The S-Matrix[1]

D. E. Soper[2]
University of Oregon

Physics 634, Advanced Quantum Mechanics

November 2000

1 Notation for states

In these notes we discuss scattering nonrelativistic quantum mechanics. We will use states with the nonrelativistic normalization

$$\langle\vec{p}|\vec{k}\rangle = (2\pi)^3\delta(\vec{p}-\vec{k}). \tag{1}$$

Recall that in a relativistic theory there is an extra factor of $2E$ on the right hand side of this relation, where $E = [\vec{k}^2 + m^2]^{1/2}$.

We will use states in the "Heisenberg picture," in which states $|\psi(t)\rangle$ do not depend on time. Often in quantum mechanics one uses the Schrödinger picture, with time dependent states $|\psi(t)\rangle_S$. The relation between these is

$$|\psi(t)\rangle_S = e^{-iHt}\,|\psi\rangle. \tag{2}$$

Thus these are the same at time zero, and the Schrdinger states obey

$$i\frac{d}{dt}\,|\psi(t)\rangle_S = H\,|\psi(t)\rangle_S \tag{3}$$

In the Heisenberg picture, the states do not depend on time but the operators do depend on time. A Heisenberg operator $\mathcal{O}(t)$ is related to the corresponding Schrödinger operator $\mathcal{O}_S$ by

$$\mathcal{O}(t) = e^{iHt}\,\mathcal{O}_S\,e^{-iHt} \tag{4}$$

Thus

$$\langle\psi|\mathcal{O}(t)|\psi\rangle = {}_S\langle\psi(t)|\mathcal{O}_S|\psi(t)\rangle_S. \tag{5}$$

The Heisenberg picture is favored over the Schrödinger picture in the case of relativistic quantum mechanics: we don't have to say which reference

[2] soper@bovine.uoregon.edu

frame we use to define t in $|\psi(t)\rangle_S$. For operators, we can deal with local operators like, for instance, the electric field $F^{\mu\nu}(\vec{x},t)$. The $\{\vec{x},t\}$ dependence is given by a covariant relation

$$F^{\mu\nu}(\vec{x},t) = e^{iP^\mu x_\mu} F^{\mu\nu}(\vec{0},0) e^{-iP^\mu x_\mu}. \tag{6}$$

where $P^0 = H$ and $x^0 = t$. We use the Heisenberg picture here even though we discuss nonrelativistic quantum mechanics.

2 In and out states

We deal here with the simplest version of scattering theory. We imagine that there is a free particle hamiltonian H_0 that consists of the kinetic energy operators for all of the particles in the theory but does not contain any terms that cause the particles to interact. The full hamiltonian is

$$H = H_0 + V \tag{7}$$

where V contains interactions among the particles. For example, in a nonrelativistic description of two particles we might have

$$\langle \vec{x}_1, \vec{x}_2 | H_0 | \psi \rangle = \left(-\frac{1}{2m_1} \vec{\nabla}_1^2 - \frac{1}{2m_2} \vec{\nabla}_2^2 \right) \langle \vec{x}_1, \vec{x}_2 | \psi \rangle \tag{8}$$

and

$$\langle \vec{x}_1, \vec{x}_2 | V | \psi \rangle = \mathcal{V}(|\vec{x}_1 - \vec{x}_2|) \langle \vec{x}_1, \vec{x}_2 | \psi \rangle \tag{9}$$

for some potential function $\mathcal{V}$. We consider potential functions with the property that $\mathcal{V}(|\vec{x}_1 - \vec{x}_2|) \to 0$ as $|\vec{x}_1 - \vec{x}_2| \to \infty$.

In scattering theory, we consider shooting particles at each other and then seeing what happens. With the kind of nonrelativistic theory just mentioned, what can happen is that the particles emerging with different momenta in a fashion consistent with conservation of the total energy and momentum. The main idea is that when the particles scatter, after awhile they are far apart and V doesn't act anymore. In addition, before they scatter they are also are far apart and V doesn't do anything.

Consider a state $|\psi_F\rangle_f$ whose corresponding Schrödinger wave function $\psi_F(\vec{x}_1, \vec{x}_2)$ consists of approximately plane waves in "wave packets". If we were using the *free* theory, this state would consist of two particles that propagate freely into the far future, with their wave packets separating from each other. But we are using interacting theory rather than the free theory. We let $|\psi_F\rangle_{\rm out}$ denote the state in the full theory that, in the far future, looks like $|\psi_F\rangle_f$ would look if we used the free hamiltonian. That is

$$e^{-iHt}\,|\psi_F\rangle_{\rm out} \approx e^{-iH_0 t}\,|\psi_F\rangle_f \tag{10}$$

for very large positive t. The wave function for the out state is not at all simple. But based on this physical argument, we may hope to construct the out state as a limit:

$$|\psi_F\rangle_{\rm out} = \lim_{t\to\infty} e^{iHt}\,e^{-iH_0 t}\,|\psi_F\rangle_f \tag{11}$$

