Scattering in quantum mechanics[1]

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1 Introduction

In these notes, we develop what is usually called time dependent scattering theory and use it to find the perturbative expansion for the S-matrix in what is often called time-ordered perturbation theory. We consider the scattering of a single particle from a fixed potential. With a few changes, the same formalism can handle much more complicated situations.

2 The S-matrix

The operator of interest for scattering theory is the scattering operator S. If we make a matrix $\langle p_F | S | p_I \rangle$ from it, we have the S matrix. We define

$$S = \lim_{\substack{t_I \to -\infty \\ t_F \to +\infty}} U(t_F, t_I) \quad . \tag{1}$$

Here $U(t_F, t_I)$ takes the system, in a certain sense to be defined, from an initial time t_I to a final time t_F. We define $U(t_F, t_I)$ as

$$U(t_F, t_I) = e^{iH_0 t_F} e^{-i(H_0+V)(t_F - t_I)} e^{-iH_0 t_I} \quad . \tag{2}$$

Here H_0 is the free particle hamiltonian, $p^2/(2m)$, and H_0+V is the full hamiltonian including a potential $V(\vec{x})$. The operator $\exp(-i(H_0+V)(t_F - t_I)$ propagates the system from time t_I to time t_F. When t_F is very large, we have an outgoing wave that is mostly propagating according to H_0 because the particle has moved far from the region where the potential acts. We do not, however, get a finite limit as $t_F \to \infty$ because the particle keeps on propagating: behind the moon, out past Jupiter, on to Pluto, *etc.* The trick is to bring it back to earth with $\exp(iH_0 t_F)$. Then we don't lose any information and we have a finite limit. For the same reason we multiply by $\exp(-iH_0 t_I)$ on the right hand side.

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3 Differential equation for U

Given the definition, we have

$$\frac{d}{dt}U(t,t_I) = -iV(t)U(t,t_I) \quad , \tag{3}$$

where

$$V(t) = e^{iH_0 t} V e^{-iH_0 t} \quad . \tag{4}$$

(Be sure to verify this, including the proper ordering of the operators.) The boundary condition for U is

$$U(t_I,t_I) = 1 \quad . \tag{5}$$

4 Solution of the differential equation

The solution for this differential equation and boundary condition is

$$U(t,t_I) = T\exp\left(-i\int_{t_I}^{t} d\tau\ V(\tau)\right) \quad . \tag{6}$$

If $V(\tau)$ were just a numerical-valued function, this would be simple. Since we deal with quantum mechanics, we have operators $V(\tau)$ and $V(\tau_1)$ may not commute with $V(\tau_2)$. We have therefore supplied a symbol T that says to "time order" the operators $V(\tau)$ by putting the operators for the latest values of τ to the left. To define what this means, expand $U(t,t_I)$ in powers of V. The nth term is

$$U_n = \frac{(-i)^n}{n!}\, T\int_{t_I}^{t} d\tau_n \ldots \int_{t_I}^{t} d\tau_2 \int_{t_I}^{t} d\tau_1\ V(\tau_n)\cdots V(\tau_2)V(\tau_1) \quad . \tag{7}$$

There are $n!$ possible orderings of the time variables τ_i. Let's relable the τ_i so that the earliest is called τ_1, the next earliest is called τ_2, *etc.* Then

$$U_n = (-i)^n T\int_{t_I}^{t} d\tau_n \ldots \int_{t_I}^{\tau_3} d\tau_2 \int_{t_I}^{\tau_2} d\tau_1\ V(\tau_n)\cdots V(\tau_2)V(\tau_1) \quad . \tag{8}$$

This is just a relabeling of dummy variables. We haven't said anything about operator ordering yet. Now we can specify the operator ordering: the $V(\tau)$ with the latest values of τ go to the left. Thus

$$U_n = (-i)^n \int_{t_I}^{t} d\tau_n \ldots \int_{t_I}^{\tau_3} d\tau_2 \int_{t_I}^{\tau_2} d\tau_1\ V(\tau_n)\cdots V(\tau_2)V(\tau_1) \quad . \tag{9}$$

With this form, we can directly differentiate with respect to t and verify that we have a solution of the original differential equation.

