7 Scattering

Physics is becoming so unbelievably complex that it is taking longer and longer to train a physicist. It is taking so long, in fact, to train a physicist to the place where he understands the nature of physical problems that he is already too old to solve them.
Eugene P. Wigner

Finding solutions of the time-dependent Schrödinger equation (6.87) is incredibly difficult, even for the simplest models. However, nature had mercy on us and created a very important class of experiments, where a description of dynamics by equation (6.87) is completely unnecessary, because it is too detailed. Here we are talking about scattering experiments, which are the topic of this chapter.

A typical scattering experiment is designed in such a way that free particles (or their bound states, such as atoms or nuclei) are prepared at a great distance from each other and directed into collision. Then experimentalists study the properties of free particles or stable bound states leaving the collision region. In these experiments, as a rule, it is impossible to see evolution during the interaction process: particle reactions occur almost instantaneously, and we can observe only reactants and products moving freely before and after the collision. In such situations, the theory is not required to describe the true dynamics of the particles during the short interval of interaction. It is sufficient to understand only the mapping of free states before the collision to free states after the collision. This mapping is described by the so-called S-operator, which we are going to discuss in the next section.

In Section 7.2 we will consider the situation of scattering equivalence when two different Hamiltonians have exactly the same scattering properties.

7.1 Scattering operators

7.1.1 Physical meaning of S-operator

Let us consider a scattering experiment in which the free states of the reactants were prepared in the distant past, so $t = -\infty$. The collision itself occurred within a short interval $[\eta', \eta]$ near time zero.[1] Free states of the collision products are registered in the distant future, $t = \infty$, so that the inequalities $-\infty \ll \eta' < 0 < \eta \ll \infty$ are satisfied. For simplicity, we assume that the two colliding particles do not form bound states either before or after the collision. Therefore, at asymptotically distant times, the exact

1 The short interaction time interval (and the applicability of the scattering theory) is guaranteed if three conditions are satisfied. First, the interaction between particles is short-range or, in a more general setting, cluster-separable. Second, the states of particles are describable by localized wave packets, for example, as in Section 6.6.1. Third, the velocities (or momenta) of the particles are high enough.

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time evolution of the system is well approximated by the noninteracting operators $U_0(\eta' \leftarrow -\infty)$ and $U_0(\infty \leftarrow \eta)$.[2] Then the full evolution operator from the remote past to the distant future is (here we use properties (6.84) and (6.85))

$$\begin{aligned} U(\infty \leftarrow -\infty) &\approx U_0(\infty \leftarrow \eta) U(\eta \leftarrow \eta') U_0(\eta' \leftarrow -\infty) \\ &= U_0(\infty \leftarrow \eta) U_0(\eta \leftarrow 0) [U_0(0 \leftarrow \eta) U(\eta \leftarrow \eta') U_0(\eta' \leftarrow 0)] \\ &\quad \times U_0(0 \leftarrow \eta') U_0(\eta' \leftarrow -\infty) \\ &= U_0(\infty \leftarrow 0) S_{\eta,\eta'} U_0(0 \leftarrow -\infty), \end{aligned} \tag{7.1}$$

where we denote

$$S_{\eta,\eta'} \equiv U_0(0 \leftarrow \eta) U(\eta \leftarrow \eta') U_0(\eta' \leftarrow 0). \tag{7.2}$$

Equation (7.1) means that it is possible to formulate a simplified description for the time evolution in collision processes. In this description, the evolution is always free, except for a sudden change of state at the time $t = 0$. This change is described by the unitary operator $S_{\eta,\eta'}$. Approximation (7.1) becomes more accurate if we increase the time interval $[\eta', \eta]$, during which the exact time evolution is taken into account, i. e., in the limits $\eta' \to -\infty$ and $\eta \to \infty$.[3] Therefore, the exact formula for the time evolution from $-\infty$ to ∞ has the form

$$U(\infty \leftarrow -\infty) = U_0(\infty \leftarrow 0) S U_0(0 \leftarrow -\infty), \tag{7.3}$$

where the S-operator (or *scattering operator*) is defined by

$$\begin{aligned} S &= \lim_{\eta' \to -\infty, \eta \to \infty} S_{\eta,\eta'} = \lim_{\eta' \to -\infty, \eta \to \infty} U_0(0 \leftarrow \eta) U(\eta \leftarrow \eta') U_0(\eta' \leftarrow 0) \\ &= \lim_{\eta' \to -\infty, \eta \to \infty} e^{\frac{i}{\hbar} H_0 \eta} e^{-\frac{i}{\hbar} H(\eta - \eta')} e^{-\frac{i}{\hbar} H_0 \eta'} \\ &= \lim_{\eta \to \infty} S(\eta), \end{aligned} \tag{7.4}$$

where

$$S(\eta) \equiv \lim_{\eta' \to -\infty} e^{\frac{i}{\hbar} H_0 \eta} e^{-\frac{i}{\hbar} H(\eta - \eta')} e^{-\frac{i}{\hbar} H_0 \eta'}. \tag{7.5}$$

To better understand how scattering theory describes the time evolution, we turn to Figure 7.1. In this figure, we have plotted the state of the physical system (represented

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2 Here we denote by $U_0(t \leftarrow t_0) \equiv \exp(-\frac{i}{\hbar} H_0 (t - t_0))$ the time evolution operator associated with the noninteracting Hamiltonian H_0. The interaction evolution operator will be denoted by $U(t \leftarrow t_0) \equiv \exp(-\frac{i}{\hbar} H (t - t_0))$. In the Schrödinger representation, this operator acts on state vectors, as in (6.86).

3 Of course, we assume that the right-hand side of (7.2) converges in these limits. The question of convergence will be discussed briefly in Section 7.1.4.