Consider a different state $|\psi_I\rangle_f$ whose corresponding Schrödinger wave function $\psi_I(\vec{x}_1, \vec{x}_2)$ also consists of approximately plane waves in "wave packets". This state represents a description of the wave packets for the particles entering the collision. We let $|\psi_I\rangle_{\rm in}$ denote the state in the full theory that, in the far past, looks like $|\psi_I\rangle_f$ would look if we used the free hamiltonian. That is

$$e^{-iHt}\,|\psi_I\rangle_{\rm in} \approx e^{-iH_0 t}\,|\psi_I\rangle_f \tag{12}$$

for very large negative t. Based on this physical argument, we may hope to construct the in state as a limit:

$$|\psi_I\rangle_{\rm in} = \lim_{t\to-\infty} e^{iHt}\,e^{-iH_0 t}\,|\psi_I\rangle_f \tag{13}$$

The S-matrix is defined to be the amplitude that a state that looks like $|\psi_I\rangle_f$ in the far past will look like $|\psi_F\rangle_f$ in the far future. That is

$$S_{FI} = {}_{\rm out}\langle\psi_F|\psi_I\rangle_{\rm in}. \tag{14}$$

3 Analysis of the S-matrix

With our definition, we have

$$S_{FI} = {}_{\rm out}\langle\psi_F|\psi_I\rangle_{\rm in} = \lim_{\substack{T_F\to+\infty \\ T_I\to-\infty}} \langle\psi_F|U(T_F,T_I)|\psi_I\rangle \tag{15}$$

where

$$U(T_F,T_I) = e^{iH_0 T_F}\,e^{-iH(T_F-T_I)}\,e^{-iH_0 T_I}. \tag{16}$$

We can write this in a better form by writing a differential equation for U:

$$
\begin{aligned}
i\frac{d}{dt}U(t,T_I) &= e^{iH_0 t}\,(H-H_0)\,e^{-iH(t-T_I)}\,e^{-iH_0 T_I} \\
&= e^{iH_0 t}\,V\,e^{-iH_0 t}\,e^{iH_0 t}\,e^{-iH(t-T_I)}\,e^{-iH_0 T_I} \\
&= V(t)\,U(t,T_I),
\end{aligned}
\tag{17}
$$

where

$$
V(t) \equiv e^{iH_0 t}\,V\,e^{-iH_0 t}. \tag{18}
$$

The solution of this is

$$
U(t,T_I) = T\,\exp\left(-i\int_{T_I}^{t} d\tau\,V(\tau)\right). \tag{19}
$$

Here the T is a time ordering instruction that tells us what order the non-commuting operators $V(\tau)$ belong in. We should expand the exponential and then put the $V(\tau)$ operators with the later values of the time argument to the left. That is

$$
\begin{aligned}
T\,\exp\left(-i\int_{T_I}^{t} d\tau\,V(\tau)\right) &= 1 - i\int_{T_I}^{t} d\tau\,V(\tau) \\
&\quad -\frac{1}{2}\,T\int_{T_I}^{t} d\tau_2\,\int_{T_I}^{t} d\tau_1\,V(\tau_2)\,V(\tau_1) \\
&\quad +\frac{i}{3!}\,T\int_{T_I}^{t} d\tau_3\,\int_{T_I}^{t} d\tau_2\,\int_{T_I}^{t} d\tau_1\,V(\tau_3)\,V(\tau_2)\,V(\tau_1) \\
&\quad +\cdots \\
&= 1 - i\int_{T_I}^{t} d\tau\,V(\tau) \\
&\quad -\int_{T_I}^{t} d\tau_2\,\int_{T_I}^{\tau_2} d\tau_1\,V(\tau_2)\,V(\tau_1) \\
&\quad +i\int_{T_I}^{t} d\tau_3\,\int_{T_I}^{\tau_3} d\tau_2\,\int_{T_I}^{\tau_2} d\tau_1\,V(\tau_3)\,V(\tau_2)\,V(\tau_1) \\
&\quad +\cdots.
\end{aligned}
\tag{20}
$$

Exercise. Show that this series actually solves the operator differential equation for $U(t,T_I)$.

Thus the operator appearing in the S-matrix is

$$U(T_F, T_I) = T\ \exp\left(-i\int_{T_I}^{T_F} d\tau\, V(\tau)\right). \tag{21}$$

4 Perturbative expansion for the S-matrix

We started by thinking of $|\psi_F\rangle$ as a product wave-packet states for the two particles, so that we could be sure that after a long time the wave functions for the two final state particles would not overlap in space. That way, the potential energy operator V could be neglected in the far future. Similarly, we wanted wave-packet states for $|\psi_I\rangle$. Now, however, let's let the momentum spread of the wave functions approach zero, so that we have momentum eigenstates. That will make calculation feasible.

