Scattering Notes

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Abstract

In these notes I provide an overview of time-dependent scattering theory.

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1 Classical Scattering

I begin with a discussion of scattering of a particle by a potential in classical mechanics. This discussion is based primarily on the textbook by Araki (chapter 6) and the article by Hunziker (see also the text by Thirring).

I assume that the dynamics is given by a classical Hamiltonian that is the sum of a kinetic energy term and a potential that vanishes for large values of the particle coordinate:

$$H = H_0 + V \qquad H_0 = \frac{p^2}{2m}, \quad V = V(\vec{x}). \tag{1}$$

The dynamics of the particle is given by Hamilton's equations

$$\frac{d\vec{p}}{dt} = -\{H, \vec{p}\} = -\frac{\partial H}{\partial \vec{x}} = -\frac{\partial V}{\partial \vec{x}} \tag{2}$$

$$\frac{d\vec{x}}{dt} = -\{H, \vec{x}\} = \frac{\partial H}{\partial \vec{p}} = \frac{\partial H_0}{\partial \vec{p}} = \frac{\vec{p}}{m} \tag{3}$$

where $\{A, B\}$ is the classical Poisson bracket of A and B.

These are ordinary differential equations. I call a potential *acceptable* if for each initial condition these equation have a unique solution for all time. While local solutions are guaranteed by standard existence and uniqueness theorems for ordinary differential equations, the question of when these equations can be extended to all times is more difficult. I will not attempt to classify acceptable potentials, however every potential that describes a physical system is acceptable.

I use the following notation for phase space variables:

$$\vec{f} := (\vec{x}, \vec{p}) \tag{4}$$

In terms of these variables the differential equations can be written in the form

$$\frac{d\vec{f}}{dt} = -\{H, \vec{f}\} := -D_H \vec{f} \tag{5}$$

where D_H is the first-order differential operator

$$D_H = \sum_i \left(\frac{\partial H}{\partial x_i}\frac{\partial}{\partial p_i} - \frac{\partial H}{\partial p_i}\frac{\partial}{\partial x_i} \right) \tag{6}$$

The unique solution of the above equations satisfying $\vec{f} = \vec{f_0}$ at $t = t_0$ is denoted by

$$\vec{F}(t; \vec{f_0}, t_0) \tag{7}$$

which can be formally written as

$$\vec{F}(t; \vec{f_0}, t_0) = e^{-D_H(t-t_0)} \vec{f}_{|f=f_0}$$

Here the condition $f = f_0$ means that one should compute all partial derivatives first and then evaluate the expression at $x = x_0$ and $p = p_0$. A simple calculation shows that if the exponential function is expanded in powers of $t - t_0$ this generates the Taylor series in time.

When $V(\vec{x}) = 0$ the solution of this system of equations is

$$\vec{F_0}(t, \vec{f_0}, t_0) = (\vec{x}_0 + \frac{\vec{p_0}}{m}(t - t_0), \vec{p_0}) \tag{8}$$

which is the solution of Hamilton's equations for constant velocity motion.

Scattering concerns Hamiltonians H where the potential $V(\vec{x})$ vanishes for sufficiently large finite $\vec{x}$. To be specific I assume that the potential satisfies

$$V(\vec{x}) = 0 \qquad |\vec{x}| < R < \infty. \tag{9}$$

If a particle has a coordinate $\vec{x}_0$ with $|\vec{x}_0| > R$ at time t_0 then it also satisfies the free particle equations of motion. As mentioned above, as long as the particle does not feel the interaction, the motion is in a straight line. There are three possibilities:

1. The particle is moving towards the target. This means that the straight-line trajectory will intersect the region where the potential is non-zero in the future.

2. The particle is moving away from the target. This means that the straight-line trajectory intersected the region where the potential is non-zero in the past.

3. The straight line trajectory never intersects the region where the potential is non-zero.

For case 1 there is a solution of Hamilton's equations, $\vec{F}_-(t; f_0, t_0)$, satisfying the asymptotic condition

$$\lim_{t\to-\infty} |\vec{F}_-(t; f_0, t_0) - \vec{F}_0(t; f_0', t_0')| = 0. \tag{10}$$

I can also write this in the equivalent form

$$\lim_{t\to-\infty} |[e^{-D_H(t-t_0)}\vec{f}_{|_{f=f_0}} - e^{-D_{H_0}(t-t_0')}\vec{f}_{|_{f=f_0'}}| = 0 \tag{11}$$

Note the initial times and coordinates do not have to be the same in these two solutions, however they are constrained because for sufficiently large negative time the coordinates and moment of these solutions agree. In this case when $t < -t_0$ the right hand side is *identically* zero. The $-$ sign denotes the solution of the interacting problem that asymptotically looks like a free particle in past.

For case 2 there is a solution of Hamilton's equations,

$$\vec{F}_+(t; \vec{f}_i, t_i) \tag{12}$$

satisfying the asymptotic condition

$$\lim_{t\to+\infty} |\vec{F}_+(t; f_0, t_0) - \vec{F}_0(t; f_0', t_0')| = 0 \tag{13}$$

or equivalently

$$\lim_{t\to-\infty} |[e^{-D_H(t-t_0)}\vec{f}_{|_{f=f_0}} - e^{-D_{H_0}(t-t_0')}\vec{f}_{|_{f=f_0'}}| = 0 \tag{14}$$

The + sign denotes the solution of the interacting problem that asymptotically looks like a free particle in future.

Equations (10) and (13) are called scattering asymptotic conditions. Generalizations of these equations will be important for the entire course. They relate the unique solution of the non-interacting system that agrees with the interacting systems for large positive or negative time.

One formulation of the scattering problem is to relate the initial and final scattering asymptotes. This can be done if the particle trajectory is such that it both enters and exits the interaction region. This does not have to happen. A particle coming into the interaction region along a straight line trajectory could be trapped by the potential. Likewise a particle that was always in the interaction region could be ejected in a straight-line trajectory.

In the case that the particle both enters and exits the interaction region then at some time t_i it will have phase-space coordinates $\vec{f_i}$ in the interaction region. Since Hamilton's equations have unique solutions for each initial condition we necessarily have

$$\vec{F}_-(t; \vec{f_i}, t_i) = \vec{F}_+(t; \vec{f_i}, t_i) \tag{15}$$

for all time t.

Choose a time t_l that is sufficiently large that

$$(\vec{x}_+, \vec{p}_+) = \vec{f_+} := \vec{F}_+(t_l; \vec{f_i}, t_i) \tag{16}$$

and

$$(\vec{x}_-, \vec{p}_-) = \vec{f_-} := \vec{F}_-(-t_l; \vec{f_i}, t_i) \tag{17}$$

is out of the range of the potential.

The corresponding free particle solutions that satisfy the asymptotic condition (10) and (13) are

$$F_{0+}(t; \vec{f_+}, t_l) := (\vec{x}_+ + \frac{\vec{p}_+}{m}(t - t_l), \vec{p}_+) \tag{18}$$

$$F_{0-}(t;\vec{f}_-,-t_l) := (\vec{x}_- + \frac{\vec{p}_-}{m}(t+t_l),\vec{p}_-). \tag{19}$$

The scattering operator is the mapping that maps the initial scattering asymptote to the final scattering asymptote

$$S[F_{0+}(t;\vec{f}_+,t_l)] = F_{0-}(t;\vec{f}_-,-t_l). \tag{20}$$

From the above this relation is determined by the solution of the dynamical equations.

Another property of the scattering operator concerns symmetries. In classical mechanics the condition

$$\{G,H\} = 0 \tag{21}$$

means

$$\frac{dG}{dt} = \frac{\partial G}{\partial \vec{q}}\cdot\frac{d\vec{q}}{dt} + \frac{\partial G}{\partial \vec{p}}\cdot\frac{d\vec{p}}{dt} = \tag{22}$$

$$\frac{\partial G}{\partial \vec{q}}\cdot\frac{\partial H}{\partial \vec{p}} + \frac{\partial G}{\partial \vec{p}}\cdot\frac{-\partial H}{\partial \vec{q}} = \{G,H\} = 0 \tag{23}$$

which shows that $G(t)$ does not change in time. This means that the value of G does not change along the trajectory of the particle in phase space. Since the physical trajectory is identical to the asymptotic trajectories for $|t| > |t_l|$, this means that it has the same value on each asymptote. It follows that the scattering operator has the same symmetry.

A simple example is the case that $G = H$, which shows that the a particle moving along the initial and final scattering asymptote have the same energy.

In this classical case the scattering operator maps any incoming asymptote to the associated outgoing asymptote. Many of the concepts discussed in this classical case will be reformulated in the quantum mechanical case.

2 Quantum Theory

I begin with a brief discussion of the essential elements of quantum theory.

In quantum theory the state of a system is described by a ray, or one-dimensional subspace in a complex vector space, or Hilbert space. In most applications rays are represented by unit normalized vectors. In what follows I will use Dirac notation to denote states, $|\psi\rangle$.

If a physical system is prepared in a state represented by a vector $|\psi\rangle$ and a measurement is made to determine if the systems is in a different state, $|\phi\rangle$, the result of a given experiment will be "yes" or "no". If the same experiment is repeated a large number of times the ratio of the "yes" outcomes ,N_y, to the total number of measurements N approaches the probability

$$\lim_{N\to\infty} \frac{N_y}{N} = |\langle\phi|\psi\rangle|^2. \tag{24}$$

This probability on the right-hand side of this equation is a prediction of quantum theory.

In a scattering experiment a typical goal is to measure of the probability that in a large ensemble of scattering experiments that a given detector will register a "count". Additional care is needed because the detector will register "yes" for several quantum states. Likewise the ensemble of beam-target states will normally contain different states.

This discussion is abstract. The structure of the Hilbert space is fixed by the experiment. The construction of the relevant Hilbert space is done by defining a complete measurement of the state of the physical system. A complete measurement involves measuring the eigenvalues of a maximal set of mutually commuting Hermitian operators. For an N-particle system a complete measurement involves a measurement of the mass, linear momentum, total spin, and magnetic quantum number of each particle. These measurements are normally done when the particles are separated beyond the range of their mutual interaction. These measurements are compatible in the sense that the outcome of each measurement does not depend on the order of the measurements. More generally if the commuting operators are $O_1 \cdots O_N$ with eigenvalues $\eta_1 \cdots \eta_N$, then the "wave function" of the state $|\psi\rangle$ is

$$\langle \eta_1, \cdots, \eta_N|\psi\rangle \tag{25}$$

The wave function has the interpretation that

$$|\langle \eta_1, \cdots, \eta_N|\psi\rangle|^2 \tag{26}$$

is the probability that if the system is prepared in the state $|\psi\rangle$ that a measurement of O_1, $O_2, \cdots$, and O_N will yield values $\eta_1, \eta_2, \cdots$ and η_N.

The requirement that a measurement of all of these quantities has to be in the set of eigenvalues of these operators with probability 1 gives the

normalization condition

$$1 = \sum_{\eta_1 \cdots \eta_N} |\langle \eta_1 \cdots \eta_N | \psi \rangle|^2. \tag{27}$$

This also yields an explicit representation for the Hilbert-space scalar product

$$\langle \phi | \psi \rangle = \sum_{\eta_1, \cdots, \eta_N} \langle \phi | \eta_1, \cdots, \eta_N \rangle \langle \eta_1, \cdots, \eta_N | \psi \rangle. \tag{28}$$

In theses two expressions the sum over η_i ranges over all possible eigenvalues of O_i. When some of the operators have a continuous eigenvalue spectrum the sum over eigenvalues is replaced by an integral over the eigenvalues.

While one can in principle formulate quantum mechanics using any set of commuting observables, nature limits the set of commuting observables that can be used to label the states of realistic systems. The relevant macroscopic observables are related to the behavior of free particles after they enter classical electromagnetic and gravitational fields. These fields, along with conservation laws, can be used to measure the momentum and magnetic quantum numbers of free particles. This is relevant because these are the normal observables of the scattering matrix in both classical and quantum mechanics.

3 Quantum Dynamics

The previous section discussed quantum measurements. In this section I introduce dynamics. It is a reasonable physical requirement that the laws of physics do not change with time. This is the simplest formulation of the principle of relativity.

Classically this means that if the time is shifted in the classical equation of motion, the solutions (as functions of initial conditions) do not change. In Hamilton's equations this means that the potentials do not have an explicit time dependence. This is the appropriate form of the relativity condition because the solution of the equations of motion, which are the coordinates and momenta of the particles, are experimental observables.

The above discussion applies only to isolated systems, where there are no externally applied forces. For isolated systems the relevant forces are the fundamental forces of nature associated with the electromagnetic, weak,

strong, and gravitational interactions. This statement means that these basic forces do not change in time.

This principle has to be modified in quantum mechanics because the prediction of the theory is a probability. The time translation invariance of the measurement requires that the probabilities are time independent, *not the equations of motion.*

In quantum mechanics I formulate this condition by assuming an abstract correspondence between equivalent states at different times:

$$|\psi(t)\rangle \to |\psi(t')\rangle. \tag{29}$$

Time translation invariance is the requirement

$$|\langle\psi(t)|\phi(t)\rangle|^2 = |\langle\psi(t')|\phi(t')\rangle|^2 \tag{30}$$

for all time. This means that I cannot experimentally distinguish the results of equivalent experiments done at different times.

If this is true for all vectors then Wigner's theorem [**?**] [**?**] requires

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle \tag{31}$$

$$|\phi(t)\rangle = U(t)|\phi(0)\rangle \tag{32}$$

where $U(t)$ is a unitary or anti-unitary operator. Consistency of

$$|\psi(t+t')\rangle = U(t+t')|\psi(0)\rangle = U(t)U(t')|\psi(0)\rangle = U(t')U(t)|\psi(0)\rangle \tag{33}$$

for all $|\psi(0)\rangle$ implies

$$U(t+t') = U(t)U(t') = U(t')U(t) \tag{34}$$

and

$$U(t) = U(t/2)U(t/2). \tag{35}$$

Since the composition of two anti-unitary transformations is unitary, equation (35) means the $U(t)$ must be unitary. Technically because the physical states are described by rays, these relations only have to hold up to a phase. In the simplest cases [**?**] the phases can be absorbed into the unitary operators. Similar arguments give

$$U(0) = I \qquad U(-t) = U^\dagger(t) = U^{-1}(t). \tag{36}$$

If I let $t'' = t + t'$ it is easy to calculate

$$\frac{dU(t'')}{dt''}U^\dagger(t'') = \frac{dt''}{dt}\frac{dU(t+t')}{dt}U^\dagger(t+t') = \tag{37}$$

$$\frac{dU(t)}{dt}U(t')U^\dagger(t')U^\dagger(t) = \frac{dU(t)}{dt}U^\dagger(t) \tag{38}$$

which shows explicitly that $\frac{dU(t)}{dt}U^\dagger(t)$ is independent of time t.

If I differentiate

$$0 = \frac{d}{dt}I = \frac{d}{dt}U(t)U^\dagger(t) = \frac{dU(t)}{dt}U^\dagger(t) + U(t)\frac{dU^\dagger(t)}{dt} \tag{39}$$

I get

$$i\frac{dU(t)}{dt}U^\dagger(t) = -iU(t)\frac{dU^\dagger(t)}{dt}[i\frac{dU(t)}{dt}U^\dagger(t)]^\dagger \tag{40}$$

which shows that

$$i\frac{dU(t)}{dt}U^\dagger(t) \tag{41}$$

is a time independent Hermitian operator. It has units of inverse time. The quantity

$$H := i\hbar\frac{dU(t)}{dt}U^\dagger(t) \tag{42}$$

has units of energy. It is the Hamiltonian of the quantum mechanical system. In all that follows I use units where $\hbar = c = 1$.

Equation (42) can be written as a differential equation for $U(t)$:

$$\frac{dU(t)}{dt} = -iHU(t) \qquad U(0) = I \tag{43}$$

This has the formal solution

$$U(t) = e^{-iHt} \tag{44}$$

which is the standard expression for the time evolution operator. The Schrödinger is obtained by noting that

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle. \tag{45}$$

With this identification (43) becomes the Schrödinger equation for the state vector $|\psi(t)\rangle$:

$$i\frac{d|\psi(t)\rangle}{dt} = H|\psi(t)\rangle. \tag{46}$$

Stone's theorem [**?**] implies that if the time translation operator $U(t)$ is (strongly) continuous that Hamiltonians constructed in this manner are necessarily self-adjoint operators on the Hilbert space.

4 Hilbert Space Topologies

In this section I look at properties of free particles to discuss the proper formulation of the asymptotic conditions in quantum mechanics. In this section I take consider a Hamiltonian of the form that was discussed in the classical example:

$$H = \frac{p^2}{2m} + V(\vec{x}), \qquad V(\vec{x}) = 0, \quad |\vec{x}| > R \tag{47}$$

In a quantum theory Hamilton's equations are replaced by the Schrödinger equation:

$$i\frac{d|\psi(t)\rangle}{dt} = H|\psi(t)\rangle. \tag{48}$$

When the interaction is turned off this becomes the Schrödinger equation for a free particle:

$$i\frac{d|\psi_0(t)\rangle}{dt} = H_0|\psi_0(t)\rangle. \tag{49}$$

The expectation, based on the classical example, is that a solution of (48) should approach a solution of (49) as $t \to \pm\infty$. The formulation of how this happens is not entirely trivial. It depends on how we define convergence of operators in the Hilbert space.

Before I can properly formulate the asymptotic condition it is instructive to consider solutions of (49) corresponding to a particle moving with a linear momentum $\vec{p}_0$. The initial state can be described by a wave function of the form

$$\langle\vec{p}|\psi_0(0)\rangle = Ne^{-\frac{(\vec{p}-\vec{p}_0)^2}{2a^2}} \tag{50}$$

where a is a constant with units of momentum that fixes the width of the wave packet and N is a normalization constant. The vector $\vec{p}_0$ is a constant that describes the momentum of the wave packet. I use the Gaussian form for the purpose of illustration. It has the advantage that integrals can be done analytically and it has the additional feature that it is a minimal uncertainty state.

The solution of the configuration space Schrödinger equation with this initial condition is

$$\langle\vec{x}|\psi_0(t)\rangle = \frac{N}{(2\pi)^{3/2}}\int e^{i\vec{p}\cdot\vec{x}}e^{-i\frac{\vec{p}\cdot\vec{p}}{2m}t}e^{-\frac{(\vec{p}-\vec{p}_0)^2}{2a^2}}d^3p. \tag{51}$$

This is a Gaussian integral that can be done using the standard integral

$$\int_{-\infty}^{\infty} e^{-au^2+bu+c}du = \sqrt{\frac{\pi}{a}}e^{\frac{b^2}{4a}+c} \tag{52}$$

The integral (51) breaks up into a product of three identical Gaussian integrals. To compute the integral we write it in the standard form:

$$\langle\vec{x}|\psi_0(t)\rangle = \frac{N}{(2\pi)^{3/2}}\int e^{-(\frac{1}{2a^2}+i\frac{t}{2m})\vec{p}\cdot\vec{p}+\vec{p}\cdot(i\vec{x}+\frac{\vec{p}_0}{a^2})-\frac{\vec{p}_0\cdot\vec{p}_0}{2a^2}}d^3p. \tag{53}$$

Using the standard Gaussian integral this becomes

$$\langle\vec{x}|\psi_0(t)\rangle = \frac{N}{(2\pi)^{3/2}}\frac{2a^2\pi}{(1+i\frac{ta^2}{m})^{3/2}}e^{-\frac{a^2}{2}\frac{1}{1+\frac{t^2a^4}{m^2}}(\vec{x}-\frac{\vec{p}_0t}{m})^2}e^{i\phi(\vec{x},t)} \tag{54}$$

where $\phi(\vec{x},t)$ is the real phase factor:

$$\phi(\vec{x}.t) = \vec{x}\cdot\vec{p}_0 - \frac{\vec{p}_0\cdot\vec{p}_2}{2m}t + \frac{a^4\vec{x}\cdot\vec{x}t}{2m}. \tag{55}$$

This expression has two important properties. First, because the time-evolution is unitary this remains normalized to unity for all time. The second property is that the wave packed spreads out. The peak of the wave function moves with the classical velocity $\vec{p}_0/m$ but the maximum amplitude falls off like $t^{-3/2}$ for large values of t, while the width of the wave packet gets correspondingly wide.

These observations have important consequences for the formulation of the asymptotic condition in quantum mechanics. The naive requirement that

$$\lim_{t\to\pm\infty}|\langle\vec{x}|\psi(t)\rangle - \langle\vec{x}|\psi_0(t)\rangle| = 0 \tag{56}$$

is useless for scattering. This is because for any value of x both terms separately vanish for large times. So far we have only shown this for $\langle\vec{x}|\psi_0(t)\rangle$, but we will establish it for both terms shortly.

So while the condition is true, it vanishes because both terms go to zero rather than having non-zero terms that asymptotically become identical.

It is also true if the wave function is replaced by a limit involving matrix elements of the form

$$\lim_{t\to\pm\infty}|\langle\phi|\psi(t)\rangle - \langle\phi|\psi_0(t)\rangle| = 0 \tag{57}$$

where $|\phi\rangle$ is any other vector in the space. Again, for any fixed $|\phi\rangle$ both terms vanish separately.

This behavior can be easily understood in the general case by noting that

$$\langle\phi|\psi(t)\rangle = \int dE e^{-iEt} \int du \langle\phi|E,u\rangle\langle E,u|\psi\rangle \tag{58}$$

where E is the free energy eigenvalue and u indicates any other quantum numbers that are needed to get a complete set of commuting observables. The normalizability of the wave functions means that

$$f(E) = \int du \langle\phi|E,u\rangle\langle E,u|\psi\rangle \tag{59}$$

is absolutely integrable. The Riemann-Lebesgue lemma then requires that

$$\lim_{t\to\pm\infty} \int dE e^{-iEt} f(E) = 0. \tag{60}$$

The same argument applies in the interacting case.

The limit in equation (57) is called a weak limit. It is a limit involving matrix elements. Formally $|\psi_n\rangle$ converges weakly to $|\psi\rangle$ provided

$$\lim_{n\to\infty} |\langle\phi|\psi_n\rangle - \langle\phi|\psi\rangle| = 0 \tag{61}$$

for every normalizable vector ϕ. What is relevant for weak limits is that the rate of convergence can be different for different choices of $\langle\phi|$.

To understand how to proceed, we note that even though the peak value of the time evolved state becomes smaller, this is exactly compensated for by an increase in the width of the wave function for large time. This is easy to see because

$$\langle\psi(t)|\psi(t)\rangle = \langle\psi(0)|U_0^\dagger(t)U_0(t)\psi(0)\rangle = \langle\psi(0)|\psi(0)\rangle \tag{62}$$

is time independent by unitarity. This suggests that the asymptotic condition can be formulated using limits involving the Hilbert space norm rather than matrix elements:

$$\lim_{t\to\pm\infty} \||\psi_\pm(t)\rangle - |\psi_0(t)\rangle\| = 0 \tag{63}$$

This limit is called a **strong limit**. If the limit is a strong limit it means that the rate of convergence of different matrix elements in (61) is independent

of $\langle\phi|$. It is obvious from this characterization that if something converges strongly it also converges weakly. The converse is not true.

In what follows I show that the strong limit leads to a non-trivial formulation of the asymptotic condition in quantum mechanics. I will use this form of the asymptotic condition to formulate quantum scattering theory.

While strong limit can be used to formulate a scattering theory, it is not the only possible formulation of the asymptotic condition. Some alternate formulations [**?**] involve the strong Abelian limit:

$$\lim_{\epsilon\to 0}\epsilon\int_0^\infty e^{-\epsilon t}\||\psi_\pm(t)\rangle - |\psi_0(t)\rangle\|dt = 0 \tag{64}$$

and the Cesaro mean

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T \||\psi_\pm(t)\rangle - |\psi_0(t)\rangle\|dt = 0. \tag{65}$$

Most results that can be proved with one type of limit can also be proved with one of the other limits. Note that both the Cesaro mean and the strong Abelian limit involve vector norms.

Finally there is one more type of limit that is important for scattering. This is the uniform limit, which applies to operators. To illustrate the difference in all three limits consider a set of operators W_n and a limiting operator W.

The operators W_n converge weakly to W if

$$\lim_{t\to\infty}|\langle\phi|W_n|\psi\rangle - \langle\phi|W|\psi\rangle| = 0 \tag{66}$$

for all $\langle\phi|$ and $|\psi\rangle$.

The operators W_n converge strongly to W if

$$\lim_{t\to\infty}\|W_n|\psi\rangle - W|\psi\rangle\| = 0 \tag{67}$$

for all $|\psi\rangle$.

The operators W_n converge uniformly to W if

$$\lim_{t\to\infty}\|W_n - W\| = 0. \tag{68}$$

In the uniform case the rate of convergence is independent of any states, and only depends on the operator.

Uniform convergence plays an important role in solving the equations of scattering theory.

5 Møller wave operators

In this section I show that the strong limits defined in the previous section lead to non-trivial asymptotic conditions. Before getting started, I discuss the physics of the asymptotic condition.

As in the classical case, long before the particle is within the range of the potential, it looks like a free particle. The state of this particle should be described by a localized wave packet with a mean momentum $\vec{p}_0$ directed at the target. The Gaussian wave function of the previous section is a suitable candidate for such a wave function. There are two relevant state vectors. One satisfies the Schrödinger with the interacting Hamiltonian and the other satisfies the Schrödinger equation with a free particle Hamiltonian:

$$i\frac{d|\psi_-(t)\rangle}{dt} = H|\psi_-(t)\rangle \tag{69}$$

$$i\frac{d|\psi_{-0}(t)\rangle}{dt} = H_0|\psi_{-0}(t)\rangle. \tag{70}$$

The Schrödinger equation is first order in time, so to obtain a solution it is necessary to specify an initial condition. This is done by demanding that the non-interacting and interacting solutions of the Schrödinger equation agree for some sufficiently large negative time:

$$\lim_{t\to-\infty} \|U(t)|\psi_-(0)\rangle - U_0(t)|\psi_0(0)\rangle\| = 0. \tag{71}$$

Note that in a real scattering experiment this condition is well satisfied for finite times, however the value of the finite time depends on the initial wave packet. Letting $t \to -\infty$ provides a means to treat all states simultaneously. The price for doing this is that in the limit that $t \to -\infty$ all of the wave functions spread out. This is why the strong limits are needed. It is important to note however in a real experiment the wave packets associated with the beam and detector remain highly localized over experimental time scales.

It is possible to use the unitarity of $U(t)$ to rewrite the asymptotic condition (71) in the equivalent form

$$\lim_{t\to-\infty} \||\psi_-(0)\rangle - U(-t)U_0(t)|\psi_0(0)\rangle\| = 0 \tag{72}$$

The relevant limiting operator

$$\boxed{\Omega_- = \Omega_-(H, H_0) := s\lim_{t\to-\infty} U(-t)U_0(t)} \tag{73}$$

is called the Møller wave operator. The s is a reminder that the relevant limit is a strong limit.

The wave operator Ω_- satisfies

$$|\psi_-(0)\rangle = \Omega_-|\phi_{0-}(0)\rangle. \tag{74}$$

The solutions of the interacting and non-interacting Schrödinger equations at time zero are expected to be localized states. The wave operators relate these states. If all of the limits exist it should be a well behaved operator.

As in the classical case, it is also useful to formulate an asymptotic condition as $t \to +\infty$. This leads to the asymptotic condition

$$\lim_{t\to+\infty} \||\psi_+(0)\rangle - U(-t)U_0(t)|\psi_{0+}(0)\rangle\| = 0 \tag{75}$$

and

$$\Omega_+(H, H_0) := s \lim_{t\to+\infty} U(-t)U_0(t) \tag{76}$$

The wave operator Ω_+ satisfies

$$|\psi_+(0)\rangle = \Omega_+|\phi_{0+}(0)\rangle. \tag{77}$$

Given the solution of the Schrödinger equation at time zero that looked like a free particle moving towards the target in the past and another solution that looks like a free particle moving towards the detector in the future, we can calculate the probability amplitude for the corresponding transition:

$$S_{fi} := \langle\psi_+(0)|\psi_-(0)\rangle = \langle\psi_{0+}(0)|\Omega_+^\dagger(H, H_0)\Omega_-(H, H_0)|\psi_{0-}(0)\rangle. \tag{78}$$

The quantity S_{fi} is called **scattering matrix**. The associated operator

$$\boxed{S = S(H, H_0) := \Omega_+^\dagger(H, H_0)\Omega_-(H, H_0)} \tag{79}$$

is called the **scattering operator**. The quantity

$$P_{fi} := |S_{fi}|^2 \tag{80}$$

represents the probability that a particle in a state that looks like $|\psi_{0-}(t)\rangle$ as $t \to -\infty$ transitions to a state that looks the $|\psi_{0+}(t)\rangle$ as $t \to \infty$.

This can be used to calculate the probability that a given detector will detect the particle if the beam is prepared with a sharply peaked momentum heading towards the target,

In what follows I establish sufficient conditions for the existence of the strong limits that define the wave operators: Consider

$$\lim_{t\to\pm\infty} \|U(-t)U_0(t)|\psi(0)\rangle\| = \|[\int_0^{\pm\infty} \frac{d}{dt}U(-t)U_0(t) - I]|\psi(0)\rangle\|dt \tag{81}$$

To show that this integral converges note that if I think of the integral as a limit of Riemann sums and then use the triangle inequality

$$\||\phi\rangle + |\psi\rangle\| \leq \||\phi\rangle\| + \||\psi\rangle\| \tag{82}$$

on each term in the sum I obtain

$$\| \int_0^{\pm\infty} \frac{d}{dt}U(-t)U_0(t)|\psi(0)\rangle dt\| \leq \tag{83}$$

$$\int_0^{\pm\infty} \|U(-t)VU_0(t)|\psi(0)\rangle\|dt = \int_0^{\pm\infty} \|V|\psi(t)\rangle\|dt. \tag{84}$$

In the last step I used the unitarity of $U(-t)$ for all t to get:

$$\|U(-t)VU_0(t)|\psi(0)\rangle\| = \|VU_0(t)|\psi(0)\rangle.\| \tag{85}$$

The condition that

$$\boxed{\int_0^{\pm\infty} \|V|\psi(t)\rangle\|dt < \infty} \tag{86}$$

for a dense set of vectors is called Cook's condition.

Note that a dense set of vectors is a set of vectors $|\psi_n\rangle$ that can be used to approximate any vector $|\psi\rangle$ in the sense that for any $\epsilon > 0$ there is an N such that for any $n > N$

$$\||\psi_n\rangle - |\psi\rangle\| < \epsilon \tag{87}$$

To use this in the above note

$$\|[U(-t)U_0(t)-U(-t')U_0(t')]|\psi_0(0)\rangle\| \leq \|[U(-t)U_0(t)-U(-t')U_0(t')]|\psi_{n0}(0)\rangle\|+$$

$$\|[U(-t)U_0(t)[|\psi_0(0)\rangle - |\psi_{n0}(0)\rangle]\|+$$

$$\|[U(-t')U_0(t')[|\psi_0(0)\rangle - |\psi_{n0}(0)\rangle]\| = \tag{88}$$

$$\|[U(-t)U_0(t) - U(-t')U_0(t')]|\psi_{n0}(0)\rangle\| + 2\||\psi_0(0)\rangle|\psi_{n0}(0)\rangle\| \tag{89}$$

The first term involves a vector in the dense set and can be made as small as desired by choosing t sufficiently large while the second term can be made as small as desired by choosing n large enough. This is done by first choosing n large enough to make the second term sufficiently small; for that value of n I choose t large enough to make the first term small. It follows that the left side of this equation can be made as small as desired.

A necessary and sufficient way to to check if a sequence $\|f_n - f\| \to 0$ is convergent is to check that the sequence is a Cauchy sequence. This means for every $\epsilon > 0$ I can find a large enough N such that for every $m, n > N$

$$\|f_m - f_n\| < \epsilon$$

The proof shows that the sequence itself has all of the properties of a vector and actually coincides with f if the limit is given. Showing that the time integral is bounded is equivalent to showing that the time sequences is a Cauchy sequence. Formally the sequence can be shown to define an element in the Hilbert space with all of the expected properties of the limiting vector.

The Gaussian wave functions are dense. I use them to show that a finite-range bounded potential satisfy Cook's condition. To estimate this integral note that V has a finite range, which cuts off the spatial integral. If the potential is bounded by a constant $V(x) \leq v$, inspection of the Gaussian wave function shows that for $\vec{x} < R$ the wave function is bounded by

$$\frac{c_1}{c_2 + t^{3/2}}. \tag{90}$$

It follows that

$$\|V|\psi(t)\rangle\| \leq v\sqrt{\langle\psi(t)|\Pi_R|\psi(t)\rangle} \tag{91}$$

where Π_R is the projection on the space of functions that vanish for $|x| > R$ where R is the the range of the potential. This in turn is bounded by

$$\|V|\psi(t)\rangle\| \leq v(\frac{4}{3}\pi R^3)^{1/2}\frac{c_1}{c_2 + t^{3/2}} \tag{92}$$

This is clearly integrable with respect to t

$$\int_0^\infty \frac{vc_1 dt}{c_2 + t^{3/2}} < \infty. \tag{93}$$

For more general potentials (86) can be checked directly. This shows that bounded finite range potentials satisfy the Cook condition. In this example R is the range of the potential and v is the bound on the potential.

In existence of wave operators can be proved by a variety of methods. Typically the interaction must fall off faster than the Coulomb interaction for large x for wave operators to exist. Cook's condition is only a sufficient condition for the existence of the Møller wave operators; failure of Cook's condition does not necessarily imply that the wave operators do not exist.

The Møller wave operators have some important properties that follow directly from the definitions. An important property is the intertwining relation. The intertwining relation is

$$H\Omega_{\pm}(H,H_0) = \Omega_{\pm}(H,H_0)H_0. \tag{94}$$

To prove this consider

$$\begin{aligned} U(s)\Omega_{\pm}(H,H_0) = s - \lim_{t\to\pm\infty} U(s)U(-t)U_0(t) = \\ s - \lim_{t\to\pm\infty} U(s-t)U_0(t-s+s) = \\ s - \lim_{t\to\pm\infty} U(s-t)U_0(t-s)U_0(s) = \\ s - \lim_{t'\to\pm\infty} U(-t')U_0(t')U_0(s) = \Omega_{\pm}(H,H_0)U_0(s) \end{aligned} \tag{95}$$

where $t' = t - s$ for fixed s.