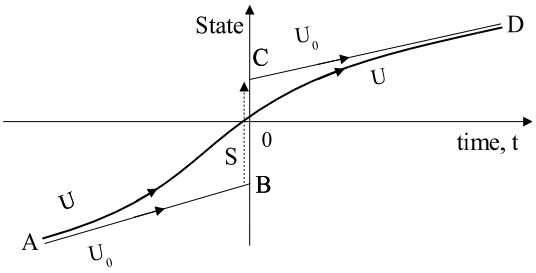

Figure 7.1: Schematic representation of the scattering process.

abstractly as a point on the vertical axis) as a function of time. The exact development of the system, governed by the complete evolution operator U, is shown by the thick line $A \to D$. In asymptotic regions (when the time t is either very negative or very positive), the interaction between the colliding parts of the system is weak. In these regions, the exact time evolution can be rather well approximated by the free operator U_0. These free "trajectories" are shown in the figure by two thin straight lines with arrows: one for very positive times $C \to D$ and the other for very negative times $A \to B$. The thick line (the exact interacting time evolution) asymptotically approaches these thin lines (free evolution) in the remote past (near A) and in the distant future (near D).

If we extrapolate the future and past free evolutions to the time $t = 0$, we will realize that there is a gap B–C between these extrapolated states. The S-operator is defined precisely in such a way as to close this gap, i. e., to connect the free extrapolated states B and C, as shown by the dashed arrow in the figure.

So, in the theory of scattering, the exact time evolution $A \to D$ is approximated in three stages: first the system develops freely up to the time instant $t = 0$, i. e., from A to B. Then there is a sharp jump $B \to C$, represented by the S-operator. Finally, the system again goes into the free evolution mode $C \to D$. As can be seen from the figure, this description of the scattering process is absolutely accurate, as long as we are interested only in the mapping of asymptotically free states from the remote past (A) into asymptotically free states in the distant future (D).

It should also be clear that the scattering operator S contains information about particle interactions in an averaged form integrated over the infinite time interval $t \in (-\infty, \infty)$. This operator is not designed to describe the interacting time evolution during the short interval of collision ($t \approx 0$). For these purposes, we would need the complete interacting time evolution operator U.

In applications, we are mainly interested in matrix elements of the S-operator

$$S_{i \to f} = \langle f|S|i\rangle, \tag{7.6}$$

where $|i\rangle$ is the initial state of the colliding particles and $|f\rangle$ is their final state. Such matrix elements are called the *S-matrix*. Formulas relating the S-matrix to observable quantities, such as scattering cross sections, can be found in any textbook on scattering theory [33, 83].

An important property of the S-operator is its "Poincaré invariance," i. e., zero commutators with generators of the noninteracting representation of the Poincaré group [89, 43],

$$[S, H_0] = [S, \boldsymbol{P}_0] = [S, \boldsymbol{J}_0] = [S, \boldsymbol{K}_0] = 0. \tag{7.7}$$

In particular, the commutator $[S, H_0] = 0$ implies that in (7.3) we can interchange U_0 and S, so that the full interacting time evolution can be represented as the following product of the free evolution and the S-operator:

$$U(\infty \leftarrow -\infty) = SU_0(\infty \leftarrow -\infty) = U_0(\infty \leftarrow -\infty)S. \tag{7.8}$$

7.1.2 *S*-operator in perturbation theory

There are many methods for calculating the S-operator. In this book, we will mainly use perturbation theory. To derive the perturbation theory series for the S-operator, we first note that the operator $S(t)$ in (7.5) satisfies the equation

$$\begin{aligned}
\frac{d}{dt}S(t) &= \frac{d}{dt}\lim_{t'\to-\infty} e^{\frac{i}{\hbar}H_0 t}e^{-\frac{i}{\hbar}H(t-t')}e^{-\frac{i}{\hbar}H_0 t'} \\
&= \lim_{t'\to-\infty}\left(e^{\frac{i}{\hbar}H_0 t}\left(\frac{i}{\hbar}H_0\right)e^{-\frac{i}{\hbar}H(t-t')}e^{-\frac{i}{\hbar}H_0 t'} + e^{\frac{i}{\hbar}H_0 t}\left(-\frac{i}{\hbar}H\right)e^{-\frac{i}{\hbar}H(t-t')}e^{-\frac{i}{\hbar}H_0 t'}\right) \\
&= -\frac{i}{\hbar}\lim_{t'\to-\infty} e^{\frac{i}{\hbar}H_0 t}(H - H_0)e^{-\frac{i}{\hbar}H(t-t')}e^{-\frac{i}{\hbar}H_0 t'} \\
&= -\frac{i}{\hbar}\lim_{t'\to-\infty} e^{\frac{i}{\hbar}H_0 t}Ve^{-\frac{i}{\hbar}H(t-t')}e^{-\frac{i}{\hbar}H_0 t'} \\
&= -\frac{i}{\hbar}\lim_{t'\to-\infty} e^{\frac{i}{\hbar}H_0 t}Ve^{-\frac{i}{\hbar}H_0 t}e^{\frac{i}{\hbar}H_0 t}e^{-\frac{i}{\hbar}H(t-t')}e^{-\frac{i}{\hbar}H_0 t'} \\
&= -\frac{i}{\hbar}\lim_{t'\to-\infty} V(t)e^{\frac{i}{\hbar}H_0 t}e^{-\frac{i}{\hbar}H(t-t')}e^{-\frac{i}{\hbar}H_0 t'} \\
&= -\frac{i}{\hbar}V(t)S(t),
\end{aligned} \tag{7.9}$$

where we denote[4]

$$V(t) = e^{\frac{i}{\hbar}H_0 t}Ve^{-\frac{i}{\hbar}H_0 t}. \tag{7.10}$$

4 Note that the t-dependence in $V(t)$ does not mean that we are considering time-dependent interactions. The argument t has no relation with the true *time* dependence of operators in the Heisenberg representation. The latter must be generated by the full interacting Hamiltonian H, not by the free Hamiltonian H_0, as in equation (7.10). To emphasize this difference, in cases like (7.10) we will talk about "t-dependence" instead of "time-dependence".

