Non-relativistic and Relativistic Scattering Theory

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Dramatis Personae

Baryons	Mass (MeV)	Mesons	Mass (MeV)
p, n	938.926	π	138.03
Λ	1116.0	η	548.8
Σ	1197.3	σ	≈ 550.0
Δ	1232.0	ρ	770
		ω	782.6
		δ	983.0
		K	495.8
		$K^\star$	895.0

Components of the force and quantum numbers

Before we proceed, we will look into specific quantum numbers of the relative system and study expectation vaues of the various terms of

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

$$\left. + C_{SL} \left(\frac{1}{m_\alpha r} + \frac{1}{(m_\alpha r)^2} \right) \mathbf{L} \cdot \mathbf{S} \right\} \frac{e^{-m_\alpha r}}{m_\alpha r}$$

Relative and CoM system, quantum numbers

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

$$\mathbf{K} = \sum_{i=1}^{A} \mathbf{k}_i,$$

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

$$\mathbf{k}_{ij} = \frac{1}{2}(\mathbf{k}_i - \mathbf{k}_j).$$

We will below skip the indices ij and simply write $\mathbf{k}$

Relative and CoM system, quantum numbers

In a similar fashion we can define the CoM coordinate

$$\mathbf{R} = \frac{1}{A}\sum_{i=1}^{A} \mathbf{r}_i,$$

and the relative distance

$$\mathbf{r}_{ij} = (\mathbf{r}_i - \mathbf{r}_j).$$

Relative and CoM system, quantum numbers

With the definitions

$$\mathbf{K} = \sum_{i=1}^{A} \mathbf{k}_i,$$

and

$$\mathbf{k}_{ij} = \frac{1}{2}(\mathbf{k}_i - \mathbf{k}_j).$$

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

$$\frac{\mathbf{k}_1^2}{2m_n} + \frac{\mathbf{k}_2^2}{2m_n} = \frac{\mathbf{k}^2}{m_n} + \frac{\mathbf{K}^2}{4m_n},$$

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

Relative and CoM system, quantum numbers

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 $|(j_1j_2)JM_J\rangle$ 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

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

where $\mathcal{J}$ is the total angular momentum of the relative motion.

Phenomenology of nuclear forces

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 $|\mathbf{l} - \mathbf{S}| \leq |\mathbf{J}| \leq |\mathbf{l} + \mathbf{S}|$,

${}^{2S+1}l_J$	J	l	S	T	$\|pp\rangle$	$\|pn\rangle$	$\|nn\rangle$
${}^1S_0$	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

Prelude to the Lippmann-Schwinger equation: Interaction, Heisenberg and Schroedinger pictures

In order to derive the various rules for computing diagrams, we find it easier, in particular with respect to the computation of energy denominators, to use time-dependent perturbation theory. This is normally used as a starting point for Green's function based methods as well. In addition it links the formalism to what is done in quantum field theory. Before we start we will find it convenient to define various representations of Schroedinger's equation.

The Schroedinger picture

The time-dependent Schroedinger equation (or equation of motion) reads

The time-dependent Schroedinger equation (or equation of motion) reads

$$\imath\hbar\frac{\partial}{\partial t}|\Psi_S(t)\rangle = \hat{H}\Psi_S(t)\rangle,$$

where the subscript S stands for Schroedinger here.

The Schroedinger picture, formal solution

A formal solution is given by

$$|\Psi_S(t)\rangle = \exp\left(-\imath\hat{H}(t-t_0)/\hbar\right)|\Psi_S(t_0)\rangle.$$

The Hamiltonian $\hat{H}$ is hermitian and the exponent represents a unitary operator with an operation carried ut on the wave function at a time t_0.

Our Hamiltonian is normally written out as the sum of an unperturbed part $\hat{H}_0$ and an interaction part $\hat{H}_I$, that is

$$\hat{H} = \hat{H}_0 + \hat{H}_I.$$

In general we have $[\hat{H}_0, \hat{H}_I] \neq 0$ since $[\hat{T}, \hat{V}] \neq 0$.

The Schroedinger picture, unitary transformation

We wish now to define a unitary transformation in terms of $\hat{H}_0$ by defining

$$|\Psi_I(t)\rangle = \exp\left(\imath\hat{H}_0 t/\hbar\right)|\Psi_S(t)\rangle,$$

which is again a unitary transformation carried out now at the time t on the wave function in the Schroedinger picture.

We can easily find the equation of motion by taking the time derivative

$$\imath\hbar\frac{\partial}{\partial t}|\Psi_I(t)\rangle = -\hat{H}_0\exp\left(\imath\hat{H}_0 t/\hbar\right)\Psi_S(t)\rangle + \exp\left(\imath\hat{H}_0 t/\hbar\right)\imath\hbar\frac{\partial}{\partial t}\Psi_S(t)\rangle.$$

The Schroedinger picture, final manipulation

Using the definition of the Schroedinger equation, we can rewrite the last equation as

$$\imath\hbar\frac{\partial}{\partial t}|\Psi_I(t)\rangle = \exp\left(\imath\hat{H}_0 t/\hbar\right)\left[-\hat{H}_0+\hat{H}_0+\hat{H}_I\right]\exp\left(-\imath\hat{H}_0 t/\hbar\right)\Psi_I(t)\rangle,$$

which gives us

$$\imath\hbar\frac{\partial}{\partial t}|\Psi_I(t)\rangle = \hat{H}_I(t)\Psi_I(t)\rangle,$$

with

$$\hat{H}_I(t) = \exp\left(\imath\hat{H}_0 t/\hbar\right)\hat{H}_I\exp\left(-\imath\hat{H}_0 t/\hbar\right).$$