If I differentiate this result with respect to s and set $s = 0$ I get the **intertwining relations**

$$\boxed{H\Omega_{\pm}(H,H_0) = \Omega_{\pm}(H,H_0)H_0} \tag{96}$$

If $|E_0\rangle$ is an eigenstate of H_0 with energy E_0 then

$$H\Omega_{\pm}(H,H_0)|E_0\rangle = \Omega_{\pm}(H,H_0)H_0|E_0\rangle = E_0\Omega_{\pm}(H,H_0)|E_0\rangle \tag{97}$$

which means that $\Omega_{\pm}(H,H_0)|E_0\rangle$ is an eigenstate of H with the same eigenvalue, E_0.

This is the quantum mechanical version of the energy conservation condition that was found for classical scattering. It means that the energy of the asymptotic solution is the same as the energy for the corresponding exact solution.

A second important result that follows from the intertwining relation is that the ranges of the wave operators are orthogonal to the bound states of

H. To see this let $|E_b\rangle$ be a bound state of H with energy $E_b < 0$ and let $|E_0\rangle$ be an energy eigenstate of H_0 with energy $E_0 \geq 0$. It follows that

$$0 = \langle E_b|(H - H)\Omega_\pm(H, H_0)|E_0\rangle = (E_0 - E_b)\langle E_b|\Omega_\pm(H, H_0)|E_0\rangle. \quad (98)$$

Since $(E_0 - E_b) > 0$ it follows that

$$\langle E_b|\Omega_\pm(H, H_0)|E_0\rangle = 0. \quad (99)$$

This says that the scattering eigenstates of H are necessarily orthogonal to the bound states. To prove this I used the orthogonality of the eigenstates with different eigenvalues.

This result is surprising because the wave operators are limits of products of unitary operators. When a product of unitary operators is applied to a complete set of free particle eigenstates the result will be a complete set of states.

The above calculation shows that this is no longer the case after the limit is taken, since the application of the wave operators to a complete set of free particle eigenstates is orthogonal to the bound states. This means that the Møller wave operators are not unitary.

In general the wave operators are isometric operators, this means the they preserve the norm of vectors, but their range is not the necessarily full Hilbert space.

I define the subspaces $\mathcal{H}_\pm$ to be the subspaces of vectors in the Hilbert space spanned by vectors of the form

$$|\psi_\pm\rangle = \Omega_\pm(H, H_0)|\psi_{0\pm}\rangle. \quad (100)$$

Vectors in these spaces are linear combinations of eigenstates of H with positive eigenvalues.

I define $\mathcal{H}_b$ to be the subspace of the Hilbert space spanned by the bound states of H.

I have shown that

$$\mathcal{H}_b \perp \mathcal{H}_+ \quad (101)$$

and

$$\mathcal{H}_b \perp \mathcal{H}_- \quad (102)$$

If there are no other eigenstates of H then I expect

$$\mathcal{H} = \mathcal{H}_b \oplus \mathcal{H}_- = \mathcal{H}_b \oplus \mathcal{H}_+. \quad (103)$$

When this holds the scattering theory is said to be **asymptotically complete**.

Note that I do not expect $\mathcal{H}_-$ to be orthogonal to $\mathcal{H}_+$ because these overlaps are precisely the scattering matrix elements. If these spaces were orthogonal there would be no scattering. Asymptotic completeness implies that the scattering matrix is unitary.

In the quantum mechanical case asymptotic completeness means that every particle that enters the scattering region comes out with probability 1. Mathematically asymptotic completeness is difficult to prove, however it is a standard assumption of scattering theory. I will discuss one method to test asymptotic completeness.

Before constructing the scattering operator I want to point out some additional properties of the wave operators.

The relation

$$U(s)\Omega_\pm(H,H_0) = \Omega_\pm(H,H_0)U_0(s) \tag{104}$$

means

$$\frac{1}{2\pi}\int ds f(s)U(s)\Omega_\pm(H,H_0) = \frac{1}{2\pi}\int ds \Omega_\pm(H,H_0)U_0(s)f(s) \tag{105}$$

or

$$\tilde{f}(H)\Omega_\pm(H,H_0) = \Omega_\pm(H,H_0)\tilde{f}(H_0) \tag{106}$$

where $\tilde{f}(E)$ is the Fourier transform or $f(s)$.

The means that the wave operators transform functions of H_0 to the same functions of H.

The same identity also gives

$$|\psi_\pm(t)\rangle = U(t)|\psi_\pm(0)\rangle = \tag{107}$$

$$U(t)\Omega_\pm(H,H_0)|\psi_{0\pm}(0)\rangle = \Omega_\pm(H,H_0)U_0(t)|\psi_{0\pm}(0)\rangle = \Omega_\pm(H,H_0)|\psi_{0\pm}(t)\rangle \tag{108}$$

which shows that the wave operators relate the free and interacting states at all times, not just $t = 0$.

$$\boxed{|\psi_\pm(t)\rangle = \Omega_\pm(H,H_0)|\psi_{0\pm}(t)\rangle}.$$

The next result that I discuss is called the chain rule for wave operators. I consider the special case where I have three Hamiltonians and none of them have bound states. If I assume

$$\Omega_\pm(H_1,H_2) \tag{109}$$

and

$$\Omega_{\pm}(H_2, H_3) \tag{110}$$

exist then

$$\Omega_{\pm}(H_1, H_3) \tag{111}$$

exists and is equal to

$$\Omega_{\pm}(H_1, H_3) = \Omega_{\pm}(H_1, H_2)\Omega_{\pm}(H_2, H_3) \tag{112}$$

To prove this result I note that

$$\|[e^{-iH_1t}e^{iH_3t} - \Omega_{\pm}(H_1, H_2)\Omega_{\pm}(H_2, H_3)]|\psi\rangle\| =$$

$$\|[e^{-iH_1t}e^{iH_2t}e^{-iH_2t}e^{iH_3t} - \Omega_{\pm}(H_1, H_2)\Omega_{\pm}(H_2, H_3)]|\psi\rangle\| =$$

$$\|[e^{-iH_1t}e^{iH_2t}(e^{-iH_2t}e^{iH_3t} - \Omega_{\pm}(H_2, H_3))+$$
$$\Omega_{\pm}(H_2, H_3)) - \Omega_{\pm}(H_1, H_2)\Omega_{\pm}(H_2, H_3)]|\psi\rangle\| \leq$$

$$\|e^{-iH_1t}e^{iH_2t}[e^{-iH_2t}e^{iH_3t} - \Omega_{\pm}(H_2, H_3)]|\psi\rangle\|+$$
$$\|[e^{-iH_1t}e^{iH_2t} - \Omega_{\pm}(H_1, H_2)]\Omega_{\pm}(H_2, H_3)|\psi\rangle\| =$$

$$\|[e^{-iH_2t}e^{iH_3t} - \Omega_{\pm}(H_2, H_3)]|\psi\rangle\|+$$
$$\|[e^{-iH_1t}e^{iH_2t} - \Omega_{\pm}(H_1, H_2)]\Omega_{\pm}(H_2, H_3)|\psi\rangle\|$$

This vanishes as $t \to \pm\infty$ provided $\Omega_{\pm}(H_1, H_2)$ and $\Omega_{\pm}(H_2, H_3)$ both exist. In this case the limit is

$$\Omega_{\pm}(H_1, H_3) = \Omega_{\pm}(H_1, H_2)\Omega_{\pm}(H_2, H_3)$$

This proves the chain rule in the simplest case.

We proved the chain rule for the case that there are no bound states. When there are bound states the chain rule holds provided the definition of the wave operator is generalized by

$$\Omega_{\pm}(H_i, H_j) = s\lim_{t\to\pm\infty} e^{iH_it}e^{-iH_jt}\Pi_{jc} \tag{113}$$

where Π_{jc} is the orthogonal projector on the subspace orthogonal to the bound states of H_j. This is consistent with the previous definition because the free Hamiltonian has no bound states.

A useful property of the chain rule is that is gives a simple condition for the asymptotic completeness of the wave operators which is: If $\Omega_\pm(H, H_0)$ both exist then scattering theory is asymptotically complete if and only if

$$\Omega_\pm(H_0, H) \tag{114}$$

also exist. Note that I have reversed the order of H and H_0.

A simple application of the chain rule gives for both time limits

$$\Omega_\pm(H, H_0)\Omega_\pm(H_0, H) = \Pi_c \tag{115}$$

and

$$\Omega_\pm(H_0, H)\Omega_\pm(H, H_0) = I. \tag{116}$$

The first equation means that any vector that is orthogonal to the bound states is necessarily in the range of both $\Omega_+(H, H_0)$ and $\Omega_-(H, H_0)$ or

$$\mathcal{H}_+ \supseteq \mathcal{H}_\perp \qquad \mathcal{H}_- \supseteq \mathcal{H}_\perp \tag{117}$$

which when coupled with (101) and (102) requires

$$\mathcal{H}_\perp = \mathcal{H}_- = \mathcal{H}_+.$$

Another useful property of wave operators is the Kato-Birman invariance principle. I begin with the following characterization of the limit that defines the wave operator

$$\lim_{t\to\pm\infty} \|[U(t)\Omega_\pm(H, H_0) - U_0(t)]|\psi\rangle\| = 0. \tag{118}$$

The intertwining relations imply

$$\lim_{t\to\pm\infty} \|[\Omega_\pm(H, H_0) - I]U_0(t)|\psi\rangle\| = 0 \tag{119}$$

or

$$\lim_{t\to\pm\infty} \|[\Omega_\pm(H, H_0) - I]e^{-iH_0t}|\psi\rangle\| = 0 \tag{120}$$

If I replace H_0 by a function $f(H_0)$ I can consider the limit

$$\lim_{s\to\pm\infty} \|[\Omega_\pm(H, H_0) - I]e^{-if(H_0)s}|\psi\rangle\| \tag{121}$$

If this limit vanishes then it follows that

$$\Omega_{\pm}(H,H_0) = s\lim_{s\to\pm\infty} e^{if(H)s}e^{-if(H_0)s}. \tag{122}$$

To find conditions for this replacement first note that

$$\|[\Omega_{\pm}(H,H_0)-I]e^{-if(H_0)s}|\psi\rangle\|^2 =$$

$$\langle\psi|e^{if(H_0)s}[\Omega_{\pm}^{\dagger}(H,H_0)-I][\Omega_{\pm}(H,H_0)-I]e^{-if(H_0)s}|\psi\rangle =$$

$$2 - 2Re\langle\psi|e^{if(H_0)s}\Omega_{\pm}^{\dagger}(H,H_0)e^{-if(H_0)s}|\psi\rangle =$$

$$2Re\langle\psi|e^{-if(H_0)s}\Omega_{\pm}^{\dagger}(H,H_0)[\Omega_{\pm}(H,H_0)-I]e^{if(H_0)s}|\psi\rangle. \tag{123}$$

Next I write $[\Omega_{\pm}(H,H_0)-I]$ as an integral

$$[\Omega_{\pm}(H,H_0)-I]e^{-if(H_0)s}|\psi\rangle = i\int_0^{\pm\infty} e^{iHt}Ve^{-iH_0t}e^{-if(H_0)s}|\psi\rangle dt \tag{124}$$

and use it in equation (123) to get

$$2Im\int_0^{\pm\infty}\langle\psi|e^{-if(H_0)s}\Omega_{\pm}^{\dagger}(H,H_0)e^{iHt}Ve^{-iH_0t}e^{-if(H_0)s}|\psi\rangle \tag{125}$$

The intertwining relations give

$$2Im\int_0^{\pm\infty}\langle\psi|e^{if(H_0)s}e^{iH_0t}\Omega_{\pm}^{\dagger}(H,H_0)Ve^{-iH_0t}e^{-if(H_0)s}|\psi\rangle \tag{126}$$

In what follows I assume that the potential is trace class, which means that it has the form

$$V = \sum_n |v_n\rangle\lambda_n\langle v_n| \qquad \sum_n |\lambda_n| = \mathrm{Tr}(V) < \infty \tag{127}$$

Note that the theorem is valid for a more general class of potential, the proofs are just more complicated.

Next I insert the expansion for the interaction in (126) to get

$$2Im\sum_n\int_0^{\pm\infty}\langle\psi|e^{if(H_0)s}e^{iH_0t}\Omega_{\pm}^{\dagger}(H,H_0)|v_n\rangle\lambda_n\times$$

$$\langle v_n|e^{-iH_0t}e^{-if(H_0)s}|\psi\rangle \tag{128}$$

The Schwartz inequality (considering both t and n as vector component labels) gives

$$\|[\Omega_\pm(H,H_0)-I]e^{if(H_0)s}|\psi\rangle\|^2 \leq$$
$$2\sqrt{\sum_n \int_0^{\pm\infty} dt|\lambda_n||\langle\psi|e^{if(H_0)s}e^{iH_0t}\ \Omega_\pm^\dagger(H,H_0)|v_n\rangle|^2}\times$$
$$\sqrt{\sum_n \int_0^{\pm\infty} dt|\lambda_n||\langle v_n|e^{-iH_0t}e^{-if(H_0)s}|\psi\rangle|^2}. \tag{129}$$

The term with the wave operator is bounded by

$$\sqrt{\sum_n \int_{-\infty}^{\infty} |\lambda_n|| \int \langle\psi|P(E)\Omega_\pm^\dagger(H,H_0)|v_n\rangle e^{if(E)s}e^{iEt}dE|^2}$$

where $P(E)$ is the differential projection on the spectral subspace of H_0 with eigenvalue E.

The energy integral is a Fourier transform $\hat{g}_n(t)$ of the following function of energy

$$g_n(E) = \langle\psi|P(E)e^{-if(E)s}\Omega_\pm^\dagger(H,H_0)|v_n\rangle$$

As long as

$$\int |\hat{g}_n(t)|^2dt < G^2 < \infty$$

with G independent of s and n, the first terms is bounded by $G\sqrt{\mathrm{Tr}(V)}$:

$$\|[\Omega_\pm(H,H_0)-I]e^{if(H_0)s}|\psi\rangle\|^2 \leq$$
$$G\sqrt{\mathrm{Tr}(V)}\sqrt{\sum_n \int_0^{\pm\infty} dt|\lambda_n||\langle v_n|e^{iH_0t}e^{if(H_0)s}|\psi\rangle|^2}$$

It is enough to show

$$\sqrt{\sum_n |\lambda_n| \int_0^{\infty} |\langle v_n|e^{iH_0t}e^{if(H_0)s}|\psi\rangle|^2} \tag{130}$$

vanishes as $s \to \pm\infty$.

The square of this integral is bounded by

$$\int_0^{\infty} \sum_n |\lambda_n||\langle v_n|e^{iH_0t+if(H_0)s}|\psi\rangle|^2dt \tag{131}$$

The free Hamiltonian can be replaced by its eigenfunction expansion

$$\int_0^\infty g(E)e^{iEt}e^{if(E)s}dE \tag{132}$$

To keep life simple I choose a dense set of functions ψ so $f(E)$ is constant on a small subinterval $[a,b]$ in energy and vanishes everywhere else. In this case the energy integral becomes

$$\int_a^b e^{iEt}e^{if(E)s}dE =$$

$$-i\int_a^b \frac{1}{t+f'(E)s}\frac{d}{dE}e^{iEt}e^{if(E)s}dE =$$

$$-i\frac{1}{t+f'(b)s}e^{ibt}e^{if(b)s}$$

$$+i\frac{1}{t+f'(a)s}e^{iat}e^{if(a)s}$$

$$-i\int_a^b \left(\frac{1}{t+f'(E)s}\right)^2 f''(E)e^{iEt}e^{if(E)s}dE.$$

This is bounded by

$$\frac{1}{t+f'(b)s}$$

$$\frac{1}{t+f'(a)s}$$

$$\left(\frac{1}{t+f'(E)s}\right)^2\int_a^b |f''(E)|dE$$

The square of this appears in (131). It is integrable with respect to t and the integral vanishes at $s\to\infty$ provided $f'(E)$ is positive and the integral of $|f''(E)|$ is finite on closed bounded intervals.

This shows that for trace class potentials

$$\Omega_\pm(H,H_0) = s\lim_{s\to\pm\infty} e^{if(H)s}e^{-if(H_0)s} \tag{133}$$

when f has a positive first derivative and the second derivative is locally integrable.

The invariance theorem works for a much larger class of potentials. It implies that we can replace H by $f(H)$ in computing Møller wave operators as long as $f(E)$ is reasonably nice increasing function of energy

$$\Omega_{\pm}(H, H_0) = \Omega_{\pm}(f(H), f(H_0)) \qquad f'(E) > 0 \tag{134}$$

This freedom is useful in relativistic formulations of scattering theory.

It is worth noting that this does not necessarily imply the existence of the modified wave operators, only that if both exist then they must be equal.

One of the goals of scattering theory is to learn something about microscopic interactions by looking at the results of a scattering experiments. I will show even if it is possible to experimentally measure every scattering matrix element that it is still impossible to extract a unique potential. I show this by exhibiting distinct potentials that lead to the same matrix elements.

I begin by assuming a Hamiltonian of the standard form

$$H = \frac{p^2}{2m} + V = H_0 + V$$

where H_0 represents the kinetic energy operator or free particle Hamiltonian. Let A be a unitary operator that satisfies the asymptotic condition:

$$s - \lim_{t \to \pm\infty} (I - A)U_0(t) = 0 \tag{135}$$

for both times. Unitary operators A satisfying (135) are called scattering equivalences. Operators of the form

$$A = \frac{I - iB}{I + iB}$$

where B is a finite rank Hermitian operator can be shown to be unitary and satisfy this condition, so it is clear that there are an infinite number of scattering equivalences. It is useful to express A in the form

$$A = I + \Delta$$

Let

$$H' = A^{\dagger} H A = (I + \Delta^{\dagger})(H_0 + V)(I + \Delta) = H_0 + V'$$

where V' represents all of the short range contributions to H'.

I show that H and H' lead to the same scattering operator. To see this note

$$\Omega_{\pm}(H', H_0) = s - \lim_{t\to\pm\infty} e^{-iH't} e^{iH_0 t} =$$

$$s - \lim_{t\to\pm\infty} e^{-iA^\dagger HAt} e^{iH_0 t} =$$

$$s - \lim_{t\to\pm\infty} A^\dagger e^{-iHt} A e^{iH_0 t} = s - \lim_{t\to\pm\infty} A^\dagger e^{-iHt}(A - I + I) e^{iH_0 t}$$

The term

$$\lim_{t\to\pm\infty} \| A^\dagger e^{-iHt}(A - I) e^{iH_0 t} |\psi_{0\pm}\rangle \| \leq \lim_{t\to\pm\infty} \| (A - I) e^{iH_0 t} |\psi_{0\pm}\rangle \| = 0$$

vanishes by (135). What remains is

$$\Omega_{\pm}(H', H_0) = s - \lim_{t\to\pm\infty} e^{-iH't} e^{iH_0 t} =$$

$$s - \lim_{t\to\pm\infty} e^{-iA^\dagger HAt} e^{iH_0 t} =$$

$$s - \lim_{t\to\pm\infty} A^\dagger e^{-iHt} e^{iH_0 t} A^\dagger \Omega_{\pm}(H, H_0)$$

Since this result holds for both time limits we have

$$S(H', H_0) = \Omega_+^\dagger(H', H_0)\Omega_-(H', H_0) = \Omega_+^\dagger(H, H_0) A A^\dagger \Omega_-(H, H_0) =$$

$$\Omega_+^\dagger(H, H_0)\Omega_-(H, H_0) = S(H, H_0)$$

so the scattering matrix is the same for both V and V'.

This has a number of interesting implications. First I note that the operator A was not applied to the the free particle Hamiltonian, only to the interacting Hamiltonian. The net result is to replace the original potential with a new potential. The operator A will transform the wave functions that are eigenstates of H' to different wave functions that are eigenstates of H.

- A unique potential cannot be extracted from a knowledge of the scattering operator.
- The quantum mechanical wave function is not an observable - in these examples two different wave functions give identical scattering observables.
- A single scattering matrix is associated with an infinite number of scattering equivalent theories.

6 The Transition operator

The scattering operator is the central element of scattering theory. In this section I demonstrate how to calculate the scattering operator. I develop the connection between time-dependent and time-independent scattering.

Formally the scattering matrix is defined by

$$S_{fi} := \lim_{s,t\to\infty} \langle \psi_{0+}|e^{iH_0 s}e^{-iH(t+s)}e^{iH_0 t}|\psi_{0-}\rangle$$

which can be written in terms of a single limit:

$$S_{fi} := \lim_{t\to\infty} \langle \psi_{0+}|e^{iH_0 t}e^{-iH(2t)}e^{iH_0 t}|\psi_{0-}\rangle.$$

In order to evaluate this let $\epsilon(p) := \frac{p^2}{2m}$ be the kinetic energy and expand the initial and final states in terms of momentum eigenstates:

$$S_{fi} := \lim_{t\to\infty} \int \langle \psi_{0+}|\vec{p}\rangle e^{i\epsilon(p)t}\langle \vec{p}|e^{-iH(2t)}|\vec{p}\,'\rangle e^{i\epsilon(p')t}\langle \vec{p}\,'|\psi_{0-}\rangle d^3p d^3p'.$$

This expression only makes sense if the $\vec{p}$ and $\vec{p}\,'$ integrals are performed **before** taking the time limit. I replace this with the equivalent expression:

$$S_{fi} := \lim_{\lambda\to 0^+}\lim_{t\to\infty} \int \langle \psi_{0+}|\vec{p}\rangle e^{i\epsilon(p)t}\langle \vec{p}|e^{-iH(2t)}|\vec{p}\,'\rangle e^{i\epsilon(p')t}\langle \vec{p}\,'|\psi_{0-}\rangle e^{-\lambda t} d^3p d^3p'$$

The term $e^{-\lambda t}$ has no impact on the result in the limit that $\lambda \to 0$ as long as the integrals are performed before taking the limit.

Adding this factor allows me to change the order of the limit and integral. Thus I can remove the wave functions and consider the time limit

$$S = \lim_{\lambda\to 0^+}\lim_{t\to\infty} \langle \vec{p}|e^{-iH(2t)+i(\epsilon(p)+\epsilon(p'))t-\lambda t}|\vec{p}\,'\rangle.$$

I write the limit as the integral of a derivative

$$S = \langle \vec{p}|\vec{p}\,'\rangle + \int_0^\infty \lim_{\lambda\to 0^+} \frac{d}{dt}\langle \vec{p}|e^{-iH(2t)+i(\epsilon(p)+\epsilon(p'))t-\lambda t}|\vec{p}\,'\rangle =$$

$$\langle \vec{p}|\vec{p}\,'\rangle - i\int_0^\infty \lim_{\lambda\to 0^+} [\langle \vec{p}|(H-\epsilon(p))e^{-iH(2t)+i(\epsilon(p)+\epsilon(p'))t-\lambda t}|\vec{p}\,'\rangle +$$
$$\langle \vec{p}|e^{-iH(2t)+i(\epsilon(p)+\epsilon(p'))t-\lambda t}(H-\epsilon(p'))|\vec{p}\,'\rangle$$

Performing the integral using

$$\langle\vec{p}|(H-\epsilon(p)) = \langle\vec{p}|V$$

and

$$(H-\epsilon(p'))|\vec{p}'\rangle = V|\vec{p}'\rangle$$

gives

$$\langle\vec{p}|S|\vec{p}'\rangle = \langle\vec{p}|\vec{p}'\rangle + \frac{1}{2}\lim_{\lambda\to 0^+}[\langle\vec{p}|V\frac{1}{\bar{\epsilon}+i\lambda-H}|\vec{p}'\rangle + \langle\vec{p}|V\frac{1}{\bar{\epsilon}+i\lambda-H}V|\vec{p}'\rangle]$$

where $\bar{\epsilon}$ is the average of the initial and final energy. Next I use the **second resolvent identities**

$$\frac{1}{z-H} = \frac{1}{z-H_0} + \frac{1}{z-H_0}(H-H_0)\frac{1}{z-H} =$$

$$\frac{1}{z-H_0} + \frac{1}{z-H}(H-H_0)\frac{1}{z-H_0} \tag{136}$$

which can be easily derived. Let $z := \bar{\epsilon}+i\lambda$ then

$$\langle\vec{p}|S|\vec{p}'\rangle = \langle\vec{p}|\vec{p}'\rangle + \frac{1}{2}\lim_{\lambda\to 0^+}[\langle\vec{p}|V\frac{1}{z-H}|\vec{p}'\rangle + \langle\vec{p}|V\frac{1}{z-H}V|\vec{p}'\rangle] =$$

$$= \langle\vec{p}|\vec{p}'\rangle + \frac{1}{2}\lim_{\lambda\to 0^+}[\langle\vec{p}|V[1+\frac{1}{z-H}V]\frac{1}{z-H_0}|\vec{p}'\rangle +$$

$$\langle\vec{p}|V\frac{1}{z-H_0}[1+V\frac{1}{z-H}]V|\vec{p}'\rangle] =$$

$$= \langle\vec{p}|\vec{p}'\rangle + \frac{1}{2}\lim_{\lambda\to 0^+}[\langle\vec{p}|V[1+\frac{1}{z-H}V]\frac{1}{z-\epsilon'}|\vec{p}'\rangle +$$

$$\langle\vec{p}|V\frac{1}{z-\epsilon}[1+V\frac{1}{z-H}]V|\vec{p}'\rangle] =$$

$$= \langle\vec{p}|\vec{p}'\rangle + \frac{1}{2}\lim_{\lambda\to 0^+}[\langle\vec{p}|T(z)|\vec{p}'\rangle[\frac{1}{z-\epsilon'}+\frac{1}{z-\epsilon}]$$

Note that

$$\frac{1}{z-\epsilon'} + \frac{1}{z-\epsilon} =$$

$$\frac{2}{\epsilon-\epsilon'+i2\lambda} + \frac{2}{\epsilon'-\epsilon+i2\lambda} =$$

$$\frac{-8i\lambda}{(\epsilon-\epsilon')^2+4\lambda^2} \to -4\pi i\delta(\epsilon-\epsilon')$$

where I have used

$$\pi\delta(x-y) = \lim_{\lambda\to 0}\frac{\lambda}{(x-y)^2+\lambda^2}.$$

This gives the final result

$$\boxed{\langle\vec{p}|S|\vec{p}'\rangle = \delta^3(\vec{p}-\vec{p}') - 2\pi i\delta(\frac{p^2}{2m}-\frac{p'^2}{2m})\langle\vec{p}|T(\frac{p'^2}{2m}+i0^+)|\vec{p}'\rangle} \tag{137}$$

where

$$\boxed{T(z) = V + V\frac{1}{z-H}V} \tag{138}$$

T is called the **transition operator**.

Equation (137) is an important equation in scattering theory. It shows that S is the sum of two terms. The delta function term corresponds to the contribution from no scattering. The second term, containing the transition operator, describes the scattering. It is the dynamical contribution to the scattering matrix.

The operator

$$R(z) := (z-H)^{-1} \tag{139}$$

is called the **resolvent operator**. In general z is a complex number. The resolvent operator does not exist for all z. The points z where $R(z)$ does not exist is called the **discrete spectrum** of H; the points where $R(z)$ exists as an unbounded operator is called the **continuous spectrum** of H, and the points where $R(z)$ has a bounded inverse is called the **resolvent set** of H. It is clear from this definition that every point in the complex plane is either in the discrete spectrum of H, the continuous spectrum of H, or the resolvent set of H.

The matrix elements of the transition operator that appear in the scattering matrix

$$\langle\vec{p}|T(\epsilon+0^+)|\vec{p}'\rangle$$

are multiplied by an energy conserving delta function which gives

$$\epsilon_i = \epsilon_f = \epsilon. \tag{140}$$

Transition matrix elements where all energies are the same are called **on energy-shell** transition matrix elements. The transition operator itself can be evaluated with all three quantities being different.

I use the second resolvent identity to obtain an equation for the transition operator. The definition (138) can be put in the form

$$\boxed{T(z) = V + VR(z)V} \tag{141}$$

while the second resolvent identities (139) can be written

$$\boxed{R(z) = R_0(z) + R_0(z)VR(z) = R_0(z) + R(z)VR_0(z)} \tag{142}$$

$$R(z) = (z - H)^{-1} \qquad R_0(z) = (z - H_0)^{-1}. \tag{143}$$

Using (142) in (141) gives

$$T(z) = V + V(R_0(z) + R_0(z)VR(z))V = V + VR_0(z)[V + VR(z)V] = \tag{144}$$

$$\boxed{T(z) = V + VR_0(z)T(z).} \tag{145}$$

This equation is called the **Lippmann-Schwinger** equation. I have it expressed as an operator equation. If this is put in a basis it becomes an integral equation. It can be expressed in either configuration space or momentum space. These equations are

$$\langle \vec{p}_i|T(z)|\vec{p}_f\rangle = \langle \vec{p}_i|V|\vec{p}_f\rangle + \int d^3p \langle \vec{p}_i|V|\vec{p}\rangle \frac{1}{z - p^2/2m + i0^+} \langle \vec{p}|T(z)|\vec{p}_f\rangle \tag{146}$$

or

$$\langle \vec{r}_i|T(z)|\vec{r}_f\rangle = \langle \vec{r}_i|V|\vec{r}_f\rangle + \int d^3r d^3r' \langle \vec{r}_i|V|\vec{r}\rangle \langle \vec{r}|R_0(z)|\vec{r}'\rangle \langle \vec{r}'|T(z)|\vec{r}_f\rangle. \tag{147}$$

Both of these equations are integral equations. I will discuss solution methods shortly.

7 Relation between $T(z)$ and $\Omega_\pm$

Recall that the interacting and non-interacting solutions of the Schrödinger equation are related in the scattering asymptotic condition by

$$|\psi_\pm(t)\rangle = \Omega_\pm |\psi_0(t)\rangle.$$

For $t = 0$ this becomes

$$|\psi_\pm\rangle = \Omega_\pm |\vec{p}\rangle d^3p \langle \vec{p}|\psi_0\rangle =$$

$$[I + i\int_0^{\pm\infty} e^{iHt}Ve^{-iH_0t}dt]|\vec{p}\rangle d^3p\langle\vec{p}|\psi_0\rangle =$$

$$[|\vec{p}\rangle + i\int_0^{\pm\infty} e^{i(H-p^2/2m)t}Vdt]|\vec{p}\rangle]d^3p\langle\vec{p}|\psi_0\rangle$$

As before, the momentum integral must be done before the time integral; however if the momentum integral is done first nothing changes if I write this as

$$[|\vec{p}\rangle + i\lim_{\lambda\to 0^+}\int_0^{\pm\infty} e^{i(H-p^2/2m)t\mp\lambda t}Vdt]|\vec{p}\rangle]d^3p\langle\vec{p}|\psi_0\rangle \tag{148}$$

With the λ in the equation I can change the order of integration and obtain:

$$[|\vec{p}\rangle + i\lim_{\lambda\to 0^+}\frac{-1}{i(H-p^2/2m\pm i\lambda)}V|\vec{p}\rangle]d^3p\langle\vec{p}|\psi_0\rangle =$$

$$[|\vec{p}\rangle + \frac{1}{p^2/2m\mp i0^+ - H}V|\vec{p}\rangle]d^3p\langle\vec{p}|\psi_0\rangle =$$

$$[|\vec{p}\rangle + R(p^2/2m\mp i0^+)V|\vec{p}\rangle]d^3p\langle\vec{p}|\psi_0\rangle \tag{149}$$

To relate this to the transition operator I use the second resolvent identity again to get

$$R(p^2/2m\mp i0^+)V =$$

$$[R_0(p^2/2m\mp i0^+) + R_0(p^2/2m\mp i0^+)VR(p^2/2m\mp i0^+)]V =$$

$$R_0(p^2/2m\mp i0^+)[V + VR(p^2/2m\mp i0^+)V] =$$

$$R_0(p^2/2m\mp i0^+)T(p^2/2m\mp i0^+). \tag{150}$$

Using (150) in (149) gives

$$|\psi_\pm\rangle = \Omega_\pm|\vec{p}\rangle d^3p\langle\vec{p}|\psi_0\rangle =$$

$$[|\vec{p}\rangle + R_0(p^2/2m\mp i0^+)T(p^2/2m\mp i0^+)|\vec{p}\rangle]d^3p\langle\vec{p}|\psi_0\rangle \tag{151}$$

I write this is the following abbreviated notation

$$\boxed{|\vec{p}_\pm\rangle = \Omega_\pm|\vec{p}\rangle = [I + R_0(p^2/2m\mp i0^+)T(p^2/2m\mp i0^+)]|\vec{p}\rangle.} \tag{152}$$

This is the desired equation relating $T(z)$ and $\Omega_\pm$ The relations are complicated because the z appearing in $T(z)$ is an integration variable in the above expression. It is also worth noting that the signs appearing in the $\mp i0^+$ are

opposite to the signs appearing in the related wave operator. Note that only one sign appears in the expression for the scattering operator. It is the $+i0^+$ sign; this is because it involves Ω_- and $\Omega_+^\dagger$ where the adjoint is responsible for the sign change in the second term.

The quantity $|\vec{p}_\pm\rangle$ is an eigenstate of the interacting Hamiltonian with energy $\vec{p}\cdot\vec{p}/2m$ and momentum $\vec{p}$. When it is integrated against a function $\langle\vec{p}|\psi_0\rangle$ of the momentum it becomes the scattering state $|\psi_\pm\rangle$ that satisfies the asymptotic condition with respect to the non-interacting wave packet at time $t = 0$:

$$\int |\vec{p}\rangle d^3p \langle\vec{p}|\psi_0\rangle$$

The generalized vector $|\vec{p}_\pm\rangle$ is called the scattering wave function. It satisfies the a Lippmann Schwinger equation which can be derived using the Lippmann Schwinger equation for the transition operator:

$$|\vec{p}_\pm\rangle = [I + R_0(p^2/2m \mp i0^+)[V + VR_0(p^2/2m \mp i0^+)T(p^2/2m \mp i0^+)]]|\vec{p}\rangle =$$
$$[I + R_0(p^2/2m \mp i0^+)V[I + R_0(p^2/2m \mp i0^+)T(p^2/2m \mp i0^+)]|\vec{p}\rangle =$$
$$|\vec{p}\rangle + R_0(p^2/2m \mp i0^+)V|\vec{p}_\pm\rangle$$

The resulting equation

$$\boxed{|\vec{p}_\pm\rangle = |\vec{p}\rangle + R_0(p^2/2m \mp i0^+)V|\vec{p}_\pm\rangle} \tag{153}$$

is the Lippmann-Schwinger equation for the wave function.