By a direct substitution, one can verify that a solution of equation (7.9) with the natural initial condition $S(-\infty) = 1$ is given by the Dyson perturbation series

$$S(t) = 1 - \frac{i}{\hbar}\int_{-\infty}^{t} V(t')dt' - \frac{1}{\hbar^2}\int_{-\infty}^{t} V(t')dt' \int_{-\infty}^{t'} V(t'')dt'' + \cdots.$$

Therefore, the S-operator can be calculated by substituting $t = +\infty$ as the upper limit of t-integrals, so we have

$$S = 1 - \frac{i}{\hbar}\int_{-\infty}^{+\infty} V(t')dt' - \frac{1}{\hbar^2}\int_{-\infty}^{+\infty} V(t')dt' \int_{-\infty}^{t'} V(t'')dt'' + \cdots. \tag{7.11}$$

As a rule, only the first few terms of this series are used in calculations, assuming, therefore, that the interaction V is so weak that it can be regarded as a small perturbation; and the scattering itself is just a small correction to the free propagation of particles. We shall say that a term in the perturbation theory series has *order n* if it contains a product of n factors V. Thus, in (7.11) we have explicit terms in the zero, first and second perturbation orders. We do not want to dwell on mathematical details related to (nontrivial) convergence properties of the expansion (7.11). Throughout this book, we will tacitly assume that all relevant perturbation series do converge.

7.1.3 Convenient notation for *t*-integrals

We shall often use the following symbols for t-integrals:

$$\underline{Y(t)} \equiv -\frac{i}{\hbar}\int_{-\infty}^{t} Y(t')dt'. \tag{7.12}$$

$$\underbrace{Y}\equiv -\frac{i}{\hbar}\int_{-\infty}^{+\infty} Y(t')dt' = \underline{Y(\infty)}. \tag{7.13}$$

In this notation, the perturbation theory series for the S-operator (7.11) has a compact form. We have

$$S = 1 + \underbrace{\Sigma}, \tag{7.14}$$

$$\Sigma(t) = V(t) + V(t)\underline{V(t')} + V(t)\underline{V(t')V(t'')} + V(t)\underline{V(t')V(t'')V(t''')} + \cdots. \tag{7.15}$$

Equations (7.14)–(7.15) do not represent the only perturbative expansion of the S-operator and perhaps not even the most convenient one. In quantum field theory,

the preference is given to the time-ordered perturbation series [89, 63], which uses time ordering of interaction operators in the following integrand[5]:

$$S = 1 - \frac{i}{\hbar}\int_{-\infty}^{+\infty} dt_1 V(t_1) - \frac{1}{2!\hbar^2}\int_{-\infty}^{+\infty} dt_1 dt_2 T\big[V(t_1)V(t_2)\big] + \frac{i}{3!\hbar^3}\int_{-\infty}^{+\infty} dt_1 dt_2 dt_3 T\big[V(t_1)V(t_2)V(t_3)\big] + \frac{1}{4!\hbar^4}\int_{-\infty}^{+\infty} dt_1 dt_2 dt_3 dt_4 T\big[V(t_1)V(t_2)V(t_3)V(t_4)\big] + \cdots . \tag{7.17}$$

In the second volume of our book, we will find another useful perturbative expression, proposed by Magnus [51, 62, 12], i. e.,

$$S = \exp(\underbrace{\Phi}). \tag{7.18}$$

In this formula, the Hermitian operator $\Phi(t)$ is called the *scattering phase*. It is represented by a series of multiple commutators with t-integrals,

$$\Phi(t) = V(t) - \frac{1}{2}\Big[\underline{V(t')}, V(t)\Big] + \frac{1}{6}\Big[\underline{\underline{V(t'')}}, \big[V(t'), V(t)\big]\Big] + \frac{1}{6}\Big[\underline{\big[V(t''), V(t')\big]}, V(t)\Big] - \frac{1}{12}\Big[\underline{\underline{\underline{V(t''')}}}, \big[\big[V(t''), V(t')\big], V(t)\big]\Big] - \frac{1}{12}\Big[\underline{\underline{\big[V(t'''), \big[V(t''), V(t')\big]\big]}}, V(t)\Big] - \frac{1}{12}\Big[\underline{\underline{\big[V(t'''), V(t'')\big]}}, \big[V(t'), V(t)\big]\Big] + \cdots . \tag{7.19}$$

An important advantage of equation (7.18) is that it explicitly preserves the unitarity of the S-operator in each perturbation order.[6] The three listed perturbation theory series (Dyson, time-ordered and Magnus) are equivalent in the sense that in the limit $n \to \infty$ they converge to the same S-operator. However, in each finite order n their terms can differ.

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5 When applied to a product of several t-dependent boson operators, the time ordering symbol T changes the order of the operators so that their t arguments increase from right to left, e. g.,

$$T\big[A(t_1)B(t_2)\big] = \begin{cases} A(t_1)B(t_2), & \text{if } t_1 > t_2, \\ B(t_2)A(t_1), & \text{if } t_1 < t_2. \end{cases} \tag{7.16}$$

6 The argument of the exponent is an anti-Hermitian operator $\underbrace{\Phi}$; therefore the exponent itself is unitary.

For brevity, we will often omit t-arguments in operator expressions. Then equations (7.15) and (7.19) simplify, even more, to

$$\Sigma = V + V\underline{V} + V\underline{V}\,\underline{V} + \cdots, \tag{7.20}$$

$$\Phi = V - \frac{1}{2}[\underline{V}, V] + \frac{1}{6}\Big[\underline{\underline{V}}, [V, V]\Big] + \cdots. \tag{7.21}$$

7.1.4 Adiabatic switching of interaction

In formulas for scattering operators (7.15) and (7.19), we encounter t-integrals $\underline{V(t)}$. Straightforward calculation of such integrals leads to a rather depressing result. To understand, let us introduce the complete basis $|n\rangle$ of eigenvectors of the free Hamiltonian,

$$H_0|n\rangle = E_n|n\rangle, \tag{7.22}$$

$$\sum_n |n\rangle\langle n| = 1, \tag{7.23}$$

and calculate matrix elements of $\underline{V(t)}$ in this basis. Then we have

$$\langle n|\underline{V(t)}|m\rangle \equiv -\frac{i}{\hbar}\int\limits_{-\infty}^{t} \langle n|e^{\frac{i}{\hbar}H_0 t'} V e^{-\frac{i}{\hbar}H_0 t'}|m\rangle dt' = -\frac{i}{\hbar}V_{nm}\int\limits_{-\infty}^{t} e^{\frac{i}{\hbar}(E_n - E_m)t'}dt'$$

$$= -V_{nm}\left(\frac{e^{\frac{i}{\hbar}(E_n-E_m)t}}{E_n - E_m} - \frac{e^{\frac{i}{\hbar}(E_n-E_m)(-\infty)}}{E_n - E_m}\right). \tag{7.24}$$

What can we do with the meaningless term on the right-hand side that contains $(-\infty)$?