The Schroedinger picture

The order of the operators is important since $\hat{H}_0$ and $\hat{H}_I$ do generally not commute. The expectation value of an arbitrary operator in the interaction picture can now be written as

$$\langle\Psi'_S(t)|\hat{O}_S|\Psi_S(t)\rangle = \langle\Psi'_I(t)|\exp\left(\imath\hat{H}_0 t/\hbar\right)\hat{O}_I\exp\left(-\imath\hat{H}_0 t/\hbar\right)|\Psi_I(t)\rangle,$$

and using the definition

$$\hat{O}_I(t) = \exp\left(\imath\hat{H}_0 t/\hbar\right)\hat{O}_I\exp\left(-\imath\hat{H}_0 t/\hbar\right),$$

we obtain

$$\langle\Psi'_S(t)|\hat{O}_S|\Psi_S(t)\rangle = \langle\Psi'_I(t)|\hat{O}_I(t)|\Psi_I(t)\rangle,$$

stating that a unitary transformation does not change expectation values!

The interaction picture

If the take the time derivative of the operator in the interaction picture we arrive at the following equation of motion

$$\imath\hbar\frac{\partial}{\partial t}\hat{O}_I(t) = \exp\left(\imath\hat{H}_0 t/\hbar\right)\left[\hat{O}_S\hat{H}_0-\hat{H}_0\hat{O}_S\right]\exp\left(-\imath\hat{H}_0 t/\hbar\right) = \left[\hat{O}_I(t),\hat{H}_0\right].$$

Here we have used the time-independence of the Schroedinger equation together with the observation that any function of an operator commutes with the operator itself.

The interaction picture, finding expressions

In order to solve the equation of motion equation in the interaction picture, we define a unitary operator time-development operator $\hat{U}(t,t')$. Later we will derive its connection with the linked-diagram theorem, which yields a linked expression for the actual operator. The action of the operator on the wave function is

$$|\Psi_I(t)\rangle = \hat{U}(t,t_0)|\Psi_I(t_0)\rangle,$$

with the obvious value $\hat{U}(t_0,t_0) = 1$.

The interaction picture, time-development operator

The time-development operator U has the properties that

$$\hat{U}^\dagger(t,t')\hat{U}(t,t') = \hat{U}(t,t')\hat{U}^\dagger(t,t') = 1,$$

which implies that U is unitary

$$\hat{U}^\dagger(t,t') = \hat{U}^{-1}(t,t').$$

Further,

$$\hat{U}(t,t')\hat{U}(t't'') = \hat{U}(t,t'')$$

and

$$\hat{U}(t,t')\hat{U}(t',t) = 1,$$

which leads to

$$\hat{U}(t,t') = \hat{U}^\dagger(t',t).$$

The interaction picture, equation of motion

Using our definition of Schroedinger's equation in the interaction picture, we can then construct the operator $\hat{U}$. We have defined

$$|\Psi_I(t)\rangle = \exp(\imath\hat{H}_0 t/\hbar)|\Psi_S(t)\rangle,$$

which can be rewritten as

$$|\Psi_I(t)\rangle = \exp(\imath\hat{H}_0 t/\hbar)\exp(-\imath\hat{H}(t-t_0)/\hbar)|\Psi_S(t_0)\rangle,$$

or

$$|\Psi_I(t)\rangle = \exp(\imath\hat{H}_0 t/\hbar)\exp(-\imath\hat{H}(t-t_0)/\hbar)\exp(-\imath\hat{H}_0 t_0/\hbar)|\Psi_I(t_0)\rangle.$$

The interaction picture, more equation motion stuff

From the last expression we can define

$$\hat{U}(t,t_0) = \exp(\imath\hat{H}_0 t/\hbar)\exp(-\imath\hat{H}(t-t_0)/\hbar)\exp(-\imath\hat{H}_0 t_0/\hbar).$$

It is then easy to convince oneself that the properties defined above are satisfied by the definition of $\hat{U}$.

We derive the equation of motion for $\hat{U}$ using the above definition. This results in

$$\imath\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}_I(t)\hat{U}(t,t_0),$$

which we integrate from t_0 to a time t resulting in

$$\hat{U}(t,t_0) - \hat{U}(t_0,t_0) = \hat{U}(t,t_0) - 1 = -\frac{\imath}{\hbar}\int_{t_0}^{t} dt'\hat{H}_I(t')\hat{U}(t',t_0),$$

which can be rewritten as

$$\hat{U}(t,t_0) = 1 - \frac{\imath}{\hbar}\int_{t_0}^{t} dt'\hat{H}_I(t')\hat{U}(t',t_0).$$

The interaction picture, iterative solution

We can solve this equation iteratively keeping in mind the time-ordering of the of the operators

$$\hat{U}(t,t_0) = 1 - \frac{\imath}{\hbar}\int_{t_0}^{t} dt'\hat{H}_I(t') + \left(\frac{-\imath}{\hbar}\right)^2\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\hat{H}_I(t')\hat{H}_I(t'') + \ldots$$

The third term can be written as

$$\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\hat{H}_I(t')\hat{H}_I(t'') = \frac{1}{2}\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\hat{H}_I(t')\hat{H}_I(t'') + \frac{1}{2}\int_{t_0}^{t} dt''\int_{t''}^{t} dt'\hat{H}_I(t')\hat{H}_I(t'').$$

The interaction picture, final stage

We obtain this expression by changing the integration order in the second term via a change of the integration variables t' and t'' in

$$\frac{1}{2}\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\hat{H}_I(t')\hat{H}_I(t'').$$

We can rewrite the terms which contain the double integral as

$$\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\hat{H}_I(t')\hat{H}_I(t'') =$$

$$\frac{1}{2}\int_{t_0}^{t}dt'\int_{t_0}^{t'}dt''\left[\hat{H}_I(t')\hat{H}_I(t'')\Theta(t'-t'')+\hat{H}_I(t')\hat{H}_I(t'')\Theta(t''-t')\right],$$

with $\Theta(t''-t')$ being the standard Heavyside or step function. The step function allows us to give a specific time-ordering to the above expression.

