Scattering Theory. S Matrix (S Operator)

Notes by R B Griffiths January, 1987

1. Introduction.

These notes contain some remarks on the S matrix as applied to potential scattering. For an extensive treatment of the subject see:

John R. Taylor, <u>Scattering Theory</u> (Krieger, 1983)

The intuitive significance of the S matrix is that it is a unitary transformation which when applied to the "incoming" wave in a scattering problem transforms it into the "outgoing wave". In the case of potential scattering it contains the same information as the scattering amplitude.

2. Derivation.

Let the Hamiltonian be

$$H = H_0 + V \qquad (2.1)$$

where

$$H_0 = \vec{p}^{\,2}/2m \qquad (2.2)$$

is the unperturbed or "free particle" Hamiltonian, and V is a potential which decays sufficiently rapidly for large $|\vec{r}|$ and is not too badly behaved at small $|\vec{r}|$; see Taylor for the technical conditions. Corresponding to H and H_0, both assumed to be independent of time, are the unitary time transformations

$$U(t'-t) = e^{-iH\cdot(t'-t)/\hbar} \qquad (2.3)$$

$$U_0(t'-t) = e^{-iH_0\cdot(t'-t)/\hbar} \qquad (2.4)$$

In particular, if $\psi(t)$ is a solution to the Schrödinger equation

$$i\hbar\,\partial\psi/\partial t = H\psi \qquad (2.5)$$

then

$$\psi(t_2) = U(t_2-t_1)\,\psi(t_1) \qquad (2.6)$$

~~In particular~~ Now let us imagine that $\psi(t_1)$ represents a wave packet at an early time $t_1 \ll t_0$ which is traveling towards the scattering center, and $\psi(t_2)$ the wave function at a much later time $t_2 \gg t_0$ when the particle has been scattered (or is continuing in the initial direction) and thus represents a particle traveling away from the scattering center. Define the operator $\bar{S}$ — it depends on t_1, t_0, and t_2 — by the equation

$$\mathcal{U}(t_2 - t_1) = \mathcal{U}_0(t_2 - t_0)\,\bar{S}\,\mathcal{U}_0(t_0 - t_1) \qquad (2.7)$$

Then (2.6) is equivalent to

$$\psi(t_2) = \mathcal{U}_0(t_2 - t_0)\,\bar{S}\,\mathcal{U}_0(t_0 - t_1)\,\psi(t_1) \qquad (2.8)$$

One can think of (2.8) intuitively in the following way. The particle moves forward in time, from t_1 to t_0, following the <u>free particle dynamics</u>

determined by H_0 and embodied in U_0. At time t_0 there is an instantaneous "magical" transformation induced by $\bar{S}$, which is chosen so that when the resulting transformed wave packet develops in time from t_0 to t_2, the net result is the same as it would have been had we simply used the correct (complete) dynamics determined by H, and embodied in U, at <u>all</u> times. That is, $\bar{S}$ is an artificial ~~object~~ operator which is chosen to mimic, in conjunction with U_0, the results of an exact calculation.

Solving (2.7), noting that

$$U_0^{-1}(t-t') = U_0(t'-t), \qquad (2.9)$$

gives us

$$\bar{S}(t_1, t_0, t_2) = \cancel{U_0^{-1}}\, U_0(t_0-t_2)\, U(t_2-t_1)\, U_0(t_1-t_0) \qquad (2.10)$$

We then <u>define</u> the S operator or S matrix by

$$S = \lim_{t_1 \to -\infty} \; \lim_{t_2 \to +\infty} \bar{S}(t_1, t_0, t_2) \qquad (2.11)$$