Normally this equation is derived from the Schrödinger equation. That derivation is not very satisfying because the underlying asymptotic condition emerges as something that comes out of the equation rather than as physical input. As in the case with the transition operator, matrix elements give integral equations:

$$\langle\vec{p}'|\vec{p}_\pm\rangle = \delta(\vec{p} - \vec{p}') + \int d^3p'' \frac{1}{p^2/2m \mp i0^+ - (p')^2/2m}\langle\vec{p}'|V|\vec{p}''\rangle\langle\vec{p}''|\vec{p}_\pm\rangle \tag{154}$$

$$\langle\vec{r}|\vec{p}_\pm\rangle = (2\pi)^{-3/2} + \int d^3r' d^3r'' \langle\vec{r}|R_0(p^2/2m \mp i0^+)|\vec{r}'\rangle\langle\vec{r}'|V|\vec{r}''\rangle\langle\vec{r}''|\vec{p}_\pm\rangle \tag{155}$$

In many cases of interest the interaction is modeled by a local potential,

$$\langle\vec{r}'|V|\vec{r}\rangle = V(r)\delta^3(\vec{r}' - \vec{r}). \tag{156}$$

For a local potential one of the integrals in the radial integral equation disappears when it is integrated against the delta function.

8 K matrix

The non-interacting resolvent operator $R_0(\frac{p^2}{2m\mp i0^+})$ has simple momentum space matrix elements:

$$\langle \vec{p}\,'|R_0(\frac{p^2}{2m\mp i0^+})|\vec{p}\,''\rangle = \delta(\vec{p}\,'-\vec{p}\,'')\frac{2m}{p^2-p'^2\mp 2mi0^+}.$$

Since 0^+ represents a small positive terms that eventually goes to zero, I replace $2mi0^+$ by $i0^+$. (*in general this must be done with care in the cases where the small terms conspire to give something singular that leads to a delta function*).

When this is integrated against a nice function of p it can be expressed in the form

$$\int f(\vec{p}\,')\frac{2m}{p^2-p'^2\mp i0^+}p'^2dp'd\Omega(\hat{p}\,').$$

I define

$$\int f(\vec{p})d\Omega(\hat{p}) = \tilde{f}(p)$$

so the remaining integral becomes

$$\int_0^\infty \tilde{f}(p')\frac{2m}{p^2-p'^2\mp i0^+}p'^2dp'.$$

To treat the singularity in a manner that allows me to take the limit that the small quantity $0^+\to 0$ I write this as

$$\int_0^\infty \frac{2m(p'^2\tilde{f}(p')-p^2\tilde{f}(p))}{p^2-p'^2\mp i0^+}dp' + 2mp^2\tilde{f}(p)\int_0^\infty \frac{1}{p^2-p'^2\mp i0^+}dp'.$$

In the first term the integrand in not singular as $p\to p'$ as long as $\hat{f}(p)$ is differentiable at p. This term is continuous as $0^+\to 0$. As a practical matter the first term contains $0/0$ so some care is needed to compute it. The second term can be computed using the residue theorem

$$2mp^2\tilde{f}(p)\int_0^\infty \frac{1}{p^2-p'^2\mp i0^+}dp' =$$

$$mp^2\tilde{f}(p)\int_{-\infty}^\infty \frac{1}{p^2-p'^2\mp i0^+}dp' =$$

$$-mp^2\tilde{f}(p)\int_{-\infty}^{\infty}\frac{1}{(p'-p\pm i0^+)(p'+p\mp i0^+)}dp=$$
$$\mp 2\pi i(-\frac{m}{2}p)\tilde{f}(p)=\pm i\pi mp\tilde{f}(p)$$

It is customary to write this as

$$\frac{1}{p^2-p'^2\mp i0^+}=$$

$$P\frac{1}{p^2-p'^2\mp i0^+}\pm i\delta(p^2-p'^2)$$

where the P stands for the principal value. It is defined as follows

$$P\int_a^b\frac{f(x)}{x-y}dx=\lim_{\epsilon\to 0}[\int_a^{y-\epsilon}+\int_{y+\epsilon}^b]\frac{f(x)}{x-y}$$

To see that the first integral is equivalent to the principal value note that

$$P\int_0^{\infty}\frac{1}{x^2-y^2}dx=\lim_{\epsilon\to 0}[\int_0^{y-\epsilon}+\int_{y+\epsilon}^{\infty}]\frac{1}{x^2-y^2}$$

To evaluate this let $x=uy$ in the first integral and let $x=y/v$ in the second integral. With these substitutions

$$\lim_{\epsilon\to 0}[\int_0^{y-\epsilon}+\int_{y+\epsilon}^{\infty}]\frac{1}{x^2-y^2}$$

$$\frac{1}{y}\lim_{\epsilon\to 0}\int_0^{1-\epsilon/y}\frac{du}{u^2-1}$$
$$\frac{1}{y}\lim_{\epsilon\to 0}\int_{1-\epsilon/y+\cdots}^{0}\frac{dv}{1^2-v^2}]$$
$$\frac{1}{y}\lim_{\epsilon\to 0}\int_{1-\epsilon/y+\cdots}^{1-\epsilon/y}\frac{du}{u^2-1}]$$

Expanding this out shows that it vanishes linearly in ϵ as $\epsilon\to 0$.

This shows that subtracted term has 0 principal value. This means that the first term is equal to the principal value of the original integral.

There are a few things to observe. The delta function term changes sign depending on the sign of $i0^+$. This means that the transition operator $T(z)$ is discontinuous

$$\lim_{y\to 0} T(x+iy) \neq \lim_{y\to 0} T(x-iy)$$

This discontinuity is an important element of scattering theory. The second thing to note is that because of this discontinuity the integral equation for the T matrix elements is a complex equation, even for real potentials.

It is easier to solve real integral or differential equations. To transform the Lippmann-Schwinger equation to a real equation note that the above implies

$$R_0(E \pm i0^+) = PR_0(E) \mp i\pi\delta(E - H_0)$$

which separates the real and imaginary parts of the non-interacting resolvent operator. Using this in the Lippmann-Schwinger equation gives

$$T(E \pm i0^+) = V + V[PR_0(E) \mp i\pi\delta(E - H_0)]T(E \pm i0^+)$$

It is an easy exercise to show that this is equivalent to the following pair of equations

$$K(E) = V + VPR_0(E)K(E)$$

$$T(E \pm i0^+) = K(E) \mp i\pi K(E)\delta(E - H_0)T(E \pm i0^+)$$

The operator $K(E)$ is called the K operator and its matrix elements are K-matrix elements. The equation for the K matrix has the advantage that the integral equation is real. The equation to construct T from K is complex, but the dimensionality of the integral is reduced by the delta function.

It is useful to relate the K operator directly to the S operator. Formally

$$S = I - 2\pi i\delta(E - E')T(E + i0^+)$$

$$T(E + i0^+) = \frac{1}{1 + i\pi K(E)\delta(E - H_0)}K(E)$$

$$S = I - 2\pi i\frac{1}{1 + i\pi K(E)\delta(E - H_0)}K(E)\delta(E - E') =$$

$$I - 2\pi i\frac{1}{1 + i\pi K(E)\delta(E - H_0)}K(E)\delta(E - H_)) =$$

$$\frac{1 + i\pi K(E)\delta(E - H_0) - 2\pi iK(E)\delta(E - H_0)}{1 + i\pi K(E)\delta(E - H_0)} =$$

$$\frac{1 - i\pi K(E)\delta(E - H_0)}{1 + i\pi K(E)\delta(E - H_0)}$$

or

$$\boxed{S = \frac{1 - i\pi K(E)\delta(E - H_0)}{1 + i\pi K(E)\delta(E - H_0)}} \tag{157}$$

which shows that the scattering operator is a Cayley transform of $K(E)\delta(E - H_0)$. This means that the scattering operator can be obtained directly from the K matrix. In addition K is approximated, but is Hermitian, then the corresponding approximate S matrix is unitary.

I comment that the K matrix defined in the text is defined with a $-$ sign. Both signs appear in the literature so it is important to check conventions.

Note that (157) shows that the Hermiticity of K implies the unitarity of S. We can derive a similar unitarity condition for the transition operator. We start by writing

$$\langle p_f|I|p_i\rangle = \langle p_f|S^\dagger S|p_i\rangle =$$

$$\int \langle p_f|S^\dagger|p\langle d^3p\rangle p|S|p_i\rangle =$$

$$\langle p_f|(I+2\pi i\delta(E_f-E_p)[T(E+i0^+)]^\dagger)|p\rangle d^3p\langle p|(I-2\pi iT(E+i0^+)\delta(E_p-E_i))|p_i\rangle =$$

$$\langle p_f|I|p_i\rangle +$$

$$2\pi i\delta(E_f - E_i)\langle p_f|(T(E - i0^+) - T(E + i0^+))|p_i\rangle + y$$

$$4\pi^2\delta(E_f - E_i)T(E - i0^+)\delta(E_i - H_0)T(E + i0^+)$$

Unitarity requires that the last line vanishes when $E = E_i = E_f$. If we factor out the delta function we are left with

$$\boxed{\langle p_f|(T(E - i0^+) - T(E + i0^+))|p_i\rangle = 2\pi i\langle p_f|T(E - i0^+)\delta(E - H_0)T(E + i0^+)|p_i\rangle} \tag{158}$$

This is called the generalized optical theorem. It can also be derived directly from the definition of T using the second resolvent equations. In this derivation it is important to be careful about the $i0^+$ factors. The generalized optical theorem expresses the unitarity of the scattering operator in terms of the transition operator.

For completeness I give the derivation below

$$T(E-i0^+)-T(E+i0^+) = T(E-i0^+)R_0(E-i0^+)V-VR_0(E-i0^+)T(E+i0^+)$$

Next use the Lippmann Schwinger equation to write

$$V = T(E + i0^+) - VR_0(E + i0^+)T(E + i0^+)$$

and

$$V = T(E - i0^+) - T(E - i0^+)R_0(E - i0^+)V$$

and substitute in the above to get

$$T(E-i0^+)-T(E+i0^+) = T(E-i0^+)[R_0(E-i0^+)-R_0(E+i0^+)]T(E+i0^+)$$

Finally we use

$$[R_0(E - i0^+) - R_0(E + i0^+)] = \frac{-2i\epsilon}{(E - H_0)^2 + \epsilon^2} \rightarrow = 2\pi i\delta(E - H_0)$$

as $\epsilon \rightarrow 0$ to get

$$\boxed{T(E - i0^+) - T(E + i0^+) = 2\pi i T(E - i0^+)\delta(E - H_0)T(E + i0^+)} \quad (159)$$

This is a stronger version of our previous result because I have not used the on-shell assumption in the above derivation.

9 Cross Sections

In this section I define the scattering cross section. This is the quantity that is measured in laboratory scattering experiments. I begin by assuming that a scattering experiment is repeated many times. The number of scattered particles, N_{sc} is directly proportional to the number n_{inc} of particles incident per unit area in a direction perpendicular to the initial momentum. The constant of proportionality has units of area and is called the cross section σ

$$N_{sc} = n_{inc}\sigma \quad (160)$$

I can select the number of particles that are scattered in a cone of solid angle $\Delta\Omega$ as

$$N_{sc}(\Delta\Omega) = n_{inc}\sigma(\Delta\Omega) \quad (161)$$

I write this as an integral of a *differential cross section* over the solid angle

$$N_{sc}(\Delta\Omega) = n_{inc}\int_{\Delta\Omega} \frac{d\sigma}{d\Omega}d\Omega \quad (162)$$

where I have assumed a uniform density n_{inc} over the size of the target.

For a given initial wave packet the probability of scattering into a cone solid angle $d\Omega$ is

$$P(d\Omega \leftarrow \psi_{0-}) =$$
$$d\Omega \int_0^\infty p^2 dp | \int d^3p' \langle \vec{p}|S|\vec{p}'\rangle \langle \vec{p}'|\psi_{0-}\rangle|^2 \tag{163}$$

By integrating over p I am only concerned with the particles that eventually hit the detector. I assume that every particle in the cone triggers the detector, independent of momentum.

The total number of particles scattering into a given cone will be the sum over the number of incident particles times the probability of scattering into a given cone with solid angle $d\Omega$:

$$N_{sc}(d\Omega) = \sum_i P(d\Omega \leftarrow \psi_{i0-}) \tag{164}$$

In a real experiment the wave packets $|\psi_{i0-}\rangle$ will all be different. Typically they will all have an average momentum approximately equal to the beam momentum,

I treat this in two steps. I begin by assuming that the wave packets only differ by impact parameter $\vec{b}$, where $\vec{b}$ is a two dimensional vector in the plane perpendicular to the incident beam, which I call the 3-direction. An initial state shifted by an amount $\vec{b}$ relative to a reference state $\langle \vec{p}'|\psi_{0-}\rangle$ is

$$\langle \vec{p}'|\psi_{\vec{b}0-}\rangle = e^{i\vec{b}\cdot\vec{p}'}\langle \vec{p}'|\psi_{0-}\rangle. \tag{165}$$

Next I assume that the impact parameters are uniformly distributed over the cross sectional area subtended by the target with density n_{inc}. The sum over states can be replaced by a density n_{inc} times an integral over impact area:

$$N_{sc}(d\Omega) = \int d^2b n_{inc} P(d\Omega \leftarrow \psi_{\vec{b}0-}) \tag{166}$$

The integral over impact area can be extended over the entire plane because the probability of a scattering event is essentially zero for an event with a sufficiently large impact parameter. The incident density n_{inc} can be factored out of the integral if it is uniform:

$$N_{sc}(d\Omega) = n_{inc} d\Omega \int d^2b P(d\Omega \leftarrow \psi_{\vec{b}0-}). \tag{167}$$

This gives the following expression for the cross section

$$\sigma(d\Omega \leftarrow \cdot) = d\Omega \int d^2b P(d\Omega \leftarrow \psi_{\vec{b}0-}). \tag{168}$$

Next I use the expression for the scattering operator. I assume that the differential cone of interest does not include the beam direction, so S can be replaced the transition operator term:

$$\sigma(d\Omega \leftarrow \cdot) = \int d^2b P(d\Omega \leftarrow \psi_{\vec{b}0-})$$

$$\sigma(d\Omega \leftarrow \cdot) = d\Omega \int d^2b d\Omega \int_0^\infty p^2 dp| \int d^3p' \langle \vec{p}|S|\vec{p}'\rangle e^{i\vec{b}\cdot\vec{p}'} \langle \vec{p}'|\psi_{0-}\rangle|^2 =$$

$$d\Omega \int d^2b \int_0^\infty p^2 dp| \int d^3p'|(-2\pi i\delta(E-E')\langle \vec{p}|T(E+i0^+)|\vec{p}'\rangle e^{i\vec{b}\cdot\vec{p}'} \langle \vec{p}'|\psi_{0-}\rangle|^2. \tag{169}$$

Expanding everything out gives:

$$d\Omega \int d^2b \int_0^\infty p^2 dp \int d^3p' d^3p''$$

$$4\pi^2 \delta(E_{p''} - E)\delta(E_{p'} - E)\langle \vec{p}|T(E+i0^+)|\vec{p}'\rangle \langle \vec{p}''|T(E-i0^+)|\vec{p}\rangle \times$$

$$e^{i\vec{b}\cdot(\vec{p}'-\vec{p}''')} \langle \vec{p}'|\psi_{0-}\rangle \langle \vec{p}''|\psi_{0-}\rangle \tag{170}$$

The integral over the impact parameters can be done with the result that

$$\int d^2b e^{-i\vec{b}\cdot(\vec{p}'-\vec{p}'')} = 4\pi^2 \delta(\vec{p}_\perp{}' - \vec{p}_\perp{}'')$$

The product of the energy delta functions

$$\delta(E_{p''} - E)\delta(E_{p'} - E) = \delta(E_{p''} - E_{p'})\delta(E_{p'} - E) =$$

$$2m\delta((p'')^2 - (p')^2)\delta(E_{p'} - E) \tag{171}$$

When this is coupled with the constraint from the delta function that comes from the integration over impact parameter, it becomes

$$2m\delta((p_3'')^2 - (p_3')^2)\delta(E_{p'} - E) \tag{172}$$

If the wave packet are sharply peaked about the beam momentum so only one root survives. I get

$$\frac{m}{p_3}\delta(p_3'' - p_3')\delta(E_{p'} - E) \tag{173}$$

Combining this with the other delta function gives

$$\frac{m}{p_3}\delta(\vec{p}'' - \vec{p}')\delta(E_{p'} - E) \tag{174}$$

Using these identities in the original expression for the cross section gives

$$d\Omega \int p^2 dp \int d^3p'$$

$$16\pi^4\delta(E_{p'} - E)\frac{m}{p_3'}|\langle\vec{p}|T(E + i0^+)|\vec{p}'\rangle|^2|\langle\vec{p}'|\psi_{0-}\rangle|^2 \tag{175}$$

I can also evaluate

$$\int p^2 dp\delta(E_{p'} - E) = 2m\int p^2 dp\delta(p'^2 - p^2) = mp' \tag{176}$$

The last step is to *assume that the transition matrix elements are approximately constant* on the region where the momentum wave packets are non-vanishing. This can always be achieved with sufficiently sharply peaked wave packets. When this holds I can factor the T-matrix elements out of the integral and replace the initial momentum $\vec{p}$ by the average value.

$$d\Omega \int 16\pi^4 m'p'\frac{m}{p_3'}|\langle\vec{p}|T(E + i0^+)|\vec{p}'\rangle|^2|\langle\vec{p}'|\psi_{0-}\rangle|^2 d^3p' \approx$$

$$d\Omega 16\pi^4\frac{m}{\bar{p}_3'}|\langle\vec{p}|T(E + i0^+)|\vec{p}'\rangle|^2 m\bar{p}\int |\langle\vec{p}'|\psi_{0-}\rangle|^2 d^3p' \tag{177}$$

Using the normalization integral for the wave function gives

$$d\Omega 16\pi^4\frac{m}{\bar{p}_3}|\langle\vec{p}|T(E + i0^+)|\vec{p}'\rangle|^2 m'\bar{p} \tag{178}$$

or

$$d\sigma = \frac{(2\pi)^4}{v_{inc}}|\langle\vec{p}|T(E + i0^+)|\bar{\vec{p}}'\rangle|^2 p^2\frac{dp}{dE}d\Omega \tag{179}$$

where $v_{inc} := \bar{p}_3/m$ is the mean incident speed. This is the standard expression for the differential cross section in terms of the transition operator.

The key observation is that as long as the wave packet is sharply peaked, this result is independent of the shape of the wave packet. This is important because is would be very difficult to repeat experiments that were very sensitive to the structure of the initial wave packets. I also note that this derivation assumes that the beam and target densities are sufficiently low that a given beam particle has a very small probability of scattering from more than one target particle.

The differential cross section is a useful quantity because its ratio in two different cones is equal to the ratio of the number of particles detected in each cone for a large enough set of scattering experiments.

Unlike standard textbook derivations that rely heavily on a wave interpretation of quantum mechanics, this derivation emphasizes the particle interpretation of quantum mechanics.

I also note that the assumption that the beam is in the 3-direction and the energy conservation enforced by the delta functions means

$$1 = \frac{\bar{p}}{\bar{p}_3}. \tag{180}$$

This allows me to write the cross section as

$$\frac{d\sigma}{d\Omega} = |(2\pi)^2 m \langle \vec{p}|T(E + i0^+)|\bar{\vec{p}}'\rangle|^2 = |f|^2 \tag{181}$$

where the scattering amplitude f is defined by

$$f := -4\pi^2 m \langle \vec{p}|T(E + i0^+)|\bar{\vec{p}}'\rangle \tag{182}$$

The $-$ arises when this quantity is derived by looking at asymptotic properties of scattering wave functions.

10 Two-Body Scattering

So far I have only considered scattering of an incoming projectile from a fixed source, which was represented by a potential. This is an idealized setting. Normally a projectile of mass m_1 scatters off of a target particle of mass m_2. In this case the projectile scatters and the target recoils.

Two-particle scattering normally means two isolated particles. For isolated the dynamics is Galilean invariant. This means that result of any experiment is invariant with respect to rotations. translations, time translations and Galilean boosts (changes in the overall velocity of the system).

Using these principles I discuss the general form of the Hamiltonian. I start with two free particles. The kinetic energy is

$$H_0 = \frac{\vec{p}_1 \cdot \vec{p}_1}{2m_1} + \frac{\vec{p}_2 \cdot \vec{p}_2}{2m_2}. \tag{183}$$

The total momentum is defined by

$$\vec{P} = \vec{p}_1 + \vec{p}_2 \tag{184}$$

The momentum of particle 1 in the center of momentum frame is obtained by applying a the Galilean boost that takes $\vec{P}$ to zero, to the momentum of particle 1:

$$\vec{k}_1 = \vec{p}_1 - m_1\vec{v} = \vec{p}_1 - \frac{m_1}{m_1+m_2}(\vec{p}_1 + \vec{p}_2) =$$

$$\frac{m_2\vec{p}_1 - m_1\vec{p}_2}{m_1+m_2.}$$

Note that this *operator is defined in any frame*, but its eigenvalue represents the value of the momentum of particle 1 if it was boosted to the zero momentum frame. The operator $\vec{k}_1$ is constructed to be invariant with respect to Galilean boosts.

These relations can be inverted to obtain

$$\vec{p}_1 = \vec{k}_1 + \frac{m_1}{m_1+m_2}\vec{P} \tag{185}$$

$$\vec{p}_2 = -\vec{k}_1 + \frac{m_2}{m_1+m_2}\vec{P}. \tag{186}$$

Using these equations in the expression for the kinetic energy gives

$$H_0 = \frac{\vec{k}_1 \cdot \vec{k}_1}{2m_1} + \frac{m_1}{2(m_1+m_2)^2}\vec{P}\cdot\vec{P} + \frac{\vec{k}_1 \cdot \vec{k}_1}{2m_2} + \frac{m_2}{2(m_1+m_2)^2}\vec{P}\cdot\vec{P} =$$

$$H_0 = \frac{1}{2}(\frac{1}{m_1} + \frac{1}{m_2})\vec{k}_1 \cdot \vec{k}_1 + \frac{1}{2(m_1+m_2)}\vec{P}\cdot\vec{P}. \tag{187}$$

I define the total mass m and the reduced mass μ by

$$m = m_1 + m_2$$

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} \qquad \mu = \frac{m_1 m_2}{m}. \tag{188}$$

The kinetic energy can be expressed as

$$H_0 = \frac{\vec{k_1} \cdot \vec{k_1}}{2\mu} + \frac{\vec{P} \cdot \vec{P}}{2m}. \tag{189}$$

At this stage it does not look like anything has been accomplished. The new free Hamiltonian has the same form as the initial Hamiltonian.

This transformed form becomes interesting because of the symmetries of the potential. If I write

$$V(\vec{k_1}\,, \vec{P}\,; \vec{k_1}\,', \vec{P}\,', t) := \langle \vec{k_1}\,, \vec{p}\,|V(t)|\vec{k_1}\,', \vec{P}\,'\rangle \tag{190}$$

Galilean invariance of the interaction requires

$$V(\vec{k_1}\,, \vec{P}\,; \vec{k_1}\,', \vec{P}\,', t) \tag{191}$$

$$e^{i(\vec{P}-\vec{P}\,')\cdot\vec{c}} V(R\vec{k_1}\,, R\vec{P} + m\vec{v}\,; R\vec{k_1}\,', R\vec{P}\,' + m\vec{v}, t + t_0)$$

for any $\vec{c}$, $\vec{v}$, t_0 or rotation R. Independence on $\vec{c}$ means that the potential matrix elements vanishes unless $\vec{P} - \vec{P}\,' = 0$. Independence on $\vec{v}$ (for $\vec{P} = \vec{P}\,'$) means that the matrix element is independent of $\vec{P}$. Independence on t_0 means that the potential matrix element is independent of t. What remains is a rotationally invariant function of $\vec{k_1}$ and $\vec{k_1}\,'$ or

$$V(\vec{k}_1\,, \vec{P}\,; \vec{k}_1\,', \vec{P}\,', t) := \langle \vec{k}_1\,, \vec{P}\,|V(t)|\vec{k}_1\,', \vec{P}\,'\rangle =$$

$$\delta(\vec{P} - \vec{P}\,')v(\vec{k}_1 \cdot \vec{k}_1, \vec{k}_1' \cdot \vec{k}_1', \cdot\vec{k}_1 \cdot \vec{k}_1\,'). \tag{192}$$

It is clear that Galilean invariance puts strong constraints on the interactions. The Hamiltonian takes on the form

$$H = \frac{\vec{P} \cdot \vec{P}}{2m} + h$$

$$h = \frac{\vec{k}_1 \cdot \vec{k}_1}{2\mu} + v$$

The Galilean invariant Hamiltonian h looks just the Hamiltonian for a single particle scattering off of a fixed source, except the mass is replaced by the reduced mass. The total kinetic energy separates from the problem. The eigenvalue of h represents the total energy of the system in the zero momentum frame of the system.

To treat two particle scattering the first step is to realize that the starting point for treating scattering is the formulation of the asymptotic condition. The only change is that the initial wave packet depends on both $\vec{p}_1$ and $\vec{p}_2$ or $\vec{P}$ and $\vec{k}$.

The Møller wave operators become

$$\Omega_{\pm}(H, H_0) = s - \lim_{t\to\pm\infty} e^{iHt}e^{-iH_0t} = s - \lim_{t\to\pm\infty} e^{i\frac{\vec{P}\cdot\vec{P}t}{2m}+iht}e^{-i\frac{\vec{P}\cdot\vec{P}t}{2m}-ih_0t} =$$

$$s - \lim_{t\to\pm\infty} e^{iht}e^{-ih_0t} = I_P \otimes \Omega_{\pm}(h, h_0) \tag{193}$$

where I_P is the identity on the space of square integrable functions of $\vec{P}$. This holds because $\frac{\vec{P}\cdot\vec{P}}{2m}$ commutes with both h and h_0. Matrix elements of the wave operators have the form

$$\langle \vec{P}\,', \vec{k}_1\,'|\Omega_{\pm}(H, H_0)|\vec{P}, \vec{k}_1\rangle = \delta^3(\vec{P} - \vec{P}\,')\langle \vec{k}_1\,'|\Omega_{\pm}(h, h_0)|\vec{k}_1\rangle.$$

This can also be expressed in terms of single particle variables, but the expression is more complicated.

Similarly, the scattering matrix elements are

$$\langle \vec{P}\,', \vec{k}_1\,'|S(H, H_0)|\vec{P}, \vec{k}_1\rangle = \delta^3(\vec{P} - \vec{P}\,')\langle \vec{k}_1\,'|S(h, h_0)|\vec{k}_1\rangle \tag{194}$$

The relation between the scattering operator and the transition operator becomes

$$\langle \vec{P}\,', \vec{k}_1\,'|S(H, H_0)|\vec{P}, \vec{k}_1\rangle =$$

$$\delta^3(\vec{P} - \vec{P}\,')[\delta^3(\vec{k}_1 - \vec{k}_1\,') - 2\pi i\langle \vec{k}_1\,'|[v + v\frac{1}{\frac{\vec{k}_1\cdot\vec{k}_1}{2\mu} - h_0 - +i0^+}v]|\vec{k}_1\rangle]. \tag{195}$$

Similar remarks apply to the K matrix. In general replace the one-body expression by the corresponding center of momentum expression, multiplied by a three dimensional momentum conserving delta function.

This is also true when I construct the scattering cross section. The new features are

a. The initial wave packet $\langle\vec{p}|\psi_{0-}\rangle$ is replaced by $\langle\vec{P},\vec{k},|\psi_{0-}\rangle$

b. There are three-dimensional delta functions multiplying in the total momentum connecting the initial and final momenta in each appearance of S. There are also accompanying integrations over the initial momenta.

c. The cone is associated with final momenta in a volume d^3P, d^3k. If we are only measuring the center of momentum angles of particle 1, then is it necessary to integrate over k^2dkd^3P.

These modifications lead to the following expression for the differential cross section:

$$\frac{d\sigma}{d\Omega} = |(2\pi)^2 m\langle\vec{k}_1|T(\frac{\vec{k}_1\,'\cdot\vec{k}_1\,'}{2\mu}+i0^+)|\vec{k}_1\,'\rangle|^2$$

Since the total cross section is a ratio of numbers, it is obviously invariant. When I consider the differential cross section some additional care is needed.

A more useful form of the expression for the cross section is

$$d\sigma = \frac{(2\pi)^4}{k_1'/\mu}|\langle\vec{k}_1|T(\frac{\vec{k}_1\,'\cdot\vec{k}_1\,'}{2\mu}+i0^+)|\vec{k}_1\,'\rangle|^2 d^3k_1 d^3P\delta^3(P-P')\delta(E-E') \quad (196)$$

The previous expression is recovered by integrating over all of the unmeasured variables, k^2dkd^3P.

This expression is more general than the previous one because I can choose to measure an observable other than $d\Omega(k)$. For example I could replace $d^3k_1d^3P = d^3p_1d^3p_1$. If I wanted to measure the angular distribution of particle 1 in the lab frame it is enough to integrate over the 3-momentum of particle two and the magnitude of the momentum of particle 1.

Here v_{inc} is always $\frac{\vec{k}\cdot\hat{z}}{\mu}$ where $\hat{z}$ is a unit vector in the beam direction.

The text and the article by Brenig and Haag give a direct derivation of the two-body cross section that does not utilize the equivalent one-body center of momentum solution. The results are identical to the above.

11 Spin

A structureless point particle is characterized by its mass, spin, linear momentum, and magnetic quantum number. Spin plays an important role in

scattering experiments. It is an additional degree of freedom that can be measured and is relevant for understanding the spin dependence of the interactions.

I assume that you have studied spin in quantum mechanics. The spin is a triple of hermitian operators $\vec{j}$ that satisfy the commutation relations

$$[j^i, j^j] = i\epsilon_{ijk} j^k.$$

In addition, for particles with spin, the spin vector commutes with all components of the linear momentum

$$[p^i, j^k] = 0.$$

Since the different components of the spin do not commute, only one component can be taken as a commuting observable. If is customary to include the 3-component of the spin as a commuting observable that describes the state of a particle.

A single particle wave functions is

$$\langle (m, j)\vec{p}, \mu | \psi \rangle \tag{197}$$

where m and j are fixed invariant quantum numbers, and μ runs from $-j$ to j in integer steps.

When the state of the target of beam is prepared it can be in an eigenstate of j_3 or in a superposition of eigenstates.

The simplest theoretical situation is when all of initial and final states are prepared or measured to be in specific spin states. I use the notation

$$|\vec{p}_1, \mu_1, \vec{p}_2, \mu_2\rangle = |\vec{P}, \vec{k}_1, \mu_1, \mu_2\rangle \tag{198}$$

to denote the initial and final plane wave states.

With these variables the transition matrix elements for Galilean invariant interaction have the form

$$\langle \vec{P}, \vec{k}_1, \mu_1, \mu_2 | T(E^+) | \vec{P}\,', \vec{k}_1\,', \mu_1', \mu_2' \rangle = \delta^3(\vec{P} - \vec{P}\,') \langle \vec{k}_1, \mu_1, \mu_2 | t(E^+) |, \vec{k}_1\,', \mu_1', \mu_2' \rangle \tag{199}$$

where $\langle \vec{k}_1, \mu_1, \mu_2 | t(E^+) |, \vec{k}_1\,', \mu_1', \mu_2' \rangle$ is the solution to the Lippmann-Schwinger equation

$$\langle \vec{k}, \mu_1, \mu_2 | t(E^+) |, \vec{k}\,', \mu_1', \mu_2' \rangle = \langle \vec{k}, \mu_1, \mu_2 | v |, \vec{k}\,', \mu_1', \mu_2' \rangle + \int d^3k'' \sum_{\mu_1'', \mu_2''}$$

$$\frac{\langle \vec{k}, \mu_1, \mu_2 | v |, \vec{k}\,'', \mu_1'', \mu_2'' \rangle}{\frac{k'^2}{2\mu} - \frac{k''^2}{2\mu} + i0^+} \langle \vec{k}\,'', \mu_1'', \mu_2'' | t(E^+) |, \vec{k}\,', \mu_1', \mu_2' \rangle. \tag{200}$$

This differs form the previous version of the Lippmann-Schwinger equation by the spin sums. The operator form is identical to the previous case. Note that while there are two magnetic quantum numbers, only the relative momentum is needed in the dynamical equation.

Building on the derivation in the previous section the differential cross sections becomes

$$d\sigma =$$

$$\frac{(2\pi)^4}{k_1'/\mu} |\langle \vec{k}_1, \mu_1, \mu_2 | T(\frac{\vec{k}_1\,' \cdot \vec{k}_1\,'}{2\mu} + i0^+) | \vec{k}_1\,', \mu_1', \mu_2' \rangle|^2 d^3k_1 d^3P \delta^3(P - P') \delta(E - E') \tag{201}$$

The opposite extreme is to make the experiment as simple as possible. This corresponds to the situation where the beam and target are unpolarized and the final spins are not measured.

By unpolarized we mean that any measurement of the z component of spin will have identical probabilities for measuring each eigenvalue. For the beam there are $2j_1+1$ possible eigenvalues and for the target there are $2j_2+1$ possible eigenstates.

It follows that the incoming scattering asymptote have $N_i = (2j_1 + 1)(2j_2 + 1)$ possible polarization states. Each one appears in the initial state with probability $1/N_i$. For spin $1/2$ there are four, with two spin states for the beam and two spins states for the target.

In the cross section I treat this by considering an ensemble of initial states where the continuous wave function is localized and each system is in one of the N_i possible states of initial polarization. I assume that each polarization occurs in the initial state with probability $1/N$.