The interaction picture, rewriting the wave operator

With the Θ-function we can rewrite the last expression as

$$\int_{t_0}^{t}dt'\int_{t_0}^{t'}dt''\hat{H}_I(t')\hat{H}_I(t'')=\frac{1}{2}\int_{t_0}^{t}dt'\int_{t_0}^{t'}dt''\hat{T}\left[\hat{H}_I(t')\hat{H}_I(t'')\right],$$

where $\hat{T}$ is the so-called time-ordering operator.

With this definition, we can rewrite the expression for $\hat{U}$ as

$$\hat{U}(t,t_0)=\sum_{n=0}^{\infty}\left(\frac{-\imath}{\hbar}\right)^n\frac{1}{n1}\int_{t_0}^{t}dt_1\cdots\int_{t_0}^{t}dt_N\hat{T}\left[\hat{H}_I(t_1)\dots\hat{H}_I(t_n)\right]=\hat{T}\exp\left[\frac{-\imath}{\hbar}\int_{t_0}^{t}dt'\hat{H}_I(t')\right].$$

The above time-evolution operator in the interaction picture will be used to derive various contributions to many-body perturbation theory.

The Heisenberg picture

We wish now to define a unitary transformation in terms of $\hat{H}$ by defining

$$|\Psi_H(t)\rangle=\exp\left(\imath\hat{H}t/\hbar\right)|\Psi_S(t)\rangle,$$

which is again a unitary transformation carried out now at the time t on the wave function in the Schroedinger picture. If we combine this equation with Schroedinger's equation we obtain the following equation of motion

$$\imath\hbar\frac{\partial}{\partial t}|\Psi_H(t)\rangle=0,$$

meaning that $|\Psi_H(t)\rangle$ is time independent. An operator in this picture is defined as

$$\hat{O}_H(t)=\exp\left(\imath\hat{H}t/\hbar\right)\hat{O}_S\exp\left(-\imath\hat{H}t/\hbar\right).$$

The time dependence in the Heisenberg picture

The time dependence is then in the operator itself, and this yields in turn the following equation of motion

$$\imath\hbar\frac{\partial}{\partial t}\hat{O}_H(t) = \exp(\imath\hat{H}t/\hbar)\left[\hat{O}_H\hat{H} - \hat{H}\hat{O}_H\right]\exp(-\imath\hat{H}t/\hbar) = \left[\hat{O}_H(t), \hat{H}\right].$$

We note that an operator in the Heisenberg picture can be related to the corresponding operator in the interaction picture as

$$\hat{O}_H(t) = \exp(\imath\hat{H}t/\hbar)\hat{O}_S\exp(-\imath\hat{H}t/\hbar) =$$

$$\exp(\imath\hat{H}_I t/\hbar)\exp(-\imath\hat{H}_0 t/\hbar)\hat{O}_I\exp(\imath\hat{H}_0 t/\hbar)\exp(-\imath\hat{H}_I t/\hbar).$$

The Heisenberg picture

With our definition of the time evolution operator we see that

$$\hat{O}_H(t) = \hat{U}(0,t)\hat{O}_I\hat{U}(t,0),$$

which in turn implies that $\hat{O}_S = \hat{O}_I(0) = \hat{O}_H(0)$, all operators are equal at $t = 0$. The wave function in the Heisenberg formalism is related to the other pictures as

$$|\Psi_H\rangle = |\Psi_S(0)\rangle = |\Psi_I(0)\rangle,$$

since the wave function in the Heisenberg picture is time independent.

The Heisenberg picture and the time evolution operator

We can relate this wave function to that a given time t via the time evolution operator as

$$|\Psi_H\rangle = \hat{U}(0,t)|\Psi_I(t)\rangle.$$

We assume that the interaction term is switched on gradually. Our wave function at time $t = -\infty$ and $t = \infty$ is supposed to represent a non-interacting system given by the solution to the unperturbed part of our Hamiltonian $\hat{H}_0$. We assume the ground state is given by $|\Phi_0\rangle$, which could be a Slater determinant.

The adiabatic hypothesis

We define our Hamiltonian as

$$\hat{H} = \hat{H}_0 + \exp(-\varepsilon t/\hbar)\hat{H}_I,$$

where ε is a small number. The way we write the Hamiltonian and its interaction term is meant to simulate the switching of the interaction.