Assuming that we are dealing with plane wave states, the states $|\psi_I\rangle$ and $|\psi_F\rangle$ are eigenstates of H_0, with eigenvalues E_I and E_F respectively. With this assumption, let's expand the S-matrix in powers of V:

$$S_{FI} = \sum_{n=0}^{\infty} S_{FI}^{(n)}. \tag{22}$$

We have

$$S_{FI}^{(0)} = \langle\psi_F|\psi_I\rangle. \tag{23}$$

This is the no-scattering term. The Born approximation is

$$\begin{aligned} S_{FI}^{(1)} &= -i\int_{-\infty}^{\infty} d\tau\, \langle\psi_F|e^{iH_0\tau}\, V\, e^{-iH_0\tau}|\psi_I\rangle \\ &= -i\int_{-\infty}^{\infty} d\tau\, e^{i(E_F-E_I)\tau}\, \langle\psi_F|V|\psi_I\rangle \\ &= -i\, 2\pi\, \delta(E_F - E_I)\, \langle\psi_F|V|\psi_I\rangle. \end{aligned} \tag{24}$$

That's pretty simple. We just need to calculate the matrix element of V in plane wave states.

The order V^2 approximation is

$$\begin{aligned} S_{FI}^{(2)} &= -\int_{-\infty}^{\infty} d\tau_2 \int_{-\infty}^{\tau_2} d\tau_1\, \langle\psi_F|e^{iH_0\tau_2}\, V\, e^{-iH_0(\tau_2-\tau_1)}\, V\, e^{-iH_0\tau_1}|\psi_I\rangle \\ &= -\int_{-\infty}^{\infty} d\tau_1 \int_{0}^{\infty} d\tau\, \langle\psi_F|e^{iH_0(\tau+\tau_1)}\, V\, e^{-iH_0\tau}\, V\, e^{-iH_0\tau_1}|\psi_I\rangle \end{aligned}$$

$$
\begin{aligned}
&= -\int_{-\infty}^{\infty} d\tau_1 \int_0^{\infty} d\tau\, e^{i(E_F-E_I)\tau_1} \langle\psi_F|V\, e^{i(E_F-H_0)\tau}\, V|\psi_I\rangle \\
&= -i\, 2\pi\delta(E_F-E_I)\, \langle\psi_F|V\, \frac{1}{E_F-H_0+i\epsilon}\, V|\psi_I\rangle
\end{aligned}
\tag{25}
$$

This is characteristic of the higher order terms. We have factors of V and energy denominator factors $1/(E_F - H_0 + i\epsilon)$.

Let us summarize this result. One defines the T-matrix as

$$
S_{FI} = \langle\psi_F|\psi_I\rangle - i(2\pi)\delta(E_F-E_I)\, T_{FI}. \tag{26}
$$

Then we expand T_{FI} in powers of V:

$$
T_{FI} = \sum T_{FI}^{(n)}, \tag{27}
$$

where $T_{FI}^{(n)}$ is the contribution to T_{FI} proportional to n powers of V. The result just derived is

$$
-iT_{FI}^{(n)} = \langle\psi_F|(-iV)\, \frac{i}{E_F-H_0+i\epsilon}\, (-iV)\, \frac{i}{E_F-H_0+i\epsilon} \cdots (-iV)|\psi_I\rangle. \tag{28}
$$

Let us see what this is for plane wave initial and final states,

$$
\begin{aligned}
|\psi_I\rangle &= |\vec{p}_I, \vec{k}_I\rangle \\
|\psi_F\rangle &= |\vec{p}_F, \vec{k}_F\rangle.
\end{aligned}
\tag{29}
$$

Wherever we see an energy denominator factor we can insert a sum over a complete set of plane wave states. For the ith such sum over intermediate states, we can write

$$
1 = \int \frac{d\vec{p}_i}{(2\pi)^3}\, \frac{d\vec{k}_i}{(2\pi)^3}\; |\vec{p}_i, \vec{k}_i\rangle\langle\vec{p}_i, \vec{k}_i|. \tag{30}
$$

When H_0 acts on one of the plane wave states it gives

$$
H_0|\vec{p}_i, \vec{k}_i\rangle = \left[\frac{p_i^2}{2m} + \frac{k_i^2}{2m}\right] |\vec{p}_i, \vec{k}_i\rangle \tag{31}
$$

(assuming that the two particles have the same mass). This gives factors

$$
\int \frac{d\vec{p}_i}{(2\pi)^3}\, \frac{d\vec{k}_i}{(2\pi)^3}\; \frac{|\vec{p}_i, \vec{k}_i\rangle\langle\vec{p}_i, \vec{k}_i|}{E_F - p_i^2/(2m) + k_i^2/(2m) + i\epsilon} \tag{32}
$$

for each intermediate state. For the V operators we can write (again writing 1 as a sum over projection operators $|n\rangle\langle n|$ onto states)