In this case the differential cross section is computed by averaging over the initial polarizations

$$d\sigma = \frac{1}{N_i} \sum_{\mu_1', \mu_2'} \frac{(2\pi)^4}{k_1'/\mu} |\langle \vec{k}_1, \mu_1, \mu_2 | T(\frac{\vec{k}_1\,' \cdot \vec{k}_1\,'}{2\mu} + i0^+) | \vec{k}_1\,', \mu_1', \mu_2' \rangle|^2 \times$$

$$d^3k_1 d^3P \delta^3(P - P') \delta(E - E') \tag{202}$$

If I do not measure the polarization of the scattered particle or the recoiling target, then it is appropriate to sum over all $N_f = N_i$ polarizations.

It follows that

$$d\sigma_{\text{unpolarized}} = \frac{1}{N_i}\sum_{\mu_1',\mu_2'}\sum_{\mu_1,\mu_2}\frac{(2\pi)^4}{k_1'/\mu}|\langle\vec{k}_1,\mu_1,\mu_2|T(\frac{\vec{k_1}'\cdot\vec{k_1}'}{2\mu}+i0^+)|\vec{k_1}',\mu_1',\mu_2'\rangle|^2\times$$

$$d^3k_1 d^3P\delta^3(P-P')\delta(E-E') \tag{203}$$

Thus the prescription for unpolarized scattering is to average over initial polarizations and sum over final polarizations.

In most experiments what is measured falls between these two extremes. The most natural way to treat the general setting is to use a density matrix formulation. I begin by considering the description partially polarized beam. Even if one tries to make a perfectly polarized beam the result is normally partially polarized. This can be due to collisions in the beam or thermal effect.

I begin by assuming that the beam contains states with N different polarizations, $\{\lambda_i\}_{i=1}^N$. The different states do not have to be orthogonal, one could correspond to spin up in the z direction and another could be spin down in the y direction. I assume that polarization λ_i occurs with probability p_i in the beam so it follows that

$$\sum_{i=1}^N p_i = 1 \tag{204}$$

The density matrix for this beam is the operator

$$\rho := \sum_{i=1}^N |\lambda_i\rangle p_i\langle\lambda_i| \tag{205}$$

where the states λ_i are normalized to unity. General properties of the density matrix follow from this definition. The important properties are

$$\rho = \rho^\dagger \tag{206}$$

$$\rho \geq 0 \tag{207}$$

$$\text{Tr}\rho = 1 \tag{208}$$

$$\text{Tr}\rho^2 \leq 1. \tag{209}$$

The first of these results is obvious. The second follows because

$$\langle\psi|\rho|\psi\rangle = \sum_{i=1}^N |\langle\psi|\lambda_i\rangle|^2 p_i \geq 0.$$

The third follows because

$$\mathrm{Tr}(\rho) = \sum_{i=1}^{N} p_i = 1.$$

The last condition is most easily proved by multiplying both sides of ρ by an expansion of the identity in terms of orthonormal states, and then evaluating the trace. Since ρ is a positive hermitian matrix it has a complete set of non-negative eigenvalues $\bar{p}_j$ and orthonormal eigenvectors $|\bar{\lambda}_j\rangle$. It can be expressed as

$$\rho := \sum_{i=1}^{M} |\bar{\lambda}_i\rangle \bar{p}_i \langle\bar{\lambda}_i|$$

where M does not have to equal N and the states $\langle\bar{\lambda}_i|$ are orthonormal.

Since the trace is invariant it follows that

$$\mathrm{Tr}\rho = \sum_{i=1}^{N} p_i = \sum_{i=1}^{M} \bar{p}_i = 1$$

In the new representation I can compute

$$\mathrm{Tr}\rho^2 = \sum_{i=1}^{M} \bar{p}_i^2 \tag{210}$$

Since each of the $\bar{p}_i$ are between 0 and 1 I always have

$$\bar{p}_i^2 \leq \bar{p}_i \tag{211}$$

and these are only equal when $\bar{p}_i$ is zero or one. It follows that

$$\mathrm{Tr}\rho^2 \leq \mathrm{Tr}\rho = 1. \tag{212}$$

These are equal only if one of the $\bar{\lambda}_i$ is one and the others are zero. In this case ρ has the form

$$\rho = |\lambda_1\rangle\langle\lambda_1| \tag{213}$$

where the ensemble has only one state.

It is customary to call an ensemble described by a density matrix a "state". When $\mathrm{Tr}(\rho^2) = 1$ the state is called a **pure state**.

The experimental determination that beam is in a given state requires some measurements. The expectation value of an observable described by a Hermitian operator A is

$$\langle A\rangle = \mathrm{Tr}(A\rho) = \sum_{i=1}^{N} p_i \langle\lambda_i|A|\lambda_i\rangle \tag{214}$$

which is the weighted average of the expectation value of A in the states $|\lambda_i\rangle$. By making enough independent measurements on the beam it is possible to uniquely determine the state.

I first use abstract considerations. Abstractly ρ is an $N \times N$ Hermitian matrix. It is a simple matter to construct N^2 independent Hermitian matrices, Q_i with the first one being the identity. The trace defines a scalar product on these matrices

$$(O_i, O_j) := \mathrm{Tr}(O_i O_j). \tag{215}$$

Note that independence requires $(O_i, O_i) > 0$. This is because the trace is the sum of the eigenvalues, and this is a matrix with non-negative eigenvalues. If the trace were zero all eigenvalues would be zero and the operator would be zero.

Starting with $O_1 = I/\sqrt{N}$ I can use the Gram-Schmidt method to construct linear combinations of these matrices, $\bar{O}_i$ with real coefficients that satisfy

$$(\bar{O}_i, \bar{O}_j) := \mathrm{Tr}(\bar{O}_i \bar{O}_j) = \delta_{ij}. \tag{216}$$

Note that because $\bar{O}_1 = O_1 = I/\sqrt{N}$ all of the $\bar{O}_i$ with $i > 1$ are traceless.

The operators $\bar{O}_i$ are independent spin observables that need to be measured to determine the density matrix. Note that in general, ρ is Hermitian

$$\rho = \sum_{i=1}^{N^2} \rho_i \bar{O}_i \tag{217}$$

The expectation values of each of the observables $\bar{O}_j$ is

$$\langle \bar{O}_j\rangle = \mathrm{Tr}(\rho \bar{O}_j) = \sum_{i=1}^{N^2} \rho_i \mathrm{Tr}(\bar{O}_i \bar{O}_j) = \rho_j \tag{218}$$

This leads to the representation

$$\rho = \sum_{i=1}^{N^2} \langle \bar{O}_j \rangle \bar{O}_i \tag{219}$$

Note that

$$\langle \bar{O}_1 \rangle = \frac{1}{\sqrt{N}} \mathrm{Tr}\rho = \frac{1}{\sqrt{N}}$$

which gives the alternate expression

$$\frac{1}{N}[I + \sum_{i=2}^{N^2} \frac{\sqrt{N}}{\mathrm{Tr}\rho} \langle O_i \rangle O_i]$$

To illustrate this consider the example of a spin 1/2 particle. The particle has two spin states. The density matrix is a 2×2 Hermitian matrix. Orthonormal Hermitian matrices with respect to the trace norm can taken to be the 2×2 identity and the three Pauli spin matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{220}$$

The density matrix for a spin $\frac{1}{2}$ beam has the form

$$\rho = \frac{1}{2}(I + \vec{\pi} \cdot \vec{\sigma}) \tag{221}$$

The quantity $\vec{\pi}$ is called the polarization vector of the beam. Note

$$\pi_i = \mathrm{Tr}(\rho \sigma_i) = 2\mathrm{Tr}(\rho j_i) \tag{222}$$

Thus we can determine the polarization of the beam measuring the expectation value of each component of the spin in the beam.

Note that if all of the spin expectation values vanish then ρ is proportional to the identity. This corresponds to an unpolarized beam. Clearly the identity is the only one four matrices that is invariant with respect to rotations. This implies that if the beam is unpolarized, this condition is rotationally invariant, as it should be.

In order to treat scattering involving polarization I assume an initial density matrix ρ_i describing an ensemble of beam and target polarizations.

The differential cross section for a beam described by density matrix ρ beam is

$$d\sigma = \frac{(2\pi)^4}{k_1'/\mu}\langle \vec{k}_1, \mu_1, \mu_2 | T(\frac{\vec{k_1}' \cdot \vec{k_1}'}{2\mu} + i0^+) | \vec{k_1}', \mu_1', \mu_2' \rangle \rho_{\mu_1'\mu_2';\mu_1''\mu_1''} \times$$
$$\langle \vec{k}_1', \mu_1'', \mu_2'' | T(\frac{\vec{k_1}' \cdot \vec{k_1}'}{2\mu} - i0^+) | \vec{k_1}, \mu_1, \mu_2 \rangle \times$$
$$d^3k_1 d^3P \delta^3(P - P')\delta(E - E') \tag{223}$$

It is customary to put this in the form spin scattering amplitude F which is defined by

$$F = -4\pi^2 \mu \langle k_1, \mu_1, \mu_2 | T(\frac{k_1^2}{2\mu} + i0^+) | k_1', \mu_1', \mu_2' \rangle$$

This gives

$$\frac{d\sigma}{d\Omega} = F\rho_i F^\dagger \tag{224}$$

If the polarizations of the final states are not measured then I sum over all of the final polarizations. This is equivalent to

$$\frac{d\sigma}{d\Omega} = \mathrm{Tr}(F\rho_i F^\dagger) \tag{225}$$

where the trace is over spin quantum numbers.

To calculate the expectation value of a spin observable $\bar{O}_j$ in the final state it is enough to compute

$$\langle \bar{O}_j \rangle = \frac{\mathrm{Tr}(\bar{O}_i F \rho_i F^\dagger)}{\mathrm{Tr}(F\rho_i F^\dagger)} \tag{226}$$

The general picture is that I start with an initial density matrix ρ_i that describes the state of the beam and target. Using this density matrix I compute a density matrix for the outgoing scattering asymptotes

$$\rho_f := \frac{F\rho_i F^\dagger}{\mathrm{Tr}(F\rho_i F^\dagger)} \tag{227}$$

Given this matrix it is possible to compute any final sate spin observable.

A case of importance is the scattering of two spin 1/2 particles. In this case the matrices

$$O_n = \sigma_{\mu_1}^{(1)} \otimes \sigma_{\mu_2}^{(2)} \tag{228}$$

where $\mu_i \in \{0,1,2,3\}$ with $\sigma_0 = I$, satisfy the orthogonality relations

$$\mathrm{Tr}(O_n O_m) = \delta_{mn} \tag{229}$$

The trace can be computed in any basis

$$\mathrm{Tr}(O_n O_m) = \sum_{\alpha\beta} \langle \alpha \otimes \beta | O_n O_m | \alpha \otimes \beta \rangle =$$

$$\sum_{\alpha\beta} \langle \alpha | \sigma_{\mu_1} \sigma_{\nu_1} | \alpha \rangle \langle \beta | \sigma_{\mu_2} \sigma_{\nu_2} | \beta \rangle. \tag{230}$$

This calculation leads to the desired result. It follows that the polarization state of the target and beam is determined by measuring the x, y, and z components of the spin for the beam and target.

The most general observable for two nucleon scattering is

$$\langle \bar{O}_n \rangle = \frac{\mathrm{Tr}(\bar{O}_n F \rho_i F^\dagger)}{\mathrm{Tr}(F^\dagger \rho_i F)} \tag{231}$$

At first glance there are 4×4 parameters that define the polarization of the initial state and 4×4 that determine the polarization of the final state. A complete measurement requires determining 256 parameters at each beam energy and scattering angle.

Things are not this bad because F has symmetries. For example if F were proportional to the identity in spin space 16 measurements in the initial state completely characterize the final state.

To illustrate this I discuss the Wolfenstein parameterization of the scattering amplitude in nucleon-nucleon scattering. This is used in many calculations and provides a constructive illustration of the simplifications in F that follow from dynamical assumptions.

In nuclear physics Heisenberg introduced the concept of isospin. The basic assumption is that the proton and neutron behave like a spin up and spin down state of a single spin one half particle called the nucleon. This spin is not a real spin - it just mathematically looks like a spin and is called isospin. If the neutron and proton were really different internal states of the same particle,the would have the same mass. The neutron and proton masses are very close and the difference is attributed to the fact the proton has charge and interacts with its own electromagnetic field. Rotations is

isospin space correspond to a relabeling of the states identifies as protons or neutrons.

Heisenberg assumed that isospin is an exact symmetry of the strong interaction. The neutron has isospin $\tau_z = -1/2$ and the proton has isospin $\tau_z = -1/2$.

A two nucleon system can be described by its total isospin, which is obtained by adding the single nucleon isospins in the same way that one adds angular momenta. When two spin 1/2 particle are coupled the result is either a spin-1 (spin triplet) or spin-zero (spin singlet) particle.

A similar thing happens with isospin. The two nucleon system can be in a total isospin 1 states (iso-triplet) or a total isospin zero (iso singlet) state. These states can be constructed from products of single nucleon states using Clebsch-Gordan coefficients

$$|\tau, \tau_z\rangle = \sum_{\tau_{1z}, \tau_{2z}} |\frac{1}{2}, \tau_{1z}\rangle \otimes |\frac{1}{2}, \tau_{2z}\rangle \langle \frac{1}{2}, \tau_{2z}, \frac{1}{2}, \tau_{1z} | \tau, \tau_z\rangle \tag{232}$$

The $|1, 1\rangle$ state corresponds to two neutrons, the $|1, -1\rangle$ state corresponds to two protons, and the $|1, 0\rangle$ and $|0, 0\rangle$ states are symmetric and antisymmetric combinations of one neutron and one proton.

Conservation of τ_z is equivalent to charge conservation so it must be respected in any interaction. Conservation of τ^2 is and assumed property of the strong interaction (isospin invariance). This interaction is charge independent if the interaction is independent of τ_z.

Since identical nucleons are fermions the overall wave function must be antisymmetric. The wave functions has an orbital part, a spin part, and an isospin part. Only the overall wave function needs to be antisymmetric with respect to particle exchange.

The scattering amplitude has the general structure

$$F = -(2\pi)^2 \mu \langle \vec{k}, \mu_1, \mu_2, \tau, \tau_z | T(\frac{\vec{k} \cdot \vec{k}}{2\mu} + i0^+) | \vec{k}', \mu_1', \mu_2', \tau', \tau_z' \rangle$$

Isospin and charge conservation require that this is proportional to

$$\delta_{\tau_z \tau_z'} \delta_{\tau \tau'}$$

For fixed τ and τ_z I investigate the dependence on the following quantities

$$\{\vec{k}, \vec{k}\,', \mu_1, \mu_2, \mu_1', \mu_2'\}$$

I begin by defining orthogonal basis vectors in a right-handed coordinate system:

$$\hat{K} := \frac{\vec{k} - \vec{k}\,'}{|\vec{k} - \vec{k}\,'|}$$

$$\hat{P} := \frac{\vec{k} + \vec{k}\,'}{|\vec{k} + \vec{k}\,'|}$$

$$\hat{N} := \frac{\vec{k} \times \vec{k}\,'}{|\vec{k} \times \vec{k}\,'|}$$

The vectors $\hat{K}$ and $\hat{P}$ span the scattering plane while $\hat{N}$ is normal to the scattering plane.

The operators $O_n = \sigma^{(1)}_{\mu_1} \otimes \sigma^{(2)}_{\mu_2}$ are a basis for the Hermitian operators in spin space. If the interaction is rotationally invariant it can be built up out of scalars constructed out of

$$\{\hat{K}, \hat{P}, \hat{N}, \vec{\sigma}^{(1)}, \vec{\sigma}^{(2)}\}$$

with coefficients that depend on

$$k^2 = \vec{k} \cdot \vec{k}, k'^2 = \vec{k}\,' \cdot \vec{k}\,', \cos(\theta) = \frac{\vec{k} \cdot \vec{k}\,'}{kk'}$$

Since F is also rotationally invariant the same consideration apply to F, except because F is evaluated on-shell, $k' = k$, so the coefficients only depend on k and $\cos(\theta)$.

The independent operators are the identity and the operators

$$\vec{\sigma}^{(i)} \cdot \hat{K}, \qquad \vec{\sigma}^{(i)} \cdot \hat{P}, \qquad \vec{\sigma}^{(i)} \cdot \hat{N}$$

$$(\vec{\sigma}^{(1)} \times \vec{\sigma}^{(2)}) \cdot \hat{K}, \qquad (\vec{\sigma}^{(1)} \times \vec{\sigma}^{(2)}) \cdot \hat{P}, \qquad (\vec{\sigma}^{(1)} \times \vec{\sigma}^{(2)}) \cdot \hat{P},$$

$$(\vec{\sigma}^{(1)} \cdot \hat{N}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{N}) \qquad (\vec{\sigma}^{(1)} \cdot \hat{P}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{P}) \qquad (\vec{\sigma}^{(1)} \cdot \hat{K}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{K})$$

$$(\vec{\sigma}^{(1)} \cdot \hat{N}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{P}) \qquad (\vec{\sigma}^{(1)} \cdot \hat{P}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{N}) \qquad (\vec{\sigma}^{(1)} \cdot \hat{N}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{K})$$

$$(\vec{\sigma}^{(1)} \cdot \hat{K}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{N}) \qquad (\vec{\sigma}^{(1)} \cdot \hat{P}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{K}) \qquad (\vec{\sigma}^{(1)} \cdot \hat{K}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{P})$$

Under space reflection invariance

$$\hat{K} \to -\hat{K} \qquad \hat{P} \to -\hat{P} \qquad \hat{N} \to -\hat{N} \qquad \vec{\sigma}^{(i)} \to \vec{\sigma}^{(i)}$$

If the interaction is space reflection invariant only scalar combinations of these quantities that do not change sign under parity are allowed. This eliminates terms of the form

$$\vec{\sigma}^{(i)} \cdot \hat{K}, \qquad \vec{\sigma}^{(i)} \cdot \hat{P}, \qquad (\vec{\sigma}^{(1)} \times \vec{\sigma}^{(2)}) \cdot \hat{K}, \qquad (\vec{\sigma}^{(1)} \times \vec{\sigma}^{(2)}) \cdot \hat{P}$$

$$(\vec{\sigma}^{(i)} \cdot \hat{K}) \cdot (\vec{\sigma}^{(j)} \cdot \hat{N}) \qquad (\vec{\sigma}^{(i)} \cdot \hat{P}) \cdot (\vec{\sigma}^{(j)} \cdot \hat{N})$$

Next I consider invariance with respect to time reversal. Recall that time reversal, Θ, is an antiunitary operator. I also recall

$$\Theta|\vec{k}\mu_1\mu_2\rangle = (-)^{1-\mu_1-\mu_2}|-\vec{k}-\mu_1-\mu_2\rangle$$

where the phase is one of several possible conventions. Applying Θ to the scattering amplitude I get

$$F = -(2\pi)^2\mu\langle\vec{k},\mu_1,\mu_2,\tau,\tau_z|T(\frac{\vec{k}\cdot\vec{k}}{2\mu}+i0^+)|\vec{k}',\mu_1',\mu_2',\tau',\tau_z'\rangle =$$

$$-(2\pi)^2\mu\langle\Theta(\vec{k},\mu_1,\mu_2,\tau,\tau_z)|\Theta(T(\frac{\vec{k}\cdot\vec{k}}{2\mu}+i0^+)|\vec{k}',\mu_1',\mu_2',\tau',\tau_z')\rangle^* =$$

$$-(-)^{2-\mu_1-\mu_2-\mu_1'-\mu_2'}(2\pi)^2\mu\langle-\vec{k}',-\mu_1',-\mu_2',\tau,\tau_z|T(\frac{\vec{k}\cdot\vec{k}}{2\mu}+i0^+)|-\vec{k},-\mu_1,-\mu_2,\tau,\tau_z\rangle$$

Since the amplitude is expanded in terms of Pauli matrices it is useful to express the above transformation properties in terms of the spin matrices:

$$(-)^{1-\mu_1-\mu_1'}\langle-\mu_1'|\vec{\sigma}^{(1)}|-\mu_1\rangle =$$

$$\langle\Theta(\mu_1')|\vec{\sigma}^{(1)}|\Theta(\mu_1)\rangle =$$
$$-\langle\Theta(\mu_1')|\Theta\vec{\sigma}^{(1)}|(\mu_1)\rangle =$$
$$-\langle\mu_1|\vec{\sigma}^{(1)}|\mu_1'\rangle$$

which corresponds to changing the sign of the $\vec{\sigma}^{(i)}$. Since $\vec{k} \to -\vec{k}'$ and $\vec{k}' \to -\vec{k}$ I also have

$$\hat{K} \to \hat{K} \qquad \hat{P} \to -\hat{P} \qquad \hat{N} \to -\hat{N}$$

Time reversal eliminates the terms the change sign under time reversal:

$$\vec{\sigma}^{(i)} \cdot \hat{K}, \qquad (\vec{\sigma}^{(1)} \times \vec{\sigma}^{(2)}) \cdot \hat{N} \qquad (\vec{\sigma}^{(1)} \times \vec{\sigma}^{(2)}) \cdot \hat{P}$$
$$(\vec{\sigma}^{(i)} \cdot \hat{K}) \cdot (\vec{\sigma}^{(j)} \cdot \hat{N}) \qquad (\vec{\sigma}^{(i)} \cdot \hat{K}) \cdot (\vec{\sigma}^{(j)} \cdot \hat{P})$$

The surviving term after requiring rotational invariance, time reversal invariance, and parity are

$$\vec{\sigma}^{(i)} \cdot \hat{N} \qquad (\vec{\sigma}^{(1)} \cdot \hat{N}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{N}) \qquad (\vec{\sigma}^{(1)} \cdot \hat{P}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{P}) \qquad (\vec{\sigma}^{(1)} \cdot \hat{K}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{K})$$

It follows that the most general F consistent with rotational invariance, parity and time reversal has the general structure:

$$F = aI + b(\vec{\sigma}^{(1)} - \vec{\sigma}^{(2)}) \cdot \hat{N} + c(\vec{\sigma}^{(1)} + \vec{\sigma}^{(2)}) \cdot \hat{N} m(\vec{\sigma}^{(1)} \cdot \hat{N}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{N}) +$$
$$(g+h)(\vec{\sigma}^{(1)} \cdot \hat{P}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{P}) + (g-h)(\vec{\sigma}^{(1)} \cdot \hat{K}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{K}) \tag{233}$$

where $\{a, b, c, m, g, h\}$ are functions of k^2 and $\cos(\theta)$. These parameters are called the Wolfenstein parameters.

There is one additional simplification that follows from isospin invariance if the system is also invariant with respect to parity.

Parity changes the sign of $\vec{k}$. In an eigenstate of parity the parity of the space part of the wave function has a definite parity and thus symmetry with respect to exchange of identical particles. Since the two particle system is a Fermion the spin and isospin parts of the wave function must be symmetric or antisymmetric depending on the parity. The parity plus the isospin fixed the total spin (single or triplet) which must be preserved if isospin is preserved. The term $(\vec{\sigma}^{(1)} - \vec{\sigma}^{(2)})$ changes the spin symmetry (exchanging triplet and singlets) which is not allowed if there is isospin conservation. This eliminates the b parameter giving the general form of the scattering amplitude

$$F = aI + c(\vec{\sigma}^{(1)} + \vec{\sigma}^{(2)}) \cdot \hat{N} + m(\vec{\sigma}^{(1)} \cdot \hat{N}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{N}) +$$
$$(g+h)(\vec{\sigma}^{(1)} \cdot \hat{P}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{P}) + (g-h)(\vec{\sigma}^{(1)} \cdot \hat{K}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{K}) \tag{234}$$

The goal of a theorist is then to compute the Wolfenstein parameters. This leads to a useful form of the scattering amplitude to extract spin observables.

The following relations are useful:

$$\mathrm{Tr}(\vec{\sigma} \cdot \vec{A}) = \mathrm{Tr}(\vec{\sigma}) \cdot \vec{A} = 0 \tag{235}$$

$$\mathrm{Tr}((\vec{\sigma}\cdot\vec{A})(\vec{\sigma}\cdot\vec{B})) = 4\vec{A}\cdot\vec{B} \tag{236}$$

$$\mathrm{Tr}((\vec{\sigma}\cdot\vec{A})(\vec{\sigma}\cdot\vec{B})(\vec{\sigma}\cdot\vec{C})) = 4i(\vec{A}\times\vec{B})\cdot\vec{C} \tag{237}$$

In addition, the trace of a tensor product of operators is the product of the traces:

$$\mathrm{Tr}(A\otimes B) = \sum_{mn}\langle m|\otimes\langle n|A\otimes B|n\rangle\otimes|m\rangle = \sum_{n}\langle n|B|n\rangle\langle m|A|m\rangle = \mathrm{Tr}(A)\mathrm{Tr}(B)$$

Applying this last relation to the expression for F in terms of the Wolfenstein parameters gives the following expressions for the parameters in terms of the scattering amplitude:

$$a = \frac{1}{4}\mathrm{Tr}(F)$$

$$c = \frac{1}{4}\mathrm{Tr}(F\vec{\sigma}^{(1)}\cdot\hat{N}) = \frac{1}{4}\mathrm{Tr}(F\vec{\sigma}^{(2)}\cdot\hat{N}) = \frac{1}{8}\mathrm{Tr}(F(\vec{\sigma}^{(1)}+\vec{\sigma}^{(2)})\cdot\hat{N})$$

$$m = \frac{1}{4}\mathrm{Tr}(F(\vec{\sigma}^{(1)}\cdot\hat{N})(\vec{\sigma}^{(2)}\cdot\hat{N}))$$

$$(g+h) = \frac{1}{4}\mathrm{Tr}(F(\vec{\sigma}^{(1)}\cdot\hat{P})(\vec{\sigma}^{(2)}\cdot\hat{P}))$$

$$(g-h) = \frac{1}{4}\mathrm{Tr}(F(\vec{\sigma}^{(1)}\cdot\hat{K})(\vec{\sigma}^{(2)}\cdot\hat{K}))$$

I give an example that utilizes the Wolfenstein parameterization.

I consider the case the incident beam has a polarization $\vec{\pi}$. The initial density matrix is (assuming that beam is labeled by 1)

$$\rho_i = \frac{1}{4}(\sigma_0^{(1)} + \vec{\pi}\cdot\vec{\sigma}^{(1)})\otimes\sigma_0^{(2)} \tag{238}$$

This gives the following expression for the final density matrix

$$\rho_f := F\rho_i F^\dagger \tag{239}$$

The trace of this gives the differential cross section the where the beam has polarization $\vec{\pi}$ and the target is not polarized and final spins are not measured:

$$\frac{d\sigma}{d\Omega} = \mathrm{Tr}(F\rho_i F^\dagger) =$$

$$\mathrm{Tr}[(aI + c(\vec{\sigma}^{(1)} + \vec{\sigma}^{(2)}) \cdot \hat{N} + m(\vec{\sigma}^{(1)} \cdot \hat{N}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{N}) +$$
$$(g+h)(\vec{\sigma}^{(1)} \cdot \hat{P}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{P}) + (g-h)(\vec{\sigma}^{(1)} \cdot \hat{K}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{K})) \times$$
$$(\frac{1}{4}(\sigma_0^{(1)} + \vec{\pi} \cdot \vec{\sigma}^{(1)}) \otimes \sigma_0^{(2)}) \times$$
$$(a^* I + c^*(\vec{\sigma}^{(1)} + \vec{\sigma}^{(2)}) \cdot \hat{N} + m^*(\vec{\sigma}^{(1)} \cdot \hat{N}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{N}) +$$
$$(g+h)^*(\vec{\sigma}^{(1)} \cdot \hat{P}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{P}) + (g-h)^*(\vec{\sigma}^{(1)} \cdot \hat{K}) \cdot (\vec{\sigma}^{(2)} \cdot \hat{K}))]$$

Here it is enough to have the patience to compute the traces. This calculation can be easily automated by computer. The result is a sum of products of traces on the particle 1 and 2 Hilbert spaces.

For the manual computation I first compute the identity contribution: I get

$$aa^* + 2cc^* + mm^* + 2gg^* + 2hh^*.$$

For the polarization term the surviving pairings involve ca^*, a^*c, cm^*, c^*m which leads to the following expression:

$$\vec{\pi} \cdot \hat{N} \times (ca^* + c^*a + cm^* + c^*m) = 2\vec{\pi} \cdot \hat{N} \times Re(c^*(a+m))$$

The entire cross section becomes

$$\frac{d\sigma}{d\Omega} = a * a + 2c * c + m * m + 2g * g + 2h * h + 2\vec{\pi} \cdot \hat{N} \times Re(c^*(a+m))$$

which shows an enhancement of the cross section if the beam is polarized in the direction $\hat{N}$ perpendicular to the scattering plane.

These same ideas can be used to compute more complex spin observables. Clearly there are 5 non-trivial Wolfenstein parameters. Ten independent experiments are needed to extract the real and imaginary parts of these coefficients in the lab. The full set of experiments has to be performed for many momenta and scattering angles.

12 The Lippmann Schwinger Equation

In this section I discuss methods for solving the Lippmann Schwinger equation. Much of what I plan to discuss follows because the kernel of the Lippmann Schwinger equation is a compact operator. Since compact operators are also important in the many-body problem, I discuss compact operators first.

The Lippmann Schwinger equation has the formal structure

$$T = D + KT$$

where the driving term $D = V$ and the kernel $K = V\frac{1}{z-H_0}$. The norm of an operator A is defined by

$$\|A\| = \sup_{|\psi\rangle \neq 0} \frac{\|A|\psi\rangle\|}{\||\psi\rangle\|}$$

where sup is the least upper bound. It follows from this definition that

$$\|A|\psi\rangle\| \leq \|A\|\||\psi\rangle\|$$

for *any* vector $|\psi\rangle$.

An operator A is **bounded** (equivalently strongly continuous) if $\|A\| < \infty$.

An operator A is called **contractive** if $\|A\| < 1$. Contractive operators reduce the norm of any vector. Any bounded operator can be made contractive by multiplication by a sufficiently small constant. For example if A is bounded then $B := A/(2\|A\|)$ is contractive.

If the Lippmann Schwinger kernel is contractive then the series

$$T = D + \sum_{n=1}^{\infty} K^n D \tag{240}$$

converges in norm

$$\|T\| < \frac{1}{1 - \|K\|}\|D\| < \infty$$

and satisfies the Lippmann Schwinger equation. This means that the Lippmann Schwinger equation can be solved by convergent perturbation theory. The series defined in (**??**) is called the Born series; the first term $D = V$ is called the first Born approximation to T

A bounded operator is **compact** if it can be approximated in operator norm by a finite rank operator F. Specifically for any $\epsilon > 0$ there is a F of the form

$$F = \sum_{n=1}^{N} |\phi_n\rangle \lambda_n \langle\psi_n|$$

with the property that

$$\|A - F\| < \epsilon$$

Here $\{|\phi\rangle_n\}$ and $\{|\psi\rangle_n\}$ are separately orthonormal, and $\lambda_n > 0$, and N is finite. As ϵ is reduced the number of terms in F will generally increase, however N is finite for any non-zero ϵ.

Compactness is a restrictive condition. The identity is clearly a bounded operator, but it is not compact. Likewise $\frac{1}{2}I$ is contractive, but it is not compact.

One important property of a compact operator is that the product of a compact operator and a bounded operator is a compact operator. To see this let B be bounded and A be compact. It follows that

$$\|BA - BF\| < \|B\|\epsilon = \epsilon'$$

Clearly if F is finite rank, so is BF. Also, because $\|B\|$ is a positive constant, ϵ' and be made as small as desired by choosing ϵ sufficiently small. A similar argument can be used to show that right multiplication by a bounded operator is also compact (i.e. AB).

Note there are many more mathematical characterizations of compact operators. The one I use emphasizes the most important property for scattering theory. All of the characterization are equivalent.

The simplest kind of compact operator is a positive Hermitian compact operator. These operators have complete sets of eigenvectors and non-negative eigenvalues. If the dimension of the subspace spanned by the eigenvalues with value greater than a given $\epsilon > 0$ is not finite, then the operator cannot be compact. It follows that either there are a finite number of non-zero eigenvalues or the eigenvalues have an accumulation point at zero. This means that that the operator can be expressed in the form

$$A = \sum_{n=1}^{N} |\psi_n\rangle \lambda_n \langle\psi_n|$$

where either N is finite or $\lim_{n\to\infty} \lambda_n \to 0$ and $|\psi_n\rangle$ are orthonormal. It is also clear that any operator of this form is a compact, positive, Hermitian operator.

If A is an arbitrary compact operator $A^\dagger$ is bounded and $A^\dagger A$ is a positive, Hermitian compact operator which has the form

$$A^\dagger A = \sum_{n=1}^{N} |\psi_n\rangle \lambda_n^2 \langle\psi_n|$$

Define

$$|\phi_n\rangle = A|\psi_n\rangle\lambda_n^{-1}$$

for $\lambda_n \neq 0$. By definition

$$\langle\phi_n|\phi_m\rangle = \langle\psi_n|A^\dagger A\psi_m\rangle/(\lambda_m\lambda_n) =$$

$$\delta_{nm}\frac{\lambda_n^2}{\lambda_n^2} = \delta_{mn}$$

Define

$$A' = \sum |\phi_n\rangle\lambda_n\langle\psi_n|$$

If this is applied to any for the eigenstates of $A^\dagger A$ I get

$$A'|\psi_m\rangle =$$

$$\sum_{n=1}^{N} |\phi_n\rangle\lambda_n\langle\psi_n|\psi_m\rangle =$$

$$\sum_{n=1}^{N} A|\psi_n\rangle\delta_{nm}.$$

This is zero if $m > N$, and is $A|\psi_m\rangle$ otherwise. If $m > N$ I get

$$\|A|\psi_m\rangle\|^2 = \langle\psi_m|A^\dagger A|\psi_m\rangle = 0.$$

It follows that A' and A agree on an orthonormal basis and are consequently equal. The recovers the formula that was initially used to define the compact operator:

$$A = \sum_{n=1}^{N} |\phi_n\rangle\lambda_n\langle\psi_n|$$

In this expression all of the quantities are defined in terms of A

To understand the value of having a compact kernel in an integral equation let

$$T = D + KT$$

and write

$$K = F + C$$

where F is finite rank and C is contractive. Then I can write the equation

$$T = D + (F + C)T$$

$$(I - C)T = D + FT.$$

Since C is contractive $(I - C)^{-1}$ exists and is given by the convergent power series

$$(I - C)^{-1} = I + \sum_{n=1}^{\infty} C^n.$$

The integral equation can be replaced by

$$T = (I - C)^{-1}D + (I - C)^{-1}FT.$$

Since

$$F' := (I - C)^{-1}F$$

is finite rank this equation becomes

$$T = D' + F'T$$

with

$$D' := (I - C)^{-1}D$$

which can be solved by finite matrix algebra.