The time evolution of the wave function in the interaction picture is then

$$|\Psi_I(t)\rangle = \hat{U}_\varepsilon(t,t_0)|\Psi_I(t_0)\rangle,$$

with

$$\hat{U}_\varepsilon(t,t_0) = \sum_{n=0}^{\infty}\left(\frac{-\imath}{\hbar}\right)^n \frac{1}{n!}\int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_N \exp\left(-\varepsilon(t_1+\cdots+t_n)/\hbar\right)\hat{T}\left[\hat{H}_I(t_1)\ldots\hat{H}_I(t_n)\right]$$

The adiabatic hypothesis and the wave operator

In the limit $t_0 \to -\infty$, the solution ot Schroedinger's equation is $|\Phi_0\rangle$, and the eigenenergies are given by

$$\hat{H}_0|\Phi_0\rangle = W_0|\Phi_0\rangle,$$

meaning that

$$|\Psi_S(t_0)\rangle = \exp\left(-\imath W_0 t_0/\hbar\right)|\Phi_0\rangle,$$

with the corresponding interaction picture wave function given by

$$|\Psi_I(t_0)\rangle = \exp\left(\imath\hat{H}_0 t_0/\hbar\right)|\Psi_S(t_0)\rangle = |\Phi_0\rangle.$$

The adiabatic hypothesis and the wave operator, more details

The solution becomes time independent in the limit $t_0 \to -\infty$. The same conclusion can be reached by looking at

$$\imath\hbar\frac{\partial}{\partial t}|\Psi_I(t)\rangle = \exp\left(-\varepsilon|t|/\hbar\right)\hat{H}_I|\Psi_I(t)\rangle$$

and taking the limit $t \to \pm\infty$. We can rewrite the equation for the wave function at a time $t = 0$ as

$$|\Psi_I(0)\rangle = \hat{U}_\varepsilon(0,-\infty)|\Phi_0\rangle.$$

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

$$\left(\hat{H}_0 + \hat{V}\right)|\psi_n\rangle = E_n|\psi_n\rangle.$$

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

$$\left(\hat{H}_0 - E_n\right)|\psi_n\rangle = -\hat{V}|\psi_n\rangle.$$

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

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

The Lippman-Schwinger equation for two-nucleon scattering

The equation

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

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.

The Lippman-Schwinger equation for two-nucleon scattering

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

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

as our first iteration. Reinserting again gives

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

and continuing we obtain

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

The Lippman-Schwinger equation for two-nucleon scattering

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

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

which we rewrite as

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

The Lippman-Schwinger equation for two-nucleon scattering

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 Lippman-Schwinger equation for two-nucleon scattering

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

$$\mathbf{1} = \sum_n |\phi_n\rangle\langle\phi_n|, \;\; \langle\phi_n|\phi_{n'}\rangle = \delta_{n,n'}$$

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.

The Lippman-Schwinger equation for two-nucleon scattering

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

$$\mathbf{1} = \sum_n |\psi_n\rangle\langle\psi_n|, \;\; \langle\psi_n|\psi_{n'}\rangle = \delta_{n,n'}$$

The Lippman-Schwinger equation for two-nucleon scattering

The most commonly used representations are the coordinate and the momentum space representations. They define the completeness relations

$$\begin{aligned}
\mathbf{1} &= \int d\mathbf{r}\,|\mathbf{r}\rangle\langle\mathbf{r}|, \;\; \langle\mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}') \\
\mathbf{1} &= \int d\mathbf{k}\,|\mathbf{k}\rangle\langle\mathbf{k}|, \;\; \langle\mathbf{k}|\mathbf{k}'\rangle = \delta(\mathbf{k}-\mathbf{k}')
\end{aligned}$$

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,

$$\langle \mathbf{r}|\mathbf{k}\rangle = \left(\frac{1}{2\pi}\right)^{3/2} \exp\left(i\mathbf{k}\cdot\mathbf{r}\right)$$

which is a transformation function defining the mapping from the abstract $|\mathbf{k}\rangle$ to the abstract $|\mathbf{r}\rangle$ space.

The Lippman-Schwinger equation for two-nucleon scattering

That the **r**-space basis states are delta-function normalized follows from

$$\delta(\mathbf{r}-\mathbf{r}') = \langle \mathbf{r}|\mathbf{r}'\rangle = \langle \mathbf{r}|\mathbf{1}|\mathbf{r}'\rangle = \int d\mathbf{k}\langle \mathbf{r}|\mathbf{k}\rangle\langle \mathbf{k}|\mathbf{r}'\rangle = \left(\frac{1}{2\pi}\right)^3 \int d\mathbf{k} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')}$$

and the same for the momentum space basis states,

$$\delta(\mathbf{k}-\mathbf{k}') = \langle \mathbf{k}|\mathbf{k}'\rangle = \langle \mathbf{k}|\mathbf{1}|\mathbf{k}'\rangle = \int d\mathbf{r}\langle \mathbf{k}|\mathbf{r}\rangle\langle \mathbf{r}|\mathbf{k}'\rangle = \left(\frac{1}{2\pi}\right)^3 \int d\mathbf{r} e^{i\mathbf{r}(\mathbf{k}-\mathbf{k}')}$$

The Lippman-Schwinger equation for two-nucleon scattering

Projecting on momentum states, we obtain the momentum space Schroedinger equation as

$$\frac{\hbar^2}{2\mu}k^2\psi_n(\mathbf{k}) + \int d\mathbf{k}' V(\mathbf{k},\mathbf{k}')\psi_n(\mathbf{k}') = E_n\psi_n(\mathbf{k}) \tag{1}$$

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

$$V(\mathbf{k},\mathbf{k}') = \left(\frac{1}{2\pi}\right)^3 \int d\mathbf{r} \int d\mathbf{r}' \exp -i\mathbf{k}\mathbf{r} V(\mathbf{r},\mathbf{r}') \exp i\mathbf{k}'\mathbf{r}'$$

The Lippman-Schwinger equation for two-nucleon scattering

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 Lippman-Schwinger equation for two-nucleon scattering

