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THE THREE-BODY TIME-DELAY OPERATOR*

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ABSTRACT

Using Faddeev's form of time-dependent scattering theory we give an abstract definition of time-delay valid for multichannel scattering. For the three-body scattering problem we find an explicit relation, that is valid on the energy shell, between the time-delay operator and the S-operators and their energy derivatives.

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I. INTRODUCTION

This paper studies the time-delay problem as it occurs in three-body scattering.[1] Roughly speaking, the time-delay effect is the advancement or retardation of wavepacket motion due to the presence of interactions not contained in the asymptotic Hamiltonians. In the following we first give a rigorous definition of multichannel time delay. This definition is an extension to the multichannel case of the one employed by Goldberger and Watson.[2] Using then Faddeev's[3] results in time-dependent scattering theory, together with the primary singularity structure[4,5] of the exact stationary wavefunction, we construct an explicit solution of the time-delay problem by following an approach similar to Jauch and Marchand's treatment[6] of two-body time delay. Specifically we obtain a relation between the time-delay operator and the different S-operators and their energy derivatives, that is valid on the energy shell. It is the proof of this relation that is the main objective of this paper.

The physical interpretation of the time-delay operator we define is only touched upon very briefly. Because of the controversy that clearly exists already for two particle time-delay regarding the different definition,[2,6,7] which might or might not be equivalent,[8] that are given in the literature, and because of the length of the present paper, we like to discuss the physical aspects of the problem elsewhere.

This paper is organized into five sections. Section II introduces those features of three-body time-dependent scattering theory which are necessary in this problem. In Section III we define a set of reduced S-operators which have an explicit energy dependence because the solution of the time-delay problem cannot be expressed directly in terms of the usual S-operators. In Section IV we construct the time-delay operator starting from first principles and state the problem we want to solve. Section V gives the main body of the derivation of the time-delay relation. Finally, Appendix A contains a discussion of the projection operators and their momentum-space representations. Appendix B collects some of the details needed in Section V. Appendix C discusses a class of terms which vanish and do not contribute to the result derived in Section V.

II. TIME-DEPENDENT SCATTERING THEORY

This section gives an outline of the aspects of three-body time-dependent theory that are necessary in the analysis of our problem. The physical scattering problem is taken to be that studies by Faddeev, namely the scattering of three distinct nonrelativistic particles interacting via short range forces. Furthermore, the interaction in each two-body channel is assumed to be such that there is only one two-body boundstate.

Let us briefly describe the coordinate systems we employ. After the center-of-mass motion has been eliminated from our problem there remain six degrees of freedom. In coordinate space we choose the Jacobi variables[9] $\vec{x}_\alpha, \vec{y}_\alpha$ to describe these. The variable $\vec{x}_\alpha$ is the separation of particle α from the center-of-mass of the $(\beta\gamma)$ cluster. The independent variable $\vec{y}_\alpha$ gives the vector separation of the constituents of the α cluster namely the spatial separation of particles β and γ. The canonically conjugate momenta related to $\vec{x}_\alpha$ and $\vec{y}_\alpha$ are denoted by $\vec{p}_\alpha$ and $\vec{q}_\alpha$. The momenta $\vec{p}_\alpha$ describes the relative motion of particle α and cluster α. The kinetic energy of this motion is given by $\vec{p}_\alpha^{\,2}/2n_\alpha$ where $n_\alpha = m_\alpha(m_\beta + m_\gamma)/(m_\alpha + m_\beta + m_\gamma)$ represents the reduced mass of particle α and cluster α. The internal momentum of cluster α is just $\vec{q}_\alpha$. The kinetic energy associated with this motion is $\vec{q}_\alpha^{\,2}/2\mu_\alpha$ where $\mu_\alpha = m_\beta m_\gamma/(m_\beta + m_\gamma)$ is now the reduced mass for particles β and γ relative to their own center-of-mass system. It is clear that we have three distinct $(\alpha = 1, 2, 3)$ Jacobi coordinate systems each of which provides a complete description of the degrees of freedom.

The behavior of any physical system is determined by its Hamiltonian. The free Hamiltonian related to the total kinetic energy is given by

$$H_0 = \frac{\vec{p}_\alpha^{\,2}}{2n_\alpha} + \frac{\vec{q}_\alpha^{\,2}}{2\mu_\alpha} \quad , \qquad \alpha = 1, 2, 3 \quad . \tag{2.1}$$

We shall employ an abbreviated notation for these kinetic energies, viz.

$$\tilde{p}_\alpha^2 = \frac{\vec{p}_\alpha^{\,2}}{2n_\alpha} \quad , \qquad \tilde{q}_\alpha^2 = \frac{\vec{q}_\alpha^{\,2}}{2\mu_\alpha} \quad . \tag{2.2}$$

The right-hand side of Eq. (2.1) is independent of the index α. We shall take notational advantage of this invariance of H_0 by frequently omitting the α label. There is a similar invariant quantity in coordinate space. If we define

$$\tilde{x}_\alpha^2 = 2n_\alpha \vec{x}_\alpha^{\,2} \quad , \qquad \tilde{y}_\alpha^2 = 2\mu_\alpha \vec{y}_\alpha^{\,2} \tag{2.3a}$$

and

$$\tilde{\rho}^2 = \tilde{x}_\alpha^2 + \tilde{y}_\alpha^2 \quad . \tag{2.3b}$$

then $\tilde{\rho}$ is a coordinate space invariant for all α.