This term can be made harmless if we take into account the important fact that the S-operator cannot be applied to all states in the Hilbert space. According to our discussion in Section 7.1.1, scattering theory is applicable in its entirety only to *scattering states* $|\Psi\rangle$, in which free particles are far apart in the asymptotic limits $t \to \pm\infty$, so that the time evolution of these states coincides with free evolution in the remote past and in the distant future. Naturally, these assumptions are inapplicable to all states in the Hilbert space. For example, the time evolution of bound states of the full Hamiltonian H does not resemble the free evolution in any time interval. It turns out that if we restrict our theory only to scattering states,[7] then there are no problems with t-integrals.

Indeed, for scattering states $|\Psi\rangle$, the interaction operator effectively vanishes in asymptotic regions, so we can write

7 Usually, such states can be constructed from asymptotic wave packets, which are well localized in both the position and momentum spaces; see, for example, Section 6.6.1.

$$\lim_{t\to\pm\infty} Ve^{-\frac{i}{\hbar}H_0 t}|\Psi\rangle = 0,$$
$$\lim_{t\to\pm\infty} V(t)|\Psi\rangle = \lim_{t\to\pm\infty} e^{\frac{i}{\hbar}H_0 t}\left(Ve^{-\frac{i}{\hbar}H_0 t}|\Psi\rangle\right) = 0. \tag{7.25}$$

How can we apply this condition to calculations of integrals like (7.24)?

One approach to a rigorous formulation of scattering theory is the explicit consideration of localized wave packets [33]. Then, the cluster separability (= short range) of the interaction V ensures the correct asymptotic behavior of colliding particles and the validity of equation (7.25). However, this approach is rather complicated, and we prefer to keep away from wave packets.

There is another, less rigorous, but shorter way to achieve the same goal – to use a trick known as the *adiabatic switching*. The idea is to add the property (7.25) "by hands." To do this, we multiply $V(t)$ by a real nonnegative function of t that grows slowly from zero (= interaction is "off") at $t = -\infty$ to 1 in the vicinity of $t \approx 0$ (interaction is "on") and then slowly decreases back to zero at $t = +\infty$ (interaction "switches off" again). For example, one convenient choice for such a function is the exponent

$$V(t) = e^{\frac{i}{\hbar}H_0 t} V e^{-\frac{i}{\hbar}H_0 t} e^{-\epsilon|t|}. \tag{7.26}$$

If the parameter ϵ is small and positive, then such a modification of the interaction operator will have no effect on the movement of wave packets and on the S-matrix.[8] For the integral (7.24), we then get

$$\langle n|\underline{V(t)}|m\rangle \approx -V_{nm}\left(\frac{e^{\frac{i}{\hbar}(E_n-E_m)t-\epsilon|t|}}{E_n-E_m} - \frac{e^{\frac{i}{\hbar}(E_n-E_m)(-\infty)-\epsilon(\infty)}}{E_n-E_m}\right)$$
$$= -V_{nm}\frac{e^{\frac{i}{\hbar}(E_n-E_m)t-\epsilon|t|}}{E_n-E_m}.$$

At the end of the calculations, we have to go to the limit $\epsilon \to +0$. Then the t-integral becomes

$$\langle n|\underline{V(t)}|m\rangle \longrightarrow -V_{nm}\frac{e^{\frac{i}{\hbar}(E_n-E_m)t}}{E_n-E_m} \tag{7.27}$$

and the unpleasant expression $e^{i\infty}$ vanishes.

The "adiabatic switching" trick makes possible an alternative derivation of equation (7.11). Take equation (6.89) with the initial time in the remote past $t_0 = -\infty$ and the final time in the distant future $t = +\infty$. Then we have

$$|\Psi(+\infty)\rangle = \lim_{t\to+\infty} e^{-\frac{i}{\hbar}H_0(t-t_0)}\left(1 - \frac{i}{\hbar}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}H_0(t'-t_0)} V e^{-\frac{i}{\hbar}H_0(t'-t_0)} dt'\right.$$

8 Indeed, when the interaction is "off," the wave packets are far from each other, anyway.

$$
\left. - \frac{1}{\hbar^2} \int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}H_0(t'-t_0)} V e^{-\frac{i}{\hbar}H_0(t'-t_0)} dt' \int\limits_{-\infty}^{t'} e^{\frac{i}{\hbar}H_0(t''-t_0)} V e^{-\frac{i}{\hbar}H_0(t''-t_0)} dt'' + \cdots \right)
$$
$$
\times |\Psi(-\infty)\rangle.
$$

Then change the integration variables $t' - t_0 = \tau'$ and $t'' - t_0 = \tau''$ so that[9]

$$
\begin{aligned}
|\Psi(+\infty)\rangle &= U_0(\infty \leftarrow -\infty) \lim_{t\to+\infty} \left(1 - \frac{i}{\hbar} \int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}H_0\tau'} V e^{-\frac{i}{\hbar}H_0\tau'} d\tau' \right. \\
&\left. - \frac{1}{\hbar^2} \int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}H_0\tau'} V e^{-\frac{i}{\hbar}H_0\tau'} d\tau' \int\limits_{-\infty}^{\tau'} e^{\frac{i}{\hbar}H_0\tau''} V e^{-\frac{i}{\hbar}H_0\tau''} d\tau'' + \cdots \right) |\Psi(-\infty)\rangle \\
&= U_0(\infty \leftarrow -\infty) S |\Psi(-\infty)\rangle.
\end{aligned}
$$

Comparing this formula with equation (7.8), we conclude that the S-factor is exactly as in (7.11).