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

$$\psi_n(\mathbf{k}) = \sum_{lm} \psi_{nlm}(k) Y_{lm}(\hat{k}) \qquad \psi_{nlm}(k) = \int d\hat{k} Y^*_{lm}(\hat{k}) \psi_n(\mathbf{k}).\,, \tag{2}$$

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

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

where the angular momentum projected potential takes the form,

$$V_{lm,l'm'}(k,k') = \int d\hat{k} \int d\hat{k}' Y^*_{lm}(\hat{k}) V(\mathbf{k}\mathbf{k}') Y_{l'm'}(\hat{k}') \tag{4}$$

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

The Lippman-Schwinger equation for two-nucleon scattering

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

$$V = \int d\mathbf{r} \int d\mathbf{r}' \left\{ \int d\hat{k} Y^*_{lm}(\hat{k}) \langle \mathbf{k}|\mathbf{r}\rangle \right\} \langle \mathbf{r}|V|\mathbf{r}'\rangle \left\{ \int d\hat{k}' Y_{lm}(\hat{k}') \langle \mathbf{r}'|\mathbf{k}'\rangle \right\} \tag{5}$$

The Lippman-Schwinger equation for two-nucleon scattering

Since the plane waves depend only on the absolute values of position and momentum, $|\mathbf{k}|$ and $|\mathbf{r}|$, and the angle between them, θ_{kr}, they may be expanded in terms of bipolar harmonics of zero rank, i.e.

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

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,

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

The Lippman-Schwinger equation for two-nucleon scattering

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

$$\begin{aligned} \int d\hat{k} Y^*_{lm}(\hat{k}) \langle \mathbf{k}|\mathbf{r}\rangle &= \left(\frac{1}{2\pi}\right)^{3/2} 4\pi i^{-l} j_l(kr) Y^*_{lm}(\hat{r}), \\ \int d\hat{k}'\, Y_{lm}(\hat{k}') \langle \mathbf{r}'|\mathbf{k}'\rangle &= \left(\frac{1}{2\pi}\right)^{3/2} 4\pi i^{l'} j_{l'}(k'r') Y_{l'm'}(\hat{r}). \end{aligned}$$

The Lippman-Schwinger equation for two-nucleon scattering

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

$$V_{lm,l'm'}(k,k') = \frac{2}{\pi} i^{l'-l} \int_0^\infty dr r^2 \int_0^\infty dr' r'^2 j_l(kr) V_{lm,l'm'}(r,r') j_{l'}(k'r') \qquad (6)$$

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

$$V_{lm,l'm'}(r,r') = \int d\hat{r} \int d\hat{r}' Y^*_{lm}(\hat{r}) V(\mathbf{r},\mathbf{r}') Y_{l'm'}(\hat{r}'). \qquad (7)$$

The Lippman-Schwinger equation for two-nucleon scattering

No assumptions of locality/non-locality and deformation of the interaction has so far been made, and the result in equation (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 equation (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.

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

then equation (6) reduces to

$$V_{lm,l'm'}(r,r') = \frac{\delta(r-r')}{r^2}\int d\hat{r}\; Y^*_{lm}(\hat{r})V(\mathbf{r})Y_{l'm'}(\hat{r}), \tag{8}$$

The Lippman-Schwinger equation for two-nucleon scattering

and equation (6) reduces to

$$V_{lm,l'm'}(k,k') = \frac{2}{\pi}i^{l'-l}\int_0^\infty drr^2 j_l(kr)V_{lm,l'm'}(r)j_{l'}(k'r) \tag{9}$$

where

$$V_{lm,l'm'}(r) = \int d\hat{r}Y^*_{lm}(\hat{r})V(\mathbf{r})Y_{l'm'}(\hat{r}), \tag{10}$$

The Lippman-Schwinger equation for two-nucleon scattering

In the case that the interaction is central, $V(\mathbf{r}) = V(r)$, then

$$V_{lm,l'm'}(r) = V(r)\int d\hat{r}Y^*_{lm}(\hat{r})Y_{l'm'}(\hat{r}) = V(r)\delta_{l,l'}\delta_{m,m'}, \tag{11}$$

and

$$V_{lm,l'm'}(k,k') = \frac{2}{\pi}\int_0^\infty drr^2 j_l(kr)V(r)j_{l'}(k'r)\delta_{l,l'}\delta_{m,m'} = V_l(k,k')\delta_{l,l'}\delta_{m,m'} \tag{12}$$

where the momentum space representation of the interaction finally reads,

$$V_l(k,k') = \frac{2}{\pi}\int_0^\infty dr\; r^2\; j_l(kr)V(r)j_l(k'r). \tag{13}$$

The Lippman-Schwinger equation for two-nucleon scattering

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

$$\frac{\hbar^2}{2\mu}k^2\psi_{nl}(k) + \int_0^\infty dk'k'^2 V_l(k,k')\psi_{nl}(k') = E_{nl}\psi_{nl}(k) \tag{14}$$

Where we have written $\psi_{nl}(k) = \psi_{nlm}(k)$, 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

$$\phi_{nl}(r) = \sqrt{\frac{2}{\pi}}\int dkk^2 j_l(kr)\psi_{nl}(k)$$

The Lippman-Schwinger equation for two-nucleon scattering

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

$$\exp(\imath\mathbf{kr}) = \langle\mathbf{r}|\mathbf{k}\rangle = 4\pi\sum_{lm}\imath^l j_l(kr)Y^*_{lm}(\hat{\mathbf{k}})Y_{lm}(\hat{\mathbf{r}}),$$

where j_l is a spherical Bessel function and Y_{lm} the spherical harmonics.