Thus the scattering operator is

$$S = 1 + \sum_{n=1}^{\infty} (-i)^n \int_{-\infty}^{\infty} d\tau_n \ldots \int_{-\infty}^{\tau_3} d\tau_2 \int_{-\infty}^{\tau_2} d\tau_1 \; V(\tau_n) \cdots V(\tau_2) V(\tau_1) \quad . \tag{10}$$

5 Perturbation expansion for the S-matrix

Let's take the matrix element of S between an initial momentum eigenstate $\big|p_I\big\rangle$ and a final momentum eigenstate $\big\langle p_F\big|$.

$$\begin{aligned} \big\langle p_F\big|S\big|p_I\big\rangle = \big\langle p_F\big|p_I\big\rangle & \\ & + \sum_{n=1}^{\infty} (-i)^n \int_{-\infty}^{\infty} d\tau_n \ldots \int_{-\infty}^{\tau_3} d\tau_2 \int_{-\infty}^{\tau_2} d\tau_1 \\ & \times \big\langle p_F\big|V(\tau_n) \cdots V(\tau_2) V(\tau_1)\big|p_I\big\rangle \quad . \end{aligned} \tag{11}$$

If we insert the definition of $V(\tau)$ into this, we have

$$\begin{aligned} \big\langle p_F\big|S\big|p_I\big\rangle = \big\langle p_F\big|p_I\big\rangle & \\ & + \sum_{n=1}^{\infty} (-i)^n \int_{-\infty}^{\infty} d\tau_n \ldots \int_{-\infty}^{\tau_3} d\tau_2 \int_{-\infty}^{\tau_2} d\tau_1 \\ & \times \big\langle p_F\big|e^{iH_0\tau_n} V e^{-iH_0(\tau_n - \tau_{n-1})} \\ & \quad \times \cdots e^{-iH_0(\tau_3-\tau_2)} V e^{-iH_0(\tau_2-\tau_1)} V e^{-iH_0\tau_1}\big|p_I\big\rangle \quad . \end{aligned} \tag{12}$$

It proves useful to change integration variables to

$$\begin{aligned} \tilde{\tau}_1 &= \tau_2 - \tau_1 \\ \tilde{\tau}_2 &= \tau_3 - \tau_2 \\ &\cdots \\ \tilde{\tau}_{n-1} &= \tau_n - \tau_{n-1} \\ \tilde{\tau}_n &= \tau_n \ . \end{aligned} \tag{13}$$

The inverse transformation is

$$\begin{aligned}
\tau_1 &= \tilde{\tau}_n - \tilde{\tau}_{n-1} - \cdots - \tilde{\tau}_1 \\
\tau_2 &= \tilde{\tau}_n - \tilde{\tau}_{n-1} - \cdots - \tilde{\tau}_2 \\
&\cdots \\
\tau_{n-1} &= \tilde{\tau}_n - \tilde{\tau}_{n-1} \\
\tau_n &= \tilde{\tau}_n \ .
\end{aligned} \tag{14}$$

Thus

$$\begin{aligned}
\big\langle p_F \big| S \big| p_I \big\rangle &= \big\langle p_F \big| p_I \big\rangle \\
&\quad + \sum_{n=1}^{\infty} (-i)^n \int_{-\infty}^{\infty} d\tilde{\tau}_n \int_0^{\infty} d\tilde{\tau}_{n-1} \ \ldots \int_0^{\infty} d\tilde{\tau}_2 \int_0^{\infty} d\tilde{\tau}_1 \\
&\quad \times \big\langle p_F \big| e^{iH_0\tilde{\tau}_n} V e^{-iH_0\tilde{\tau}_{n-1}} \\
&\qquad \times \cdots e^{-iH_0\tilde{\tau}_2} V e^{-iH_0\tilde{\tau}_1} V e^{-iH_0\tilde{\tau}_n + iH_0(\tilde{\tau}_{n-1} + \cdots \tilde{\tau}_1)} \big| p_I \big\rangle \ .
\end{aligned} \tag{15}$$

The advantage of this is that now all of the $\tilde{\tau}$ variables are integrated between fixed limits.

