J \text{ and } l' = J, \end{cases}$$

and zero else.

In this exercise we will focus only on the one-pion exchange term of the nuclear force, namely

$$V_\pi(r) = -\frac{f_\pi^2}{4\pi m_\pi^2} \tau_1 \cdot \tau_2 \frac{1}{3} \left\{ \sigma_1 \cdot \sigma_2 + \left( 1 + \frac{3}{m_\pi r} + \frac{3}{(m_\pi r)^2} \right) S_{12}(\hat{r}) \right\} e^{-m_\pi r}.$$

Here the constant $f_\pi^2/4\pi \approx 0.08$ and the mass of the pion is $m_\pi \approx 140$ MeV/c².
a) Compute the expectation value of the tensor force and the spin-spin and isospin operators for the one-pion exchange potential for all partial waves you found previously. Comment your results. How does the one-pion exchange part behave as function of different $l$, $J$ and $S$ values? Do you see some patterns?

b) For the binding energy of the deuteron, with the ground state defined by the quantum numbers $l = 0$, $S = 1$ and $J = 1$, the tensor force plays an important role due to the admixture from the $l = 2$ state. Use the expectation values of the different operators of the one-pion exchange potential and plot the ratio of the tensor force component over the spin-spin component of the one-pion exchange part as function of $x = m_\pi r$ for the $l = 2$ state (that is the case $l, l' = J + 1$). Comment your results.

Exercise 4: Program for the Lippman-Schwinger equation

The aim here is to develop a program which solves the Lippman-Schwinger equation for a simple parametrization for the $^1S_0$ partial wave. This partial wave is given by a central force only and is parametrized in coordinate space as

$$V(r) = V_a e^{-ax} + V_b e^{-bx} + V_c e^{-cx}$$

with $x = \mu r$, $\mu = 0.7$ fm (the inverse of the pion mass), $V_a = -10.463$ MeV and $a = 1$, $V_b = -1650.6$ MeV and $b = 4$ and $V_c = 6484.3$ MeV and $c = 7$.

a) Find an analytical expression for the Fourier-Bessel transform (Hankel transform) to momentum space for $l = 0$ using

$$\langle k | V_l | k' \rangle = \int j_l(kr)V(r)j_l(k'r)r^2 dr.$$

b) Write a small program which calculates the latter expression and use this potential to compute the $T$-matrix at positive energies for $l = 0$. Compare your results to those obtained with a box potential given by

$$V(r) = \begin{cases} -V_0 & r < R_0 \\ 0 & r > R_0 \end{cases}$$

Make a plot of the two $T$-matrices for energies up to 300 MeV in the lab frame and comment your results.

Finally, a warning, the above central potential is fitted to data from approximately 20 MeV to some 300 MeV. This means that results outside the data set should be taken seriously.

Solution. The following Fortran 95 program solves the above Lippmann-Schwinger equation. Python and C++ codes will be added later. Discussions of the results will also be added.
Example program used to evaluate the T-matrix following Kowalski's method (eqs V88 & V89 in Brown and Jackson) for positive energies only. The program is set up for S-waves only.

Coded by: Morten Hjorth-Jensen
Language: FORTRAN 90

*********************************************************
obtain the t-mtx
vkk is the box potential
f_mtx is equation V88 og Brown & Jackson
*********************************************************

SUBROUTINE t_channel
USE mesh_variables
IMPLICIT NONE
INTEGER istat, i,j
DIMENSION vkk(:,:),f_mtx(:,:),t_mtx(:,:)
DOUBLE PRECISION, ALLOCATABLE :: vkk,t_mtx,f_mtx
DOUBLE PRECISION t_shell