The Lippman-Schwinger equation for two-nucleon scattering

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

$$\langle\mathbf{k}'\mathbf{K}'|V|\mathbf{k}\mathbf{K}\rangle = \int d\mathbf{r}d\mathbf{r}'\exp-(\imath\mathbf{k}'\mathbf{r}')V(\mathbf{r}',\mathbf{r})\exp\imath\mathbf{k}\mathbf{r}\delta(\mathbf{K},\mathbf{K}').$$

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

$$\exp(\imath\mathbf{kr}) = \langle\mathbf{r}|\mathbf{k}\rangle = 4\pi\sum_{lm}\imath^l j_l(kr)Y^*_{lm}(\hat{\mathbf{k}})Y_{lm}(\hat{\mathbf{r}}),$$

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

The Lippman-Schwinger equation for two-nucleon scattering

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

$$\langle\mathbf{k}'|V|\mathbf{k}\rangle = (4\pi)^2\sum_{STll'm_lm_{l'}\mathcal{J}}\imath^{l+l'}Y^*_{lm}(\hat{\mathbf{k}})Y_{l'm'}(\hat{\mathbf{k}}')$$

$$\langle lm_lSm_S|\mathcal{J}M\rangle\langle l'm_{l'}Sm_S|\mathcal{J}M\rangle\langle k'l'S\mathcal{J}M|V|klS\mathcal{J}M\rangle,$$

where we have defined

$$\langle k'l'S\mathcal{J}M|V|klS\mathcal{J}M\rangle = \int j_{l'}(k'r')\langle l'S\mathcal{J}M|V(r',r)|lS\mathcal{J}M\rangle j_l(kr)r'^2dr'r^2dr.$$

We have omitted the momentum of the center-of-mass motion **K** and the corresponding orbital momentum L, since the interaction is diagonal in these variables.

The Lippman-Schwinger equation for two-nucleon scattering

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 Lippman-Schwinger equation for two-nucleon scattering

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

$$T^{\alpha}_{ll'}(kk'K\omega) = V^{\alpha}_{ll'}(kk')$$

$$+\frac{2}{\pi}\sum_{l''m_{l''}M_S}\int_0^{\infty} d\mathbf{q}(\langle l''m_{l''}Sm_S|\mathcal{J}M\rangle)^2 \frac{Y^*_{l''m_{l''}}(\hat{\mathbf{q}})Y_{l''m_{l''}}(\hat{\mathbf{q}})V^{\alpha}_{ll''}(kq)T^{\alpha}_{l''l'}(qk'K\omega)}{\omega - H_0}, \tag{15}$$

The Lippman-Schwinger equation for two-nucleon scattering

The shorthand notation

$$T^{\alpha}_{ll'}(kk'K\omega) = \langle kKlL\mathcal{J}S|T(\omega)|k'Kl'L\mathcal{J}S\rangle,$$

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, $\mathcal{J}$, 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'.

The Lippman-Schwinger equation for two-nucleon scattering

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

$$T^{\alpha}_{ll'}(kk'K\omega) = V^{\alpha}_{ll'}(kk') + \frac{2}{\pi}\sum_{l''}\int_0^{\infty} dqq^2 \frac{V^{\alpha}_{ll''}(kq)T^{\alpha}_{l''l'}(qk'K\omega)}{\omega - H_0}.$$

Inserting the denominator we arrive at

$$\hat{T}^{\alpha}_{ll'}(kk'K) = \hat{V}^{\alpha}_{ll'}(kk') + \frac{2}{\pi}\sum_{l''}\int_0^{\infty} dqq^2\hat{V}^{\alpha}_{ll''}(kq)\frac{1}{k^2-q^2+i\epsilon}\hat{T}^{\alpha}_{l''l'}(qk'K).$$

The Lippman-Schwinger equation for two-nucleon scattering

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

$$T^{\alpha}_{ll'}(kk'K) = V^{\alpha}_{ll'}(kk') + \frac{2}{\pi}\sum_{l''}\int_0^{\infty} dqq^2V^{\alpha}_{ll''}(kq)\frac{1}{k^2-q^2+i\epsilon}T^{\alpha}_{l''l'}(qk'K).$$

The shorthand notation

$$T(\hat{V})^{\alpha}_{ll'}(kk'K\omega) = \langle kKlL\mathcal{J}S|T(\omega)|k'Kl'L\mathcal{J}S\rangle,$$

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, $\mathcal{J}$, 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.

The Lippman-Schwinger equation for two-nucleon scattering

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)

$$R_l(k,k') = V_l(k,k') + \frac{2}{\pi}\mathcal{P}\int_0^{\infty} dqq^2V_l(k,q)\frac{1}{E-q^2/m}R_l(q,k'). \qquad (16)$$

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

The Lippman-Schwinger equation for two-nucleon scattering

The symbol $\mathcal{P}$ 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 Lippman-Schwinger equation for two-nucleon scattering

The matrix $R_l(k,k')$ relates to the the phase shifts through its diagonal elements as

$$R_l(k_0,k_0) = -\frac{tan\delta_l}{mk_0}. \tag{17}$$

The Lippman-Schwinger equation for two-nucleon scattering

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.

The Lippman-Schwinger equation for two-nucleon scattering

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

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

and

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

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

The Lippman-Schwinger equation for two-nucleon scattering

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

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

The Lippman-Schwinger equation for two-nucleon scattering

We can then express a principal values integral as

$$\mathcal{P}\int_0^\infty \frac{f(k)dk}{k^2-k_0^2} = \int_0^\infty \frac{(f(k)-f(k_0))dk}{k^2-k_0^2}, \tag{18}$$

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.