7.1.5 *T*-matrix

In this subsection we will get acquainted with a useful concept of the T matrix.[10] Let us calculate matrix elements of the S-operator (7.11) in the basis of eigenvectors of the free Hamiltonian (7.22)–(7.23).[11] We have

$$
\begin{aligned}
\langle n|S|m\rangle &= \delta_{nm} - \frac{i}{\hbar} \int\limits_{-\infty}^{\infty} \langle n| e^{\frac{i}{\hbar}H_0 t'} V e^{-\frac{i}{\hbar}H_0 t'} |m\rangle dt' \\
&\quad - \frac{1}{\hbar^2} \int\limits_{-\infty}^{\infty} \langle n| e^{\frac{i}{\hbar}H_0 t'} V e^{-\frac{i}{\hbar}H_0 t'} |k\rangle dt' \int\limits_{-\infty}^{t'} \langle k| e^{\frac{i}{\hbar}H_0 t''} V e^{-\frac{i}{\hbar}H_0 t''} |m\rangle dt'' + \cdots \\
&= \delta_{nm} - \frac{i}{\hbar} \int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(E_n - E_m)t'} V_{nm} dt' \\
&\quad - \frac{1}{\hbar^2} \int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(E_n - E_k)t'} V_{nk} dt' \int\limits_{-\infty}^{t'} e^{\frac{i}{\hbar}(E_k - E_m)t''} V_{km} dt'' + \cdots
\end{aligned}
$$

---

9 For brevity, we do not show the "adiabatic switching" factors explicitly. They force the integrands to vanish at $\pm\infty$ asymptotics. So, they allow us to leave the infinite integration limits ($-\infty$ and ∞) unchanged.

10 I am grateful to Cao Bin for online communications that led to the writing of this subsection.

11 Summation over repeated indices k and l is implied. Equation (7.27) is used for t-integrals.

$$
\begin{aligned}
&= \delta_{nm} - 2\pi i\delta(E_n - E_m)V_{nm} + \frac{i}{\hbar}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}(E_n-E_k)t'}dt'\frac{e^{\frac{i}{\hbar}(E_k-E_m)t'}}{E_m - E_k}V_{nk}V_{km} + \cdots \\
&= \delta_{nm} - 2\pi i\delta(E_n - E_m)V_{nm} + 2\pi i\delta(E_n - E_m)\frac{1}{E_m - E_k}V_{nk}V_{km} + \cdots \\
&= \delta_{nm} - 2\pi i\delta(E_n - E_m)V_{nk} \\
&\quad \times \left(\delta_{km} + \frac{1}{E_m - E_k}V_{km} + \frac{1}{E_m - E_k}V_{kl}\frac{1}{E_m - E_l}V_{lm} + \cdots\right) \\
&= \delta_{nm} - 2\pi i\delta(E_n - E_m)T_{nm}. \qquad (7.28)
\end{aligned}
$$

The first term is the unit matrix expressing the free propagation of particles. The matrix in the second term is called the *transition matrix* (or *T-matrix*).[12] We have

$$
\begin{aligned}
T_{nm} &\equiv V_{nk}\left(\delta_{km} + \frac{1}{E_m - E_k}V_{km} + \frac{1}{E_m - E_k}V_{kl}\frac{1}{E_m - E_l}V_{lm} + \cdots\right) \\
&= \langle n|V|k\rangle\langle k|m\rangle + \langle n|V(E_m - E_k)^{-1}|k\rangle\langle k|V|m\rangle \\
&\quad + \langle n|V(E_m - E_k)^{-1}|k\rangle\langle k|V(E_m - E_l)^{-1}|l\rangle\langle l|V|m\rangle + \cdots \\
&= \langle n|V|k\rangle\langle k|m\rangle + \langle n|V(E - H_0)^{-1}|k\rangle\langle k|V|m\rangle \\
&\quad + \langle n|V(E - H_0)^{-1}|k\rangle\langle k|V(E - H_0)^{-1}|l\rangle\langle l|V|m\rangle + \cdots \\
&= \langle n|V|m\rangle + \langle n|V(E - H_0)^{-1}V|m\rangle \\
&\quad + \langle n|V(E - H_0)^{-1}V(E - H_0)^{-1}V|m\rangle + \cdots \\
&= \langle n|V\left(1 + \frac{1}{E - H_0}V + \frac{1}{E - H_0}V\frac{1}{E - H_0}V + \cdots\right)|m\rangle.
\end{aligned}
$$

The infinite series in the parenthesis can be summed by the standard formula $(1-x)^{-1} = 1 + x + x^2 + \cdots$, so we have

$$
\begin{aligned}
T_{nm} &= \langle n|V\frac{1}{1 - (E - H_0)^{-1}V}|m\rangle = \langle n|V(E - H_0)(E - H_0 - V)^{-1}|m\rangle \\
&= \langle n|V(E - H_0)(E - H)^{-1}|m\rangle = \langle n|T(E)|m\rangle.
\end{aligned}
$$

Thus, the T-matrix is represented by matrix elements of the energy-dependent $T(E)$-operator and we have

$$
T(E) \equiv V(E - H_0)(E - H)^{-1}. \qquad (7.29)
$$

The beauty of this result is that it provides a closed expression for the S-operator that goes beyond perturbation theory. This result is widely used in numerical calculations [69, 13, 48, 24].

12 Taking into account the fact that the T-matrix enters the S-matrix multiplied by the delta-function of energy $\delta(E_n - E_m)$, we have denoted $E = E_m = E_n$.

7.1.6 *S*-matrix and bound states

The formal expression (7.29) can be used to derive an important connection between poles of the *S*-matrix and energies of bound states. Our derivation will be formally heuristic. More rigorous reasoning can be found in textbooks on scattering theory [33, 83].

We already mentioned that scattering theory can be formulated only for states that behave asymptotically as free ones. The energy E of such states exceeds the energy E_0 of separated reactants at rest, for which we have

$$E_0 = \sum_{a=1}^{N} m_a c^2.$$

Therefore, the operator $T(E)$ introduced in (7.29) has a well-defined meaning only in the energy interval

$$E \in [E_0, \infty). \tag{7.30}$$

There are reasons to believe that this operator is an analytic function of energy E. Therefore, it would be interesting to find out where the poles of this function are located. We can expect the appearance of poles at those values of E, where the denominator of the expression $(E - H_0)(E - H)^{-1}$ in (7.29) vanishes. Hence (at least some of) the poles E_α can be found as solutions of the eigenvalue equation

$$(H - E_\alpha)|\Psi_\alpha\rangle = 0.$$

Obviously, this is the familiar stationary Schrödinger equation (6.79) for bound states. This means that there is a connection between poles of the T-operator and energies of bound states E_α of the full Hamiltonian H.[13] These energies are always lower than E_0, i. e., formally they are outside the domain of the operator $T(E)$. Therefore, the above-mentioned connection (poles of the T-operator) $\leftrightarrow$ (energies of bound states) can be established only in the sense of analytic continuation of the operator $T(E)$ from its natural domain (7.30) to values below E_0.