It can happen that the finite dimensional equation does of have a solution. This will happen when

$$(I - F')|\psi\rangle = 0$$

has a not trivial solution. Using the definitions

$$(I - F')^{-1} := (I - (I - C)^{-1}F) = (I - C)^{-1}(I - C - F) = (I - C)^{-1}(I - K)$$

Since $(I - C)$ has a bounded inverse the condition that the matrix equation cannot be solved is

$$(I - K)|\psi\rangle = 0$$

or the homogeneous form of the equation has a non-trivial solution. Thus I have that either a solution to the problem or a solution to the homogeneous equation. This is called the Fredholm Alternative.

What I have shown is that if the kernel is compact it is possible to write the kernel as the sum of a contractive and finite dimensional term. The

contractive part can be solved by convergent perturbation theory. The remainder of the problem is reduced to algebra.

What is most impressive is the the convergence is in operator norm, which means that the errors are independent of the initial state.

There are several tests to see if an linear operators is compact. Sufficient conditions for an operator A to be compact are that A is a trace class or a Hilbert Schmidt operator. A linear operator is trace class if

$$\mathrm{Tr}(|A|) <= \infty$$

where

$$|A|^2 := A^\dagger A.$$

The operator is Hilbert Schmidt if

$$\mathrm{Tr}(|A|^2) <= \infty.$$

It is worth noting that what is meant by compact depends on the choice of operator norm. The finite rank operator is made up out of vectors and linear functionals on the associated normed linear space. Weinberg showed that the kernel is Hilbert Schmidt for z not strictly on the real line. Normally a slight change in norm is needed to allow one the take the limit that z approached the real line. What is necessary that the norm excludes functions that make the principal value integral badly behaved. There are many such spaces, and the implication is the final solution is in this space. These are not a concern in practical applications.

A formal method for performing this decomposition is due to Weinberg, and is called the quasi-particle method. Weinberg begins by defining "quasi-particles" as solutions of the eigenvalue problem:

$$R_0(z)V|\eta_n(z)\rangle = \eta_n(z)|\eta_n(z)\rangle$$

Note that these are eigenstates of the adjoint of the kernel of the Lippmann Schwinger equation. The eigenvalues $\eta_n(z)$ are in general complex and accumulate at zero. It follows that

$$VR_0(z)[V|\eta_n(z)\rangle] = \eta_n(z)[V|\eta_n(z)\rangle]$$

which shows

$$|\xi_n(z)\rangle := V|\eta_n(z)\rangle$$

is an eigenvector of the kernel with the same eigenvalue.

The eigenvectors satisfy the following orthogonality conditions

$$\langle \eta_n(z^*)|V|\eta_m * (z)\rangle = 0 \quad \text{if} \quad \eta_m(z) \neq \eta_n(z)$$

This follows by taking adjoints and replacing $z \rightarrow z^*$:

$$\langle \eta_n(z)|VR_0(z^*) = \eta_n(z*)\langle \eta_n(z)|$$

$$\langle \eta_n(z^*)|VR_0(z) = \eta_n(z)\langle \eta_n(z^*)|$$

It is clear that if the largest eigenvalue $\eta(z)$ is less than one in magnitude, then the kernel is contractive; conversely if one of the eigenvalues lies outside the unit circle the Born series will diverge.

If I define the reduced kernel:

$$\bar{V}(z)R_0(z) := VR_0(z) - \sum_{n=1}^{N} \frac{V|\eta_n(z)\rangle\langle\eta_n(z^*)|VR_0(z)}{\langle\eta_n(z^*)|V|\eta_n(z)\rangle}$$

where is sum is over a finite number of quasi-particle states

If this kernel is applied to any of the $|\xi_n\rangle$ I get

$$\bar{V}(z)R_0(z)|\xi_n\rangle = 0$$

by the orthogonality condition, assuming all of the quasi-particle states have different eigenvalues. It follows that by subtracting the quasi-particle states from the original kernel a new kernel is obtained that has smaller eigenvalues.

Weinberg's approach to this problem is to find the solution to the Lippmann Schwinger equation in two steps. I give a slight modification of his procedure. First I define the reduced potential

$$V_c = V - \sum_{n=1}^{N} \frac{V|\eta_n(z)\rangle\langle\eta_n(z^*)|V}{\langle\eta_n(z^*)|V|\eta_n(z)\rangle}$$

where the subtracted term contains enough quasi-particle states so the kernel

$$K_c(z) = V_c(z)R_0(z)$$

is contractive. This can alway be done if the original kernel is compact. The exact potential has the form

$$V = V_c + V_f$$

where V_f is finite rank.

The equation

$$T(z) = (V_c(z) + V_f(z)) + (V_c(z) + V_f(z))R_0(z)T(z)$$

can be put in the form

$$(I - V_c(z)R_0(z))T(z) = (V_c(z) + V_f(z)) + V_f(z)R_0(z)T(z).$$

I define

$$T_c(z) = V_c(z) + V_c(z)R_0(z)T_c(z)$$

and

$$T_2(z) = V_f(z) + V_c(z)R_0(z)T_f(z).$$

Because these equations have the same contractive kernel the series solution converges

$$T_c(z) = \Omega_c(z)V_c; \qquad T_2(z) = \Omega_c(z)V_f$$

where

$$\Omega_c(z) = I + \sum_{n=1}^{\infty}[V_c(z)R_0(z)]^n$$

Given $T_c(z)$ and $T_2(z)$ the solution for $T(z)$ becomes

$$T(z) = T_c(z) + T_2(z) + T_2(z)R_0(z)T(z).$$

The important feature of the equation for $T(z)$ is that the kernel $T_2(z)R_0(z)$ is finite rank, so the solution of this equation is algebraically equivalent to solving equations for a finite linear system.

What I have shown you is that if the kernel is compact then the solution of the Lippmann Schwinger equation can be reduced to convergent perturbation theory and finite algebra.

While the quasi-particle method is powerful, it still requires solving complex eigenvalue problems at each energy. In practice one does not have to be that systematic.

While two-body problems can be solved directly with with modest computational effort, the Lippmann Schwinger equation provides a simple laboratory to test methods that are useful for large problems.

A large class of these methods utilize a basis generated by applying powers of the kernel to a random vector. For compact operators this works

because powers of the kernel tend to emphasize quasi-particle states with the largest eigenvalues. This class of methods usually lead to very efficient approximations.

I give one method that illustrates these ideas. I begin by writing the Lippmann Schwinger equation in the form

$$T = D + KT.$$

Normally the potential is applied to a plane wave state,

$$|\bar{\phi}_1\rangle := D|\vec{k}_i\rangle.$$

If the potential has finite range this state can be normalized to unity. I define

$$|\phi_1\rangle := |\bar{\phi}_1\rangle(\langle\bar{\phi}_1|\bar{\phi}_1\rangle)^{-1/2}$$

$$\langle\phi'_1| = \langle\phi_i|.$$

The next step is to generate a bi-orthogonal set of vectors: I defined

$$|\phi_2\rangle = \alpha|\phi_1\rangle + \beta K|\phi_1\rangle$$

and

$$\langle\phi'_2| = \gamma\langle\phi'_1\rangle + \eta\langle\phi'_1|K.$$

The coefficients are determined by the requirements

$$\langle\phi'_2|\phi_2\rangle = 1$$

$$\langle\phi'_2|\phi_1\rangle = \langle\phi'_1|\phi_2\rangle = 0$$

and $\beta = \eta$. These conditions uniquely fix all coefficients.

This can be repeated recursively to generate

$$\{|\phi_n\rangle\} \qquad \text{and} \qquad \{\langle\phi'_n|\}$$

with the properties

$$\langle\phi'_m|\phi_n\rangle = \delta_{mm'}$$

and

$$\langle\phi'_m|K|\phi_n\rangle = 0 \qquad \text{unless} \qquad |m-n| \leq 1.$$

This second condition is because by construction $K|\phi_m\rangle$ is a linear combination of the $|\phi_m\rangle$ with $m \leq n+1$, which are orthogonal to the $\langle\phi'_m|$ with $m > n+1$. An identical argument holds if K is applied on the left of $\langle\phi'_n|$

To solve the Lippmann Schwinger equation

$$T|\vec{k}\rangle = |\phi_1\rangle + KT|\vec{k}\rangle$$

assume that the solution can be expressed in the form

$$T|\vec{k}\rangle = \sum_{n=1}^{\infty} |\phi_n\rangle t_n.$$

At this stage I do not know if the states $|\phi_n\rangle$ form a basis, I simply process as if that is the case. Using this in the equation gives

$$\sum_n |\phi_n\rangle t_n = |\phi_1\rangle + \sum_n K|\phi_n\rangle t_n.$$

Taking overlaps with the dual basis gives the algebraic equations for the expansion coefficients t_m:

$$t_m = \delta_{m1} + \langle\phi'_m|K|\phi_{m-1}\rangle t_{m-1} + \langle\phi'_m|K|\phi_m\rangle t_m + \langle\phi'_m|K|\phi_{m+1}\rangle t_{m+1}$$

Which are a simple tridiagonal set of equations for the coefficients t_m. The only input is the first state and the matrix elements $\langle\phi'_m|K|\phi_n\rangle$ for $|m-n| \leq 1$.

If I define the matrix elements

$$\kappa_{mn} = \langle\phi'_m|K|\phi_n\rangle$$

and truncate the series at N the solution is a continued fraction generated by

$$t_1 = \frac{1}{1 - \kappa_{11} - \kappa_{12}\frac{t_2}{t_1}}$$

$$\frac{t_2}{t_1} = \frac{\kappa_{21}}{1 - \kappa_{22} - \kappa_{23}\frac{t_3}{t_2}}$$

$$\frac{t_3}{t_2} = \frac{\kappa_{32}}{1 - \kappa_{33} - \kappa_{34}\frac{t_4}{t_3}}$$

$$\vdots$$

$$\frac{t_N}{t_{N-1}} = \frac{\kappa_{N,N-1}}{1 - \kappa_{N-1,N-1} - \kappa_{N-1,N}\frac{t_N}{t_{N-1}}}$$

$$\frac{t_N}{t_{N-1}} = \frac{\kappa_{N,N-1}}{1 - \kappa_{NN}}$$

This system can be written as one large continued fraction. The required input are the non-zero matrix elements of the kernel in the biorthogonal basis.

This leads to a fairly efficient method for solving the Lippmann Schwinger equation. In practice this method and related methods are more useful in three body problems which involve larger matrices. Direct methods are normally employed for solving the two-body Lippmann-Schwinger equation.

13 Partial Waves

Direct numerical computation of the solution of the Lippmann Schwinger equation can be done most efficiently by exploiting symmetries. One important symmetries is rotational invariance. If the interaction is rotationally invariant it commutes with the total angular momentum operator. When the Lippmann Schwinger equation is expressed in a basis of angular momentum eigenstates, it decouples into an infinite set of uncoupled equations. The uncoupled equations involve a one dimensional integration while the original equation involves a three dimensional integral. For finite range potentials with fixed beam momentum only a finite number of angular momentum channels are relevant. Classically, the maximum angular momentum resulting in a collision in the lab frame is $p_b R$ were p_b is the beam momentum and R is the range of the interaction.

The total angular momentum of the two body system is the sum

$$\vec{J} = \vec{L} + \vec{l} + \vec{S}_1 + \vec{S}_2$$

$\vec{L}$ is the orbital angular momentum associated with the center of mass coordinate and momentum. It is conserved independent of $\vec{J}$. The total intrinsic angular momentum

$$\vec{j} = \vec{J} - \vec{L} = \vec{l} + \vec{S}_1 + \vec{S}_2$$

is also conserved. Eigenstates of $\vec{j}$ are constructed using the usual rules of angular momentum addition in quantum mechanics. Starting with the plane

wave states $|\vec{k},\mu_1,\mu_2\rangle$ I define

$$|k,j,\mu_j;l_1,s,s_1,s_2\rangle =$$

$$\int \sum |\vec{k},\mu_1,\mu_2\rangle d\Omega(\hat{k})\langle\hat{k}|l,m_l\rangle\langle s_1,\mu_2,s_2,\mu_2|s,\mu_s\rangle\langle l,m_l,s,\mu_s|j,\mu_j\rangle$$

where the sum is over all repeated magnetic quantum numbers and

$$\langle\hat{k}|l,m_l\rangle = Y_{lm_l}(\hat{k})$$

is a standard spherical harmonic.

In this basis a Galilean invariant potential has the form

$$\langle\vec{P},k,j,\mu_j;l,s,s_1,s_2|V|\vec{P}',k',j',\mu_j';l',s',s_1',s_2'\rangle =$$

$$\delta(\vec{P}-\vec{P}\,')\delta_{jj'}\delta_{\mu_j\mu_j'}\langle k,l,s,s_1,s_2|V^j|k',l',s',s_1',s_2'\rangle$$

The transition matrix elements can be expressed in terms of a reduced transition operator

$$\langle\vec{P},k,j,\mu_j;l,s,s_1,s_2|T(z)|\vec{P}',k',j',\mu_j';l',s',s_1',s_2'\rangle =$$

$$\delta(\vec{P}-\vec{P}\,')\delta_{jj'}\delta_{\mu_j\mu_j'}\langle k,l,s,s_1,s_2|T^j(z)|k',l',s',s_1',s_2'\rangle$$

The Lippmann Schwinger equation takes on the form

$$\langle k,l,s,s_1,s_2|T^j(z)|k',l',s',s_1,s_2\rangle = \langle k,l,s,s_1,s_2|V^j|k',l',s',s_1,s_2\rangle +$$

$$\int_0^\infty \sum_{s'',l''}\langle k,l,s,s_1,s_2|V^j|k'',l'',s'',s_1,s_2\rangle\frac{k''^2dk''}{z-k''^2/2\mu}\times$$

$$\langle k'',l'',s'',s_1,s_2|T^j(z)|k',l',s',s_1,s_2\rangle$$

This notation can be simplified by observing that the final variables remain unchanged. Defining

$$t^j(k,l,s) := \langle k,l,s,s_1,s_2|T^j(z)|k',l',s',s_1,s_2\rangle =$$

$$v^j(k,l,s;k',l',s') := \langle k,l,s,s_1,s_2|V^j|k',l',s',s_1,s_2\rangle +$$

$$z = \frac{k'^2}{2\mu} + i0^+$$

this equation takes on the form

$$t^j(k,l,s) = v^j(k,l,s;k',l',s')+$$

$$\int_0^\infty \sum_{s=|s_1-s_2|}^{|s_1+s_2|} \sum_{l=|j-s|}^{|j+l|} v^j(k,l,s;k'',l'',s'')\frac{2\mu k''^2 dk''}{k'^2-k''^2+i0^+}t^j(k,l,s)$$

The methods discussed in the previous section can be used to solve this equation, however this is a simple enough equation that normally direct methods can be employed. The part that needs to be done with the most care is the integration over the singularity. This is also true in methods discussed in the last section. Also, this is generally a complex equations which can be simplified using the K-matrix.

The K matrix method breaks this up into two equations; one for the partial wave K-matrix:

$$k^j(k,l,s;k',l',s') = v^j(k,l,s;k',l',s')+$$

$$P\int_0^\infty \sum_{s=|s_1-s_2|}^{|s_1+s_2|} \sum_{l=|j-s|}^{|j+l|} v^j(k,l,s;k'',l'',s'')\frac{2\mu k''^2 dk''}{k'^2-k''^2}k^j(k'',l'',s'',k'l's')$$

and one that expresses the partial wave transition matrix elements in terms of the k matrix

$$t^j(k,l,s) = k^j(k,l,s;k',l',s')$$
$$-2\mu\pi i k' \sum_{s=|s_1-s_2|}^{|s_1+s_2|} \sum_{l=|j-s|}^{|j+l|} k^j(k,l,s;k',l'',s'')t^j(k',l,s). \qquad (241)$$

To solve the last equation set $k = k'$ to obtain a finite linear system for $t^j(k',l,s)$:

$$t^j(k',l,s) = k^j(k',l,s;k',l',s')$$
$$-2\mu\pi i k' \sum_{s=|s_1-s_2|}^{|s_1+s_2|} \sum_{l=|j-s|}^{|j+l|} k^j(k',l,s;k',l'',s'')t^j(k',l,s)$$

Once this algebraic equation is solved it can be substituted in the right hand side of (241) to get an expression for the partial wave transition matrix elements.

This is all very elementary. The next step is solve for the partial wave k matrix. This is a real, singular integral equation. In order to make the equation non singular it is useful to use

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

I proved this result earlier. This allows me to replace the singular k-matrix equation by the regular equation

$$k^j(k,l,s;k',l',s')=v^j(k,l,s;k',l',s')+$$

$$2\mu\int_0^\infty k''^2dk''\sum_{s=|s_1-s_2|}^{|s_1+s_2|}\sum_{l=|j-s|}^{|j+l|}\times$$

$$\frac{v^j(k,l,s;k'',l'',s'')k^j(k'',l'',s'',k'l's')-v^j(k,l,s;k',l'',s'')k^j(k',l'',s'',k'l's')}{k'^2-k''^2}$$

This equation is normally solved by direct integration or expansion methods. Expansion methods express the k-matrix elements as linear combinations of know orthonormal basis functions $\phi_n(k)$ with unknown coefficients:

$$k^j(k,l,s;k',l',s')=\sum_n c_{n,l,s}\phi_n(k)$$

The equations become

$$\sum_n c_{n,l,s}\phi_n(k)=v^j(k,l,s;k',l',s')+$$

$$2\mu\int_0^\infty k''^2dk''\sum_n\sum_{s=|s_1-s_2|}^{|s_1+s_2|}\sum_{l=|j-s|}^{|j+l|}\frac{v^j(k,l,s;k'',l'',s'')\phi_n(k'')-v^j(k,l,s;k',l'',s'')\phi_n(k')}{k'^2-k''^2}c_{n,l'',s''}$$

If I approximate the solution by truncating after a finite number of basis functions (N), there are two methods to solve the resulting equations.

The Galerkin methods multiplies the above by $\phi_m(k)k^2dk$ and integrates using the orthonormality. This gives the following linear equations for the coefficients

$$c_{m,l,s}=\int_0^\infty k^2\phi_m(k)v^j(k,l,s;k',l',s')+$$

$$2\mu \int_0^\infty k^2 k''^2 dk dk'' \sum_n \sum_{s=|s_1-s_2|}^{|s_1+s_2|} \sum_{l=|j-s|}^{|j+l|} \times$$

$$\phi_m(k) \frac{v^j(k,l,s;k'',l'',s'')\phi_n(k'') - v^j(k,l,s;k',l'',s'')\phi_n(k')}{k'^2 - k''^2} c_{n,l'',s''}$$

The price paid for doing this is that an integration over k is required.

This integration can be avoided using the collocation method; which simply demands that the equation hold exactly at N points, $\{k_m\}$. this gives the alternative equation:

$$\sum_n c_{n,l,s}\phi_n(k_m) = v^j(k_m,l,s;k',l',s') +$$

$$2\mu \int_0^\infty k''^2 dk'' \sum_n \sum_{s=|s_1-s_2|}^{|s_1+s_2|} \sum_{l=|j-s|}^{|j+l|} \times$$

$$\frac{v^j(k_m,l,s;k'',l'',s'')\phi_n(k'') - v^j(k_m,l,s;k',l'',s'')\phi_n(k')}{k'^2 - k''^2} c_{n,l'',s''}$$

With either method, after the coefficients are obtained an improved solution is obtained by interpolation:

$$k^j(k,l,s;k',l',s') = v^j(k,l,s;k',l',s') +$$

$$2\mu \sum_n \int_0^\infty k''^2 dk'' \sum_{s=|s_1-s_2|}^{|s_1+s_2|} \sum_{l=|j-s|}^{|j+l|} \times$$

$$\frac{v^j(k,l,s;k'',l'',s'')\phi_n(k'') - v^j(k,l,s;k',l'',s'')\phi_n(k')}{k'^2 - k''^2} c_{n,l'',s''} \qquad (242)$$

An alternative to the expansion methods is direct integration. in this case the integration is replaced by an approximate sum with weights

$$\int_0^\infty f(k)dk = \sum f(k_i)\Delta_i.$$

The k_n are chosen to not include the singular point (usually symmetrically around the singular point)

$$k^j(k,l,s;k',l',s') = v^j(k,l,s;k',l',s') +$$

$$\sum_n 2\mu \int_0^\infty k''^2 dk'' \sum_{s=|s_1-s_2|}^{|s_1+s_2|} \sum_{l=|j-s|}^{|j+l|} \times$$

$$\frac{v^j(k,l,s;k_n,l'',s'')k^j(kN,l'',s'',k'l's') - v^j(k,l,s;k',l'',s'')k^j(k',l'',s'',k'l's')}{k'^2 - k_n^2}\Delta_n$$

This equation can also be solved by collocation, but one additional equation is needed where $k \to k'$, since $k^j(k',l',s';k',l',s')$ appears on the right side of the equation. This done by using the on shell point as an additional collocation point. The integrals are often transformed to a finite interval by a variable change to facilitate the solution of the equations. A transformation like

$$y = \tanh(k)$$

maps $[0,\infty]$ to $[0,1]$ is commonly used in nuclear physics problems. Once the k-matrix elements are known at the quadrature points and the on shell point (k') an interpolation like (242) can be used to get the solution a arbitrary points.

The partial wave k-matrix is used to construct the partial wave transition matrix. This is used to construct the exact transition matrix, and the cross section or Wolfenstein parameters.

14 Phase Shifts

In this section I consider scattering of spinless particles with a rotationally invariant interaction. In the interest of simplicity I consider the case of spinless particles.

A plane wave basis of eigenstates can be expressed as a linear combination of simultaneous eigenstates of the relative energy, angular momentum, and magnetic quantum number

$$|\vec{k}\rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} |E,l,m\rangle |\frac{\partial E}{k^2 \partial k}|^{1/2} Y_{lm}(\hat{k})$$

where

$$|\frac{\partial E}{k^2 \partial k}|^{1/2} = \sqrt{\frac{1}{k\mu}}$$

fixes the normalization

$$\langle E, l, m | E', l', m' \rangle = \delta(E - E') \delta_{mm'} \delta_{jj'}$$

assuming that the momentum eigenstates have delta function normalization.

In this basis the scattering matrix elements have the form

$$\langle E, l, m | S | E', l', m' \rangle = \delta(E - E') \delta_{ll'} \delta_{mm'} (1 - 2\pi i \langle E, l, m | t(E + i0^+) | E, l, m \rangle)$$

The rotational invariance of the interaction means that

$$\langle E, l, m | t(E + i0^+) | E, l', m' \rangle = \delta_{ll'} \delta_{mm'} \langle E | t_l(E + i0^+) | E \rangle := \delta_{ll'} \delta_{mm'} t_l(E)$$

This gives

$$\langle E, l, m | S | E', l', m' \rangle = \delta(E - E') \delta_{ll'} \delta_{mm'} (1 - 2\pi i t_l(E)) \tag{243}$$

Unitarily of the scattering operator means that it can be expressed as

$$\langle E, l, m | S | E', l', m' \rangle = \delta(E - E') \delta_{ll'} \delta_{mm'} e^{2i\delta_l(E)} \tag{244}$$

where the quantity $\delta_l(E)$ is a real function of E called the phase shift in the l-th partial wave. The factor of two is included because with this definition the phase shift corresponds to a shift in the phase of the scattered wave. I will show this later.

It follows from (243) and (244) that the phase shift is related to $t_l(E)$ by

$$e^{2i\delta_l(E)} = 1 - 2\pi i t_l(E) \tag{245}$$

or equivalently

$$\boxed{t_l(E) = -\frac{1}{\pi} e^{i\delta_l(E)} \sin(\delta_k(E)).} \tag{246}$$

In this expression $t_l(E)$ is the on shell transition matrix element in the energy-angular momentum basis.

I can write this in terms of a momentum-angular momentum basis using the Jacobian factor to get

$$\boxed{\langle k | t_l(E) | k \rangle = -\frac{1}{k\mu\pi} e^{i\delta_l(E)} \sin(\delta_k(E)).}$$

I can also use this to get an expression in terms of the partial wave K matrix which was shown in the last section (restricting to the spinless case)

$$\langle k|t_l(E)|k\rangle = \frac{\langle k|k_l(E)|k\rangle}{1 + i2\pi\mu k\langle k|k_l(E)|k\rangle}$$

It is most common to relate the scattering amplitude to the phase shift. Beginning with the definition

$$f = -(2\pi)^2\mu\langle\vec{k}\,'|t|\vec{k}\rangle =$$

$$-(2\pi)^2\mu\sum_{lm} Y^*_{lm}(\hat{k}\,')\langle k|t_l|k\rangle Y_{lm}(\hat{k})$$

Since $\langle k|t_l|k\rangle$ is independent of m the m sum can be done using the addition theorem for spherical harmonics

$$\sum_{m=-l}^{l} Y^*_{lm}(\hat{k}\,')Y_{lm}(\hat{k}) = \frac{2l+1}{4\pi}P_l(\hat{k}\,'\cdot\hat{k})$$

giving

$$f = -(2\pi)^2\mu\langle\vec{k}\,'|t|\vec{k}\rangle =$$

$$-\pi\mu\sum_{l}(2l+1)\langle k|t_l|k\rangle P_l(\hat{k}\,'\cdot\hat{k})$$

The quantity

$$\boxed{f_l(k) := -\pi\mu\langle k|t_l|k\rangle = -\frac{\pi}{k}t_l(E)} \tag{247}$$

is called the partial wave scattering amplitude. It is related to the phase shift by

$$\boxed{f_l(k) := \frac{1}{k}e^{i\delta_l(E)}\sin(\delta_k(E))}$$

Since the total cross section is

$$\sigma = \int\frac{d\sigma}{d\Omega}d\Omega = \int|f|^2 d\Omega =$$

$$\int dud\phi\sum_{l,l'}(2l+1)(2l'+1)f^*_l f_{l'}P_l(u)P'_l(u) =$$

$$2\pi \sum_{l,l'} \frac{2}{2l+1}(2l+1)(2l'+1) f_l^* f_{l'} \delta_{ll'} =$$

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

This shows that the total cross section can be expressed in terms of a *real* phase shift and that the maximum contribution of any partial wave to the total cross section is

$$\frac{4\pi}{k^2}(2l+1).$$

This is called the unitarity bound because it is a consequence of the parameterization of the scattering matrix in terms of a *real* phase shift.

In order to obtain additional insight into the phase shift and scattering amplitude consider the free Schrödinger equation for the partial wave radial wave function in configuration space.

For plane waves this equation is

$$-\frac{1}{2\mu}[\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{L^2}{2\mu r^2}]w_l(r) = \frac{k^2}{2\mu}w_l(r)$$

The solutions that are finite at the origin are the spherical Bessel functions:

$$w_l(r) = j_l(kr).$$

It will be important to understand the relation of these solution to the usual plane wave states. To see this expand

$$e^{i\vec{k}\cdot\vec{x}} = e^{ikr\cos(\theta)} = \sum_{l=0}^{\infty} a_l P_l(\cos(\theta))$$

The coefficients can be determined by multiplying by $P_{l'}(\cos(\theta))$ and integrating over $\sin(\theta)d\theta$ which gives

$$a_l = \frac{2l+1}{2}\int_{-1}^{1} P_l(u)e^{ikru}du$$

The integral is proportional to an integral representation of a spherical Bessel function

$$j_l(kr) = (i)^{-l}\frac{1}{2}\int_{-1}^{1} P_l(u)e^{ikru}du$$

which gives

$$e^{i\vec{k}\cdot\vec{r}} = \sum_{l=0}^{\infty}(2l+1)i^l j_l(kr)P_l(\hat{k}\cdot\hat{r}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} 4\pi i^l j_l(kr)Y_{lm}(\hat{k})Y_{lm}^*(\hat{r})$$

For normalized plane wave states I get

$$\delta(\vec{k}-\vec{k}\,') = \frac{1}{(2\pi)^{3/2}}e^{i\vec{k}\cdot\vec{r}} =$$

$$\sum_{l=0}^{\infty}\frac{2l+1}{(2\pi)^{3/2}}i^l j_l(kr)P_l(\hat{k}\cdot\hat{r}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\sqrt{\frac{2}{\pi}}i^l j_l(kr)Y_{lm}(\hat{k})Y_{lm}^*(\hat{r})$$

Finally I calculate the normalization for the spherical Bessel functions using

$$\frac{\delta(k-k')}{k^2}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}(\hat{k})Y_{lm}^*(\hat{k}\,') =$$

$$\langle\vec{k}|\vec{r}\rangle d^3r\langle\vec{r}|\vec{k}\,'\rangle =$$

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{2}{\pi}\int_0^{\infty}r^2dr j_l(kr)j_l(k'r)Y_{lm}(\hat{k})Y_{lm}^*(\hat{k}\,')$$

From which I get

$$\int_0^{\infty}r^2dr j_l(kr)j_l(k'r) =$$

$$\frac{\pi}{2}\frac{\delta(k-k')}{k^2}$$

This can be summarized by writing

$$\langle r|k\rangle = i^l\sqrt{\frac{2}{\pi}}j_l(kr)$$

$$-\frac{1}{2\mu}[\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{L^2}{2\mu r^2} + 2\mu V_l(r)]v_{kl}(r) = \frac{k^2}{2\mu}v_{kl}(r)$$

The corresponding scattering eigenstates satisfy

$$[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - 2\mu V(r)]v_{kl}(r)$$

These can be normalized just like the spherical Bessel functions

$$\int_0^\infty r^2 dr v_{kl}(r) v_{k'l}(r) = \frac{\pi}{2}\frac{\delta(k'-k)}{k^2}$$

As r gets large the potential becomes unimportant and $v_{kl}(r)$ looks like a free particle solution, but it does not have to satisfy the same boundary condition at the origin as the free particle solution.

The simplest way to construct $v_{kl}(r)$ this is to use the Lippmann Schwinger equation:

$$v_{kl}(r) = j_l(kr) + \int_0^\infty R_{0lk}(r,r')U^l(r')v_{kl}(r')r'^2 dr'$$

where

$$\langle r,l,m|R_0(k^2+i0^+)|r',l',m'\rangle := \delta_{ll'}\delta_{mm'}R_{0lk}(r,r')$$

and the 2μ is absorbed in the potential term. This can be computed

$$\langle r,l,m|R_0(k^2+i0^+)|r',l',m'\rangle =$$

$$\frac{2}{\pi}\int \frac{j_l(kr)j_l(kr')}{k_0^2-k^2+i0^+}k^2 dk \delta_{ll'}\delta_{mm'}$$

This is an even function so the integral can be extended to the real line. The integral can be done by contour integrals. It requires knowing that

$$j_l(kr) = \frac{h_l^+(kr) - (h_l^+(kr))^*}{2i}$$

where for large r, $h_l^+(kr)$ behaves like $(i)^{-l}e^{ikr}/kr$ for large kr and like $(kr)^{-l-1}$ near the origin. The trick to doing the integral is to note that for $r' > r$ that

$$k^2 j_l(kr)j_l(kr') = \frac{k^2}{2i}(e^{ikr'}j_l(kr) - e^{-ikr'}j_l(kr))$$

Both terms on the right are entire functions and the first term has no contribution from the boundary at infinity if the k integral is closed in the upper half plane, while the second term give no contribution if it close in the lower half plane. Both terms are regular at the origin. This means that I only pick up pole contributions from the energy denominator:

$$\frac{2}{\pi}\int \frac{j_l(kr)j_l(kr')}{k_0^2-k^2+i0^+}k^2 dk =$$

$$-kj_l(kr)h_l(kr')\theta(r'-r) - kj_l(kr')h_l(kr)\theta(r-r').$$

With this integral the Lippmann-Schwinger equation takes on the form

$$v_l(r) = j_l(r) - 2\mu k \int_0^\infty j_l(kr_<)h_l(kr_>)V^l(r')v_l(r')r'^2dr'. \qquad (248)$$

For r larger than the range of the potential this becomes

$$v_l(r) \to j_l(r) - h_l(kr)2\mu k \int_0^\infty j_l(kr')V^l(r')v_l(r')r'^2dr'. \qquad (249)$$

In this expression $h_l(kr)$ behaves like a outgoing spherical wave, while $j_l(kr)$ is the plane wave part of this expression. To relate this to the scattering amplitude I use (**??**) in the full expansion of the solution in partial waves

$$\sum_l \sum_m \sqrt{\frac{2}{\pi}} i^l j_l(kr) Y_{lm}(\hat{r}) Y^*_{lm}(\hat{k}) +$$

$$-\sum_l \sum_m 2\mu k h_l(kr) \int j_l(kr')r'^2dr' \langle r'|V_l|k^+\rangle Y_{lm}(\hat{r})Y^*_{lm}(\hat{k})$$

Using

$$\langle k|r\rangle = j_l(kr)(-i)^l\sqrt{\frac{2}{\pi}}$$

in the above expression gives

$$\sum_l \sum_m \sqrt{\frac{2}{\pi}} i^l j_l(kr) Y_{lm}(\hat{r}) Y^*_{lm}(\hat{k}) -$$

$$\sum_l \sum_m 2\mu k h_l(kr) \int \sqrt{\frac{2}{\pi}} i^l j_l(kr') j_l(k''r') r'^2 dr' k''^2 dk'' \langle k''|V_l|k^+\rangle Y_{lm}(\hat{r})Y^*_{lm}(\hat{k}) =$$

Using the normlization integral for the spherical Bessel functions gives The last terms can be expressed as

$$-\sum_l \sum_m 2\mu k h_l(kr) \int \sqrt{\frac{\pi}{2}} i^l \frac{\pi}{2} \frac{\delta(k-k'')}{k^2} k''^2 dk'' \langle k''|t_l|k\rangle Y_{lm}(\hat{r})Y^*_{lm}(\hat{k}) =$$

The last terms can be expressed as

$$-\sum_l \sum_m 2\mu k h_l(kr)\sqrt{\frac{2}{\pi}} i^l \langle k|t_l|k\rangle Y_{lm}(\hat{r}) Y^*_{lm}(\hat{k})$$

Factoring out

$$\sum_l \sum_m \sqrt{\frac{2}{\pi}} 2i^l Y_{lm}(\hat{r}) Y^*_{lm}(\hat{k})[-2\mu k h_l(kr)\langle k|t_l|k\rangle$$

The entire expression can be put in the form

$$\sum_l \sum_m \sqrt{\frac{2}{\pi}} 2i^l Y_{lm}(\hat{r}) Y^*_{lm}(\hat{k})[v_l(r) - j_l(kr) + \pi\mu k h_l(kr)\langle k|t_l|k\rangle$$

Doing the integral gives

$$\sum_l (2l+1) i^l \sqrt{\frac{2}{\pi}} P_l(u)[j_l(kr) - \frac{2\pi\mu k}{2} h_l(kr)\langle k|t_l|k\rangle]. \tag{250}$$

Comparing (249) with (250) gives

$$-h_l(kr) 2\mu k \int_0^\infty j_l(kr') V^l(r') v_l(r') r'^2 dr' = -\frac{2\pi\mu k}{2} h_l(kr)\langle k|t_l|k\rangle$$

Finally I use $\langle k|t|l\rangle = -f_l/\pi\mu$ to get the asymptotic form of $v_{kl}(r)$

$$[j_l(kr) + \frac{2\pi\mu k}{2} h_l(kr)\frac{f_l(k)}{\pi\mu}]$$

or

$$[j_l(kr) + k h_l(kr) f_l(k)]$$

and

$$f_l = -2\mu \int j_l(kr) V_l(r) v_l(r) r^2 dr$$

Asymptotically this becomes

$$[\frac{\sin(kr - \frac{\pi}{2}l)}{kr} + (i)^{-l}\frac{e^{ikr}}{r} f_l(k)]$$

Using the expression for the scattering amplitude in terms of the phase shift gives

$$[\frac{\sin(kr-\frac{\pi}{2}l)}{kr}+(i)^{-l}\frac{e^{ikr}}{r}\frac{e^{i\delta_l}\sin(\delta_l)}{k}]=$$
$$\frac{1}{kr}[\sin(kr-\frac{\pi}{2}l)+e^{irk-l\frac{\pi}{2}}e^{i\delta_l}\sin(\delta_l)]$$

Writing everything out I get

$$\frac{1}{2ikr}[e^{i(kr-\frac{\pi}{2}l)}-e^{-i(kr-\frac{\pi}{2}l)}+e^{irk-il\frac{\pi}{2}}(e^{2i\delta_l}-1)]=$$
$$\frac{1}{2ikr}[e^{i(kr-\frac{\pi}{2}l)}(1+e^{2i\delta_l}-1)-e^{-i(kr-\frac{\pi}{2}l)}=$$
$$\frac{e^{i\delta_l}}{kr}\sin(kr-\frac{l\pi}{2}+\delta_l)$$

which shows that the phases shift in the l-th partial wave corresponds to a shift in the phase of the asymptotic wave function in the l-th partial wave.