The Lippman-Schwinger equation for two-nucleon scattering

We can then use this trick to obtain

$$R(k,k') = V(k,k') + \frac{2}{\pi}\int_0^\infty dq \frac{q^2V(k,q)R(q,k') - k_0^2V(k,k_0)R(k_0,k')}{(k_0^2-q^2)/m}. \tag{19}$$

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

The Lippman-Schwinger equation for two-nucleon scattering

How do we proceed?

Using the mesh points k_j and the weights ω_j, we reach

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

The Lippman-Schwinger equation for two-nucleon scattering

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

$$A_{i,j} = \delta_{i,j} - V(k_i, k_j)u_j, \tag{20}$$

The Lippman-Schwinger equation for two-nucleon scattering

where δ is the Kronecker δ and

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

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 Lippman-Schwinger equation for two-nucleon scattering

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

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

or just

$$AR = V.$$

The Lippman-Schwinger equation for two-nucleon scattering

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.,

$$R = A^{-1}V. \tag{21}$$

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.

The Lippman-Schwinger equation for two-nucleon scattering

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 δ are the phase shifts.

The Lippman-Schwinger equation for two-nucleon scattering

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 δ_l, from which we can define the S-matrix $S_l(k) = e^{2i\delta_l(k)}$. Thus, we have

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

The Lippman-Schwinger equation for two-nucleon scattering

The solution to the Schrodinger 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 δ_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 $e^{-il\pi/2}$

The Lippman-Schwinger equation for two-nucleon scattering

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 Eulers formula for the cotangent, this can also be written as

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

The Lippman-Schwinger equation for two-nucleon scattering

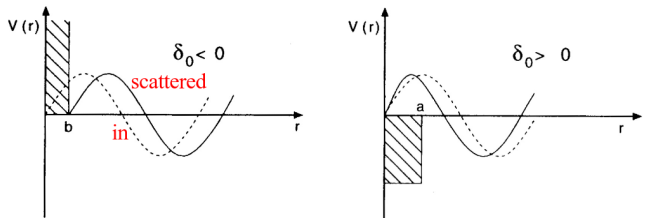

Figure 1: Examples of negative and positive phase shifts for repulsive and attractive potentials, respectively.

Interpretation of phase shifts.

The Lippman-Schwinger equation for two-nucleon scattering

The integrated cross section is given by

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

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

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

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.

The Lippman-Schwinger equation for two-nucleon scattering

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

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

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

$$k\cot\delta_0 = -\frac{1}{a} + \frac{1}{2}r_0k^2 + \dots$$

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.

The Lippman-Schwinger equation for two-nucleon scattering

Low energy scattering length.

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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),

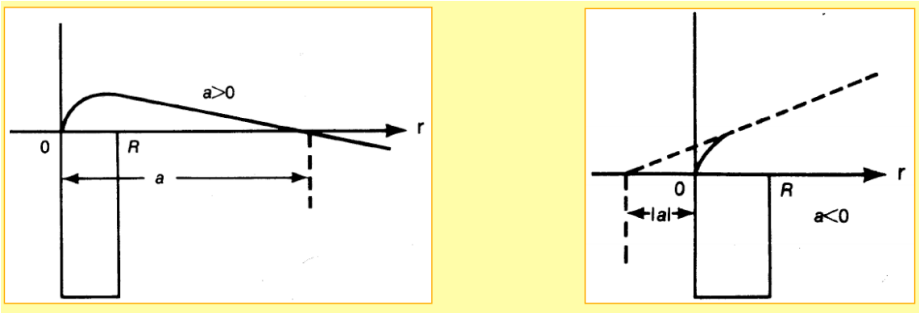

Figure 2: Examples of scattering lengths.

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!

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TABLE IV. *pp* isovector phase shifts and their multienergy error in degrees as obtained in the multienergy *pp* analysis. Errors smaller than 0.0005° are not shown. The lower part lists the phase shifts as obtained in the combined $pp+np$ analysis.