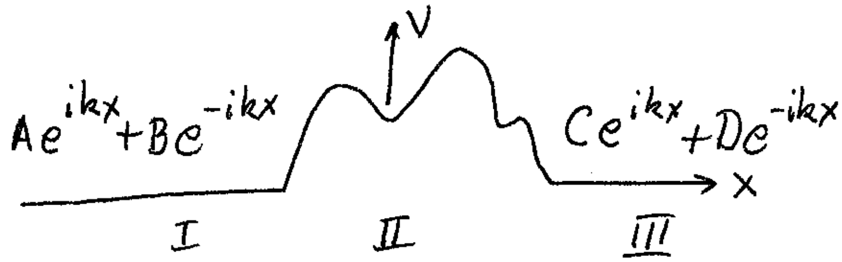
We shall assume that the limit (2.11) exists and defines a unitary operator. (Note that $\bar{S}$, as the product of three unitary operators is unitary, so it is plausible that S inherits this property.) To actually prove this is not trivial (see Taylor for further remarks). If the limit exists, it follows that

⊗ S is independent of t_0, and thus a time-independent operator.

⊗ S commutes with H_0, and therefore with $U_0(\tau)$

This means that the actual instant of time when S is applied to change the "incoming" into the "outgoing" wave is irrelevant in calculating the final result.

3. The S matrix in 1 dimensional scattering.



Consider the situation indicated in the sketch where the scattering potential is confined to region II. In regions I and III we have free particle wave functions with

$$\hbar\omega_k = E = \hbar^2 k^2/2m, \tag{3.1}$$

and the amplitudes A, B, C, and D are related by

$$\begin{pmatrix} C \\ B \end{pmatrix} = \begin{pmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix} = \underset{\sim}{S} \begin{pmatrix} A \\ D \end{pmatrix} \tag{3.2}$$

where $\underset{\sim}{S}$ is some unitary matrix whose elements <u>depend on k</u>. In what follows we shall always assume

$$k > 0 \tag{3.3}$$

so that negative wave numbers are given explicitly as $-k$.

The S *operator* is defined in terms of the matrix elements $\underset{\sim}{S}$ and the plane wave states $|k\rangle$, with

$$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}}\, e^{ikx} \qquad (3.4)$$

(note that $|k\rangle$ is a state with this functional form everywhere *including* region II), by the formulas

$$k>0: \quad \begin{aligned} S\,|k\rangle &= S_{++}(k)\,|k\rangle + S_{-+}(k)\,|-k\rangle \\ S\,|-k\rangle &= S_{+-}(k)\,|k\rangle + S_{--}(k)\,|-k\rangle \end{aligned} \qquad (3.5)$$

Exercise 3.1. Show that if $\underset{\sim}{S}$ in (3.2) is a 2×2 unitary *matrix* for all $k>0$, then the *operator* S defined by (3.5) is unitary.

Exercise 3.2. Show that if $V=0$ in region II as well (i.e., $V=0$ everywhere), then S defined by (3.5) is the identity operator.

We can also write (3.5) in the form

$$\langle \sigma k|\, S\, |\tau k'\rangle = \delta(k-k')\, S_{\sigma\tau}(k) \qquad (3.6)$$

where σ and τ are $+1$ or -1, and $k>0, k'>0$.

We now want to argue that S as defined by (3.5) has the property expected of the S operator: an incident wave packet can be changed into a scattered wave packet (which may have pieces moving both to the right and left) by a combination of free particle dynamics plus a timely application of S.

To this end let us define states $|k\rangle\hat{}$ which are solutions to the Schrödinger equation

$$H|k\rangle\hat{} = \hbar\omega_k |k\rangle\hat{} \qquad \cancel{(3.6)}\ (3.7)$$

everywhere including region II (with $V \neq 0$), with the property that (note that $k>0$):

$$\sqrt{2\pi}\,\langle x|k\rangle\hat{} = \begin{cases} e^{ikx} + S_{-+}(k)\,e^{-ikx} & \text{in region I} \\ S_{++}(k)\,e^{ikx} & \text{in region III} \end{cases} \qquad (3.8)$$

We can then form a superposition of these states representing a wave ~~fun~~ packet incident from the left by writing

$$|\psi(t)\rangle = \int_0^\infty A(k)\,e^{-i\omega_k t}\,|k\rangle\hat{}\,dk \qquad (3.9)$$

where ω_k is given by (3.1) and $A(k)$ is peaked near some $k_0>0$.