It is important to emphasize that the possibility of finding the energies of the bound states E_α from the T-operator does not mean that the eigenvectors of these states $|\Psi_\alpha\rangle$ can be found in the same way. All bound states are eigenstates of the T-operator, corresponding only to one (infinite) eigenvalue. Therefore, even knowing the exact T-operator, the most we can do is to find a subspace in $\mathscr{H}$ that is the linear span of all bound states. This ambiguity is closely related to the scattering equivalence of Hamiltonians, which we shall consider in the next section.

13 Similarly, the S-operator can be also regarded as an analytic function $S(E)$ on the complex energy plane with poles at positions $E = E_\alpha$.

7.2 Scattering equivalence

The results of the previous section indicate that even exact knowledge of the S-operator does not allow us to completely reconstruct the corresponding Hamiltonian H. In other words, many different Hamiltonians can have identical scattering properties. Here we will discuss these issues in more detail, because they will play an important role in Volume 3.

7.2.1 Equivalent Hamiltonians

The S-operator and the Hamiltonian are two fundamentally different ways of describing dynamics. From the Hamiltonian H one can obtain the evolution operator $U(t \leftarrow t_0) \equiv e^{-\frac{i}{\hbar}H(t-t_0)}$, which describes in detail the development of states in all time intervals, both large and small. On the other hand, the S-operator represents only the "integrated" time evolution in the infinite interval. In other words, if we know the state of the system in the remote past $|\Psi(-\infty)\rangle$, the free Hamiltonian H_0 and the scattering operator S, then we can find the final state of the system in the far future (7.8), i. e.,

$$|\Psi(\infty)\rangle = U(\infty \leftarrow -\infty)|\Psi(-\infty)\rangle = U_0(\infty \leftarrow -\infty)S|\Psi(-\infty)\rangle.$$

However, we cannot say anything about the system's evolution in the interacting regime.

Despite its incomplete nature, the information contained in the S-operator is fully sufficient for the analysis of most experiments in high-energy physics. In particular, from the S-operator one can obtain accurate scattering cross sections as well as energies and lifetimes of stable and metastable bound states. This situation gave the impression that an exhaustive theory of elementary particles could be constructed on the basis of the S-operator alone without resorting to the Hamiltonian and wave functions. However, this impression is deceptive, because the description of physics by means of scattering theory is incomplete, and such a theory is applicable only to a limited class of experiments.

Knowing the full interacting Hamiltonian H, we can calculate the corresponding S-operator by formulas (7.14), (7.17) or (7.18). However, the converse is not true: even if the S-operator is fully known, it is impossible to recover the unique underlying Hamiltonian. The same S-operator can be obtained from many different Hamiltonians.

Suppose that two Hamiltonians H and H' are related to each other by a unitary transformation $e^{i\Xi}$, i. e.,

$$H' = e^{i\Xi} H e^{-i\Xi}. \tag{7.31}$$

Then they have exactly the same scattering properties[14] if the following condition is satisfied:

$$\lim_{t\to\pm\infty} e^{\frac{i}{\hbar}H_0 t}\Xi e^{-\frac{i}{\hbar}H_0 t} = 0. \tag{7.32}$$

Indeed, in the limits $\eta \to +\infty$, $\eta' \to -\infty$, we obtain from (7.5) that the two scattering operators are equal [26],[15] i. e.,

$$\begin{aligned} S' &= \lim_{\eta'\to-\infty,\eta\to\infty} e^{\frac{i}{\hbar}H_0\eta}e^{-\frac{i}{\hbar}H'(\eta-\eta')}e^{-\frac{i}{\hbar}H_0\eta'} \\ &= \lim_{\eta'\to-\infty,\eta\to\infty} e^{\frac{i}{\hbar}H_0\eta}(e^{i\Xi}e^{-\frac{i}{\hbar}H(\eta-\eta')}e^{-i\Xi})e^{-\frac{i}{\hbar}H_0\eta'} \\ &= \lim_{\eta'\to-\infty,\eta\to\infty} (e^{\frac{i}{\hbar}H_0\eta}e^{i\Xi}e^{-\frac{i}{\hbar}H_0\eta})e^{\frac{i}{\hbar}H_0\eta}e^{-\frac{i}{\hbar}H(\eta-\eta')}e^{-\frac{i}{\hbar}H_0\eta'} \\ &\quad \times (e^{\frac{i}{\hbar}H_0\eta'}e^{-i\Xi}e^{-\frac{i}{\hbar}H_0\eta'}) \qquad (7.33) \\ &= \lim_{\eta'\to-\infty,\eta\to\infty} e^{\frac{i}{\hbar}H_0\eta}e^{-\frac{i}{\hbar}H(\eta-\eta')}e^{-\frac{i}{\hbar}H_0\eta'} = S. \qquad (7.34) \end{aligned}$$

Note that, due to Lemma G.9, the energy spectra of the two equivalent Hamiltonians H and H' also coincide. However, their eigenvectors could be different, and the corresponding description of dynamics (e. g., by equation (6.88)) could also differ. Therefore, two theories predicting the same scattering are not necessarily equivalent in the full physical sense.

7.2.2 Bakamjian construction of point-form dynamics

It turns out that the above statement about scattering equivalent Hamiltonians can be generalized in the sense that even two different forms of dynamics (for example, the instant and point forms) can have the same S-operators. This nontrivial fact will be discussed in Section 7.2.4. To prepare for this discussion, here we will build a specific version of the point form of dynamics, using a recipe due to Bakamjian [5]. This method is very similar to the method of Bakamjian–Thomas from Section 6.3.2.

We consider a system of $n \geq 2$ massive free particles with noninteracting operators of mass M_0, linear momentum $\boldsymbol{P}_0$, angular momentum $\boldsymbol{J}_0$, center-of-energy position

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14 We say that such Hamiltonians are *scattering-equivalent*.