So far, we just rearranged things. But now we can recognize that when we have H_0 next to $\big|p_I\big\rangle$, it becomes $E_I = p_I^2/(2m)$ and when we have H_0 next to $\big\langle p_F\big|$, it becomes $E_F = p_F^2/(2m)$. Thus

$$\begin{aligned}
\big\langle p_F \big| S \big| p_I \big\rangle &= \big\langle p_F \big| p_I \big\rangle \\
&\quad + \sum_{n=1}^{\infty} (-i)^n \int_{-\infty}^{\infty} d\tilde{\tau}_n \int_0^{\infty} d\tilde{\tau}_{n-1} \ \ldots \int_0^{\infty} d\tilde{\tau}_1 \ e^{i(E_F - E_I)\tilde{\tau}_n} \\
&\quad \times \big\langle p_F \big| V e^{i(E_I - H_0)\tilde{\tau}_{n-1}} \cdots e^{i(E_I - H_0)\tilde{\tau}_2} V e^{i(E_I - H_0)\tilde{\tau}_1} V \big| p_I \big\rangle .
\end{aligned} \tag{16}$$

We can now perform all of the integrals. First,

$$\int_{-\infty}^{\infty} d\tilde{\tau}_n \ e^{i(E_F - E_I)\tilde{\tau}_n} = 2\pi\delta(E_F - E_I) \ . \tag{17}$$

This says that energy is conserved in the scattering. Second, we need

$$\int_0^{\infty} d\tilde{\tau}_j \ e^{i(E_I - H_0)\tilde{\tau}_j} \ . \tag{18}$$

This doesn't really converge at the $\tilde{\tau}_j \to +\infty$ end of the integration. To fix it, we can change $E_I - H_0$ to $E_I - H_0 + i\epsilon$, where ϵ is a small positive number. Then we have

$$\int_0^\infty d\tilde{\tau}_j \; e^{i(E_I - H_0)\tilde{\tau}_j} e^{-\epsilon\tau_j} \tag{19}$$

and our integral converges. We will want to take $\epsilon \to 0$, but we can do that later. Then we have

$$\int_0^\infty d\tilde{\tau}_j \; e^{i(E_I - H_0 + i\epsilon)\tilde{\tau}_j} = \frac{i}{E_I - H_0 + i\epsilon} \quad . \tag{20}$$

We thus obtain a really nice result,

$$\big\langle p_F \big| S \big| p_I \big\rangle = \big\langle p_F \big| p_I \big\rangle + 2\pi\delta(E_F - E_I)\mathcal{M} \quad , \tag{21}$$

where

$$\mathcal{M} = \sum_{n=1}^{\infty} \big\langle p_F \big| (-iV) \frac{i}{E_I - H_0 + i\epsilon} (-iV) \cdots (-iV) \big| p_I \big\rangle \quad . \tag{22}$$

In the nth term there are n factors of $-iV$. If there are more than one factors of $-iV$ then there is a factor $i/[E_I - H_0 + i\epsilon]$ between each pair of $-iV$s.

To use this, we can insert

$$1 = \int \frac{d\vec{k}_j}{(2\pi)^3} \; \big| \vec{k}_j \big\rangle \big\langle \vec{k}_j \big| \tag{23}$$

between each pair of $-iV$ factors. This gives a factor

$$\frac{i}{E_I - H_0 + i\epsilon} = \int \frac{d\vec{k}_j}{(2\pi)^3} \; \big| k_j \big\rangle \frac{i}{E_I - E_j + i\epsilon} \big\langle k_j \big| \quad , \tag{24}$$

where

$$E_j = \frac{\vec{k}_j^{\,2}}{2m} \quad . \tag{25}$$

We then need to know the matrix elements $\big\langle \vec{k}_1 \big| V \big| \vec{p}_I \big\rangle$, $\big\langle \vec{k}_2 \big| V \big| \vec{k}_1 \big\rangle$, *etc.*

6 Rules for perturbation theory

The S-matrix is related to the amplitude $\mathcal{M}$ by

$$\langle p_F | S | p_I \rangle = \langle p_F | p_I \rangle + 2\pi\delta(E_F - E_I)\mathcal{M} \quad . \tag{26}$$

The expression for $\mathcal{M}$ at nth order in perturbation theory involves n interactions with the potential and $n-1$ intermediate states. The result is

- For each intermediate state with momentum $\vec{k}_j$, an integration

$$\int \frac{d\vec{k}_j}{(2\pi)^3} \quad . \tag{27}$$

- For each intermediate state with momentum $\vec{k}_j$, a factor

$$\frac{i}{E_I - E_j + i\epsilon} \tag{28}$$

- For each interaction with the potential, a factor

$$\langle \vec{k}_{j+1} | (-iV) | \vec{k}_j \rangle \quad . \tag{29}$$

  Here the first $\vec{k}_j$ is $\vec{p}_I$ and the last is $\vec{p}_F$. Note that this is ($-i$ times) the Fourier transform of the potential.