$$\begin{aligned}
\langle \vec{p}_j, \vec{k}_j | V | \vec{p}_i, \vec{k}_i \rangle &= \int d\vec{x}\, d\vec{y}\ \langle \vec{p}_j, \vec{k}_j | \vec{x}, \vec{x}+\vec{y} \rangle \langle \vec{x}, \vec{x}+\vec{y} | V | \vec{p}_i, \vec{k}_i \rangle \\
&= \int d\vec{x}\, d\vec{y}\ \mathcal{V}(|\vec{y}|)\ \langle \vec{p}_j, \vec{k}_j | \vec{x}, \vec{x}+\vec{y} \rangle \langle \vec{x}, \vec{x}+\vec{y} | \vec{p}_i, \vec{k}_i \rangle \\
&= \int d\vec{x}\, d\vec{y}\ \mathcal{V}(|\vec{y}|) \\
&\quad \times \exp\Big(-i[(\vec{p}_j + \vec{k}_j)\cdot\vec{x} + \vec{k}_j\cdot\vec{y} - (\vec{p}_i + \vec{k}_i)\cdot\vec{x} - \vec{k}_i\cdot\vec{y}] \Big) \\
&= \int d\vec{x}\, d\vec{y}\ \mathcal{V}(|\vec{y}|) \\
&\quad \times \exp\Big(-i[(\vec{p}_j + \vec{k}_j - \vec{p}_i - \vec{k}_i)\cdot\vec{x} + (\vec{k}_j - \vec{k}_i)\cdot\vec{y}] \Big) \\
&= (2\pi)^3 \delta(\vec{p}_j + \vec{k}_j - \vec{p}_i - \vec{k}_i)\tilde{\mathcal{V}}(|\vec{k}_j - \vec{k}_i|). \qquad (33)
\end{aligned}$$

Here

$$\tilde{\mathcal{V}}(|\vec{q}|) \equiv \int d\vec{y}\ \exp(-i\vec{q}\cdot\vec{y})\, \tilde{\mathcal{V}}(|\vec{y}|). \qquad (34)$$

is the Fourier transform of the potential.

Thus we arrive at the following rules for what is sometimes called *old fashioned perturbation theory* for $-iT_{FI}$. We include the following factors:

1) For each intermediate state an integration over the momenta of the intermediate particles

$$\int \frac{d\vec{p}_i}{(2\pi)^3} \frac{d\vec{k}_i}{(2\pi)^3} \qquad (35)$$

2) For each intermediate state an energy denominator factor

$$\frac{i}{E_F - p_i^2/(2m) + k_i^2/(2m) + i\epsilon} \qquad (36)$$

3) For each interaction a delta function that conserves the momentum

$$(2\pi)^3 \delta(\vec{p}_j + \vec{k}_j - \vec{p}_i - \vec{k}_i) \qquad (37)$$

4) For each interaction a factor

$$-i\tilde{\mathcal{V}}(|\vec{q}|). \qquad (38)$$

Note that the momentum conserving delta functions cancel the integration over the total momentum for each intermediate state. In addition, we are left with a delta function that conserves the momentum between the initial and final state

$$(2\pi)^3\delta(\vec{p}_F + \vec{k}_F - \vec{p}_I - \vec{k}_I). \tag{39}$$

Exercise. Find the Born approximation for scattering two particles that each have charge e that scatter by means of the Coulomb potential:

$$\mathcal{V}(|\vec{x}_1 - \vec{x}_2|) = \frac{e^2}{4\pi}\frac{1}{|\vec{x}_1 - \vec{x}_2|} \tag{40}$$

Let the initial momenta of the particles be $\vec{p}_I$ and $\vec{k}_I$ and let the final momenta of the particles be $\vec{p}_F$ and $\vec{k}_F$. After doing all of the integrals that you encounter, you should obtain an answer that is a function of these momentum variables.

---

5 The in and out states

In this section we study the in and out states in more detail. We have

$$|\psi_I\rangle_{\text{in}} = U(0, -\infty)|\psi_I\rangle_f \tag{41}$$

where

$$U(0, -\infty) = T\exp\left(-i\int_{-\infty}^{0} dt\ V(t)\right). \tag{42}$$

Expanding this gives

$$\begin{aligned}
|\psi_I\rangle_{\text{in}} &= T\exp\left(-i\int_{-\infty}^{0} dt\ V(t)\right)|\psi_I\rangle_f \\
&= |\psi_I\rangle_f - i\int_{-\infty}^{0} dt\ e^{iH_0t}Ve^{-iH_0t}|\psi_I\rangle_f \\
&\quad +(-i)^2\int_{-\infty}^{0} dt_2\ \int_{-\infty}^{t_2} dt_1\ e^{iH_0t_2}Ve^{-iH_0(t_2-t_1)}Ve^{-iH_0t_1}|\psi_I\rangle_f \\
&\quad +\cdots
\end{aligned}$$

$$
\begin{aligned}
= \quad & |\psi_I\rangle_f - i\int_{-\infty}^{0} dt\ e^{iH_0 t} V e^{-iH_0 t}|\psi_I\rangle_f \\
& +(-i)^2 \int_{-\infty}^{0} dt_2\ \int_{0}^{\infty} d\tau\ e^{iH_0 t_2} V e^{-iH_0 \tau} V e^{-iH_0 (t_2-\tau)}|\psi_I\rangle_f \\
& + \cdots \\
= \quad & |\psi_I\rangle_f - i\int_{-\infty}^{0} dt\ e^{-i(E_I - H_0)t} V|\psi_I\rangle_f \\
& +(-i)^2 \int_{-\infty}^{0} dt_2\ \int_{0}^{\infty} d\tau\ e^{-i(E_I - H_0)t_2} V e^{i(E_I-H_0)\tau} V|\psi_I\rangle_f \\
& + \cdots \\
= \quad & |\psi_I\rangle_f + \frac{i}{E_I - H_0 + i\epsilon}(-iV)|\psi_I\rangle_f \\
& + \frac{i}{E_I - H_0 + i\epsilon}(-iV)\frac{i}{E_I - H_0 + i\epsilon}(-iV)|\psi_I\rangle_f \\
& + \cdots
\end{aligned} \tag{43}
$$