15 Analytic Properties of Partial Waves

The integral equation for the scattering solution has the form

$$v_l(r)=j_l(kr)-2\mu k\int_0^\infty j_l(kr_<)h_l(kr_>)V^l(r')v_l(r')r'^2dr'$$

This is a solution of the Schrödinger equation that has boundary conditions at zero and infinity. The solution is complex.

Since the differential equation is a second order equation I can also find a solution that looks like a spherical Bessel function at the origin. This function satisfies

$$\phi_l(r)=j_l(kr)+2\mu k\int_0^r[j_l(kr)n_l(kr')-n_l(kr)j_l(kr')]V^l(r')\phi_l(r')r'^2dr.$$

I check that this satisfies the differential equation. If I write the differential equation as

$$(L+2\mu V)\phi_l=0$$

where L is a linear differential opeartor satisfying

$$Lj_l(kr)=0$$

then it follows that

$$L\phi_l = 2\mu k^2(-\frac{1}{r^2}\frac{d}{dr}r^2)\int_0^r [j_l'(kr)n_l(kr') - n_l'(kr)j_l(kr')]V^l(r')\phi_l(r')r'^2.$$

When the second r derivative comes inside the integral I get Bessel's equation which gives zero. The only surviving terms is the one were the argument of the integral is differentiated. Then $j_l'(kr)n_l(kr) - n_l'(kr)j_l(kr)$ becomes the Wronskian, which is $1/(kr)^2$. This gives

$$L\phi_l(r) = 2\mu k^2(-\frac{1}{r^2})r^2\frac{1}{k^2r^2}V^l(r)\phi_l(r)r^2 =$$

$$-2\mu V^l(r)\phi_l(r)$$

or

$$(L + 2\mu V^l(r))\phi_l(r) = 0$$

which is exactly the differential equation. The solution to this equation has to be proportional to the solution to the scattering equation. The most elementary way to see this is to work with the reduced wave function, $u_l = r\phi_l(r)$ which must vanish at the at the origin. It is a soution of the reduced equation that is fixed by its value and the value of its derivative at the origin. Since the value vanishes, the derivative necessarily fixes the normalization.

There are two nice properties of the integral equation for the regular solution. First the solution is real. Second is that the region of integration is finite. As long a the potential is a bounded operator this equation can be solved by iteration.

It is not a hard exercise to show that this series converges for every value of r and any potential strength. The $l = 0$ case is a simple example, In this case the equation is

$$\phi_0(r) - \frac{\sin(kr)}{kr} = \frac{2\mu}{kr}\int_0^r [\sin(kr)\cos(kr') - \cos(kr)\sin(kr')]V^0(r')\phi_0(r')r'dr' =$$

$$\frac{2\mu}{kr}\int_0^r \sin(k(r-r'))V^0(r')\phi_0(r')r'dr'$$

If I consider iterates of the kernel I get

$$\frac{2\mu}{k^2r}\int_0^r \sin(k(r-r'))V^0(r')\sin(kr')dr'$$

$$\frac{2\mu}{k^n r}\int_0^r \sin(k(r-r'))V^0(r')\int_0^{r''}\sin(k(r'-r''))V^0(r'')dr'dr''$$

$$\vdots$$

It is possible to show for complex z (homework) that

$$|\sin(z)| < c\frac{|z|}{1+|z|}e^{|Im(z)|}$$

With some more work this can be show to be analytic in k with reasonable assumptions on the potential.

For large r this must look like a free particle solution. I can write

$$\phi_l(kr) \to \frac{i}{2}[J_l(k)h_l^*(kr) - J_l^*(k)h_l(kr)]$$

which is written in a manner that makes it manifestly real. (This is beacuse both the kernel and driving term of the equation are real).The coefficient function $J_l(k)$ is called the Jost function.

To see the significance of the Jost function recall that

$$v_l(r) \to j_l(kr) + kf_l h_l(kr) = [\frac{1}{2i} + kf_l]h_l(kr) - \frac{1}{2i}h_l^*(kr)$$

for large r. I express this in terms of the partial wave scattering matrix

$$s_l = 1 - 2\pi ik\mu\langle k|t_l|k\rangle = 1 + 2ikf_l$$

$$kf_l = \frac{s_l - 1}{2i}$$

which gives the asymptotic form

$$v_l(r) \to j_l(kr) + kf_l h_l(kr) = \frac{1}{2i}(h_l(kr) - h_l^*(kr) + (s_l - 1)h_l(kr)) =$$

$$\frac{1}{2i}(h_l(kr) - h_l^*(kr) + (s_l - 1)h_l(kr)) =$$

$$\frac{i}{2}(h_l^*(kr) - s_l h_l(kr))$$

Comparing the asymptotic forms of this solution and the regular solution I get the following relation between the scattering matrix elements and the Jost function:

$$\phi_l(r) \to \frac{i}{2}[J_l(k)[h_l^*(kr) - \frac{J_l^*(k)}{J_l(k)}h_l(kr)]$$

which means

$$\boxed{\phi_l(kr) = J_l(k)v_l(r)}$$

and

$$\boxed{s_l(k) = \frac{J_l^*(k)}{J_l(k)}}$$

These equation show that the Jost function is closely related to the scattering operator.

The Jost function can be calculated in terms of the regular solution as follows. Note for large r the regular function becomes

$$\phi_l(r) \to j_l(kr) + 2\mu k j_l(kr)\int_0^\infty [n_l(kr')V^l(r')\phi_l(r')r'^2dr$$

$$-2\mu k n_l(kr)\int_0^\infty j_l(kr')V^l(r')\phi_l(r')r'^2dr$$

the coefficient of $h_l^*(kr)$ in this expression is

$$\phi_l(r) \to -\frac{1}{2i} - 2\mu k\frac{1}{2i}\int_0^\infty n_l(kr')V^l(r')\phi_l(r')r'^2dr - 2\mu k\frac{1}{2}\int_0^\infty j_l(kr')V^l(r')\phi_l(r')r'^2dr =$$

$$\frac{i}{2}[1 + 2\mu k\int_0^\infty (n_l(kr') + ij_l(kr'))V^l(r')\phi_l(r')r'^2]dr =$$

$$\frac{i}{2}[1 + 2\mu k\int_0^\infty h_l(kr')V^l(r')\phi_l(r')r'^2dr']$$

which gives an expression for the Jost function in terms of the regular solution:

$$J_l(k) = 1 + 2\mu k\int_0^\infty h_l(kr')V^l(r')\phi_l(r')r'^2dr'$$

Although $\phi_l(r)$ is analytic in k, the Jost function $J_l(k)$ is not because of the presence of $h_l(kr')$ in the integral representation. By inspection it is apparent that $J_l(k)$ is only analytic for $Im(k) > 0$. It is also continuous as $Im(k) \to 0$.

Note that for real k

$$J_l^*(k) = 1 + 2\mu k \int_0^\infty h_l^*(kr')V^l(r')\phi_l(r')r'^2 dr' =$$

$$1 + 2\mu k \int_0^\infty (-)^l h_l(-kr')V^l(r')(-)^l \phi_{l,-k}(r')r'^2 dr' =$$

$$J_l(-k)$$

which shows that

16 Relativistic Scattering

When the underlying quantum theory is relativistically invariant changes to the scattering theory are minimal. A quantum theory is relativistically invariant if the Hilbert space has a unitary representation of the Poincaré group.

This ensures that quantum probabilities

$$P = |\langle\psi|\phi\rangle|^2 \tag{251}$$

have the same value in all reference frames related by Lorentz transformations and/or space time translations. These unitary transformations U relate states associated with different inertial coordinate systems of special relativity:

$$|\phi'\rangle = U|\phi\rangle \qquad |\psi'\rangle = U|\psi\rangle \tag{252}$$

which ensure the invariance condition

$$P = |\langle\psi|\phi\rangle|^2 = |\langle'\psi|\phi'\rangle|^2 = P'. \tag{253}$$

This clearly implies that experimental measurements on an isolated system cannot make an absolute determination of an inertial coordinate system.

The Poincaré group is the group of coordinate transformations that preserve the proper distance between space-time events. Coordinates of theses events are given by four vectors:

$$x^\mu = (ct_x, \vec{x}) = (x^0, \vec{x}) \qquad y^\mu = (ct_y, \vec{y}) = (y^0, \vec{y})$$

The invariance condition is

$$(x-y)^2 = \eta_{\mu\nu}(x^\mu - y^\mu)(x^\nu - y^\nu) = \eta_{\mu\nu}(x'^\mu - y'^\mu)(x'^\nu - y'^\nu) = (x'-y')^2 \tag{254}$$

where

$$\eta_{\mu\mu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

is the Minkowski metric tensor. In the above expression and in what follows repeated Greek indices are assumed to summed from 0 to 3.

The most general transformation satisfying (**??**) has the form

$$x^\mu \to x'^\mu = \Lambda^\mu{}_\nu x^\nu + a^\mu \tag{255}$$

where the constant matrix $\Lambda^\nu{}_\beta$ satisfies

$$\eta^{\mu\nu} = \Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta \eta^{\alpha\beta} \tag{256}$$

and a^μ is a constant four vector. This is a generalization of the classical mechanics theorem that rigid body motions are generated by translations and rotations. Here the four dimensional Minkowski metric replaces the three dimensional Euclidean metric.

Successive Poincaré transformations can be expressed as a single Poincaré transformation:

$$(\Lambda, a) = (\Lambda_2, a_2)(\Lambda_1, a_1)$$

where

$$\Lambda^\mu{}_\nu = \Lambda^\mu_{2\,\alpha}\Lambda^\alpha_{1\,\nu} \qquad a^\mu = \Lambda^\mu_{2\,\nu} a_1^\nu + a_2^\mu.$$

It is useful to express these equations in the index free notation

$$\Lambda = \Lambda_2 \Lambda_1 \qquad a = \Lambda_2 a_1 + a_2$$

A unitary representation $U(\Lambda, a)$ of the Poincaré group is a set of unitary operators labeled by elements of the Poincaré group. These operators satisfy the group representation property:

$$U(\Lambda_2, a_2)U(\Lambda_1, a_1) = U((\Lambda_2, a_2)(\Lambda_1, a_1)).$$

The operator $U(\Lambda, a)$ contains time evolution, which involves the interaction. The new feature in relativistic quantum mechanics is that it is possible to transform the time using transformations other than time translation. This means that $U(\Lambda, a)$ must have a more complex interaction dependence than

one has in Galilean invariant quantum mechanics. The interaction dependence ensures that all independent paths to the future lead to the same result.

This can be understood by considering a rotationaless Lorentz transformation about the z axis:

$$\Lambda(\omega) = \begin{pmatrix} \cosh(\omega) & 0 & 0 & \sinh(\omega) \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \sinh(\omega) & 0 & 0 & \cosh(\omega) \end{pmatrix}$$

Matrix multiplication plus hyperbolic trigonomety gives the following

$$\Lambda(\omega_1)\Lambda(\omega_2) = \Lambda(\omega_1 + \omega_2)$$

The quantity ω is called the rapidity of the Lorentz transformation. It behaves like an angle of rotation.

If I start with an initial four vector,

$$x^\mu = \begin{pmatrix} 0 \\ 0 \\ 0 \\ z \end{pmatrix}$$

The Lorentz transforamtion $\Lambda(\omega)x$ gives

$$x_1^\mu = \begin{pmatrix} z\sinh(\omega) \\ 0 \\ 0 \\ z\cosh(\omega) \end{pmatrix}$$

Space translation in the z direction by $-z\cosh(\omega)$ gives

$$x_2^\mu = \begin{pmatrix} z\sinh(\omega) \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Applying the inverse Lorentz transformation $\Lambda(\omega)^{-1}$ gives

$$x_3^\mu = \begin{pmatrix} z\cosh(\omega)\sinh(\omega) \\ 0 \\ 0 \\ 0 - z\sinh^2(\omega) \end{pmatrix}$$

A second translation in the z direction by $z(1+\sinh^2(\omega)) = z\cosh^2(\omega)$ gives

$$x_4^\mu = \begin{pmatrix} z\cosh(\omega)\sinh(\omega) \\ 0 \\ 0 \\ 0z \end{pmatrix}$$

This show that the effect of this combination of translations in the z direction and rotationless boosts in the z direction is equivalent to time evolution by an amount

$$\Delta t = z\cosh(\omega)\sinh(\omega)$$

Since time evolution involves the dynamics, consistency requires that the combination of spatial translations and rotatinless Lorentz transformation should also involve the dynamcis.

The the transformation properties imply that

$$U(\Lambda(\omega), 0) = e^{i\omega K_z}$$

form some Hermetian operator K_z. This is called the infinitesimal generator of rotationless Lorentz transformations.

The formulation of a relativistic scattering theory starts by assuming the existence of two unitary representations of the Poincare group, $U(\Lambda, a)$ and $U_0(\Lambda, a)$, where $U_0(\Lambda, a)$ is associated with the non-interacting system.

The asymptotic condition is formulated in exactly the same way that it is formulated in the non-relativistic case

$$\lim_{t\to\pm\infty} \|U(I,t)|\psi_\pm\rangle - U_0(I,t)|\phi\rangle\| = 0$$

This can be expressed in terms of Møller wave operators

$$|\psi_\pm\rangle = \Omega_\pm|\phi\rangle$$

where

$$\Omega_\pm := s - \lim_{t\to\pm\infty} U(I,(-t,\vec{0}))U_0(I,(t,\vec{0})).$$

The Scattering operator has the same relation to the wave operators

$$S := \Omega_+^\dagger\Omega_-$$

that it has in the non-relativistic case. As in the non-relativistic case the square of the scattering matrix elements,

$$|\langle\phi_f|S|\phi_i\rangle|^2 = |\langle\psi_f^+|\psi_i^-\rangle|^2$$

are quantum probabilities. In a relativistic theory they must be invariant.

Clearly while

$$|\psi^{+\prime}\rangle = U(\Lambda, a)|\psi^+\rangle \qquad |\psi^{-\prime}\rangle = U(\Lambda, a)|\psi^-\rangle$$

implies

$$|\langle\psi^{+\prime}|\psi^{-\prime}\rangle|^2 = |\langle\psi^+|\psi^-\rangle|^2.$$

In the preparation of the scattering experiment the initial state is determined when the particles are isolated beyond the range of the interactions. Likewise, the final states are determined by measuring the states of the asymptotically separated scattered particles. A reasonable scattering operator should also be invariant with respect to kinematic Poincaré transformations of the asymptotic initial and final scattering asymptotes.

This requires

$$U_0^\dagger(\Lambda, a)SU_0(\Lambda, a) = S$$

which is an invariance with respect to the asymptotic labels of the initial and final states. A sufficient condition for this to hold is that wave operators satisfy the relativistic intertwining conditions

$$\Omega_\pm U_0(\Lambda, a) = U(\Lambda, a)\Omega_\pm$$

This condition automatically holds for the Hamiltonian using the ordinary intertwining condition that was derived in the non-relativistic case. In addition, it holds for any kinematic Poincaré transformations; i.e. transformations (Λ, a) that satisfy

$$U_0(\Lambda, a)U^\dagger(\Lambda, a) = I$$

Unfortunately, there can be at most a seven parameter group of kinematic transformations, and a one parameter group of time translations. This does not exhaust the full ten parameter group of Poincaré transformation. The invariance requirement is a non-trivial condition on the remaining dynamical transformations.

For example, it is possible to formulate quantum models where rotations and spatial translations are kinematic. This generates a six parameter kinematic subgroup. In this example, the rotationless Lorentz transformations cannot be kinematic and must satisfy the non-trivial intertwining relations

$$\Omega_{\pm} U_0(\Lambda, 0) = U(\Lambda, 0)\Omega_{\pm}.$$

This is an additional condition on the interaction operators that appear in the rotationless Lorentz transforms.

In order to discuss the invariance it is useful to begin by assuming the existence of the following wave operators

$$\Omega_{\pm}(M, M_0) := \lim_{\tau \to \pm\infty} e^{iM\tau} e^{-iM_0\tau}$$

The mass operator, $M = \sqrt{H^2 - \vec{P} \cdot \vec{P}}$, is the analog of the non-relativistic center of momentum Hamiltonian. In the non-relativistic case the Hamiltonian has the form $H = \vec{P} \cdot \vec{P}/2m_t + h$, $H_0 = \vec{P} \cdot \vec{P}/2m_t + h_0$ where $\vec{P}$ commutes with H, h, H_0, and h_0. This implies

$$\Omega_{\pm}(H, H_0) = \Omega_{\pm}(h, h_0).$$

Let $g = (\Lambda, a)$ denote an arbitrary but fixed Poincaré transformation. The operator $\Omega_{\pm}(M, M_0)$ is invariant if

$$U(g)\Omega_{\pm}(M, M_0) = \Omega_{\pm}(M, M_0)U_0(g).$$

It follows from the definitions that this will hold if and only if

$$\boxed{\lim_{\tau \to \pm\infty} [I - U^{\dagger}(g)U_0(g)]e^{-iM_0\tau} = 0}$$

for all Poincaré transforms g.

To prove this note that this condition is equivalent to

$$\lim_{\tau \to \pm\infty} [U(g) - U_0(g)]e^{-iM_0\tau} = 0$$

which is equivalent to

$$\lim_{\tau \to \pm\infty} e^{iM\tau}[U(g) - U_0(g)]e^{-iM_0\tau} = 0$$

and finally

$$\lim_{\tau\to\pm\infty}[U(g)e^{iM\tau}e^{-iM_0\tau} - e^{iM\tau}e^{-iM_0\tau}U_0(g)] = 0.$$

which is the invariance condition for $\Omega(M, M_0)$.

This condition means that $A = U^\dagger(g)U_0(g)$ is a scattering equivalence.

Next I consider the relation between $\Omega_\pm(M, M_0)$ and $\Omega_\pm(H, H_0)$ assuming both operators exist and satisfy the invariance condition.

The spatial translations are generated by the linear momentum

$$U(I, \vec{a}) = e^{i\vec{a}\cdot\vec{P}}$$

Taking partial derivatives with respect to the components of $\vec{a}$ and then setting $\vec{a} = 0$ in the invariance condition gives

$$\langle\vec{P}|\vec{P}\Omega_\pm(M, M_0)|\vec{P}_0\rangle = \langle\vec{P}|\Omega_\pm(M, M_0)\vec{P}_0|\vec{P}_0\rangle$$

or equivalently

$$0 = (\vec{P} - \vec{P}_0)\langle\vec{P}|\Omega_\pm(M, M_0)|\vec{P}_0\rangle.$$

Similarly

$$0 = (\vec{P} - \vec{P}_0)\langle\vec{P}|\Omega_\pm(H, H_0)|\vec{P}_0\rangle.$$

This means that the matrix elements in the mixed representation are proportional to delta functions

$$\langle\vec{P}|\Omega_\pm(M, M_0)|\vec{P}_0\rangle\delta(\vec{P} - \vec{P}_0)\hat{\Omega}_\pm(\vec{P}, M, M_0)$$

and

$$\langle\vec{P}|\Omega_\pm(H, H_0)|\vec{P}_0\rangle\delta(\vec{P} - \vec{P}_0)\hat{\Omega}_\pm(\vec{P}, H, H_0).$$

In these expression the mass (respectively the energy) is also conserved by the intertwining relations.

If Λ is the Lorentz transformation that maps $(\sqrt{M^2 + \vec{P}\cdot\vec{P}}, \vec{P}$ to its zero momentum value then the invariance condition implies

$$\delta(\vec{P} - \vec{P}_0)\hat{\Omega}_\pm(\vec{P}, M, M_0) =$$

$$\langle\vec{P}|\Omega_\pm(M, M_0)|\vec{P}_0\rangle =$$

$$\langle\vec{P}|U^\dagger(\Lambda, 0)\Omega_\pm(M, M_0)|U^\dagger(\Lambda, 0)\vec{P}_0\rangle =$$

$$\sqrt{\frac{M}{E}}\sqrt{\frac{M_0}{E_0}}\langle\vec{P}_r|\Omega_\pm(M,M_0)|\vec{P}_{0r}\rangle =$$
$$\sqrt{\frac{M}{E}}\delta(\vec{P}_r-\vec{P}_{r0})\hat{\Omega}_\pm(\vec{0},M,M_0)$$
$$\delta(\vec{P}-\vec{P}_0)\hat{\Omega}_\pm(\vec{0},M,M_0)$$

from which I identify

$$\hat{\Omega}_\pm(\vec{0},M,M_0)=\hat{\Omega}_\pm(\vec{P},M,M_0)$$

Similarly

$$\hat{\Omega}_\pm(\vec{P},H,H_0)=\hat{\Omega}_\pm(\vec{0},H,H_0)=\hat{\Omega}_\pm(\vec{0},M,M_0)$$

The final identification is because $H(\vec{P}=\vec{0})=M$.

This shows that if both operators exist and satisfy the invariance condition that

$$\Omega_\pm(H,H_0)=\Omega_\pm(M,M_0)$$

Thus, even thought the $\vec{P}$ is not necessarily a kinematic operator, the invariance condition means that the scattering can formulated using the mass operator rather than the Hamiltonian. Note that M is the analog of the center of mass Hamiltonian that is used in non-relativistic scattering theory.

It is easy to construct a large class of models having all of the desired properties.

The next step it show how to define scattering cross sections in relativistic quantum mechanics. Rather than follow non-relativistic derivation, which began by generalizing the case of an infinitely massive target, the derivation I give for the relativistic case follows closely one given by Brenig and Haag.

I begin by considering a two-body scattering reaction. The target and projectile are described by wave packets in momentum space that are sharply peaked around the beam momentum, $\bar{p}_b$ and the target momentum $\bar{p}_t$

The probability for measuring the scattered beam particle to be within d^3p_1 of and $\vec{p}_1$ and the scattered target particle to be within d^3p_2 of $\vec{p}_2$ is given by

$$dP:=|\langle\vec{p}_1\vec{p}_2|\phi\rangle|d^3p_1d^3p_2$$

where

$$\langle\vec{p}_1\vec{p}_2|\phi\rangle =$$
$$-2\pi i\delta(E_f-E_i)\int d^3p_bd^3p_t\langle\vec{p}_1,\vec{p}_2|T(E+i0^+)|\vec{p}_b,\vec{p}_t\rangle d^3p_bd^3p_t\phi_b(\vec{p}_b)\phi_t(\vec{p}_t).$$

This assumes that the final states are not along the beam line. The previous assumption about sharply peaked momentum distributions are important here.

The invariance of the wave operators with respect to the linear momentum means that the scattering operator is diagonal in the free linear momentum. I can take advantage of this by factoring out the momentum conserving delta function in the expression above to obtain

$$\langle \vec{p}_1, \vec{p}_2 | \phi \rangle =$$

$$-2\pi i \delta(E_f - E_i) \delta^3(p_b + p_t - p_1 - p_2) \langle \vec{p}_1, \vec{p}_2 \| T(E + i0^+) \| \vec{p}_b \vec{p}_t \rangle d^3 p_b d^3 p_t \phi_b(\vec{p}_b) \phi_t(\vec{p}_t).$$

Writing out the probability density explicitly gives

$$|\langle \vec{p}_1, \vec{p}_2 | \phi \rangle|^2 =$$

$$4\pi^2 \delta(E_f - E_i) \delta^3(p_b + p_t - p_1 - p_2) \delta(E_f - E_i') \delta^3(p_b' + p_t' - p_1' - p_2) \times$$
$$\langle \vec{p}_1, \vec{p}_2 \| T(E + i0^+) \| \vec{p}_b \vec{p}_t \rangle \langle \vec{p}_b', \vec{p}_t' \| T(E - i0^+) \| \vec{p}_1, \vec{p}_2 \rangle \times$$
$$d^3 p_b d^3 p_t \phi_b(\vec{p}_b) \phi_t(\vec{p}_t) d^3 p_b' d^3 p_t' \phi_b(\vec{p}_b') \phi_t(\vec{p}_t')$$

The delta functions can be expressed in a Fourier representation

$$\delta(E_f - E_i) \delta^3(p_b + p_t - p_1 - p_2) \delta(E_i - E_i') \delta^3(p_b' + p_t' - p_b - p_t) =$$

$$\delta(E_f - E_i) \delta^3(p_b + p_t - p_1 - p_2) (2\pi)^{-4} \int e^{i(p_b + p_t - p_b' - p_t') \cdot x} e^{i(E_i' - E_i) \cdot t} d^3 x dt$$

Assume that the transition matrix elements are essentially constant on the support of the initial wave packets. Under this assumption the arguments of the transition operators can he replaced by their peak values. With this replacement it becomes possible to do the momentum integrals over the beam and target momenta, which gives

$$|\langle \vec{p}_1, \vec{p}_2 | \phi \rangle|^2 =$$

$$(2\pi)^{2-4+6} \delta(E_f - \bar{E}_i) \delta^3(\bar{p}_b + \bar{p}_t - p_1 - p_2) |\langle \vec{p}_1, \vec{p}_2 \| T(E + i0^+) \| \bar{p}_b, \bar{p}_t \rangle|^2 \times$$
$$\int |\phi_b(\vec{x}, t) \phi_t(\vec{x}, t)|^2 d^3 x dt$$

This expresses the probability density of a scattering with final momenta $\vec{p}_1$ and $\vec{p}_2$ on terms of the the probability density of finding a target and beam

particle at the point $\vec{x}$ and time t. It is clear proportional to the product of these densities, and there is only a contribution to the total probability when both probability densities are non-zero at the same point and time. There is a contribution for all times when the particles have an appreciable probability for being found at the same point. The total contribution can be found by integrating over time.

With the factorization assumption, it is clear that all of the dependence on the shape of the target or beam wave function this through this last term. If I remove the space and time integrals I get a differential probability per unit volume per unit time (or equivalently a transition rate per unit volume).

The total number of particles that scatter is obviously Lorentz invariant. Similarly the 4-volume, d^3ddt is an invariant volume (note that the determinant of the Lorentz transformation is 1).

We divide this by a Lorentz invariant quantity that is equal to the target density multiplied by the beam density times the relative speed of the target and beam in the center of momentum frame. To find the desired invariant quantity consider

$$F = \frac{\rho_b}{\omega_b}\frac{\rho_t}{\omega_t}\sqrt{\frac{1}{2}(p_b^\mu p_t^\nu - p_b^\mu p_t^\nu)(p_{b\mu}p_{t\nu} - p_{b\mu}p_{t\nu})}$$

which is manifestly Lorentz invariant. In the center of momentum frame this becomes

$$\frac{\rho_{cm-b}}{\omega_b}\frac{\rho_{cm-t}}{\omega_t}\sqrt{(\omega_b+\omega_t)^2k^2} =$$

$$\rho_{cm-b}\rho_{cm-t}|\frac{k}{\omega_b} - \frac{-k}{\omega_t}|$$

which reduces to the desired quantity. Dividing the transition rate per unity volume by this invariant quantity gives Møller's invariant differential cross section

$$d\sigma = (2\pi)^4|\langle\vec{p}_1,\vec{p}_2\|T(E+i0^+)\|\bar{p}_b\bar{p}_t\rangle|^2\times$$

$$\delta(E_f - E_i)\delta^3(\bar{p}_b + \bar{p}_t - p_1 - p_2)\frac{d^3p_1d^3p_2E_pE_b}{B}$$

In this the energies and momenta are related to each other by kinematic relativistic dispersion relations.

It is customary to write the above in the form

$$d\sigma = |M_{fi}|^2dL$$

where

$$M_{fi} := (2\pi)^4 |\langle \vec{p}_1, \vec{p}_2 \| T(E + i0^+) \| \bar{p}_b \bar{p}_t \rangle|^2 \times \frac{E_1 E_2 E_p E_b}{B}$$

and

$$dL := \delta(E_f - E_i)\delta^3(\bar{p}_b + \bar{p}_t - p_1 - p_2)\frac{d^3p_1 d^3p_2}{E_1 E_2}$$

The quantity M is called the invariant transition amplitude and L is called the Lorentz invariant phase space.

In this form the differential cross section is manifestly invariant.

While we did not talk about the relation between the scattering operator and the transition operator, the previously derived formulas give

$$T(z) = (M - M_0) + (M - M_0)\frac{1}{z - M_0}T(z)$$

along with the standard relation

$$S_{fi} = \langle f|i\rangle - 2\pi i \delta(E_f - E_i)\langle f|T(z)|i\rangle$$

There is an interesting question concerning the relationship between relativistic and non-relativistic quantum mechanics. In many instances interactions are designed by a fitting procedure.

Normally the way that this works is that the laboratory cross section is measured. The angular distributions and asymptotic spin observables are transformed to the center of momentum frame using relativistic transformation laws. The result is that center of momentum cross section given as a function of either relative energy or relative momentum.

The cross section is computed by solving the non-relativistic Lippmann Schwinger equation. The potential is adjusted until the non-relativistic center of mass cross section agrees with the "measured" cross section as a function of the relative momentum. (this could alternatively be fit as a function of the relative energy). Of course the relation between energy and momentum in the relativistic and non-relativistic theories is different, so these two possible fitting procedures are not equivalent.

One thing is apparent is that the notion of a non-relativistic limit does not make sense when the interaction is determined in this manner. Specifically the non-relativistic, relativistic, and experimental cross sections all agree (by definition) in zero momentum frame as functions of relative momentum. Differences in the two formalisms are only relevant in other frames.

17 Multiparticle Scattering

For systems of more than two particles the possible outcomes of a scattering experiment are complex. Both the target and projectile can be bound states of constituent particles. In addition, the reaction products can involve rearrangements of the constituent particles, or the target and projectile can break up into different fragments, or emerge in excited states.

I begin by assuming an N-particle Hamiltonian of the form

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \cdots \tag{257}$$

where V_{ij} are two-body interactions between particles i and j and V_{ijk} are three-body interactions. The formulation of multiparticle scattering is similar to two-body scattering.

In order to keep book keeping simple I introduce the following short hand notation. I let a denote a partition of the N particles into n_a disjoint subsets or equivalence classes. I let $\mathcal{P}(N)$ denote the set of all partitions of the N particles. For example

$$\mathcal{P}(3) = \{(1)(2)(3), (12)(3), (23)(1), (31)(2), (123)\}. \tag{258}$$

The partition $a = (12)(3)$ is a two-cluster partition ($n_a = 2$), while $a = (1)(2)(3)$ is a three cluster partition ($n_a = 3$).

For each partition a, I let V_a denote the sum of all interactions between particles in the same cluster of a. For example

$$V_{(13)(245)} := V_{12} + V_{24} + V_{45} + V_{25} + V_{245}. \tag{259}$$

This includes both two and three-body interactions. Let

$$V^a := V - V_a \tag{260}$$

denote the residual interaction. These are the interactions that should vanish when the clusters of a are asymptotically separated. I also define

$$H_a = H_0 + V_a = \sum_{i=1}^{n_a} H_{a_i} \tag{261}$$

where H_{a_i} is the subsystem Hamiltonian for the particles in the $i-th$ cluster of the partition a. It is an immediate consequence of the definitions that

$$H = H_a + V^a \tag{262}$$

for any partition a. This decomposition leads to resolvent relations of the form

$$\frac{1}{z-H} - \frac{1}{z-H_a} = \frac{1}{z-H_a} V^a \frac{1}{z-H} = \frac{1}{z-H} V^a \frac{1}{z-H_a}. \tag{263}$$

These equations hold for any partition a.