7 Relation to the cross section

The differential probability to find the system to have momentum $\vec{p}_F$ is

$$dP = \frac{d\vec{p}_F}{(2\pi)^3} \left| \langle p_F | S | p_I \rangle \right|^2 \quad . \tag{30}$$

The differential cross section is this dP divided by the observation time and divided by the luminosity. By the the luminosity, we mean the number of beam particles striking the target potential per unit area per unit time:

$$\mathcal{L} = \rho v \quad , \tag{31}$$

where ρ is the density of particles in the beam and v is their velocity. With our convention of having an incoming plane wave e^{ikz}, the density is 1. Thus $\mathcal{L} = v$ so

$$d\sigma = \frac{1}{v\Delta T}\frac{d\vec{p}_F}{(2\pi)^3}\ \left|\langle p_F|S|p_I\rangle\right|^2 \ . \tag{32}$$

Using Eq. (26) and supposing that $\vec{p}_F \neq \vec{p}_I$ this is

$$d\sigma = \frac{1}{v\Delta T}\frac{d\vec{p}_F}{(2\pi)^3}\ \left|\mathcal{M}\right|^2\ 2\pi\delta(E_F - E_I) \times 2\pi\delta(E_F - E_I)_{E_F=E_I} \ . \tag{33}$$

Note that

$$2\pi\delta(E_F - E_I)_{E_F=E_I} = \int_{-\infty}^{\infty} dt \ . \tag{34}$$

We really should have used finite wave packets instead of plane waves. I omit the proof, but if we had, we would have a definite expression for how long the observation lasts, ΔT and we would replace

$$\int_{-\infty}^{\infty} dt \to \Delta T \tag{35}$$

Then

$$d\sigma = \frac{1}{v\Delta T}\frac{d\vec{p}_F}{(2\pi)^3}\ \left|\mathcal{M}\right|^2\ 2\pi\delta(E_F - E_I) \times \Delta T \ . \tag{36}$$

That is

$$d\sigma = \frac{1}{v}\frac{d\vec{p}_F}{(2\pi)^3}\ \left|\mathcal{M}\right|^2\ 2\pi\delta(E_F - E_I) \ . \tag{37}$$

8 Eliminating the energy integration

Eq. (37) has a simple intuitive meaning: a $1/v$ for the initial state luminosity, an differential $d\vec{p}_F/(2\pi)^3$ reflecting an integration over final state momenta, a squared matrix element $|\mathcal{M}|^2$ and an energy conserving delta function. However, if we want $d\sigma/d\Omega$, we need to do a little more calculation.

Write

$$d\vec{p}_F = p_F^2 dp_F d\Omega \ . \tag{38}$$

Then

$$p_F^2 dp_F d\Omega = \frac{1}{2}\, p_F dp_F^2 d\Omega = m p_F d(p_F^2/(2m))d\Omega = m^2 v dE_F d\Omega \ . \tag{39}$$

We can use the $2\pi\delta(E_F - E_I)$ to eliminate an integration $\int dE_F$. This leaves

$$d\sigma = \frac{m^2}{(2\pi)^2} d\Omega \big|\mathcal{M}\big|^2 \ . \tag{40}$$

That is

$$\frac{d\sigma}{d\Omega} = \left(\frac{m}{2\pi}\right)^2 \big|\mathcal{M}\big|^2 \ . \tag{41}$$

This is consistent with the relation

$$\mathcal{M} = \frac{2\pi i}{m} \ f(\theta, \phi) \ , \tag{42}$$

where $f(\theta, \phi)$ is the scattering amplitude in the conventions of Griffiths, with

$$\frac{d\sigma}{d\Omega} = \big|f(\theta, \phi)\big|^2 \ . \tag{43}$$

9 The optical theorem

There is a remarkable relation, known as the optical theorem, between the total scattering cross section and the amplitude for forward scattering. Griffiths derives this theorem using the partial wave decomposition. We can derive it in a simpler way using our expression for the scattering operator and its relation to the total cross section.

