Bound States and the Formal Theory of Scattering

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(Received May 20, 1954)

The exact expression for the transition rate for quantum-mechanical scattering problems is derived formally without recourse to adiabatically switching on the interaction or averaging the initial state in time. The equivalence is shown of the stationary definition of the S matrix and an appropriate definition by the time-dependent method.

INTRODUCTION

IN the derivation of the expression for the transition rate in the formal theory of scattering, a certain difficulty arises in connection with oscillatory terms in the time development of the state vector, which is due to the assumption of an initial "plane wave state" for the incident system, and which has sometimes been circumvented by a mathematical device usually described as "adiabatically switching on the interaction." This has been avoided in a recent treatment by Gell-Mann and Goldberger,[1] in which they introduced instead an averaging of the initial state in time. This has the effect of removing the oscillatory terms, which arise from the presence of bound states (if any) of the total Hamiltonian. In the following formal derivation of the expression for the transition rate, neither of the above devices, which are artificial from the standpoint of their physical interpretation in terms of the principles of quantum mechanics, is employed.

We assume that the total Hamiltonian H is the sum of two parts,

$$H=K+V, \tag{1}$$

where K, the "noninteracting part," and V, the "interacting part" of the total Hamiltonian are Hermitian time-independent operators in the Schroedinger representation. We will denote by φ_a a continuum eigenfunction of K of energy E_a,

$$K\varphi_a=E_a\varphi_a. \tag{2}$$

H is assumed to have the same continuous spectrum as K; and ψ_a^+ and ψ_a^-, the outgoing and incoming wave eigenfunctions of H corresponding to φ_a, satisfy the Lippmann-Schwinger equations[2]

$$\psi_a^{\pm}=\varphi_a+\lim_{\epsilon\to 0+}\frac{1}{E_a-K\pm i\epsilon}V\psi_a^{\pm}, \tag{3}$$

and

$$H\psi_a^{\pm}=E_a\psi_a^{\pm}. \tag{4}$$

H may have in addition discrete eigenstates ψ_l,

$$H\psi_l=E_l\psi_l, \tag{5}$$

where the ψ_l will be assumed not to overlap the continuous spectrum.

THE TRANSITION RATE

We start from the general relation (in units $\hbar=1$),

$$U(t_2,t_1)=e^{iKt_2}e^{-iH(t_2-t_1)}e^{-iKt_1}, \tag{6}$$

where $U(t_2,t_1)$ is the operator that generates the wave function at time t_2 from the wave function at time t_1 in the interaction representation,[3] and are interested in the convergence as $t\to-\infty$ of

$$U(0,t)\varphi_a=e^{iHt}e^{-iE_at}\varphi_a.$$

Expanding[4] φ_a in the complete set of eigenfunctions of H,

$$\varphi_a=\int dc\psi_c^+(\psi_c^+,\varphi_a)+\sum_l\psi_l(\psi_l,\varphi_a),$$

we obtain

$$U(0,t)\varphi_a=\gamma_a(t)+\beta_a(t),$$
$$\beta_a(t)=\sum_l e^{i(E_l-E_a)t}\psi_l(\psi_l,\varphi_a) \tag{7}$$
$$\gamma_a(t)=\int dc\left(\varphi_c+\frac{1}{E_c+i\epsilon-K}V\psi_c^+,\varphi_a\right)\psi_c^+e^{i(E_c-E_a)t},$$

where in the last line we have substituted from (3) and the limit as $\epsilon\to 0+$ is understood. By the orthonormality of the φ_c's, we have

$$\gamma_a(t)=\psi_a^+ +\rho_a^+(t), \tag{8}$$

$$\rho_a^+(t)=\int dc^0\int dE_c\frac{1}{E_c-i\epsilon-E_a}\times(V\psi_c^+,\varphi_a)\psi_c^+e^{i(E_c-E_a)t}, \tag{9}$$

where, following Watson,[5] we have explicitly separated out the integration over the energy in the integration over all physical quantities needed to specify the states

[1] M. Gell-Mann and M. L. Goldberger, Phys. Rev. **91**, 398 (1953).
[2] B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950).
[3] See, e.g., reference 1, Sec. III.
[4] The expansion coefficients (ψ_c^+,φ_a) are singular. However, see below where a wave packet is taken for initial state; this introduces an integration over these quantities.
[5] K. M. Watson and K. A. Brueckner, U. S. Atomic Energy Commission Document AECU-2765 (unpublished).