Allocate(vkk (n_rel,n_rel), STAT=istat)
CALL v_pot_yukawa(vkk) ! set up the box potential in routine vpot
ALLOCATE(t_mtx (n_rel), STAT=istat) ! allocate space in heap for T
ALLOCATE(f_mtx (n_rel), STAT=istat) ! allocate space for f
DO i=1,n_rel ! loop over positive energies e=k^2
   CALL f_mtx_eq(f_mtx,vkk,i) ! solve eq. V88
   CALL principal_value(vkk,f_mtx,i,t_shell) ! solve Eq. V89
   DO j=1,n_rel ! the t-matrix
      t_mtx(j)=f_mtx(j)*t_shell
      IF(j == i) WRITE(6,*) ra(i) ,t_mtx(i)
   ENDDO
ENDDO
DEALLOCATE(vkk , STAT=istat)
DEALLOCATE(t_mtx, f_mtx, STAT=istat)
1000 FORMAT( I3, 2F12.6)
END SUBROUTINE t_channel

C ***********************************************************
C The analytical expression for the box potential
C of exercise 1 and 12
C vkk is in units of fm^-2 (14 MeV/41.47Mevfm^2, where
C 41.47= \hbarc^2/mass_nucleon),
C ra are mesh points in rel coordinates, units of fm^-1
C ***********************************************************

SUBROUTINE v_pot_box(vkk)
USE mesh_variables
USE constants
IMPLICIT NONE
INTEGER i,j
DOUBLE PRECISION vkk, r_0, v_0, a, b, fac
PARAMETER(r_0=2.7d0,v_0=0.33759d0) !r_0 in fm, v_0 in fm^-2
DIMENSION vkk(n_rel,n_rel)
DO i=1,n_rel ! set up the free potential
   DO j=1,i-1
      a=ra(i)+ra(j)
      b=ra(i)-ra(j)
      fac=v_0/(2.d0*ra(i)*ra(j))
      vkk(j,i)=fac*(DSIN(a*r_0)/a-DSIN(b*r_0)/b)
      vkk(i,j)=vkk(j,i)
   ENDDO
   fac=v_0/(2.d0*(ra(i)**2))
   vkk(i,i)=fac*(DSIN(2.d0*ra(i)*r_0)/(2.d0*ra(i))-r_0)
ENDDO
END SUBROUTINE v_pot_box

C ***********************************************************
C The analytical expression for a Yukawa potential
C in the l=0 channel
C vkk is in units of fm^-2,
C ra are mesh points in rel coordinates, units of fm^-1
C The parameters here are those of the Reid-Soft core
C potential, see Brown and Jackson eq. A(4)
C ***********************************************************

SUBROUTINE v_pot_yukawa(vkk)
USE mesh_variables
USE constants
IMPLICIT NONE
INTEGER i, j
DOUBLE PRECISION vkk, mu1, mu2, mu3, v_1, v_2, v_3, a, b, fac
PARAMETER(mu1=0.49d0, v_1=-0.252d0)
PARAMETER(mu2=7.84d0, v_2=-39.802d0)
PARAMETER(mu3=24.01d0, v_3=156.359d0)
DIMENSION vkk(n_rel,n_rel)

DO i=1,n_rel ! set up the free potential
  DO j=1,i
    a=(ra(j)+ra(i))**2
    b=(ra(j)-ra(i))**2
    fac=1./(4.d0*ra(i)*ra(j))
    vkk(j,i)=v_1*fac*DLOG((a+mu1)/(b+mu1)) +
      v_2*fac*DLOG((a+mu2)/(b+mu2)) +
      v_3*fac*DLOG((a+mu3)/(b+mu3))
  ENDDO
ENDDO

END SUBROUTINE v_pot_yukawa

C **************************************************
C Solves eq. V88
C and returns < p | f_mtx | n_pole =k>
C **************************************************
SUBROUTINE f_mtx_eq(f_mtx,vkk,n_pole)
USE mesh_variables
USE constants
IMPLICIT NONE
INTEGER i, j, int, istat, n_pole
DOUBLE PRECISION f_mtx,vkk,dp,deriv,pih,xsum
DIMENSION dp(1),deriv(1)
DIMENSION f_mtx(n_rel),vkk(n_rel,n_rel),a(:,:),fu(:),q(:),au(:)
DOUBLE PRECISION, ALLOCATABLE :: fu, q, au, a