We can write this as an equation one could solve for $|\psi_I\rangle_{\rm in}$:

$$
|\psi_I\rangle_{\rm in} = |\psi_I\rangle_f + \frac{i}{E_I - H_0 + i\epsilon}(-iV)|\psi_I\rangle_{\rm in}. \tag{44}
$$

If we operate with $E_I - H_0$ and use $E_I - H_0|\psi_I\rangle_f = 0$ we have

$$
(E_I - H_0)|\psi_I\rangle_{\rm in} = V|\psi_I\rangle_{\rm in}. \tag{45}
$$

or

$$
(H_0 + V)|\psi_I\rangle_{\rm in} = E_I|\psi_I\rangle_{\rm in}. \tag{46}
$$

That is, $|\psi_I\rangle_{\rm in}$ obeys the Schrödinger equation. However, Eq. 44, which is often called the Lippman-Schwinger equation, carries more information because of the $|\psi_I\rangle_f$ term and the $i\epsilon$.

The out state $|\psi_I\rangle_{\rm in}$ obeys a similar equation with the $i\epsilon$ reversed:

$$
|\psi_F\rangle_{\rm out} = |\psi_F\rangle_f + \frac{i}{E_I - H_0 - i\epsilon}(-iV)|\psi_F\rangle_{\rm out}. \tag{47}
$$

6 One particle scattering from a potential

Let's go further, simplifying the calculations by considering one particle that scatters from a fixed potential instead of two particles that scatter from each other by means of a potential. We let the initial state be a plane wave state with momentum $\vec{p}$.

Our equation for $|\psi_I\rangle_{\rm in}$ is

$$\langle\vec{x}|\psi_I\rangle_{\rm in} = \langle\vec{x}|\vec{p}\rangle_f + \int d\vec{y}\;\langle\vec{x}|\frac{i}{E_I - H_0 + i\epsilon}|\vec{y}\rangle\langle\vec{y}|(-iV)|\psi_I\rangle_{\rm in}. \tag{48}$$

Define

$$G(\vec{x}-\vec{y}) = \langle\vec{x}|\frac{1}{E_I - H_0 + i\epsilon}|\vec{y}\rangle. \tag{49}$$

Then

$$\psi_I^{(\rm in)}(\vec{x}) = e^{i\vec{p}\cdot\vec{x}} + \int d\vec{y}\; G(\vec{x}-\vec{y})\,\mathcal{V}(\vec{y})\,\psi_I^{(\rm in)}(\vec{y}). \tag{50}$$

Note that this is the complete equation, without approximation. It is good to keep in mind that the lowest order approximation is obtained by substituting

$$\psi_I^{(\rm in)}(\vec{y}) \to e^{i\vec{p}\cdot\vec{y}} \tag{51}$$

on the right hand side.

Evidently, we should study $G(\vec{x}-\vec{y})$, which is often called the Green function. Using $\vec{r} = \vec{x}-\vec{y}$ we have

$$\begin{aligned}
G(\vec{x}-\vec{y}) &= \int \frac{d\vec{k}}{(2\pi)^3}\langle\vec{x}|\vec{k}\rangle\langle\vec{k}|\frac{1}{\vec{p}^2/(2m) - H_0 + i\epsilon}|\vec{y}\rangle \\
&= \int \frac{d\vec{k}}{(2\pi)^3}\langle\vec{x}|\vec{k}\rangle\langle\vec{k}|\frac{1}{\vec{p}^2/(2m) - \vec{k}^2/(2m) + i\epsilon}\langle\vec{k}|\vec{y}\rangle \\
&= \int \frac{d\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}}\frac{1}{\vec{p}^2/(2m) - \vec{k}^2/(2m) + i\epsilon} \\
&= (2\pi)^{-2}\int_0^\infty k^2 dk\;\int_{-1}^1 d\cos\theta\; e^{ikr\cos\theta}\frac{1}{\vec{p}^2/(2m) - \vec{k}^2/(2m) + i\epsilon} \\
&= (2\pi)^{-2}\int_0^\infty dk\;\frac{-ik}{r}\left[e^{ikr} - e^{-ikr}\right]\frac{1}{\vec{p}^2/(2m) - \vec{k}^2/(2m) + i\epsilon} \\
&= (2\pi)^{-2}\int_{-\infty}^\infty dk\;\frac{-ik}{r}e^{ikr}\frac{1}{\vec{p}^2/(2m) - \vec{k}^2/(2m) + i\epsilon} \\
&= (2\pi)^{-2}\;\frac{-ip}{r}e^{ipr}\frac{2\pi i}{-p/m} \\
&= -\frac{m}{2\pi}\;\frac{1}{r}\,e^{ipr}
\end{aligned} \tag{52}$$

Note that we have closed the contour in the upper half k plane in the second to last step.