15 In (7.33) we use condition (7.32) to make replacements

$$\begin{aligned} &\lim_{\eta\to\infty}\left[\exp\left(\frac{i}{\hbar}H_0\eta\right)\exp(i\Xi)\exp\left(-\frac{i}{\hbar}H_0\eta\right)\right] \\ &\quad = \lim_{\eta'\to-\infty}\left[\exp\left(\frac{i}{\hbar}H_0\eta'\right)\exp(-i\Xi)\exp\left(-\frac{i}{\hbar}H_0\eta'\right)\right] = 1. \end{aligned}$$

.

$\boldsymbol{R}_0$ and spin $\boldsymbol{S}_0 = \boldsymbol{J}_0 - [\boldsymbol{R}_0 \times \boldsymbol{P}_0]$. Then we introduce two new operators,

$$\boldsymbol{Q}_0 \equiv \frac{\boldsymbol{P}_0}{M_0 c^2},$$
$$\boldsymbol{X}_0 \equiv M_0 c^2 \boldsymbol{R}_0,$$

which satisfy the canonical commutation relations

$$[X_{0i}, Q_{0i}] = [X_{0i}, X_{0j}] = [Q_{0i}, Q_{0j}] = 0,$$
$$[X_{0i}, Q_{0j}] = i\hbar\delta_{ij}.$$

Next, we express the generators $\{H_0, \boldsymbol{P}_0, \boldsymbol{J}_0, \boldsymbol{K}_0\}$ of the noninteracting representation of the Poincaré group through the alternative set of operators $\{M_0, \boldsymbol{Q}_0, \boldsymbol{X}_0, \boldsymbol{S}_0\}$ as follows (compare with (6.37)–(6.38)):

$$\boldsymbol{P}_0 = M_0 c^2 \boldsymbol{Q}_0,$$
$$\boldsymbol{K}_0 = -\frac{1}{2}\left(\sqrt{1 + Q_0^2 c^2}\boldsymbol{X}_0 + \boldsymbol{X}_0\sqrt{1 + Q_0^2 c^2}\right) - \frac{[\boldsymbol{Q}_0 \times \boldsymbol{S}_0]}{1 + \sqrt{1 + Q_0^2 c^2}},$$
$$\boldsymbol{J}_0 = [\boldsymbol{X}_0 \times \boldsymbol{Q}_0] + \boldsymbol{S}_0,$$
$$H_0 = M_0 c^2 \sqrt{1 + Q_0^2 c^2}.$$

Now, a point-form interaction can be introduced by modifying the mass operator

$$M_0 \to M \tag{7.35}$$

so as to satisfy the following conditions[16]:

$$[M, \boldsymbol{Q}_0] = [M, \boldsymbol{X}_0] = [M, \boldsymbol{S}_0] = 0.$$

These conditions guarantee, in particular, that the mass operator M is invariant under transformations from the Lorentz subgroup, i. e.,

$$[M, \boldsymbol{K}_0] = [M, \boldsymbol{J}_0] = 0.$$

The mass modification (7.35) introduces interaction in generators of the translation subgroup,

$$\boldsymbol{P} = Mc^2 \boldsymbol{Q}_0,$$
$$H = Mc^2\sqrt{1 + Q_0^2 c^2}, \tag{7.36}$$

while Lorentz subgroup generators $\boldsymbol{K}_0$ and $\boldsymbol{J}_0$ remain interaction-free. So, we succeeded in defining a nontrivial interaction $\{H, \boldsymbol{P}, \boldsymbol{J}_0, \boldsymbol{K}_0\}$ in the point form of dynamics.

16 As in Section 6.3.2, these conditions can be fulfilled by defining $M = M_0 + N$, where N is a rotationally invariant function of operators of the relative position and momentum that commute with both $\boldsymbol{Q}_0$ and $\boldsymbol{X}_0$.

7.2.3 Unitary link between point and instant forms of dynamics

The S-matrix equivalence of Hamiltonians established in Section 7.2.1 remains valid even if the transformation $e^{i\Xi}$ (7.31) changes the relativistic form of dynamics [76, 77]. Here we are going to demonstrate this equivalence using the example of the Dirac instant and point forms [76].

To begin with, suppose that we are given a Bakamjian point form of dynamics with operators

$$\begin{aligned} M &\neq M_0, \\ \boldsymbol{P} &= \boldsymbol{Q}_0 M c^2, \\ \boldsymbol{J} &= \boldsymbol{J}_0, \\ \boldsymbol{R} &= \boldsymbol{X}_0 M^{-1} c^{-2}, \end{aligned}$$

specified in Section 7.2.2. Then we define a unitary operator

$$\Theta = \zeta_0 \zeta^{-1},$$

where

$$\begin{aligned} \zeta_0 &\equiv \exp(-i \ln(M_0 c^2) \mathfrak{Z}), \\ \zeta &\equiv \exp(-i \ln(M c^2) \mathfrak{Z}) \end{aligned}$$

and operator

$$\mathfrak{Z} \equiv \frac{1}{2\hbar}(\boldsymbol{R} \cdot \boldsymbol{P} + \boldsymbol{P} \cdot \boldsymbol{R}) = \frac{1}{2\hbar}(\boldsymbol{Q}_0 \cdot \boldsymbol{X}_0 + \boldsymbol{X}_0 \cdot \boldsymbol{Q}_0)$$

was defined in (4.53). Our goal is to show that the set of operators $\Theta M \Theta^{-1}$, $\Theta \boldsymbol{P} \Theta^{-1}$, $\Theta \boldsymbol{J}_0 \Theta^{-1}$ and $\Theta \boldsymbol{R} \Theta^{-1}$ generates a Poincaré group representation in the Bakamjian–Thomas instant form.