ψ_c^+. We put (suppressing the dependence on a):

$$(V\psi_c^+,\varphi_a)\psi_c^+=f(c^0,E_c),$$

and

$$x=(E_a-E_c)t.$$

Using the limit-integration theorem denoted symbolically by

$$\lim_{\eta\to 0+}\frac{1}{x\mp i\eta}=\mathrm{P}\left(\frac{1}{x}\right)\pm i\pi\delta(x), \tag{10}$$

where P denotes principal-value integration, we have for fixed $t<0$:

$$\rho_a^+(t)=\int dc^0\mathrm{P}\int_{E_at}^{\infty}dx\frac{e^{-ix}}{x}f\left(c^0,E_a-\frac{x}{t}\right)$$

$$+i\pi\int dc^0\int_{E_at}^{\infty}dx\delta(x)e^{-ix}f\left(c^0,E_a-\frac{x}{t}\right).$$

The second integral is immediately

$$+i\pi\int dc^0 f(c^0,E_a).$$

(We have assumed E_a definitely greater than the lower limit of the continuous spectrum, which we have taken, without loss of generality, equal to zero.) The principal value term is, in the limit $t\to-\infty$,

$$-i\pi\int dc^0 f(c^0,E_a).$$

Thus

$$\lim_{t\to-\infty}\rho_a^+(t)=0. \tag{11}$$

It remains to look at the contribution (7) from the bound states. This oscillates as $t\to-\infty$, unless all the (ψ_l,φ_a) vanish. Thus in the case where the total Hamiltonian H admits bound states, the limit of $U(0,t)\varphi_a$ as $t\to-\infty$ does not exist in general.[6]

Suppose, however, we take as initial state a wave packet $\bar{\varphi}_i$ which being normalizable can therefore be expanded in the φ_a's. We shall assume that this expansion contains a superposition of φ_a's over a small range of energies. We have

$$U(0,t)\bar{\varphi}_i=\int da(\varphi_a,\bar{\varphi}_i)[\psi_a^+ +\rho_a^+(t)+\beta_a(t)]$$

$$\equiv\bar{\psi}_i^+ +\bar{\rho}_i^+(t)+\bar{\beta}_i(t), \tag{12}$$

where the last equality defines the barred quantities. Now

$$E_l(\psi_l,\varphi_a)=(H\psi_l,\varphi_a)=(\psi_l,H\varphi_a)=E_a(\psi_l,\varphi_a)+(\psi_l,V\varphi_a),$$

so that, by (12) and (7),

$$\bar{\beta}_i(t)=\sum_l\int da\frac{e^{i(E_l-E_a)t}}{E_l-E_a}\psi_l(\psi_l,V\varphi_a)(\varphi_a,\bar{\varphi}_i).$$

Since we assume that the bound states do not overlap the continuous spectrum, the denominator never vanishes. By our assumption that $\bar{\varphi}_i$ involves a superposition of φ_a's over a range of energies, we therefore obtain, because of the rapidly varying exponential,

$$\lim_{t\to-\infty}\bar{\beta}_i(t)=0. \tag{13}$$

Also

$$\lim_{t\to-\infty}\bar{\rho}_i^+(t)=0, \tag{14}$$

so that

$$\lim_{t\to-\infty}U(0,t)\bar{\varphi}_i=\bar{\psi}_i^+. \tag{15}$$

By the definition (12) of $\bar{\psi}_i^+$,

$$(\varphi_b,e^{iKt}e^{-iHt}\bar{\psi}_i^+)=\left(\varphi_b,e^{iEbt}\int da(\varphi_a,\bar{\varphi}_i)\psi_a^+e^{-iEat}\right)$$

$$=\int da(\varphi_b,\psi_a^+)(\varphi_a,\bar{\varphi}_i)e^{i(Eb-Ea)t}, \tag{16}$$

$$(\varphi_b,e^{iKt}Ve^{-iHt}\bar{\psi}_i^+)$$

$$=\int da(\varphi_b,V\psi_a^+)(\varphi_a,\bar{\varphi}_i)e^{i(Eb-Ea)t}. \tag{17}$$