Inserting this in our formula, we have

$$\psi_I^{(\mathrm{in})}(\vec{x}) = e^{i\vec{p}\cdot\vec{x}} - \frac{m}{2\pi}\int d\vec{y}\,\frac{1}{|\vec{x}-\vec{y}|}\,e^{ip|\vec{x}-\vec{y}|}\,\mathcal{V}(\vec{y})\,\psi_I^{(\mathrm{in})}(\vec{y}). \tag{53}$$

Note that $\exp(+ip|\vec{x}|)$ is an outgoing wave; the sign in the exponent was determined by the sign of the $i\epsilon$ in the energy denominator. Thus $\psi_I^{(\mathrm{in})}(\vec{x})$ consists of the incoming plane wave plus an outgoing wave that emanates from positions $\vec{y}$ where the potential is big. This is an integral equation that, in principle, we could solve for $\psi_I^{(\mathrm{in})}(\vec{x})$. If $\mathcal{V}$ is small, we can approximate the solution by substituting a plane wave for $\psi_I^{(\mathrm{in})}(\vec{x})$.

We will want to know something about how $\psi_I^{\mathrm{in}}(\vec{x})$ behaves for large $|\vec{x}|$. For this, we need to expand our equation for $|\vec{x}|/|\vec{y}| \ll 1$. We use

$$\begin{aligned}
|\vec{x}-\vec{y}| &= [\vec{x}^2 - 2\vec{x}\cdot\vec{y} + \vec{y}^2]^{1/2} \\
&= |\vec{x}|\left[1 - 2\frac{|\vec{y}|}{|\vec{x}|}\hat{x}\cdot\hat{y} + \frac{|\vec{y}|^2}{|\vec{x}|^2}\right]^{1/2} \\
&\sim |\vec{x}|\left[1 - \frac{|\vec{y}|}{|\vec{x}|}\hat{x}\cdot\hat{y} + \cdots\right] \\
&\sim |\vec{x}| - |\vec{y}|\,\hat{x}\cdot\hat{y} + \cdots .
\end{aligned} \tag{54}$$

Thus

$$\psi_I^{(\mathrm{in})}(\vec{x}) \sim e^{i\vec{p}\cdot\vec{x}} - \frac{m}{2\pi}\,\frac{1}{|\vec{x}|}\,e^{ip|\vec{x}|}\int d\vec{y}\;e^{-ip|\vec{y}|\hat{x}\cdot\hat{y}}\,\mathcal{V}(\vec{y})\,\psi_I^{(\mathrm{in})}(\vec{y}). \tag{55}$$

(I use p for $|\vec{p}|$ here.) We could write this as

$$\psi_I^{(\mathrm{in})}(\vec{x}) = e^{i\vec{p}\cdot\vec{x}} + f(\hat{x})\,\frac{1}{|\vec{x}|}\,e^{ip|\vec{x}|}. \tag{56}$$

where f is a function of the direction of $\vec{x}$ only and is given by

$$f(\hat{x}) = -\frac{m}{2\pi}\int d\vec{y}\;e^{-ip|\vec{y}|\hat{x}\cdot\hat{y}}\,\mathcal{V}(\vec{y})\,\psi_I^{(\mathrm{in})}(\vec{y}). \tag{57}$$

Note that this is just telling us about how $\psi_I^{(\mathrm{in})}(\vec{x})$ behaves for large $|\vec{x}|$ – that it is an outgoing spherical wave times a function of $\hat{x}$. Unless we know $\psi_I^{(\mathrm{in})}(\vec{y})$ exactly, we cannot evaluate the integral. But this formula does become directly useful if we want the lowest order perturbative result, which we obtain by substituting $\exp(i\vec{p}\cdot\vec{y})$ for $\psi_I^{(\mathrm{in})}(\vec{y})$.

7 The T-matrix and $\psi_I^{\rm in}(\vec{x})$

One might think that the scattering matrix might have something to do with the behavior of the wave function $\psi_I^{\rm in}(\vec{x})$ for large $|\vec{x}|$ and thus might be related to the function $f(\hat{x})$ introduced above. Let's see.

We take the final state to be a plane wave state with momentum $\vec{k}$. Then

$$\begin{aligned} T_{FI} &= \langle\vec{k}|V\left[1+\frac{1}{E_I-H_0+i\epsilon}V+\cdots\right]|\vec{p}\rangle \\ &= \langle\vec{k}|V|\vec{p}\rangle_{\rm in} \\ &= \int d\vec{x}\; e^{-i\vec{k}\cdot\vec{x}}\,\mathcal{V}(\vec{x})\,\psi_I^{(\rm in)}(\vec{x}) \\ &= \int d\vec{x}\; e^{-i\vec{k}\cdot\vec{x}}\left[\frac{1}{2m}\vec{\nabla}^2+E_I\right]\psi_I^{(\rm in)}(\vec{x}). \end{aligned} \tag{58}$$