Start with our general formula

$$\big\langle p_F \big| S \big| p_I \big\rangle = \big\langle p_F \big| p_I \big\rangle + 2\pi\delta(E_F - E_I)\mathcal{M}(p_F, p_I) \ . \tag{44}$$

Write this as

$$\big\langle p_F \big| S \big| p_I \big\rangle = \big\langle p_F \big| p_I \big\rangle + \big\langle p_F \big| S - 1 \big| p_I \big\rangle \ , \tag{45}$$

where

$$\big\langle p_F \big| S - 1 \big| p_I \big\rangle = 2\pi\delta(E_F - E_I)\mathcal{M}(p_F, p_I) \ . \tag{46}$$

Thus

$$S = 1 + (S - 1) \ . \tag{47}$$

Nothing could be simpler than that.

By its definition, S is unitary,

$$S^\dagger S = 1 \ . \tag{48}$$

Thus

$$[1 + (S-1)]^\dagger [1 + (S-1)] = 1 \ . \tag{49}$$

That is,

$$(S-1)^\dagger (S-1) = -(S-1) - (S-1)^\dagger \ . \tag{50}$$

Take the matrix element of this between states $\langle p_I' |$ and $| p_I \rangle$ and insert a sum over all possible final states between $(S-1)^\dagger$ and $(S-1)$. This gives,

$$\begin{aligned} \int \frac{dp_F}{(2\pi)^3} \ \langle p_I' | (S-1)^\dagger | p_F \rangle \langle p_F | (S-1) | p_I \rangle = \\ - \langle p_I' | (S-1) | p_I \rangle - \langle p_I' | (S-1)^\dagger | p_I \rangle \ . \end{aligned} \tag{51}$$

Using the relation of matrix elements of $(S-1)$ to $\mathcal{M}$, this is

$$\begin{aligned} 2\pi\delta(E_I' - E_I) \int \frac{dp_F}{(2\pi)^3} \ 2\pi\delta(E_F - E_I) \ \mathcal{M}(p_F, p_I')^* \mathcal{M}(p_F, p_I) = \\ - 2\pi\delta(E_I' - E_I) \mathcal{M}(p_I', p_I) - 2\pi\delta(E_I' - E_I) \mathcal{M}(p_I, p_I')^* \ . \end{aligned} \tag{52}$$

There is a common factor of $2\pi\delta(E_I' - E_I)$. Taking the coefficient of that factor, we have (under the assumption that $E_I' = E_I$)

$$\begin{aligned} \int \frac{dp_F}{(2\pi)^3} \ 2\pi\delta(E_F - E_I) \ \mathcal{M}(p_F, p_I')^* \mathcal{M}(p_F, p_I) = \\ - \mathcal{M}(p_I', p_I) - \mathcal{M}(p_I, p_I')^* \ . \end{aligned} \tag{53}$$

Now we can simply set $p_I' = p_I$, giving

$$\int \frac{dp_F}{(2\pi)^3} \ 2\pi\delta(E_F - E_I) \ |\mathcal{M}(p_F, p_I)|^2 = -\mathcal{M}(p_I, p_I) - \mathcal{M}(p_I, p_I)^* \ . \tag{54}$$

Now we can use general relation (37) between $|\mathcal{M}|^2$ and cross sections to obtain the optical theorem, which is

$$\sigma_T = -\frac{2}{v_I} \ \mathrm{Re}\, \mathcal{M}(p_I, p_I) \ , \tag{55}$$

where σ_T is the total cross section and v_I is the velocity of the beam particles. On the right hand side, we have the real part of the scattering amplitude $\mathcal{M}$ for forward scattering.

If we like, this can be restated using $\mathcal{M} = (2\pi i/m)\ f(\theta, \phi)$ and $mv_I = p_I$. Stated this way, the optical theorem is

$$\sigma_T = \frac{4\pi}{p_I} \operatorname{Im} f(0, \phi) \quad . \tag{56}$$

(Note that at $\theta = 0$, $f(\theta, \phi)$ does not depend on ϕ).