Let us define

$$\boldsymbol{Q}_0(b) \equiv e^{ib\mathfrak{Z}} \boldsymbol{Q}_0 e^{-ib\mathfrak{Z}}, \quad b \in \mathbb{R}.$$

From the commutator

$$[\mathfrak{Z}, \boldsymbol{Q}_0] = i\boldsymbol{Q}_0,$$

it follows that

$$\begin{aligned} \frac{d}{db}\boldsymbol{Q}_0(b) &= i[\mathfrak{Z}, \boldsymbol{Q}_0] = -\boldsymbol{Q}_0, \\ \boldsymbol{Q}_0(b) &= e^{-b}\boldsymbol{Q}_0. \end{aligned}$$

This formula remains valid even if b is not a number but any Hermitian operator commuting with both $\boldsymbol{Q}_0$ and $\boldsymbol{X}_0$. For example, if $b = \ln(M_0c^2)$, then

$$\zeta_0^{-1}\boldsymbol{Q}_0\zeta_0 = e^{i\ln(M_0c^2)\mathfrak{Z}}\boldsymbol{Q}_0 e^{-i\ln(M_0c^2)\mathfrak{Z}} = e^{-\ln(M_0c^2)}\boldsymbol{Q}_0 = \boldsymbol{Q}_0/(M_0c^2).$$

Similarly, one can show

$$\begin{aligned}
\zeta^{-1}\boldsymbol{Q}_0\zeta &= e^{i\ln(Mc^2)\mathfrak{Z}}\boldsymbol{Q}_0 e^{-i\ln(Mc^2)\mathfrak{Z}} = \boldsymbol{Q}_0/(Mc^2),\\
\zeta_0^{-1}\boldsymbol{X}_0\zeta_0 &= e^{i\ln(M_0c^2)\mathfrak{Z}}\boldsymbol{X}_0 e^{-i\ln(M_0c^2)\mathfrak{Z}} = \boldsymbol{X}_0 M_0c^2,\\
\zeta^{-1}\boldsymbol{X}_0\zeta &= e^{i\ln(Mc^2)\mathfrak{Z}}\boldsymbol{X}_0 e^{-i\ln(Mc^2)\mathfrak{Z}} = \boldsymbol{X}_0 Mc^2,
\end{aligned}$$

which implies

$$\begin{aligned}
\Theta\boldsymbol{P}\Theta^{-1} &= \zeta_0\zeta^{-1}(\boldsymbol{Q}_0Mc^2)\zeta\zeta_0^{-1} = \zeta_0\boldsymbol{Q}_0\zeta_0^{-1} = \boldsymbol{Q}_0M_0c^2 = \boldsymbol{P}_0,\\
\Theta\boldsymbol{J}_0\Theta^{-1} &= \boldsymbol{J}_0,\\
\Theta\boldsymbol{R}\Theta^{-1} &= \zeta_0\zeta^{-1}(\boldsymbol{X}_0/(Mc^2))\zeta\zeta_0^{-1} = \zeta_0\boldsymbol{X}_0\zeta_0^{-1} = \boldsymbol{X}_0/(M_0c^2) = \boldsymbol{R}_0.
\end{aligned}$$

From these formulas, it is clear that the transformation Θ really changes dynamics from the Bakamjian point form to the Bakamjian–Thomas instant form.

7.2.4 Scattering equivalence of forms of dynamics

Let us now verify that the scattering operator S, calculated with the point-form Hamiltonian $H = Mc^2\sqrt{1 + c^2Q_0^2}$, is the same as the operator S' calculated with the instant-form Hamiltonian $H' = \Theta H\Theta^{-1}$. Notice that we can rewrite equation (7.4) as

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

where operators

$$\Omega^\pm(H, H_0) \equiv \lim_{t\to\pm\infty} e^{\frac{i}{\hbar}H_0t}e^{-\frac{i}{\hbar}Ht}$$

are called *Möller wave operators*. Next we use the so-called *Birman–Kato invariance principle* [23], which states that $\Omega^\pm(H, H_0) = \Omega^\pm(f(H), f(H_0))$, where f can be any smooth function with positive derivative. Using the relationship between mass operators in the point (M) and instant (M') forms

$$M = \zeta^{-1}M\zeta = \zeta^{-1}\Theta^{-1}M'\Theta\zeta = \zeta^{-1}\zeta\zeta_0^{-1}M'\zeta_0\zeta^{-1}\zeta = \zeta_0^{-1}M'\zeta_0,$$

we obtain

$$\Omega^\pm(H, H_0) \equiv \Omega^\pm\left(Mc^2\sqrt{1 + Q_0^2c^2}, M_0c^2\sqrt{1 + Q_0^2c^2}\right) = \Omega^\pm(Mc^2, M_0c^2)$$

$$= \Omega^{\pm}(\zeta_0^{-1}M'\zeta_0 c^2, M_0c^2) = \zeta_0^{-1}\Omega^{\pm}(M'c^2, M_0c^2)\zeta_0$$
$$= \zeta_0^{-1}\Omega^{\pm}\Big(\sqrt{(M')^2c^4 + P_0^2c^2}, \sqrt{M_0^2c^4 + P_0^2c^2}\Big)\zeta_0$$
$$= \zeta_0^{-1}\Omega^{\pm}(H', H_0)\zeta_0,$$

$$S' = \Omega^{+}(H', H_0)\Omega^{-}(H', H_0) = \zeta_0\Omega^{+}(H, H_0)\zeta_0^{-1}\zeta_0\Omega^{-}(H, H_0)\zeta_0^{-1}$$
$$= \zeta_0\Omega^{+}(H, H_0)\Omega^{-}(H, H_0)\zeta_0^{-1} = \zeta_0 S\zeta_0^{-1}.$$

Then we notice that S commutes with free generators (7.7) and therefore with ζ_0 as well. Hence, $S' = S$ and the transformation Θ conserves the S-matrix. This completes the proof.

In addition to the above results, Sokolov and Shatnii [76, 77] established the mutual scattering equivalence of all three basic forms of dynamics – instant, point and front. Then it seems reasonable to assume that the S-operator is not sensitive to the form of dynamics at all.

The scattering equivalence of Hamiltonians and forms of dynamics gives us great advantages in calculations. If we are only interested in scattering amplitudes, energies and lifetimes of bound states,[17] then we can choose the Hamiltonian and the form of dynamics from a wide selection, as convenient. However, as we have already said, the scattering equivalence does not mean full physical equivalence of different theories. In the third volume of our book, we will see that an adequate description of the time evolution and other inertial transformations is possible only within the instant-form framework.

17 That is, the properties directly related to the scattering matrix.