We integrate by parts, watching the surface term:

$$\begin{aligned} T_{FI} &= \int d\vec{x}\;\left\{\left[\frac{1}{2m}\vec{\nabla}^2+E_I\right]e^{-i\vec{k}\cdot\vec{x}}\right\}\psi_I^{(\rm in)}(\vec{x}) \\ &\quad+\frac{1}{2m}\int d\vec{x}\;\vec{\nabla}\cdot\left\{e^{-i\vec{k}\cdot\vec{x}}\vec{\nabla}\psi_I^{(\rm in)}(\vec{x})-\left(\vec{\nabla}e^{-i\vec{k}\cdot\vec{x}}\right)\psi_I^{(\rm in)}(\vec{x})\right\} \\ &= 0+\frac{1}{2m}\int d\vec{x}\;\vec{\nabla}\cdot\left\{e^{-i\vec{k}\cdot\vec{x}}\vec{\nabla}\psi_I^{(\rm in)}(\vec{x})+i\vec{k}e^{-i\vec{k}\cdot\vec{x}}\,\psi_I^{(\rm in)}(\vec{x})\right\} \\ &= \frac{1}{2m}\lim_{R\to\infty}\int d\Omega_x\,R^2e^{-i\vec{k}\cdot\vec{x}}\;\hat{x}\cdot(i\vec{k}+\vec{\nabla})\,\psi_I^{(\rm in)}(\vec{x}) \end{aligned} \tag{59}$$

Here we are integrating over a sphere whose radius should go to infinity. If we substitute our large $|\vec{x}|$ form for $\psi_I^{(\rm in)}(\vec{x})$ we have

$$\begin{aligned} T_{FI} &= \frac{1}{2m}\lim_{R\to\infty}\int d\Omega_x\,R^2e^{-i\vec{k}\cdot\vec{x}}\;\hat{x}\cdot(i\vec{k}+\vec{\nabla})\left[e^{i\vec{p}\cdot\vec{x}}+f(\hat{x})\,\frac{1}{|\vec{x}|}\;e^{ip|\vec{x}|}\right] \\ &= \frac{i}{2m}\lim_{R\to\infty}\int d\Omega_x\,R^2e^{-i\vec{k}\cdot\vec{x}}\;\hat{x}\cdot(\vec{k}+\vec{p})e^{i\vec{p}\cdot\vec{x}} \\ &\quad+\frac{i}{2m}\lim_{R\to\infty}\int d\Omega_x\,R^2e^{-i\vec{k}\cdot\vec{x}}\;\hat{x}\cdot(\vec{k}+p\hat{x})f(\hat{x})\,\frac{1}{|\vec{x}|}\;e^{ip|\vec{x}|} \end{aligned} \tag{60}$$

In the second term, I have thrown away the term in which the $\vec{\nabla}$ differentiates the $1/|\vec{x}|$ since that term gives a non-leading contribution for large $|\vec{x}|$.

Now the first term is

$$\frac{i}{2m}\int d\vec{x}\;\nabla\cdot\left\{e^{-i\vec{k}\cdot\vec{x}}\;(\vec{k}+\vec{p})e^{i\vec{p}\cdot\vec{x}}\right\} \;=\; \frac{1}{2m}\int d\vec{x}\;\left\{e^{-i\vec{k}\cdot\vec{x}}\;(\vec{k}-\vec{p})\cdot(\vec{k}+\vec{p})e^{i\vec{p}\cdot\vec{x}}\right\}$$

$$
\begin{aligned}
&= \frac{1}{2m}\int d\vec{x}\ \left\{ e^{-i\vec{k}\cdot\vec{x}}\ (\vec{k}^2 - \vec{p}^2) e^{i\vec{p}\cdot\vec{x}} \right\} \\
&= 0 \qquad (61)
\end{aligned}
$$

Thus we are left with

$$
T_{FI} = \frac{i}{2m}\lim_{R\to\infty}\int d\Omega_x\, R e^{-i\vec{k}\cdot\vec{x}}\ (\hat{x}\cdot\vec{k}+p) f(\hat{x})\, e^{ip|\vec{x}|}. \qquad (62)
$$

What is this? I claim that the important contributions for large R can come only from $\hat{x}$ in the direction of $\vec{k}$. To see why, let θ, ϕ be the angles of $\vec{x}$ in a coordinate system in which the z-axis is along $\vec{k}$. Then

$$
T_{FI} = \frac{ip}{2m}\lim_{R\to\infty} R\int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\phi\, e^{ipR(1-\cos\theta)}\ (1+\cos\theta) f(\cos\theta,\phi). \qquad (63)
$$

For large R, the rapid oscillations of the exponential make the contributions small and the dominant contributions come from the endpoints.

Exercise. If $f(\cos\theta,\phi) = A$, a constant, show that

$$
T_{FI} = -\frac{2\pi A}{m}. \qquad (64)
$$

Exercise. If you expand $f(\cos\theta,\phi)$ around $\cos\theta = 1$, the Nth term will have a factor $(1-\cos\theta)^N$. Show that these terms contribute zero in the limit $R \to \infty$.

Applying the lesson of the exercises above, we have

$$
T_{FI} = -\frac{2\pi}{m} f(\hat{k}). \qquad (65)
$$

Thus the function $f(\hat{x})$ that gives the strength of the outgoing wave at large distances is (up to a factor) the quantum mechanical scattering matrix as given by our operator definitions.