T_{lab}	$^1S_0$	$^1D_2$	$^1G_4$	$^3P_0$	$^3P_1$	$^3F_3$	$^3P_2$	ϵ_2	$^3F_2$	$^3F_4$	ϵ_4	$^3H_4$
1	32.684	0.001	0.000	0.134	−0.081	−0.000	0.014	−0.001	0.000	0.000	−0.000	0.000
	±0.005											
5	54.832	0.043	0.000	1.582	−0.902	−0.005	0.214	−0.052	0.002	0.000	−0.000	0.000
	±0.017			±0.006	±0.001		±0.001					
10	55.219	0.165	0.003	3.729	−2.060	−0.032	0.651	−0.200	0.013	0.001	−0.004	0.000
	±0.025			±0.017	±0.002		±0.002					
25	48.672	0.696	0.040	8.575	−4.932	−0.231	2.491	−0.810	0.105	0.020	−0.049	0.004
	±0.039	±0.001		±0.053	±0.008		±0.008	±0.001				
50	38.899	1.711	0.152	11.47	−8.317	−0.690	5.855	−1.712	0.338	0.108	−0.195	0.026
	±0.049	±0.004		±0.09	±0.017		±0.016	±0.004		±0.001		
100	24.97	3.790	0.418	9.45	−13.258	−1.517	11.013	−2.659	0.817	0.478	−0.539	0.108
	±0.08	±0.018	±0.001	±0.11	±0.032	±0.003	±0.025	±0.017	±0.004	±0.007		
150	14.75	5.606	0.700	4.74	−17.434	−2.100	13.982	−2.873	1.197	1.032	−0.849	0.211
	±0.13	±0.033	±0.003	±0.14	±0.045	±0.010	±0.039	±0.029	±0.014	±0.022		
200	6.55	7.058	0.993	−0.37	−21.25	−2.487	15.63	−2.759	1.424	1.678	−1.108	0.321
	±0.16	±0.045	±0.010	±0.17	±0.07	±0.025	±0.052	±0.037	±0.034	±0.039		
250	−0.31	8.27	1.272	−5.43	−24.77	−2.724	16.59	−2.542	1.47	2.325	−1.314	0.428
	±0.18	±0.06	±0.024	±0.21	±0.12	±0.049	±0.07	±0.046	±0.06	±0.051		
300	−6.15	9.42	1.503	−10.39	−27.99	−2.84	17.17	−2.34	1.34	2.89	−1.47	0.526
	±0.25	±0.08	±0.048	±0.33	±0.19	±0.11	±0.10	±0.09	±0.11	±0.06		
350	−11.13	10.69	1.64	−15.30	−30.89	−2.87	17.54	−2.21	1.04	3.30	−1.588	0.608
	±0.46	±0.14	±0.08	±0.57	±0.27	±0.13	±0.15	±0.11	±0.16	±0.11	±0.001	
100	24.97	3.782	0.418	9.55	−13.245	−1.518	11.013	−2.654	0.816	0.471	−0.539	0.108
	±0.08	±0.017		±0.09	±0.030	±0.002	±0.021	±0.016	±0.003	±0.006		
200	6.55	7.039	0.993	−0.27	−21.18	−2.499	15.65	−2.731	1.414	1.656	−1.107	0.321
	±0.16	±0.043	±0.008	±0.17	±0.06	±0.021	±0.05	±0.035	±0.029	±0.034		
300	−6.22	9.42	1.501	−10.44	−27.80	−2.89	17.15	−2.27	1.30	2.95	−1.473	0.526
	±0.23	±0.08	±0.040	±0.29	±0.16	±0.07	±0.09	±0.06	±0.09	±0.05		

Figure 3: Nijmegen phase shifts for selected partial waves.

Nijmegen multi-energy *pp* PWA phase shifts. 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 χ^2/datum with respect to the scattering data base

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Nijmegen multi-energy *pp* PWA phase shifts.

$T_{\rm lab}$ bin (MeV)	N3LO[1]	NNLO[2]	NLO[2]	AV18[3]
0-100	1.05	1.7	4.5	0.95
100-190	1.08	22	100	1.10
190-290	1.15	47	180	1.11
0 – 290	**1.10**	**20**	**86**	**1.04**

- R. Machleidt et al., Phys. Rev. C68, 041001(R) (2003)
- E. Epelbaum et al., Eur. Phys. J. A19, 401 (2004)
- R. B. Wiringa et al., Phys. Rev. C5, 38 (1995)

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An example: chiral twobody interactions.

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

- R. Machleidt, D. R. Entem, Phys. Rep. 503, 1 (2011)
- E. Epelbaum, H.-W. Hammer, Ulf-G. Meißner, Rev. Mod. Phys. 81, 1773 (2009)

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Proton-neutron $^1S_0$ phase shift. Note that the Nijm93 PWA phase shift becomes negative at $\rm T_{lab} > 250$MeV. This indicates that the nucleon-nucleon potential is repulsive at short distances

The Lippman-Schwinger equation for two-nucleon scattering

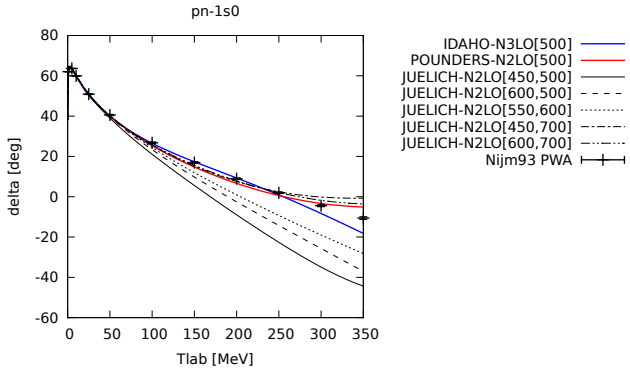

Figure 4: Proton-neutron $^1S_0$ phase shift.

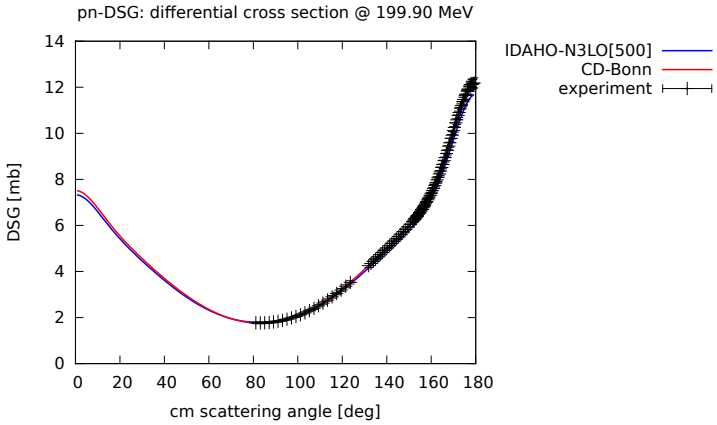

Figure 5: Proton-neutron $^1S_0$ phase shift.

Differential cross section.