I use partitions to define scattering channels. Consider a partition a. As an example I consider $a = (1)(24)(3)$. There is a scattering channel α_a associated with the partition a if the subsystem Hamiltonian, H_{a_i}, for each cluster with more than one particle, has a bound state. For example, for $a = (1)(24)(3)$ there is a scattering channel associated with each bound state of

$$H_{24} = \frac{p_2^2}{2m_2} + \frac{p_4^2}{2m_4} + V_{24}. \tag{264}$$

If I assume that each H_{a_i} is invariant with respect to rotations and translations it is possible to find simultaneous eigenstate of the form

$$|\vec{p}_i, \mu_i(j_i, \alpha_i)\rangle \tag{265}$$

where α_i labels the bound state of the particles in the i^{th} cluster of a, j_i and μ_i are the spin and magnetic quantum number of the bound state, and $\vec{p}_i$ is the linear momentum of bound state. If the cluster has only one particle these labels define the state of the particle.

A channel for the N particle system has an α_i corresponding to each cluster of the partition a. Channels are labels for the possible stable asymptotic fragments of a scattering experiment, which looks like n_a bound fragments moving with definite momenta and spins. The analog of the two-body plane-wave state corresponding to a channel α is the tensor product state

$$|\alpha\rangle = \otimes_{i=1}^{n_a} |\vec{p}_i, \mu_i(j_i, \alpha_i)\rangle. \tag{266}$$

This is an eigenstate of H_a and $\vec{P}$ with eigenvalues

$$E_a = \sum_{i=1}^{n_a} E_{\alpha_i} \qquad \vec{p} = \sum_{i=1}^{n_a} \vec{p}_{a_i} = sum_{k=1}^{N} \vec{p}_k. \tag{267}$$

In this channel the interaction V_a acts asymptotically, holding the bound fragments together, while the residual interaction, V^a, vanishes when the fragments are asymptotically separated.

For each partition a there can many channels or no channels. It depends entirely on the interaction. The states (**??**) behave like plane waves in the momentum of each asymptotic cluster. In a real experiment these are replaced by wave packets with sharply peaked momenta. This replacement is most easily accomplished by defining a channel Hilbert space which is the n_a-fold tensor product of square integrable functions of the single cluster spin and linear momentum variables. I denote this channel Hilbert space by $\mathcal{H}_\alpha$ which is spanned by products of square integrable the momentum wave packets:

$$|\phi_\alpha\rangle := \prod_{i=1}^{n_a} \phi_i(\vec{p}_i, \mu_i). \tag{268}$$

For scattering the wave packets are sharply peaked about a mean momentum for each cluster of a. The space $\mathcal{H}_\alpha$ is a space of n_a "particles = bound clusters". The internal structure of the "particles" does not appear in $\mathcal{H}_\alpha$. The internal structure is introduced with mappings to the N-particle Hilbert space.

The eigenstates (**??**) define a map Φ_α from the channel space $\mathcal{H}_a$ to the N-particle Hilbert space

$$\Phi_\alpha|\phi_\alpha\rangle := -\sum_{\nu_1\cdots\mu_{n_a}} \otimes_{i=1}^{n_a} \int |\vec{p}_i, \nu_i(j_i\alpha_i)\rangle \prod_{j=1}^{n_a} \phi_j(\vec{p}_j, \mu_j) d^3p_j \tag{269}$$

This is efficient notation for a normalizable N-particle state corresponding to a set of n_a mutually non-interacting bound fragments. The channel Hilbert space and injection operator provide a useful notation for separating the internal structure from the asymptotic structure.

The time evolution operator of a scattering asymptote in channel α associated with partition a is

$$U_a(t) := e^{-iH_a t}. \tag{270}$$

It is also useful to define the corresponding Hamiltonian on $\mathcal{H}_\alpha$ which replaces each H_{a_i} by its kinetic energy plus binding energy:

$$H_\alpha = \sum_{i=1}^{n_a} (\frac{p_i^2}{2m_i} + E_{\alpha_i}). \tag{271}$$

This definition leads to the relation:

$$H_a\Phi_\alpha = \Phi_\alpha H_\alpha. \tag{272}$$

If I Define

$$U_\alpha(t) := e^{-iH_\alpha t} \tag{273}$$

on $\mathcal{H}_\alpha$ I get the following identity

$$U_a(t)\Phi_\alpha = \Phi_\alpha U_\alpha(t). \tag{274}$$

I am now in a position to define the scattering asymptotic conditions for multichannel scattering. This is the fundamental starting point of any scattering theory. A scattering solution

$$|\Psi_\pm(t)\rangle = U(t)|\Psi_\pm(0)\rangle \qquad U(t) = e^{-iHt} \tag{275}$$

of the N-particle Schrödinger equation that asymptotically looks like n_a mutually non-interacting clusters in channel α is defined by the Asymptotic condition:

$$\boxed{\lim_{t\to\pm\infty} \|U(t)|\Psi_\pm(0)\rangle - U_a(t)\Phi_\alpha|\phi_\alpha(0)\rangle\| = 0} \tag{276}$$

where the limit is a strong limit or strong abelian limit.

Using the unitarity of $U(t)$ this state can be expressed in terms of two-Hilbert space channel wave operators

$$|\Psi_\pm\rangle = \Omega_\pm|\phi_\alpha\rangle \tag{277}$$

where

$$\Omega_{\alpha\pm} := \lim_{t\to\pm\infty} U(-t)U_a(t)\Phi_\alpha = \lim_{t\to\pm\infty} U(-t)\Phi_\alpha U_\alpha(t). \tag{278}$$

These wave operators are isometric mappings from $\mathcal{H}_\alpha$ to $\mathcal{H}$:

$$\Omega_{\alpha\pm} : \mathcal{H}_\alpha \to \mathcal{H} \qquad \|\Omega_{\alpha\pm}|\phi_\alpha\rangle\| = \||\phi_\alpha\rangle\|. \tag{279}$$

The existence of the two-Hilbert space wave operators can be established using a multichannel variant of the Cook condition. Following the steps of the two-particle derivation leads to the sufficient condition for the existence of the channel wave operator:

$$\boxed{\int_0^{\pm\infty} \|[H\Phi_\alpha - \Phi_\alpha H_\alpha]U_\alpha(t)|\phi_\alpha(0)\rangle\| < \infty} \tag{280}$$

which is the two-Hilbert space multichannel version of the Cook condition. The quantity that replaces the interaction in the two-body case is

$$H\Phi_\alpha - \Phi_\alpha H_\alpha = V^a \Phi_\alpha. \tag{281}$$

Multichannel scattering is interesting because it is possible to scatter from an initial channel α to a final channel β. The probability amplitude for such a reaction is given by the scattering matrix element

$$S_{f_i\beta i_\alpha} = \langle \Psi_{+\alpha}(0) | \Phi_{-\beta}(0) \rangle = \langle \phi_\beta(0) | \Omega^\dagger_{+\beta} \Omega_{-\alpha} | \phi_\alpha(0) \rangle. \tag{282}$$

This can be expressed as a matrix element of a multichannel S-operator, $S_{\beta\alpha}$, that maps $\mathcal{H}_\alpha$ to $\mathcal{H}_\beta$:

$$S_{\beta\alpha} := \Omega^\dagger_{+\beta} \Omega_{-\alpha} \tag{283}$$

It is useful to introduce a compact notation that treats all channels simultaneously. The first step is to define the asymptotic Hilbert space to be the orthogonal direct sum of all of the channel spaces

$$\mathcal{H}_f = \oplus_\alpha \mathcal{H}_\alpha. \tag{284}$$

It is useful to include the bound states in the channel sum. The correspond to one cluster states. Vector in $\mathcal{H}_f$ can be considered as column vectors

$$|\phi_f\rangle = \begin{pmatrix} |\phi_\alpha\rangle \\ |\phi_\beta\rangle \\ |\phi_\gamma\rangle \\ \vdots \\ |\phi_\zeta\rangle \end{pmatrix} \tag{285}$$

Two-Hilbert space wave operators are defined by

$$\Omega_\pm = \sum_\alpha \Omega_{\pm\alpha} \Pi_\alpha \tag{286}$$

where Π_α is the orthogonal projection on the subspace $\mathcal{H}_\alpha$ of $\mathcal{H}_f$. In the matrix notation Π_β is the matrix

$$\Pi_\beta = \begin{pmatrix} 0, 0, 0, \cdots 0 \\ 0, I, 0, \cdots, 0 \\ 0, 0, 0, \cdots 0 \\ \vdots \\ 0, 0, 0, \cdots 0 \end{pmatrix}. \tag{287}$$

Injection operators from $\mathcal{H}_f$ to $\mathcal{H}$ are defined by

$$\Phi := \sum_\alpha \Phi_\alpha \Pi_\alpha, \tag{288}$$

and the asymptotic Hamiltonian and time evolution operator are

$$H_f = \sum_\alpha H_\alpha \Pi_\alpha \qquad U_f(t) = e^{-iH_f t}. \tag{289}$$

In this notation the multichannel scattering operator is linear operator on $\mathcal{H}_f$

$$\boxed{S = \Omega_+^\dagger \Omega_-} \tag{290}$$

with

$$\boxed{\Omega_\pm = \lim_{t\to\pm\infty} U(-t)\Phi_f U_f(t)} \tag{291}$$

While the formulation of the asymptotic conditions are important, it is necessary to know how to compute the two-Hilbert space scattering matrix elements. To illustrate this consider scattering from channel α to channel β. I let

$$H_a\Phi_\alpha = E_\alpha \Phi_\alpha \qquad H_b\Phi_\beta = E_\beta \Phi_\beta \tag{292}$$

where the energy eigenvalues include the cluster kinetic energies. I treat the cluster momenta as plane wave states. It follows that

$$\begin{aligned}
&\langle\beta|S|\alpha\rangle = \\
&= \lim_{t\to\infty} \Phi_\beta^\dagger e^{iH_b t} e^{-2iHt} e^{iH_a t}\Phi_\alpha \\
&= \Phi_\beta^\dagger\Phi_\alpha + \lim_{t\to\infty}\int_0^t dt'\,\frac{d}{dt'}\Phi_\beta^\dagger e^{i(E_\beta+E_\alpha-2H)t'}\Phi_\alpha \\
&= \Phi_\beta^\dagger\Phi_\alpha + \lim_{\epsilon\to 0^+} i\int_0^\infty dt'\,\Phi_\beta^\dagger\Big[(E_\beta - H)e^{i(E_\beta+E_\alpha-2H+i\epsilon)t'} \\
&\qquad + e^{i(E_\beta+E_\alpha-2H+i\epsilon)t'}(E_\alpha - H)\Big]\Phi_\alpha \\
&= \Phi_\beta^\dagger\Phi_\alpha + \lim_{\epsilon\to 0^+}\frac{1}{2}\Phi_\beta^\dagger\left[(H-E_\beta)\frac{1}{\bar{E}-H+i\epsilon} + \frac{1}{\bar{E}-H+i\epsilon}(H-E_\alpha)\right]\Phi_\alpha,
\end{aligned} \tag{293}$$

where $\bar{E} := \frac{1}{2}(E_\alpha + E_\beta)$ is the average energy of the initial and final asymptotic states. Using (**??**) gives

$$\Phi_\beta^\dagger \Phi_\alpha + \lim_{\epsilon \to 0^+} \frac{1}{2} \Phi_\beta^\dagger \left[(H - E_b) \frac{1}{\bar{E} - H + i\epsilon} + \frac{1}{\bar{E} - H + i\epsilon} (H - E_a) \right] \Phi_\alpha, \quad (294)$$

Next I recall that the resolvent $R(z) := (z - H)^{-1}$, and $R_a(z) := (z - H_a)^{-1}$ of H and H_a satisfies the second resolvent relations

$$R(z) - R_a(z) = R_a(z) V^a R(z) = R(z) V^a R_a(z) \qquad R_a(z) := \frac{1}{z - H_a} \quad (295)$$

for any partition a. This leads to

$$\begin{aligned}
& S_{\beta\alpha} = \\
& = \Phi_\beta^\dagger \Phi_\alpha + \lim_{\epsilon \to 0^+} \frac{1}{2} \Phi_\beta^\dagger \left[V^b \left(1 + R(\bar{E} + i\epsilon) V^a \right) R_a(\bar{E} + i\epsilon) \right. \\
& \qquad \left. + R_b(\bar{E} + i\epsilon) \left(1 + V^b R(\bar{E} + i\epsilon) \right) V^a \right] \Phi_\alpha \\
& = \Phi_\beta^\dagger \Phi_\alpha \left[1 - \lim_{\epsilon \to 0^+} \frac{E_\beta - E_\alpha}{E_\beta - E_\alpha + 2i\epsilon} \right] \\
& + \lim_{\epsilon \to 0^+} \left[\frac{1}{E_\beta - E_\alpha + 2i\epsilon} + \frac{1}{E_\alpha - E_\beta + 2i\epsilon} \right] \Phi_\beta^\dagger \left(V^a + V^b R(\bar{E} + i\epsilon) V^a \right) \Phi_\alpha \\
& = \Phi_\beta^\dagger \Phi_\alpha \lim_{\epsilon \to 0^+} \left[\frac{2i\epsilon}{E_\beta - E_\alpha + 2i\epsilon} \right] \\
& + \lim_{\epsilon \to 0^+} \left[\frac{-4i\epsilon}{(E_\beta - E_\alpha)^2 + 4\epsilon^2} \right] \Phi_\beta^\dagger \left(V^a + V^b R(\bar{E} + i\epsilon) V^a \right) \Phi_\alpha. \qquad (296)
\end{aligned}$$

It is now possible to evaluate the limit as $\epsilon \to 0$. It is important to remember that this is the kernel of an integral operator that acts on subspaces of the asymptotic Hilbert space.

The first term in square brackets is unity when the initial and final energies are identical, and zero otherwise; however, the limit in the bracket is a Kronecker delta and *not* a Dirac delta function. For $a \neq b$, I expect that $\langle \beta(E') | \alpha(E) \rangle$ will be Lebesgue measurable in E' for fixed E (i.e there is no delta function in E) , so there is no contribution from the first term in Eq. (**??**). For the case that $H_b = H_a$, I have $\Phi_\beta^\dagger(E') \Phi_\alpha(E) \propto \delta(E' - E)$. This vanishes by orthogonality unless $E_\beta = E_\alpha$, but then coefficient is unity.

Thus, the first term is $\langle\beta|\alpha\rangle$ if the initial and final channels are the same, but zero otherwise. Note that the matrix elements vanish by orthogonality for two different channels governed by the same asymptotic Hamiltonian with the same energy. The first term in (**??**) is therefore a *channel* delta function.

For the second term, the quantity in square brackets becomes $-2\pi i\delta(E_\beta - E_\alpha)$, which leads to the relation

$$S_{\beta\alpha} = \delta_{\beta\alpha} I - 2\pi i\delta(E_\beta - E_\alpha)\Phi_\beta^\dagger T^{ba}(E_a + i0^+)\Phi_\alpha, \tag{297}$$

where

$$T^{ba}(z) = V^a + V^b R(z) V^a. \tag{298}$$

This shows that the dynamics is contained in the transition operators $T^{ab}(z)$. These have partition labels as superscripts.

In the special case that initial channel α is a two-cluster channel the formula for the differential cross section for scattering into channel β becomes

$$d\sigma = \frac{(2\pi)^4 \mu_\alpha}{k\alpha} |\Phi_\beta^\dagger T^{ba}(E_a + i0^+)\Phi_\alpha|^2_{red} \delta(E_\alpha - E_\beta)\delta(\vec{p}_\alpha - \vec{p}_\beta) \prod_{i=1}^{n_b} d^3 p_{b_i} \tag{299}$$

where the subscript *red* indicates that a three momentum delta has been factored out of the transition matrix element:

$$|\Phi_\beta^\dagger T^{ba}(E_a + i0^+)\Phi_\alpha|_{red} := |\Phi_\beta^\dagger T^{ba}(E_a + i0^+)\Phi_\alpha|\delta(\vec{p}_\beta - \vec{p}_\alpha). \tag{300}$$

There is an additional statistical factor that arises if any the final asymptotes are identical.

18 The Faddeev Equations

In the last section I showed that in many-body scattering problems the two-body transition operator is replaced by the operators

$$T^{ba}(z) = V^a + V^b R(z) V^a. \tag{301}$$

In this section I consider the simplest non-trivial case of three particles, labeled $1, 2$ and 3. There are five relevant partitions:

$$(123), (12)(3), (23)(1), (31)(2) \quad \text{and} \quad (1)(2)(3). \tag{302}$$

To illustrate the problem let $b = (12)(3)$. The relevant transition operator for elastic scattering of a bound state of the (12) system from particle (3) is

$$T^{bb}(z) = V^b + V^b R(z) V^b. \tag{303}$$

Using the resolvent equation

$$R(z) = R_b(z) + R_b(z) V^b R(z) \qquad R_b(z) = (z - H_0 - V_b)^{-1}$$

in (**??**) leads to the Lippmann-Schwinger equation

$$T^{bb}(z) = V^b + V^b R_b(z) T^{bb}(z). \tag{304}$$

This looks similar to the two-body Lippmann-Schwinger equation with $V \to V^b$ and $R_0(z) \to R_b(z)$, however there are fundamental difficulties if I repeat what was done in the two particle case.

To see the problem with this equation in its most transparent form I consider the corresponding equation for the scattering wave function. To derive it I write the Schrödinger eigenvalue problem

$$H|\psi\rangle = E|\psi\rangle \tag{305}$$

which I put in the form

$$(E - H_0 - V_b)|\psi\rangle = V^b|\psi\rangle \tag{306}$$

I can invert $(E - H_0 - V_b)$ and write the above equation as

$$|\psi\rangle = |\phi_b\rangle + (E \pm i0^+ - H_0 - V_b)^{-1} V^b |\psi\rangle \tag{307}$$

where $|\phi_b\rangle$ is a solution of

$$(E - H_0 - V_b)|\phi_b\rangle = 0 \tag{308}$$

and the $\pm i0^+$ fixes the asymptotic boundary condition on the scattering eigenstate like it does in the two-body case. In this case H_b has eigenstates where all three particles are asymptotically separated and solutions where particles in the same cluster of b are bound. For example if $b = (12)(3)$ H_b might have eigenstates where particles 1 and 2 are bound. The three-body eigenstate can still have any positive energy because the relative kinetic

energy between the (12) pair and the spectator particle 3 can take on any positive value.

In addition to solutions that asymptotically look like three free particles or bound 12 pairs, the Hamiltonian can also have eigenstates that asymptotically look like bound states of particles 2 and 3 or 1 and 3. These states will satisfy the homogeneous form of the Lippmann-Schwinger equation

$$|\psi\rangle = (E \pm i0^+ - H_0 - V_b)^{-1} V^b |\psi\rangle \tag{309}$$

If I let $|\chi\rangle := V^b|\psi\rangle$ the above equation becomes

$$|\chi\rangle = V^b (E \pm i0^+ - H_0 - V_b)^{-1} |\chi\rangle \tag{310}$$

which shows that the Lippmann-Schwinger equation to $T^{bb}(z)$ also has non-trivial solutions of the homogeneous form of the equations as z approached the real axis.

The existence of these states means that Lippmann Schwinger equation does not have a unique solution. The problem is that while integral equations normally incorporate boundary conditions, the built-in boundary conditions are not enough to ensure that the solution does not include ad-mixtures of eigenstates where the (13) or (32) pairs are asymptotically bound.

The difference between the two and three body kernel of the Lippmann Schwinger equation is that the two-body kernel is compact while the three body kernel cannot be compact. This is because it contains a delta functions in the relative momentum between particle 3 and particles 1 or 2.

If the kernel were compact the number of eigenstates of K with eigenvalues 1 is finite and each one is normalizable on the space where K is compact. This is because the problems of finding eigenvalues is reduced to finite matrix algebra in the compact case.

There are several ways to fix up the problem with the Lippmann Schwinger equation. If I supplement the original equation with the additional equations

$$|\psi\rangle = R_c(z) V^c |\psi\rangle \qquad c = (23)(1), (31)(2) \tag{311}$$

the solution becomes unique because the additional equations ensure that eigenstates that asymptotically look like bound (23) or (31) states are excluded.

The same type of problems occur in the Lippmann Schwinger equation for the transition operators. In that case kernels $V^b R_b(z)$ are not compact.

Faddeev was studying the completeness properties of the eigenstates of the three-body problem. In order to get better control of the solutions he generated a new set of coupled equations for the transition operators that have a compact kernel.

The equations that I present are derived in the same spirit as the original Faddeev equations, however they differ in structure.

I begin by considering the transition operators

$$T^{ab}(z) := V^b + V^a R(z) V^b \tag{312}$$

and I note that

$$V_a = \sum_{c \neq a} V_c \tag{313}$$

where the sum is only over two-cluster partitions, c. For simplicity I consider only two-body interactions. Using the decomposition of the interaction in (**??**) gives

$$T^{ab}(z) := V^b + \sum_{c \neq a} V_c R(z) V_b.$$

Next I use the resolvent identities

$$R(z) = R_c(z) + R_c(z) V^c R(z)$$

which gives

$$T^{ab}(z) = V^b + \sum_{c \neq a} V_c [R_c(z) + R_c(z) V^c R(z)] V^b$$

or

$$\boxed{T^{ab}(z) = V^b + \sum_{c \neq a} V_c R_c(z) T^{cb}(z).} \tag{314}$$

This is a coupled system of equation for the three amplitudes

$$T^{ab}(z) \tag{315}$$

for $a = (ij)(k)$. Note that the three-body breakup transition matrix element, $T^{0b}(Z)$, $0 = (1)(2)(3)$:

$$T^{0b} = V^b + V R(z) V^b = V^b + \sum_c V_c R_c(z) T^{cb}(z) \tag{316}$$

can be obtained directly from these solutions.

The kernel of this equation also contains a delta function so it it does not have a compact kernel. On the other hand if I iterate this equation once I get the equivalent equation

$$T^{ab}(z) = V^b + \sum_{c\neq a} V_c R_c(z) V^b + \sum_{c\neq a}\sum_{d\neq c} V_c R_c(z) V_d R_d(z) T^{db}(z) \tag{317}$$

the iterated kernel

$$\sum_{d\neq c} V_c R_c(z) V_d R_d(z) \tag{318}$$

contains no delta functions and can be shown to be compact for complex z. Faddeev found a space where the fifth iterate of a similar kernel is compact on a normed space that contains nice functions. In his case he has to use a special space to ensure that the singular integrals that appear in the equations are well-behaved. General elements of the Hilbert space do not have this property.

As a practical matter, onece the delta functions are eliminated from the kernel, the equation is usually well-behaved provided the interaction are short-ranged. Coulomb like force cannot be treated with these methods.

In order to understand what has been accomplished I consider an abstract form of these equations

$$T(z) = D + K(z)T(z) \tag{319}$$

which on n-iterations becomes

$$T(z) = D + K(z)D + K(z)^2 D + K(z)^3 D + \cdots + K(z)^n T(z). \tag{320}$$

This equation can be written as

$$(I - K^n(z))T(z) = \sum_{m=0}^{n-1} K^m(z) D. \tag{321}$$

If $K^n(z)$ is compact it can be expressed as a finite dimensional matrix $K_F(z)$ plus a small matrix $\Delta(z)$ where if $\Delta(z)$ has norm less than 1

$$\frac{1}{1-\Delta(z)} = I + \sum_{m=1}^{\infty} \Delta^m(z) \tag{322}$$

converges in norm, which leads to the pair of equations

$$T(z) = \sum_{m=0}^{n-1} X(z)K^m(z)D + X(z)K_F(z)T(z) \tag{323}$$

$$X(z) = 1 + \Delta(z)X(z) \tag{324}$$

The X equation has a uniformly convergent power series solution while the $T(z)$ equation is reduced to finite matrix algebra.

This shows that it is sufficient that a finite iterate of the kernel is compact. The system of equations () have a compact iterated kernel for short ranged interactions. This is what I mean by the Faddeev equations, although these are not the equations derived by Faddeev.

This is one of many equivalent forms of the three-body scattering equations. The driving term V^b has the nice property that when the scattering is initiated in the bound state of the interacting pair in partition b then $V^b|\phi_b\rangle$ is a localized function, which should improve numerical stability.

The actual solution of these equations is very complicated, especially when they are used with realistic interactions.

19 Partial Waves

Partial Waves

The Faddeev equations to three particles, after removing the overall momentum conserving delta functions are integral equation is two vector variables. Numerical treatments of the integral equation lead to very large systems of linear equations.

In order to reduce the complexity of the Faddeev equations it is useful to decompose them into uncoupled equations for different conserved angular momentum channels.

In each arrangement the expansion of the plane wave states in partial waves has the form:

$$|\vec{q}_i, \vec{k}_i\rangle =$$

$$\sum_{J,m,L,m_L,l,m_l} |q,k,L,l,J,m\rangle\langle J,m|L,m_L,l,m_l\rangle\langle L,m_L|\hat{q}\rangle\langle l,m_l|\hat{k}\rangle =$$

$$\sum_{J,m,L,m_L,l,m_l} |q,k,L,l,J,m\rangle\langle J,m|L,m_L,l,m_l\rangle Y^*_{L,m_L}(\hat{q})Y^*_{l,m_l}(\hat{k}) \tag{325}$$

In this separable s-wave model $l = 0$ and therefore $J = L$. I also note that J is conserved by rotational invariance. I have suppressed the particle label i in l and L.

Also, to keep the formulas simple I have assumed that the particles are spinless. The method that I outline can be easily extended to particles with spin.

The amplitudes of interest are

$$\langle q_a, k_a, L_a, l_a, J, m|T^{ab}(z)|q_b, k_b, L_b, l_b, J, m\rangle \tag{326}$$

Because of the sum over c with $c \neq a$ it is necessary to to evaluate matrix elements of the form:

$$\langle q_i, k_i, L_i, l_i, J, m|q_j, k_j, L_j, l_j, J, m\rangle. \tag{327}$$

for $i \neq j$.

There are a few properties that help with the evaluation. First, under rotations

$$U(R)|q, k, L, l, J, m\rangle = \sum_{m'} |q, k, L, l, J, m'\rangle D^J_{m'm}(R) \tag{328}$$

transforms like spin J irreducible representation of the rotation group. Inserting $U^\dagger(R)U(R)$ between the initial and final matrix elements and using the above gives

$$\langle q_i, k_i, L_i, l_i, J, n|q_j, k_j, L_j, l_j, J', m\rangle =$$

$$\sum_{n'm'} \langle q_i, k_i, L_i, l_i, J, n'|q_j, k_j, L_j, l_j, J', m'\rangle D^J_{n'n}(R) D^{J'*}_{m'm}(R). \tag{329}$$

Using the $SU(2)$ identity[**?**]

$$\int dR D^J_{n'n}(R) D^{J'*}_{m'm}(R) = \frac{1}{2J+1} \delta_{n'm'} \delta_{nm} \delta_{JJ'} \tag{330}$$

where dR is the $SU(2)$ Haar measure, I get

$$\langle q_i, k_i, L_i, l_i, J, n|q_j, k_j, L_j, l_j, J', m\rangle =$$

$$\frac{1}{2J+1} \sum_{n'} \langle q_i, k_i, L_i, l_i, J, n'|q_j, k_j, L_j, l_j, J, n'\rangle \delta_{JJ'} \delta_{mn} =$$

$$R^J[q_i, L_i, k_i, l_i, q_j, L_j, k_j, l_j]\delta_{JJ'}\delta_{mn}. \tag{331}$$

Thus, the permutation matrix elements are diagonal in J and m and are independent of m. Note, the Haar measure of a compact group is the unique measure that is (1) invariant with respect to the group and (2) integrates to 1.

This reduces the problem of computing the overlap matrix element to the problem of computing the rotationally invariant coefficients:

$$R^J[q_i, L_i, k_i, l_i, q_j, L_j, k_j, l_j] \tag{332}$$

These are normally done using complicated analytical methods. I give a simple method due to Balian and Brezin [**?**].

To compute this coefficient consider

$$R^J[q_i, L_i, k_i, l_i, q_j, L_j, k_j, l_j] =$$

$$\frac{1}{2J+1}\sum_m \langle q_i, k_i, L_i, l_i, J, m | q_j, k_j, L_j, l_j, J, m\rangle =$$

$$\frac{1}{2J+1}\sum_m \int \langle J, m | L_i, M_i, l_i, m_i\rangle \langle J, m | L_j, M_j, l_j, m_j\rangle \times$$

$$Y^*_{L_i,M_i}(\hat{q}_i) Y^*_{l_i,m_i}(\hat{k}_i) Y_{L_j,M_j}(\hat{q}_j) Y_{l_j,m_j}(\hat{k}_j) \times$$

$$\delta^3(\vec{q}_i - \vec{q}_i(\vec{k}_j, \vec{q}_j))\delta^3(\vec{k}_i - \vec{k}_i(\vec{k}_j, \vec{q}_j)) d\Omega(\hat{k}_i) d\Omega(\hat{k}_j) d\Omega(\hat{q}_i) d\Omega(\hat{q}_j). \tag{333}$$

There are 6 delta functions and 8 angular integrals. One delta function survives to give overall kinetic energy conservation. The sum over m makes the remaining quantity invariant under rotations. Three of the integrals paramarterize the rotational orientation of a coordinate system. This means that three of the integrals just contribute a volume factor. What remains are 5 non-trivial angle integrals and 5 delta functions. This means that all of the angular integrals can be done explicitly.

To do this note that the integral over $\hat{k}_i$ and $\hat{q}_i$ eliminates the angular parts of both delta functions. What remains is

$$\int \frac{\delta(k_i - G_k(k_j, q_j, \hat{k}_j \cdot \hat{q}_j))}{k_i^2} \frac{\delta(q_i - G_q(k_j, q_j, \hat{k}_j \cdot \hat{q}_j))}{q_i^2} d\Omega(\hat{k}_j) d\Omega(\hat{q}_j) \tag{334}$$

where

$$G_k = \sqrt{\frac{1}{4}k^2 + \frac{9}{16}q^2 \pm \frac{3}{4}qk\cos(\theta)} \tag{335}$$

$$G_q = \sqrt{k^2 + \frac{1}{4}q^2 \mp qk\cos(\theta)}. \tag{336}$$

For $k > 0$ I have

$$\delta(k - k') = 2k\delta(k^2 - k'^2). \tag{337}$$

Using this in the above gives

$$4\int \frac{\delta(k_i^2 - \frac{1}{4}k_j^2 - \frac{9}{16}q_j^2 \mp \frac{3}{4}q_j k_k \cos(\theta_j))}{k_i} \times$$

$$\frac{\delta(q_i^2 - k_j^2 - \frac{1}{4}q_j^2 \pm q_j k_j \cos(\theta_j))}{q_i} d\phi_{k_j} d(\cos(\theta_j)) d\Omega(\hat{q}_j). \tag{338}$$

The integral over $u = \cos(\theta_j)$ can be performed by the delta function using

$$\int \delta(a - bu)du = \frac{1}{b}\delta(u - a/b) \tag{339}$$

What remains is

$$4\int \frac{\delta(k_i^2 - \frac{1}{4}k_j^2 - \frac{9}{16}q_j^2 + \frac{3}{4}(q_i^2 - k_j^2 - \frac{1}{4}q_j^2)}{q_i q_j k_i k_j} d\phi_{k_j} d\Omega(\hat{q}_j) =$$

$$4\int \frac{\delta(k_i^2 + \frac{3}{4}q_i^2 - k_j^2 - \frac{3}{4}q_j^2)}{q_i q_j k_i k_j} d\phi_{k_j} d\Omega(\hat{q}_j) \tag{340}$$

Because of the m sum the remaining quantity is rotationally invariant. The last two integrals contribute $2\pi \times 4\pi = 8\pi^2$. This gives the final expression for the recoupling coefficient

$$R^J[q_i, L_i, k_i, l_i, q_j, L_j, k_j, l_j] =$$

$$\frac{32\pi^2}{2J+1} \frac{\delta(k_i^2 + \frac{3}{4}q_i^2 - k_j^2 - \frac{3}{4}q_j^2)}{q_i q_j k_i k_j} \times$$

$$\sum_n \langle J, n | L_i, M_i, l_i, m_i \rangle \langle J, n | L_j, M_j, l_j, m_j \rangle \times$$

$$Y^*_{L_i,M_i}(\hat{q}_i) Y^*_{l_i,m_i}(\hat{k}_i) Y_{L_j,M_j}(\hat{q}_j) Y_{l_j,m_j}(\hat{k}_j) \tag{341}$$

where the spherical harmonics can be evaluated in any kinematically consistent geometry, such as

$$q_j = (0, 0, q_j) \tag{342}$$

$$k_j = (k_j \sin(\theta), 0, k_j \cos(\theta)) \tag{343}$$

$$q_i = (\mp k_j \sin(\theta), 0, \mp k_j \cos(\theta) - \frac{1}{2} q_j) \tag{344}$$

$$k_i = (-\frac{1}{2} k_j \sin(\theta), 0, -\frac{1}{2} k_j \cos(\theta) \pm \frac{3}{4} q_j) \tag{345}$$

$$q_i = (\mp k_j \sin(\theta), 0, \mp k_j \cos(\theta) - \frac{1}{2} q_j). \tag{346}$$

In this case the angle θ can be extracted from

$$q_i^2 = k_j^2 + \frac{1}{4} q_j^2 \mp q_j k_j \cos(\theta) \tag{347}$$

or

$$\cos(\theta) = \mp \frac{4q_i^2 - 4k_j^2 - q_j^2}{4 q_j k_j}. \tag{348}$$

Thus I need to fix three kinematic scalars. Fourth is fixed by the energy conserving delta function.

I define a reduced recoupliing coefficient

$$\hat{R}^J[q_i, L_i, k_i, l_i, q_j, L_j, k_j, l_j] \tag{349}$$

by

$$R^J[q_i, L_i, k_i, l_i, q_j, L_j, k_j, l_j] =$$

$$\hat{R}^J[q_i, L_i, k_i, l_i, q_j, L_j, k_j, l_j] \frac{\delta(k_i^2 + \frac{3}{4} q_i^2 - k_j^2 - \frac{3}{4} q_j^2)}{q_i q_j k_i k_j}. \tag{350}$$

The partial wave equations are for the amplitudes

$$\langle k_a, l_a, q_a, L_a | T_J^{ab}(z) | k_b, l_b, q_b, L_b \rangle \tag{351}$$

where I have used rotational invariance to eliminate the magnetic quantum numbers.