pih=2.D0/ACOS(-1.D0)
ALLOCATE( a (n_rel,n_rel), STAT=istat)
DO i=1,n_rel
  ALLOCATE(fu(n_rel), q(n_rel), au(n_rel), STAT=istat)
  DO j=1,n_rel
    fu(j)=vkk(i,j)-vkk(i,n_pole)*vkk(n_pole,j)/
      vkk(n_pole,n_pole)
  ENDDO
  DO j=1,n_rel
    IF(j /= n_pole ) THEN ! regular part
      a(j,i)=pih*fu(j)*wra(j)*(ra(j)**2)/
        (ra(j)**2-ra(n_pole)**2)
    ELSEIF(j == n_pole) THEN ! use l'Hopitals rule to get pole term
      dp(1)=ra(j)
      CALL spls3(ra,fu,n_rel,dp,deriv(1),1,q,au,2,0)
      a(j,i)=pih*wra(j)*ra(j)/2.d0*deriv(1)
    ENDIF
  ENDDO
  DEALLOCATE(fu, q, au, STAT=istat) ! free space in heap
  a(i,i)=a(i,i)+1.D0
ENDDO
CALL matinv(a, n_rel) ! Invert the matrix a
DO j=1,n_rel ! multiply inverted matrix a with dim less pot
  xsum=0.D0
DO i=1,n_rel
  xsum=xsum+a(i,j)*vkk(i,n_pole)/vkk(n_pole,n_pole)  ! gives f-matrix in V88
ENDDO
f_mtx(j)=xsum
ENDDO
DEALLOCATE (a, STAT=istat)
END SUBROUTINE

C **************************************************
C Solves the principal value integral of V89
C returns the t-matrix for k=k, t_shell
C **************************************************
SUBROUTINE principal_value(vkk,f_mtx,n_pole,t_shell)
USE mesh_variables
IMPLICIT NONE
DOUBLE PRECISION vkk, f_mtx, t_shell, sum, pih, deriv, term
DIMENSION deriv(1)
DIMENSION vkk(n_rel,n_rel), f_mtx(n_rel),fu(:), q(:), au(:)
DOUBLE PRECISION, ALLOCATABLE :: fu, q, au
INTEGER n_pole, i, istat
ALLOCATE(fu(n_rel), q(n_rel), au(n_rel), STAT=istat)
sum=0.D0
pih=2.D0/ACOS(-1.D0)
DO i=1,n_rel
  fu(i)=vkk(n_pole,i)*f_mtx(i)
ENDDO
DO i=1,n_pole-1  ! integrate up to the pole - 1 mesh
  term=fu(i)*(ra(i)**2)-fu(n_pole)*(ra(n_pole)**2)
  sum=sum+pih*wra(i)*term/(ra(i)**2-ra(n_pole)**2)
ENDDO  ! here comes the pole part
CALL spls3(ra,fu,n_rel,ra(n_pole),deriv,1,au,q,2,0)
sum=sum+pih*wra(n_pole)*(fu(n_pole)+ra(n_pole)*deriv(1)/2.d0)
DO i=n_pole+1,n_rel  ! integrate from pole + 1 mesh pt to infty
  term=fu(i)*(ra(i)**2)-fu(n_pole)*(ra(n_pole)**2)
  sum=sum+pih*wra(i)*term/(ra(i)**2-ra(n_pole)**2)
ENDDO
t_shell=vkk(n_pole,n_pole)/(1.d0+sum)
DEALLOCATE (fu, q, au, STAT=istat)
END SUBROUTINE

C **********************************************
C Set up of relative mesh and weights
C **********************************************
SUBROUTINE rel_mesh
USE mesh_variables
IMPLICIT NONE
INTEGER i
DOUBLE PRECISION pih,u,s,xx,c,h_max
PARAMETER (c=0.75)
DIMENSION u(n_rel), s(n_rel)
pih=ACOS(-1.D0)/2.D0
CALL gausslegendret (0.D0,1.d0,n_rel,u,s)
DO i=1,n_rel
  xx=pih*u(i)
  ra(i)=DTAN(xx)*c
END SUBROUTINE
wra(i)=pih*c/DCOS(xz)**2*s(i)
ENDDO

END SUBROUTINE rel_mesh

C *********************************************************
C Routines to do mtx inversion, from Numerical
C Recepies, Teukolsky et al. Routines included
C below are MATINV, LUDCMP and LUBKSB. See chap 2
C of Numerical Recepies for further details
C Recoded in FORTRAN 90 by M. Hjorth-Jensen
C *********************************************************