By (6) and (12),

$$\frac{d}{dt}|(\varphi_b,U(t,t_0)\bar{\varphi}_i)|^2$$

$$=2\,\mathrm{Re}\{-i(\varphi_b,e^{iKt}Ve^{-iHt}[\bar{\psi}_i^+ +\bar{\rho}_i^+(t_0)+\bar{\beta}_i(t_0)])$$

$$\times(\varphi_b,e^{iKt}e^{-iHt}[\bar{\psi}_i^+ +\bar{\rho}_i^+(t_0)+\bar{\beta}_i(t_0)])^*\}. \tag{18}$$

We now obtain, from (13), (14), (16), (17), and (18), and the orthonormality of the φ_a's,

$$w_{ba}\equiv\lim_{\bar{\varphi}_i\to\varphi_a}\lim_{t_0\to-\infty}\frac{d}{dt}|(\varphi_b,U(t,t_0)\bar{\varphi}_i)|^2$$

$$=2\,\mathrm{Re}\{-i(\varphi_b,V\psi_a^+)(\varphi_b,\psi_a^+)^*\},$$

[6] In their treatment of this problem, Gell-Mann and Goldberger (see reference 1) introduced an averaging of the initial state in time. They were led to define

$$U(0,-\infty)\varphi_a=\lim_{\epsilon\to 0+}\epsilon\int_{-\infty}^{0}dte^{\epsilon t}U(0,t)\varphi_a.$$

The fact that the contribution from the continuum has a limit by the ordinary definition implies that the limit exists and has the same value (ψ_a^+) by this generalized definition. However, it is clear from (7) that with this generalized limit, the contribution from the bound states vanishes.

independent of t. By (3) and (10), we have[7]

$$(\varphi_b,\psi_a^+)=\delta(b-a)+\left[\mathrm{P}\left(\frac{1}{E_a-E_b}\right)-i\pi\delta(E_a-E_b)\right](\varphi_b,V\psi_a^+).$$

Noting that the principal value term does not contribute to the real part, and defining

$$\mathbf{T}_{ba}=(\varphi_b,V\psi_a^+),$$

we finally get

$$w_{ba}=2\delta(b-a)\,\mathrm{Im}\mathbf{T}_{ba}+2\pi\delta(E_b-E_a)|\mathbf{T}_{ba}|^2, \quad (19)$$

which is the well-known exact expression for the transition rate.

EQUIVALENCE OF THE STATIONARY AND THE TIME-DEPENDENT DEFINITIONS OF THE S MATRIX

Snyder[8] has pointed out the necessity for a demonstration of the equivalence of the stationary and time-dependent definitions of the S matrix. This can be achieved by the methods of the preceding section.[9] In case we had expanded in terms of the ψ^-'s instead of the ψ^+'s,[10] we would have obtained, instead of (8) and (9),

$$\gamma_a(t)=\psi_a^-+\rho_a^-(t),$$

$$\rho_a^-(t)=\int dc\frac{1}{E_c+i\epsilon-E_a}(V\psi_c^-,\varphi_a)\psi_c^-e^{i(E_c-E_a)t}.$$

Proceeding as in the derivation of (11), we find that the principal value term and delta function term no longer cancel, but have the same sign, and we get

$$\lim_{t\to-\infty}\rho_a^-(t)=-2\pi i\int dc^0(V\psi^-(c^0,E_a),\varphi_a)\psi^-(c^0,E_a). \quad (20)$$