The equations have the form

$$\langle k_a, l_a, q_a, L_a | T_J^{ab}(z) | k_b, l_b, q_b, L_b \rangle =$$

$$\langle k_a, l_a, q_a, L_a | V_J^b | k_b, l_b, q_b, L_b \rangle +$$

$$\sum_{c \neq a} \int \hat{R}^J[q_a, L_a, k_a, l_a; q_c', L_c', k_c', l_c'] \frac{\delta(k_a^2 + \frac{3}{4} q_a^2 - k_c'^2 - \frac{3}{4} q_c' 2)}{q_a q_c' k_a k_c'} \times$$

$$\frac{t^{l_c}(k'_c,k''_c,z-\frac{3}{4}q'^2_c)}{z-k''^2_c/m-3q'^2_c/4m}k'^2_c dk'_c k''^2_c dk''_c q'^2_c dq'_c\times$$
$$\langle k''_c,l_c,q'_c,L_c|T^{ab}_J(z)|k_b,l_b,q_b,L_b\rangle \tag{352}$$

I can eliminate the delta function, and assume that that pair in the partition is bound in a state ϕ_b. Thus, I replace k_b,l_b by ϕ_b and use

$$\int\frac{\delta(k_a^2+\frac{3}{4}q_a^2-k'^2_c-\frac{3}{4}q'^2_c)}{q_aq'_ck_ak'_c}k'^2_c dk'_c=\frac{1}{2q_aq_ck_a} \tag{353}$$

with the identification

$$k'^2_c=k_a^2+\frac{3}{4}q_a^2-\frac{3}{4}q'^2_c \tag{354}$$

These changes give the equations

$$\langle k_a,l_a,q_a,L_a|T^{ab}_J(z)|\phi_b,q_b,L_b\rangle=$$

$$\langle k_a,l_a,q_a,L_a|V^b_J|\phi_b,q_b,L_b\rangle+$$
$$\sum_{c\neq a}\int\hat{R}^J[q_a,L_a,k_a,l_a;q'_c,L'_c,k'_c,l'_c]\frac{k''^2_c dk''_c q'^2_c dq'_c}{2q_aq'_ck_a}\times$$
$$\frac{t^{l_c}(k'_c,k''_c,z-\frac{3}{4}q'^2_c)}{z-k''^2_c/m-3q'^2_c/4m}\langle k''_c,l_c,q'_c,L_c|T^{ab}_J(z)|\phi_b,q_b,L_b\rangle \tag{355}$$

where it is understood that $k'_c=k'_c(q'_c)$

To reduce this to a matrix equation I expand the solution in a complete set of functions of k_a and q_a:

$$\langle k_a,l_a,q_a,L_a|T^{ab}_J(z)|\phi_b,q_b,L_b\rangle=\sum_{m_an_a}\phi_{m_a}(k_a)\phi_{n_a}(q_a)\langle m_a,l_a,n_a,L_a|T^{ab}_J(z)|\phi_b,q_b,L_b\rangle \tag{356}$$

This leads to

$$\sum_{m_an_a}\phi_{m_a}(k_a)\phi_{n_a}(q_a)\langle m_a,l_a,n_a,L_a|T^{ab}_J(z)|\phi_b,q_b,L_b\rangle=$$

$$\langle k_a,l_a,q_a,L_a|V^b_J|\phi_b,q_b,L_b\rangle+$$
$$\sum_{c\neq a}\sum_{m_cn_c}\int\hat{R}^J[q_a,L_a,k_a,l_a;q'_c,L'_c,k'_c,l'_c]\frac{k''^2_c dk''_c q'^2_c dq'_c}{2q_aq'_ck_a}\times$$

$$\frac{t^{l_c}(k_c', k_c'', z - \frac{3}{4}q_c'^2)}{z - k_c''^2/m - 3q_c'^2/4m}\phi_{m_c}(k_c'')\phi_{n_c}(q_c')\langle m_c, l_c, n_a, L_a|T_J^{ab}(z)|\phi_b, q_b, L_b\rangle \quad (357)$$

Using orthogonality of the basis functions gives the following set of matrix equations

$$\langle m_a, l_a, n_a, L_a|T_J^{ab}(z)|\phi_b, q_b, L_b\rangle =$$

$$\langle m_a, l_a, n_a, L_a|V_J^b|\phi_b, q_b, L_b\rangle +$$

$$\sum_{c\neq a}\sum_{m_c n_c}\int \phi_{m_a}(k_a)\phi_{n_a}(q_a)k_a^2 dk_a q_a^2 dq_a \hat{R}^J[q_a, L_a, k_a, l_a; q_c', L_c', k_c', l_c']\frac{k_c''^2 dk_c'' q_c'^2 dq_c'}{2q_a q_c' k_a}\times$$

$$\frac{t^{l_c}(k_c', k_c'', z - \frac{3}{4}q_c'^2)}{z - k_c''^2/m - 3q_c'^2/4m}\phi_{m_c}(k_c'')\phi_{n_c}(q_c')\langle m_c, l_c, n_a, L_a|T_J^{ab}(z)|\phi_b, q_b, L_b\rangle \quad (358)$$

where

$$\langle m_a, l_a, n_a, L_a|V_J^b|\phi_b, q_b, L_b\rangle =$$

$$\int \phi_{m_a}(k_a)\phi_{n_a}(q_a)k_a^2 dk_a q_a^2 dq_a \langle k_a, l_a, q_a, L_a|V_J^b|\phi_b, q_b, L_b\rangle \quad (359)$$

and the kernel matrix is

$$K_{m_a n_a m_c n_c}(z) :=$$

$$\int \phi_{m_a}(k_a)\phi_{n_a}(q_a)k_a dk_a q_a dq_a \hat{R}^J[q_a, L_a, k_a, l_a; q_c', L_c', k_c', l_c']\frac{k_c''^2 dk_c'' q_c' dq_c'}{2}\times$$

$$\frac{t^{l_c}(k_c', k_c'', z - \frac{3}{4}q_c'^2)}{z - k_c''^2/m - 3q_c'^2/4m}\phi_{m_c}(k_c'')\phi_{n_c}(q_c') \quad (360)$$

These equations are two-variable integral equations. In addition, for each fixed J value there can be an infinite number of L and l values, so there is an additional infinite sent of indices that need to be truncated to a finite set. In these equations the matrices can get quite large. In addition, the integrals needed to compute the matrix elements are singular as in the two-body case. Unlike the two-body case, in the three-body problem the singularities move.

20 The Relation Between S and T

I begin with a discussion of multichannel scattering.

The first step is to define a scattering channel. The simplest channel is the one-particle channel corresponding an N-particle bound state. Simultaneous eigenstates of the Hamiltonian, linear momentum, spin, and magnetic quantum number are labeled as below

$$|\alpha\rangle := |\vec{p}, \nu\,(j, \alpha)\rangle$$

To describe a multi-particle channel let a be a partition of the N particle system into n_a disjoint subsystems. There is a scattering channel associated with the partition a if *each* of the n_a subsystems has a bound state. A channel corresponds to a possible state of the system long before or long after a scattering event has taken place. The particles in each subsystem remain bound, while the particles in different subsystems are mutually non-interacting.

The state corresponding to a multi-fragment channel is the tensor product of the subsystem bound states:

$$|\alpha_s\rangle := \otimes_{i=1}^{n_a} |\vec{p}_i, \nu_i(j_i, \alpha_i)\rangle.$$

The channel states are eigenstates of the partition Hamiltonian, H_a, obtained from the N-body Hamiltonian H by turning-off interactions between particles in different clusters of the partition a

There is a channel associated with each collection of bound states in a given partition. Some partitions may have no scattering channels.

Channels are used to define scattering states. Consider a state at time $t = 0$ of the form:

$$|\phi_\alpha\rangle := \int \sum \otimes_{i=1}^{n_a} |\vec{p}_i, \nu_i(j_i, \alpha_i)\rangle \prod_{i=1}^{n_a} \phi_i(\vec{p}_i, \nu_i) d^3 p_i,$$

where $t = 0$ is the approximate time of collision. These states span the channel subspace $\mathcal{H}_\alpha$. In the absence of interactions between different cluster of a, at an earlier time $-t$, this state had the form

$$|\phi_\alpha(-t)\rangle := e^{iH_a t} |\phi_\alpha\rangle.$$

A scattering state $|\psi_{-\alpha}(-t)\rangle$ is a state that evolves under the influence of the full Hamiltonian that looks like

$$|\phi_\alpha(-t)\rangle$$

for sufficiently large t. This condition can be expressed as

$$\lim_{t\to\infty} \| |\phi_\alpha(-t)\rangle - |\psi_{-\alpha}(-t)\rangle \| = 0.$$

Using the unitarity of the time evolution operator we have the equivalent form:

$$\lim_{t\to\infty} \| |\psi_{-\alpha}(0)\rangle - e^{-iHt} e^{iH_a t} |\phi_\alpha(0)\rangle \| = 0$$

It is also possible to find solutions of the many-body Schrödinger equation that look like a system of non-interacting subsystems in the asymptotic future

$$\lim_{t\to\infty} \| |\phi_\alpha(t)\rangle - |\psi_{+\alpha}(t)\rangle \| = 0$$

and the equivalent form:

$$\lim_{t\to\infty} \| |\psi_{+\alpha}(0)\rangle - e^{iHt} e^{-iH_a t} |\phi_\alpha(0)\rangle \| = 0.$$

These equations are the asymptotic conditions of scattering theory. They replace initial and final conditions.

Channel wave operators are defined by

$$\Omega_{\pm\alpha} := \lim_{t\to\pm\infty} e^{iHt} e^{-iH_a t} \Pi_\alpha \tag{361}$$

where Π_α is the projection on the channel subspace. The channel wave operators can be used to express the scattering states in terms of the channel states:

$$|\psi_{\pm\alpha}(0)\rangle := \Omega_{\pm\alpha} |\phi_\alpha(0)\rangle$$

The multichannel scattering operator is defined in terms of channel wave operators as:

$$S_{\beta\alpha} := \Omega^\dagger_{\beta+} \Omega_{\alpha-}. \tag{362}$$

The operator S is a mapping on the orthogonal direct sum of the channel subspaces,

$$\mathcal{H}_s = \oplus_{\alpha\in\mathcal{A}} \mathcal{H}_\alpha$$

In equation (**??**), α denotes a channel in which the particles in each cluster of the partition a are separately bound. H_a is the *partition Hamiltonian,* which is obtained from the original Hamiltonian by turning off the interactions between particles in *different* clusters of the partition a. The partition

Hamiltonian is also the sum of the subsystem Hamiltonians for each cluster in a:

$$H_a = \sum_{i=1}^{n_a} H_{a_i}. \tag{363}$$

There is a scattering channel α associated with the partition a if each of the H_{a_i} has a bound state. Let $|\alpha_i\, \vec{p}_i\rangle$ denote a bound state of H_{a_i} corresponding to the channel α with total momentum $\vec{p}_i$. Now define the channel projection operator:

$$\Pi_\alpha := \int \prod_{i=1}^{n_a} d^3p_i |\vec{p}_1\, \alpha_1 \cdots \vec{p}_{n_a}\, \alpha_{n_a}\rangle\langle \vec{p}_1\, \alpha_1 \cdots \vec{p}_{n_a}\, \alpha_{n_a}|. \tag{364}$$

Channel states $|\psi_\alpha\rangle$ are normalizable vectors satisfying:

$$|\psi_\alpha\rangle = \Pi_\alpha |\psi_\alpha\rangle. \tag{365}$$

Note that a given partition a may have none or many associated scattering channels α.

To construct formulas for scattering matrix elements, let α and β denote scattering channels associated with the asymptotic partition Hamiltonians H_a and H_b, respectively. Let $|\alpha\rangle$ and $|\beta\rangle$ denote sharp eigenstates of the partition Hamiltonians:

$$H_a|\alpha\rangle = E_\alpha|\alpha\rangle; \qquad H_b|\beta\rangle = E_\beta|\beta\rangle. \tag{366}$$

Using Eqs. (**??**,**??**) the S-matrix elements can be evaluated as follows:

$$\begin{aligned}
&\langle\beta|S_{ba}|\alpha\rangle = \\
&= \lim_{t\to\infty} \langle\beta|e^{iH_bt}e^{-2iHt}e^{iH_at}|\alpha\rangle \\
&= \langle\beta|\alpha\rangle + \lim_{t\to\infty} \int_0^t dt'\, \frac{d}{dt'} \langle\beta|e^{i(E_\beta+E_\alpha-2H)t'}|\alpha\rangle \\
&= \langle\beta|\alpha\rangle + \lim_{\epsilon\to 0^+} i\int_0^\infty dt'\, \langle\beta| \Big[(E_\beta - H)e^{i(E_\beta+E_\alpha-2H+i\epsilon)t'} \\
&\qquad + e^{i(E_\beta+E_\alpha-2H+i\epsilon)t'}(E_\alpha - H)\Big] |\alpha\rangle
\end{aligned}$$

$$= \langle\beta|\alpha\rangle + \lim_{\epsilon\to 0^+} \frac{1}{2}\langle\beta| \left[(H-E_\beta)\frac{1}{\bar{E}-H+i\epsilon} + \frac{1}{\bar{E}-H+i\epsilon}(H-E_\alpha)\right]|\alpha\rangle, \tag{367}$$

where $\bar{E} := \frac{1}{2}(E_\alpha + E_\beta)$ is the average energy of the initial and final asymptotic states. Equation (**??**) is interpreted as the kernel of an integral operator. S-matrix elements are obtained by integrating the sharp eigenstates in Eq. (**??**) over normalizable functions of the energy and any other continuous variables. To simplify this expression, we introduce a more compact notation. The residual interactions V^a and V^b are defined as follows:

$$V^a := H - H_a; \qquad V^b = H - H_b, \tag{368}$$

where

$$V^a|\alpha\rangle = (H-E_\alpha)|\alpha\rangle; \qquad V^b|\beta\rangle = (H-E_\beta)|\beta\rangle. \tag{369}$$

The resolvent operators of the Hamiltonian and the partition Hamiltonian are:

$$R(z) := \frac{1}{z-H} \qquad R_a(z) := \frac{1}{z-H_a}. \tag{370}$$

These operators satisfy the second resolvent relations (Hi 57):

$$R(z) - R_a(z) = R_a(z)V^aR(z) = R(z)V^aR_a(z). \tag{371}$$

Using these identities in Eq. (**??**) gives

$$\begin{aligned}
&\langle\beta|S|\alpha\rangle \\
&= \langle\beta|\alpha\rangle + \lim_{\epsilon\to 0^+}\frac{1}{2}\langle\beta|\left[V^b\left(1+R(\bar{E}+i\epsilon)V^a\right)R_a(\bar{E}+i\epsilon)\right. \\
&\qquad \left. + R_b(\bar{E}+i\epsilon)\left(1+V^bR(\bar{E}+i\epsilon)\right)V^a\right]|\alpha\rangle \\
&= \langle\beta|\alpha\rangle\left[1 - \lim_{\epsilon\to 0^+}\frac{E_\beta-E_\alpha}{E_\beta-E_\alpha+2i\epsilon}\right] \\
&+ \lim_{\epsilon\to 0^+}\left[\frac{1}{E_\beta-E_\alpha+2i\epsilon} + \frac{1}{E_\alpha-E_\beta+2i\epsilon}\right]\langle\beta|\left(V^a+V^bR(\bar{E}+i\epsilon)V^a\right)|\alpha\rangle \\
&= \langle\beta|\alpha\rangle\lim_{\epsilon\to 0^+}\left[\frac{2i\epsilon}{E_\beta-E_\alpha+2i\epsilon}\right] \\
&+ \lim_{\epsilon\to 0^+}\left[\frac{-4i\epsilon}{(E_\beta-E_\alpha)^2+4\epsilon^2}\right]\langle\beta|\left(V^a+V^bR(\bar{E}+i\epsilon)V^a\right)|\alpha\rangle.
\end{aligned} \tag{372}$$

It is now possible to evaluate the limit as $\epsilon \to 0$. It is important to remember that this is the kernel of an integral operator.

The first term in square brackets is unity when the initial and final energies are identical, and zero otherwise; however, the limit in the bracket is a Kronecker delta and *not* a Dirac delta function. For $a \neq b$, we expect that $\langle\beta(E')|\alpha(E)\rangle$ will be Lebesgue measurable in E' for fixed E, so there is no contribution from the first term in Eq. (**??**). For the case that $H_b = H_a$, we have $\langle\beta(E')|\alpha(E)\rangle \propto \delta(E' - E)$. The matrix elements vanish by orthogonality unless $E_\beta = E_\alpha$, but then coefficient is unity. Thus, the first term is $\langle\beta|\alpha\rangle$ if the initial and final channel are the same, but zero otherwise. Note that the matrix elements vanish by orthogonality for two different channels governed by the same asymptotic Hamiltonian with the same energy. The first term in (**??**) is therefore a *channel* delta function.

For the second term, the quantity in square brackets becomes $-2\pi i\delta(E_\beta - E_\alpha)$, which leads to the relation

$$\langle\beta|S|\alpha\rangle = \langle a|b\rangle\delta_{\beta\alpha} - 2\pi i\delta(E_\beta - E_\alpha)\langle\beta|T^{ba}(E_a + i0^+)|\alpha\rangle, \tag{373}$$

where

$$T^{ba}(z) = V^a + V^b R(z) V^a. \tag{374}$$

The operator $T^{ab}(z)$ is the channel transition operator and equation (**??**) gives its explicit relation to the S matrix. This is the general expression for the transition operator in a multichannel scattering theory. It applies both to relativistic and to nonrelativistic applications. The multichannel transition operator $T^{ab}(z)$ must be constructed in a dynamical model.

In models where the residual interactions and the resolvent commute with the total linear momentum operator, and if the sharp channel states $|\alpha\rangle$ and $|\beta\rangle$ are simultaneous eigenstates of the appropriate partition Hamiltonian and the linear momentum, then a three-momentum conserving delta function can be factored out of the T-matrix element:

$$\langle\beta|T^{ba}(E_a + i0^+)|\alpha\rangle = (2\pi)^3\delta^3(p_\beta - p_\alpha)\langle\beta|T^{ba}(E_a + i0^+)|\alpha\rangle. \tag{375}$$

If this is used in Eq.(**??**), then the S-matrix elements can be expressed in terms of the *reduced channel transition operators* as follows:

$$\langle\beta|S|\alpha\rangle = \langle a|b\rangle\delta_{\beta\alpha} - i(2\pi)^4\delta^4(p_\beta - p_\alpha)\langle\beta|T^{ba}(E_a + i0^+)|\alpha\rangle \tag{376}$$

This expression has the advantage that the delta function is manifestly invariant under Poincaré transformations. The factor $(2\pi)^3$ is included by convention.

21 Cross Sections

We now discuss the relation between the scattering matrix elements and scattering cross sections The content of this section follows the classic references of Möller (Mo 45) and Brenig and Haag (Br 59).

Plane-wave states will be used with the normalization

$$\langle \mathbf{p}'|\mathbf{p}\rangle = \delta(\mathbf{p}' - \mathbf{p}). \tag{377}$$

which is simply a convention. With this choice, the square of the magnitude of the wave functions, $|\langle \mathbf{p}|\phi\rangle|^2$, will have the interpretation of probability per unit volume in momentum space. The Fourier transforms $|\langle \mathbf{r}|\phi\rangle|^2$ then have the interpretation of probability per unit volume.

Consider a reaction initiated by the collision of a projectile and target cluster. Assume that the target and projectile are described by normalizable wave functions with very sharp momentum distributions centered about $\bar{\mathbf{p}}_t$ and $\bar{\mathbf{p}}_p$, respectively. With this choice of normalization, the probability density that the system prepared with this initial state will be found in a state of N particles with momenta centered about $\mathbf{p}_1 \cdots \mathbf{p}_N$ is given by

$$|\langle \mathbf{p}_1 \cdots \mathbf{p}_N|\phi_n\rangle|^2, \tag{378}$$

where

$$\langle \mathbf{p}_1 \cdots \mathbf{p}_N|\phi_n\rangle := \int d^3p_t \int d^3p_p \, \langle \mathbf{p}_1 \cdots \mathbf{p}_N|S|\mathbf{p}_t\mathbf{p}_p\rangle\langle \mathbf{p}_t|\phi_t\rangle\langle \mathbf{p}_p|\phi_p\rangle. \tag{379}$$

If there are any identical particles in the final state, Eq. (**??**) must be multiplied by the square root of the statistical factor:

$$\frac{1}{s} = \prod_{i=1}^{k} \frac{1}{n_i!}, \tag{380}$$

where there is a factor $1/n_i!$ for each group of n_i identical particles in the final state. Note that for n identical particles, the resolution of the identity is

$$I = \frac{1}{n!} \int d^3p_1 \cdots \int d^3p_n |\mathbf{p}_1 \cdots \mathbf{p}_n\rangle\langle \mathbf{p}_1 \cdots \mathbf{p}_n|, \tag{381}$$

if the single particle states are normalized as in Eq. (**??**). In what follows, a factor of $1/s$ will be included.

This expression can be simplified by using the property that *the initial wave packets are sharply peaked, and the assumption that the transition matrix elements are smooth functions of the momenta*. If the scattering is *not* elastic or, in the case of elastic scattering, the detector is *not* along the beam line, then the scattering operator can be replaced by the transition operator term alone:

$$\begin{aligned}
&\langle \mathbf{p}_1 \cdots \mathbf{p}_N | \phi_n \rangle \\
&= -2\pi i \delta(E_N - E_i) \int d^3p_t \int d^3p_p \, \langle \mathbf{p}_1 \cdots \mathbf{p}_N | T^{ba} \left(f(E_i) + i0^+ \right) | \mathbf{p}_t \mathbf{p}_p \rangle \langle \mathbf{p}_t \mathbf{p}_p | \phi \rangle \\
&\approx -(2\pi)^4 i \langle \mathbf{p}_1 \cdots \mathbf{p}_N | T^{ba} \left(E_i + i0^+ \right) | \bar{\mathbf{p}}_t \bar{\mathbf{p}}_p \rangle \\
&\times \int d^3p_t \int d^3p_p \, \langle \mathbf{p}_t \mathbf{p}_p | \phi \rangle \delta(E_N - E_i) \delta(\mathbf{P}_N - \mathbf{P}_t - \mathbf{p}_i). \qquad (382)
\end{aligned}$$

Using Eq. (**??**) in (**??**) , we get

$$\begin{aligned}
&|\langle \mathbf{p}_1 \cdots \mathbf{p}_N | \phi_n \rangle|^2 \\
&= \frac{4\pi^2}{s} \left| \langle \mathbf{p}_1 \cdots \mathbf{p}_N \| T^{ba} \left(E_i + i0^+ \right) | \bar{\mathbf{p}}_t \bar{\mathbf{p}}_p \rangle \right|^2 \\
&\times \int d^3p'_t \int d^3p'_p \int d^3p_t \int d^3p_p \, \langle \mathbf{p}'_t | \phi_t \rangle^* \langle \mathbf{p}'_p | \phi_p \rangle^* \langle \mathbf{p}_t | \phi_t \rangle \langle \mathbf{p}_p | \phi_p \rangle \\
&\times \delta(E_N - E'_t - E'_p) \delta(\mathbf{P}_N - \mathbf{p}'_t - \mathbf{p}'_p) \delta(E_N - E_t - E_p) \delta(\mathbf{P}_N - \mathbf{p}_t - \mathbf{p}_p). \qquad (383)
\end{aligned}$$

The integral can be expressed in terms of position-space wave functions as follows:

$$\begin{aligned}
&\int d^3p'_t \int d^3p'_p \int d^3p_t \int d^3p_p \, \langle \mathbf{p}_t | \phi_p \rangle \langle \mathbf{p}_p | \phi_p \rangle \langle \mathbf{p}'_t | \phi_p \rangle^* \langle \mathbf{p}'_p | \phi_p \rangle^* \\
&\times \delta(E_N - E_t - E_p) \delta(\mathbf{P}_N - \mathbf{p}_t - \mathbf{p}_p) \delta(E_t + E_p - E'_t - E'_p) \delta(\mathbf{p}_t + \mathbf{p}_p - \mathbf{p}'_t - \mathbf{p}'_p) \\
&= (2\pi)^{-4} \int d^3r \int dt \, e^{i(\mathbf{p}_t + \mathbf{p}_p - \mathbf{p}'_t - \mathbf{p}'_p) \cdot \mathbf{r} - i(E_t + E_p - E'_t - E'_p)t} \\
&\times \int d^3p'_t \int d^3p'_p \int d^3p_t \int d^3p_p \, \langle \mathbf{p}_t | \phi_p \rangle \langle \mathbf{p}_p | \phi_p \rangle \langle \mathbf{p}'_t | \phi_p \rangle^* \langle \mathbf{p}'_p | \phi_p \rangle^* \\
&= \delta(E_N - \bar{E}_t - \bar{E}_p) \delta(\mathbf{P}_N - \bar{\mathbf{p}}_t - \bar{\vec{p}}_p) (2\pi)^2 \int d^3r \int dt \, |\langle (\mathbf{r}, t) | \phi_t \rangle \langle (\mathbf{r}, t) | \phi_p \rangle|^2 . \qquad (384)
\end{aligned}$$

This leads to the following expression for the differential probability:

$$dW = \langle \mathbf{p}_1 \cdots \mathbf{p}_N | \phi_n \rangle =$$
$$\frac{(2\pi)^4}{s} \left| \langle \mathbf{p}_1 \cdots \mathbf{p}_N | T^{ba} \left(E_i + i0^+ \right) | \bar{\mathbf{p}}_t \bar{\mathbf{p}}_p \rangle \right|^2$$
$$\times \int d^3r \int dt \, |\langle \mathbf{r}, t | \phi_t \rangle \langle \mathbf{r}, t | \phi_p \rangle|^2 \, \delta(E_N - \bar{E}_t - \bar{E}_p) \delta(\mathbf{P}_N - \bar{\vec{p}}_t - \bar{\vec{p}}_p) \prod_{i=1}^{N} d^3 p_i. \tag{385}$$

This expression is a distribution over all energies and momenta, and is integrated over all space and time. The distribution with respect to total energy and momenta (which are conserved) can be integrated out. To do this, we introduce the phase space element $d\Phi_N$ as follows:

$$\prod_{i=1}^{N} d^3 p_i = dE_n d^3 P_N d\Phi_N. \tag{386}$$

Since

$$1 = \int dE_n d^3 P \delta^4 (P - P(\mathbf{p}_1 \cdots \mathbf{p}_N)), \tag{387}$$

it is possible to write

$$d\Phi_N = \int \prod_{i=1}^{N} d^3 p_i \delta^4 (P(\bar{\vec{p}}_t \bar{\vec{p}}_p) - P(\mathbf{p}_1 \cdots \mathbf{p}_N)), \tag{388}$$

where the integral is over any four variables that eliminate the delta functions. The remaining quantities are independent measurable quantities. After integrating out the total energy and momentum, the integrand with respect to space and time represents the probability per unit time and volume that a particle will be detected in the phase space element $d\Phi_N$, independent of the specific energy-momentum distribution of the initial state. This quantity will be denoted by dw, and has been shown to be

$$dw = \frac{(2\pi)^4}{s} \left| \langle \mathbf{p}_1 \cdots \mathbf{p}_N | T^{ba} \left(E_i + i0^+ \right) | \bar{\vec{p}}_t \bar{\mathbf{p}}_p \rangle \right|^2 |\langle (\mathbf{r}, t) | \phi_t \rangle \langle (\mathbf{r}, t) | \phi_p \rangle|^2 \, d\Phi_N. \tag{389}$$

The differential cross section is the ratio of the transition rate per unit volume to the product of the incident probability current and the target density:

$$d\sigma := \frac{dw}{v_{p-t} |\langle (\mathbf{r}, t) | \phi_t \rangle \langle (\mathbf{r}, t) | \phi_p \rangle|^2} d\Phi_N$$

$$= \frac{(2\pi)^4}{s v_{p-t}} |\langle \mathbf{p}_1 \cdots \mathbf{p}_N | T^{ba} \left(E_i + i0^+ \right) | \bar{\mathbf{p}}_t \bar{\mathbf{p}}_p \rangle|^2 d\Phi_N. \tag{390}$$

This expression is valid both relativistically and nonrelativistically. In the relativistic case, $d\sigma$ is also relativistically invariant (Mo 45). To show this, we redistribute the momentum dependent factors so that the phase space factors, the transition matrix elements, and the velocity factors are separately invariant. The first step is to change the single particle plane wave normalization to a covariant normalization:

$$|\mathbf{p}_i\rangle \to |\mathbf{p}_i\rangle_{\rm cov} := K_{p_i} |\mathbf{p}_i\rangle. \tag{391}$$

Covariance requires that

$$\mathcal{K}_{p_i} = C \times \sqrt{\omega_{m_i}(\mathbf{p}_i^2)}; \qquad \omega_{m_i}(\mathbf{p}_i^2) := \sqrt{m_i^2 + \mathbf{p}_i^2} \tag{392}$$

The constant C is arbitrary. We now define an invariant reduced transition matrix element:

$$\begin{aligned} &\langle \mathbf{p}_1 \cdots \mathbf{p}_n | M^{ab} | \mathbf{p}_t \mathbf{p}_p \rangle \\ &:= {\rm cov}\langle \mathbf{p}_1 \cdots \mathbf{p}_N | T^{ba} \left(E_i + i0^+ \right) | \bar{\mathbf{p}}_t \bar{\mathbf{p}}_p \rangle_{\rm cov} \\ &:= \langle \mathbf{p}_1 \cdots \mathbf{p}_N | T^{ba} \left(f E_i + i0^+ \right) | \bar{\mathbf{p}}_t \bar{\mathbf{p}}_p \rangle (K_t K_p \prod_{i=1}^N K_{p_i}). \end{aligned} \tag{393}$$

This entire quantity is invariant (ignoring spins) because S is invariant, the basis in which S is evaluated is covariant, and the reduced transition operator is obtained from S by factoring out a four-momentum conserving delta function. This definition introduces the factor $(K_t K_p \prod_{i=1}^N K_{p_i})^2$ into the expression for the cross section. The factors associated with the final state can be included in the phase space factor

$$dL_N := \frac{d\Phi_N}{\prod_{i=1}^N K_{pi}^2} = \prod_{i=1}^N \frac{d^3 p_i}{\mathcal{K}_{pi}^2} \delta^4(P - P(\mathbf{p}_1 \cdots \mathbf{p}_N)), \tag{394}$$

which is invariant. What remains is the factor $(v_{p-t} \mathcal{K}_t^2 \mathcal{K}_p^2)^{-1}$. Direct evaluation shows that (Mo 45)

$$v_{p-t} \omega_{m_t}(\mathbf{p}_t^2) \omega_{m_p}(\mathbf{p}_p^2) = v_{p-t} \frac{\mathcal{K}_t^2}{C^2} \frac{\mathcal{K}_p^2}{C^2} = \sqrt{(p_t \cdot p_p)^2 - m_t^2 m_p^2}. \tag{395}$$

Thus, $(v_{p-t}\mathcal{K}_t^2\mathcal{K}_p^2)^{-1}$ is invariant, and we denote it by C^4F, where C is defined in Eq. **??**eq:bu), and F is invariant. The differential cross section can now be expressed as follows:

$$d\sigma := \frac{(2\pi)^4}{s}\frac{1}{C^4}\frac{|\langle \mathbf{p}_1 \cdots \mathbf{p}_n|M^{ab}|\mathbf{p}_t\mathbf{p}_p\rangle|^2}{F}dL_N. \tag{396}$$

I have not yet considered spin degrees of freedom. The suppressed spin variables lead to the modification

$$d\sigma \to \frac{(2\pi)^4}{s}\frac{1}{C^4}\frac{|\langle \mathbf{p}_1,\mu_1 \cdots \mathbf{p}_n,\mu_n|M^{ab}|\mathbf{p}_t,\nu_t,\mathbf{p}_p,\nu_p\rangle|^2}{F}dL_N. \tag{397}$$

In general, the magnetic quantum numbers can be associated with any type of spin. In applications, any type of spin can be used. However, when one finally compares a calculation to experiment, one has to know how the given spin is coupled to the device that separates different spin states. For electron scattering, one measures invariant form factors, which can be used to extract current matrix elements with different types of spins. The relation of the current matrix element to the form factor will be different for each type of spin.

The initial and final states are prepared from measured ensembles, which are properly described by a density matrix in the spin degrees of freedom. For the initial state, the target and projectile are described by the density matrices $\rho_t(\nu_t\nu_t')$ and $\rho_b(\nu_b\nu_b')$, which are positive Hermitian matrices with unit trace. The differential cross section becomes an unnormalized density matrix in the final spins:

$$\begin{aligned} d\rho_f := \frac{(2\pi)^4}{s}\frac{1}{C^4F}&\langle \mathbf{p}_1\mu_1' \cdots \mathbf{p}_n\mu_n'|M^{ab}|\mathbf{p}_t\nu_t'\mathbf{p}_p\nu_p'\rangle\rho_t(\nu_t'\nu_t) \\ &\times\rho_p(\nu_p'\nu_p)\langle \mathbf{p}_t\nu_t\mathbf{p}_p\nu_p|M^{ab\dagger}|\mathbf{p}_1\mu_1 \cdots \mathbf{p}_n\mu_n\rangle dL_N. \end{aligned} \tag{398}$$

The expectation value of a spin observable $\mathcal{O}$ in this ensemble is computed by taking the trace with respect to the renormalized density matrix:

$$\langle\mathcal{O}\rangle := \frac{\mathrm{Tr}(\mathcal{O}d\rho_f)}{\mathrm{Tr}(d\rho_f)}, \tag{399}$$

where the trace is over the spins. The kinematic factors cancel in the computation of the renormalized density matrix. In general there are $(2s+1)^2-1$ independent spin observables for a spin s final state. The total cross section is the other one, corresponding to the trace of the identity.