SUBROUTINE matinv(a,n)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION a(n,n)
INTEGER istat
DOUBLE PRECISION, ALLOCATABLE :: y(:,:)
INTEGER, ALLOCATABLE :: indx(:)
ALLOCATE (y( n, n), STAT =istat)
ALLOCATE ( indx (n), STAT =istat)
DO i=1,n
DO j=1,n
y(i,j)=0.
ENDDO
y(i,i)=1.
ENDDO
CALL ludcmp(a,n,indx,d)
DO j=1,n
call lubksb(a,n,indx,y(1,j))
ENDDO
DO i=1,n
DO j=1,n
a(i,j)=y(i,j)
ENDDO
ENDDO
DEALLOCATE ( y, STAT=istat)
DEALLOCATE ( indx, STAT=istat)
END SUBROUTINE matinv

SUBROUTINE LUDCMP(A,N,INDX,D)
IMPLICIT REAL*8(A-H,O-Z)
PARAMETER (TINY=1.0E-20)
DIMENSION A(N,N),INDX(N)
INTEGER istat
DOUBLE PRECISION, ALLOCATABLE :: vv(:)
ALLOCATE ( vv(n), STAT = istat)
D=1.
DO I=1,N
AAMAX=0.
DO J=1,N
IF (ABS(A(I,J)) > AAMAX) AAMAX=ABS(A(I,J))
ENDDO
IF (AAMAX == 0.) PAUSE 'Singular matrix.'
VV(I)=1./AAMAX
ENDDO
DO J=1,N
IF (J > 1) THEN
  DO I=1,J-1
    SUM=A(I,J)
    IF (I > 1) THEN
      DO K=1,I-1
        SUM=SUM-A(I,K)*A(K,J)
      ENDDO
    A(I,J)=SUM
  ENDDO
ENDIF
AAMAX=0.
DO I=J,N
  SUM=A(I,J)
  IF (J > 1) THEN
    DO K=1,J-1
      SUM=SUM-A(I,K)*A(K,J)
    ENDDO
    A(I,J)=SUM
  ENDDO
  DUM=VV(I)*ABS(SUM)
  IF (DUM >= AAMAX) THEN
    IMAX=I
    AAMAX=DUM
  ENDDO
ENDIF
IF (J /= IMAX) THEN
  DO K=1,N
    DUM=A(IMAX,K)
    A(IMAX,K)=A(J,K)
    A(J,K)=DUM
  ENDDO
  D=-D
  VV(IMAX)=VV(J)
ENDIF
INDX(J)=IMAX
IF (J /= N) THEN
  IF (A(J,J) == 0.) A(J,J)=TINY
  DUM=1./A(J,J)
  DO I=J+1,N
    A(I,J)=A(I,J)*DUM
  ENDDO
ENDIF
ENDIF
IF(A(N,N) == 0.) A(N,N)=TINY
DEALLOCATE ( vv, STAT = istat)
END SUBROUTINE LUDCMP

SUBROUTINE LUBKSB(A,N,INDX,B)
  implicit real*8(a-h,o-z)
  DIMENSION A(N,N),INDX(N),B(N)
  II=0
  DO I=1,N
    LL=INDX(I)
    SUM=B(LL)
    B(LL)=B(I)
    IF (II /= 0) THEN
      DO J=II,I-1
        SUM=SUM-A(I,J)*B(J)
      ENDDO
    ENDIF
  ENDDO
ELSE IF (SUM /= 0.) THEN
   II=I
   ENDF
   B(I)=SUM
ENDDO
DO I=N,1,-1
   SUM=B(I)
   IF (I < N) THEN
      DO J=I+1,N
         SUM=SUM-A(I,J)*B(J)
      ENDDO
   ENDF
   B(I)=SUM/A(I,I)
ENDDO
END SUBROUTINE lubksb

c) The parameters of the box potential are chosen to fit a potential with a bound state at zero energy. What does this mean for your $T$-matrix with this potential when $k \to 0$?