Using (3.8) we have

$$\sqrt{2\pi}\,\langle x|\psi(t)\rangle = \int_0^\infty dk\, A(k)\left[e^{i(kx-\omega_k t)} + S_{-+}(k)\,e^{-i(kx+\omega_k t)}\right] \tag{3.10}$$

for x in region I, and

$$\sqrt{2\pi}\,\langle x|\psi(t)\rangle = \int_0^\infty dk\, A(k)\, S_{++}(k)\, e^{i(kx-\omega_k t)} \tag{3.11}$$

for x in region III.

We assume that S_{-+} and S_{++} are smooth functions of k which do not vary rapidly near $k=k_0$. It is then plausible that for <u>t very negative</u>,

$$\sqrt{2\pi}\,\langle x|\psi(t)\rangle \simeq \int_0^\infty dk\, A(k)\, e^{i(kx-\omega_k t)} \tag{3.12}$$

because the right side represents a wave packet centered well to the left of the origin, i.e., in region I, whereas the corresponding S_{-+} contribution will correspond formally to a wave packet ~~at~~ centered at a large positive x, and thus outside region I, where (3.10) holds. Similarly for t large and negative, (3.11) will be essentially zero because the integral formally represents a wave packet centered at some large negative x, and thus not in region III.

By the same sort of reasoning, when <u>t is very large and positive</u>, it is plausible that

$$\sqrt{2\pi}\,\langle x|\psi(t)\rangle \simeq \int_0^\infty dk\, A(k)\,\Big[S_{-+}(k)\,e^{-i(kx+\omega_k t)} + S_{++}(k)\,e^{i(kx-\omega_k t)}\Big] \qquad (3.13)$$

since the wave packets represented by these two terms are now in regions I and III, respectively, whereas $\int_0^\infty A(k)\,e^{i(kx-\omega_k t)}\,dk$ represents a packet which is no longer in region I, and so makes a negligible contribution to (3.10). As for region II, we expect ψ to be almost zero at some time well before the collision [of the particle with the potential hill] because the wave packet has not yet arrived, and also long after the collision because the particle – or at least its wave packet – will have diffused away.

The right side of (3.12) is

$$\sqrt{2\pi}\ \langle x \mid \psi_0(t) \rangle$$

where

$$|\psi_0(t)\rangle = \int_0^\infty A(k) e^{-i\omega_k t} |k\rangle\, dk$$

is a wave function whose time development is given by free particle dynamics: $V=0$ everywhere. Hence we expect the scattering event can be imitated by applying S to $|\psi_0(t)\rangle$, and using (3.5) we find, in fact, that

$$|\bar{\psi}_0(t)\rangle := S|\psi_0(t)\rangle = \int_0^\infty dk\ A(k)\, e^{-i\omega_k t}\left[S_{++}(k)|k\rangle + S_{-+}(k)|-k\rangle\right]$$

Consequently

$$\sqrt{2\pi}\ \langle x \mid \bar{\psi}_0(t) \rangle$$

is precisely the right side of (3.13), which is the same as the actual wave function when t is very large. Thus the S operator has the expected property.

A similar argument can be used for a wave packet incident on the potential hill from the right.

Exercise 3.3.

Suppose that $V(x) \neq 0$ only near $x = 0$. Let $|\psi\rangle$ be a wave packet far to the right of the origin and traveling to the right. Discuss in qualitative terms the function

$$\langle x | e^{-iH_0 t} S | \psi \rangle$$

when t is large and positive, assuming that the transmission coefficient of barrier is small. Compare this with the case in which $|\psi\rangle$ represents a wave packet at the same position but traveling to the left.

Hint: A useful way of thinking about this problem is to use (2.10) as an approximation to S, ~~was~~ where t_1 is a very early time. What is $U_0(t_1)|\psi\rangle$ when t_1 is very negative?