Taking the limit as $t\to-\infty$ of

$$\gamma_a(t)=\psi_a^+\rho_a^+(t)=\psi_a^-+\rho_a^-(t)$$

thus provides, by (11) and (20), the relation

$$\psi_a^+=\psi_a^--2\pi i\int dc^0(V\psi^-(c^0,E_a),\varphi_a)\psi^-(c^0,E_a).$$

Because the inner product occurs between states of the same energy, we can apply the reciprocity theorem,[2]

$$(V\psi^-(c^0,E_a),\varphi_a)=(\varphi(c^0,E_a),V\psi_a^+),$$

so that

$$\psi_a^+=\psi_a^--2\pi i\int dc\delta(E_c-E_a)(\varphi_c,V\psi_a^+)\psi_c^-.$$

Making use of the orthonormality of the ψ^-'s, we obtain from the stationary definition of the S matrix introduced by Gell-Mann and Goldberger,

$$S_{ba}\equiv(\psi_b^-,\psi_a^+)=\delta(b-a)-2\pi i\delta(E_b-E_a)\mathbf{T}_{ba}.$$

In the treatment of the S matrix by the time-dependent method the same difficulty arises that was discussed in the preceding section. It is now clear that we should take a wave packet for the initial state and at the end of the calculation let the wave packet approach a plane wave. Thus we define

$$S_{ba}\equiv\lim_{\bar{\varphi}_i\to\varphi_a}\lim_{t\to\infty}\lim_{t_0\to-\infty}(\varphi_b,U(t,t_0)\bar{\varphi}_i). \quad (21)$$

By (6), (15), and (16),

$$\lim_{t_0\to-\infty}(\varphi_b,U(t,t_0)\bar{\varphi}_i)=(\varphi_b,e^{iKt}e^{-iHt}\bar{\psi}_i^+)$$

$$=(\varphi_b,\bar{\varphi}_i)+\int da\frac{e^{i(E_b-E_a)t}}{E_a+i\epsilon-E_b}(\varphi_b,V\psi_a^+)(\varphi_a,\bar{\varphi}_i),$$

where the last line follows from substituting (3) into (16), and the limit as $\epsilon\to0+$ is understood. Thus, making use again of (10),

$$\lim_{t\to\infty}\lim_{t_0\to-\infty}(\varphi_b,U(t,t_0)\bar{\varphi}_i)$$

$$=(\varphi_b,\bar{\varphi}_i)-2\pi i\int da\delta(E_b-E_a)(\varphi_b,V\psi_a^+)(\varphi_a,\bar{\varphi}_i),$$

and we therefore again obtain

$$S_{ba}=\delta(b-a)-2\pi i\delta(E_b-E_a)\mathbf{T}_{ba}. \quad (22)$$

Thus the definition (21) of the S matrix by the time-dependent method also leads to (22), whether or not there are bound states of H, provided these do not overlap the continuous spectrum.

ACKNOWLEDGMENT

It is a pleasure to thank for discussions Professor Marvin L. Goldberger, Professor Arthur S. Wightman, Dr. John S. McIntosh, and Mr. William M. MacDonald.

[7] There is still an integration over final states to be performed eventually. In fact, inserting (19) into the relation expressing conservation of probability,

$$\int dbw_{ba}=0$$

provides, as Snyder has noted (see reference 8), an immediate proof of the well-known "optical theorem" [reference 8, Eq. (45)].

[8] H. S. Snyder, Phys. Rev. **83**, 1154 (1951).

[9] S. T. Ma [Phys. Rev. **87**, 652 (1952)], has considered this problem from a different point of view, making use of a concept of "conditional equality." Necessary integrations required for the validity of "conditional equalities" arise naturally when a wave packet is taken for the initial state. (See, e.g., Eq. (36a) of reference 8, and note that an integration over E_μ is required there.)

[10] I owe this suggestion to Professor Goldberger. It is assumed here that the ψ^+'s and ψ^-'s span the same space.

Note added in proof.—After completing this work, I received unpublished notes of Professor F. Low in which Eq. (15) and Eq. (22) are derived by the same method as used here. I have also been informed that similar methods have been employed in unpublished work of Professor J. Ashkin.