8 Cross sections

Cross sections are directly related to the s-matrix an are important because they are observable. Essentially the definition is that if a beam of N_A particles of type A collides with a beam of N_B particles of type B, and if the cross sectional area of each beam is A, then the total number of events of some specified character, dN is related to the corresponding differential cross section $d\sigma$ by

$$N = \frac{N_A N_B}{A}\, d\sigma. \tag{66}$$

A much fuller discussion can be found in Peskin and Schroeder Section 4.5.

The relation between cross sections and the s-matrix is as follows. Using a covariant normalization of states, we define the "invariant amplitude " $\mathcal{M}$ by

$$\begin{aligned} {}_{\text{out}}\langle p_1, p_2, \ldots | k_A, k_B \rangle_{\text{in}} &= \langle p_1, p_2, \ldots | k_A, k_B \rangle \\ &\quad + (2\pi)^4 \delta^{(4)}(k_A + k_B - \textstyle\sum p_f)\; i\mathcal{M}. \end{aligned} \tag{67}$$

Then,

$$d\sigma = \left(\prod_f \frac{d\vec{p}_f}{(2\pi)^3\, 2p_f^0} \right) \frac{1}{2p_A^0 2p_B^0 |v_A - v_B|}\, (2\pi)^4 \delta^{(4)}(k_A + k_B - \textstyle\sum p_f)\; |\mathcal{M}|^2. \tag{68}$$

This relation is nicely proved in Peskin and Scrhoeder Section 4.5. You should study this proof carefully.

If we want to use the non-relativistic normalization of states,

$${}_{\text{nr}}\langle k' | k \rangle_{\text{nr}} = (2\pi)^3 \delta^3(\vec{k}' - \vec{k}), \tag{69}$$

instead of the relativistic normalization

$$\langle k' | k \rangle = (2\pi)^3 2k^0\, \delta^3(\vec{k}' - \vec{k}), \tag{70}$$

then we have only to define

$$|k\rangle_{\text{nr}} = 2k^0 |k\rangle \tag{71}$$

Then we get

$$d\sigma = \left(\prod_f \frac{d\vec{p}_f}{(2\pi)^3} \right) \frac{1}{|v_A - v_B|}\, (2\pi)^4 \delta^{(4)}(k_A + k_B - \textstyle\sum p_f)\; |\mathcal{M}_{\text{nr}}|^2. \tag{72}$$

Let's see how we can use this result (assuming that we have calculated $\mathcal{M}$). Let's take the relativistic case and suppose that there are two final state particles. We have integrations $d\vec{p}_1$ and $d\vec{p}_2$, but we can use the delta function for three-momentum conservation to get rid of $d\vec{p}_2$. This leaves

$$d\sigma = \frac{d\vec{p}_1}{(2\pi)^3\, 2p_1^0\, 2p_2^0}\, \frac{1}{2p_A^0 2p_B^0 |v_A - v_B|}\, (2\pi)\delta(k_A^0 + k_B^0 - p_1^0 - p_2^0)\ |\mathcal{M}|^2. \quad (73)$$

Now we can write $d\vec{p}_1 = p_1^2 dp_1 d\cos\theta\, d\phi$, where p_1 is the magnitude of $\vec{p}_1$. Then we can use the energy conserving delta function to get rid of dp_1. We can use

$$p_1^0 = [\vec{p}_1^{\,2} + m_1^2]^{1/2} \equiv [p_1^2 + m_1^2]^{1/2} \quad (74)$$

to express p_1^0 in terms of p_1. We get the differential cross section

$$\frac{d\sigma}{d\cos\theta\, d\phi} = \frac{p_1^2}{(2\pi)^2\, 2p_1^0\, 2p_2^0}\ \frac{1}{2p_A^0 2p_B^0 |v_A - v_B|}\ \frac{1}{\partial E_{12}/\partial p_1}\ |\mathcal{M}|^2. \quad (75)$$

where

$$E_{12} = p_1^0 + p_2^0 = [\vec{p}_1^{\,2} + m_1^2]^{1/2} + [(\vec{k}_A + \vec{k}_B - \vec{p}_1)^2 + m_2^2]^{1/2}. \quad (76)$$

The simplest case arises when

$$\vec{k}_A + \vec{k}_B = 0 \quad (77)$$

so that we are in the c.m. system. Then

$$E_{12} = [p_1^2 + m_1^2]^{1/2} + [p_1^2 + m_2^2]^{1/2}. \quad (78)$$

so

$$\frac{\partial E_{12}}{\partial p_1} = \frac{p_1}{[p_1^2 + m_1^2]^{1/2}} + \frac{p_1}{[p_1^2 + m_2^2]^{1/2}}. \quad (79)$$

Exercise. Calculate the cross section $d\sigma/d\cos\theta$ for electron (charge $-e$) to scatter from a nucleus with charge Ze by means of the Coulomb force between the particles considered at lowest order in e^2. Consider the whole calculation in the nonrelativistic approximation, with the nucleus at rest. Simplify the problem by considering the electron and nucleus to have spin zero. Please set up the problem for general masses of the electron and nucleus, but then take the limit $M/m \to \infty$.