4. The S Matrix for Three Dimensional Potential Scattering.

We'll simply state some results and not give the derivation, which will be found in Taylor.

The S matrix is a unitary operator which commutes with H_0. It is determined by its matrix elements which depend, of course, on the basis which is chosen. Plane wave states $|\vec{k}\rangle$, with

$$\langle \vec{r} | \vec{k} \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}} \tag{4.1}$$

are a convenient basis, and in this basis

$$\langle \vec{k}' | S | \vec{k} \rangle = \delta(\vec{k}' - \vec{k}) + \frac{i}{2\pi k} \delta(k' - k) f(\vec{k}' \leftarrow \vec{k}) \tag{4.2}$$

Here $k = |\vec{k}|$, $k' = |\vec{k}'|$, and $f(\vec{k}' \leftarrow \vec{k})$ is the scattering amplitude for an incident beam in the direction $\vec{k}$ scattering in the direction $\vec{k}'$. [For example, if $\vec{k} = k\hat{z}$, and $\vec{k}'$ makes an angle θ with the z axis, then $f(\vec{k}' \leftarrow \vec{k})$ is just the scattering amplitude $f(\theta)$ at this energy (i.e., $\hbar^2 k^2/2m$), ~~Note that~~ in the case of a spherically symmetrical potential.]

Note the difference between the two δ functions in (4.2)! The first, $\delta(\vec{k}'-\vec{k})$ is zero unless $\vec{k}'$ and $\vec{k}$ agree in magnitude and direction, while the second, $\delta(k'-k)$, means the magnitudes must be the same (this corresponds to energy conservation in the scattering), but the directions of $\vec{k}$ and $\vec{k}'$ can be different. Also note that the scattering potential need not be spherically symmetrical. However, it does have to be short ranged in some suitable sense (see Taylor, note at the bottom of his p. 42).

Equation (4.2) shows that the scattering amplitude ~~contains~~ (for all $\vec{k}$ and $\vec{k}'$) contains the same information as the S matrix. The fact that the S matrix is unitary does, however, place a condition on the scattering amplitude, which must satisfy [Taylor, p. 53]

$$\begin{aligned}&\int d\vec{k}''\, \delta(k''-k)\, f^*(\vec{k}''\leftarrow\vec{k}')\, f(\vec{k}''\leftarrow\vec{k})\\ &= 2\pi i k\, [\, f^*(\vec{k}\leftarrow\vec{k}') - f(\vec{k}'\leftarrow\vec{k})\,]\end{aligned} \tag{4.3}$$

One consequence of (4.3) is the optical theorem [Taylor, p.54]. Set $\vec{k}' = \vec{k}$ in (4.3). Then the integrand on the left is $\delta(k''-k)$ times $|f(\vec{k}'' \leftarrow \vec{k})|^2 = d\sigma/d\Omega$, and consequently the integral is equal to $k^2\sigma(\vec{k})$, where $\sigma(\vec{k})$ is the total scattering cross section for an incident beam in direction $\vec{k}$ of momentum $\hbar k$. This gives the result

$$\sigma(\vec{k}) = \frac{4\pi}{k} \operatorname{Im} f(\vec{k} \leftarrow \vec{k})$$

relating the total cross section to the imaginary part of the scattering amplitude in the forward direction.

When considering scattering from a spherically symmetrical potential it is convenient to analyze the problem in terms of partial waves and the corresponding phase shifts. For this purpose a more convenient basis than plane waves, (1.1), is provided by functions of the type

$$\psi_{k,l,m}(\vec{r}) = C_l \, j_l(kr)\, Y_l^m(\theta, \phi)$$

where C_l is some normalizing constant. The action of the S operator on such a function is then quite simple:

$$S\,\psi_{k,l,m} = e^{i2\delta_l(k)}\,\psi_{k,l,m}$$

where the l'th phaseshift δ_l depends on k, so this dependence is noted in the exponent. (See Taylor, pp 85 ff, who adopts a particular normalization and then gives matrix elements of S.)