The complete Hamiltonian is then obtained by adding to H_0 all the interactions possible in the system. So for the system Faddeev studies we get

$$H = H_0 + \sum_{\alpha=1}^{3} V_\alpha \tag{2.4}$$

where V_α is the potential acting between the particles β and γ. The Hamiltonians H and H_0 are operators acting in the Hilbert space of square integrable functions of our six degrees of freedom, i.e., $L^2(\vec{p}_\alpha, \vec{q}_\alpha)$. We shall denote this Hilbert space by $\hbar$, the inner product related to $\hbar$ by (,) and the identity operator on $\hbar$ by E. Acting on $\hbar$, H_0 and H are both self-adjoint operators.[3]

We next want to consider the different kinds of asymptotic motion because these will finally specify the solutions of the scattering problem. Because of the short-range nature of the forces we may expect that as $t \to \pm\infty$ the three-body problem is characterized by freely moving clusters. We have two distinct types of cluster motion. First, there are three possible cases of motion involving two clusters, each of which can be labeled by the index α, indicating the particle that moves in isolation. Secondly, there is a single motion involving three clusters, labeled by the index $\alpha=0$, namely when all three particles move independently. With each cluster description of the asymptotic motion there is an associated asymptotic Hamiltonian, determined by including all the intra-cluster potentials and omitting the inter-cluster potentials. For the two-cluster type of motion these Hamiltonians are given by

$$H_\alpha = H_0 + V_\alpha \quad . \tag{2.5}$$

For the three-cluster motion the asymptotic Hamiltonian is clearly H_0.

At this point we recall that each two-body interaction is capable of supporting only one boundstate. We shall let $\psi_\alpha(\vec{q}_\alpha)$ be this unit normalized two-body boundstate wavefunction in the space of square integrable functions of $\vec{q}_\alpha$, i.e., $L^2(\vec{q}_\alpha)$. The corresponding boundstate energy is $-\chi_\alpha^2$. So we have

$$(\tilde{q}_\alpha^2 + v_\alpha)\psi_\alpha = -\chi_\alpha^2\psi_\alpha \qquad \alpha = 1, 2, 3 \quad , \tag{2.6}$$

The symbol v_α represents the potential found in the two-body problem involving the particles β and γ. As we know V_α and v_α are integral operators in momentum space whose kernels are related in the following way

$$V_\alpha(\vec{p}_\alpha, \vec{q}_\alpha; \vec{p}'_\alpha, \vec{q}'_\alpha) = v_\alpha(\vec{q}_\alpha, \vec{q}')\ \delta(\vec{p}_\alpha - \vec{p}'_\alpha) \tag{2.7}$$

Because of this fact that there is only one boundstate for a pair, each of the different cluster geometries will specify a scattering channel. We now want to describe the wavepackets that characterize the asymptotic channel motion. Let us consider, e.g., the α channel ($\alpha\neq 0$). The cluster ($\beta\gamma$) will be described by the boundstate wavefunction $\psi_\alpha(\vec{q}_\alpha)$. To describe the relative motion of α and the center-of-mass of the pair ($\beta\gamma$) we shall need the appropriate wavepacket indicated by $f_\alpha(\vec{p}_\alpha)$. In effect this function f_α is like a two-particle wavepacket expect that one of the particles is a cluster. So for f_α to be an acceptable wavepacket it must lie in the Hilbert space of square integrable function of $\vec{p}_\alpha$, i.e., $L^2(\vec{p}_\alpha)$ which we denote by h_α. The inner product for this space will be $(\ ,\ )_\alpha$ and E_α will be the identity operator. So the α channel motion is described by $f_\alpha(\vec{p}_\alpha)\ \psi_\alpha(\vec{q}_\alpha)$ and since ψ_α is a known function, all the nontrivial information about this channel is given by f_α. For the three free particle cluster we have all six degrees of freedom present and the related wavepacket will have the form $f_0(\vec{p},\vec{q})$. The space for f_0 will be $L^2(\vec{p},\vec{q}) = h_0$, its inner product $(\ ,\ )_0$ and its identity E_0. Of course, h_0 is mathematically identical with h.

It is useful now to construct Hamiltonians that act in those channel spaces h_α. These new Hamiltonians are suggested by utilizing Eqs. (2.5), (2.6), and (2.7) to get

$$\begin{aligned} H_\alpha\ f_\alpha(\vec{p}_\alpha)\,\psi_\alpha(\vec{q}_\alpha) &= (\tilde{p}_\alpha^2 + \tilde{q}_\alpha^2 + V_\alpha)\ f_\alpha(\vec{p}_\alpha)\,\psi_\alpha(\vec{q}_\alpha) \\ &= (\tilde{p}_\alpha^2 - \chi_\alpha^2)\ f_\alpha(\vec{p}_\alpha)\,\psi_\alpha(\vec{q}_\alpha) \qquad \alpha > 0 \qquad (2.8) \end{aligned}$$

Eliminating the multiplicative factor $\psi_\alpha(\vec{q}_\alpha)$ we are lead to define the channel Hamiltonian $\tilde{H}_\alpha$ by

$$\tilde{H}_\alpha f_\alpha = (\tilde{p}_\alpha^2 - \chi_\alpha^2)\ f_\alpha \in h_\alpha \quad , \qquad \alpha > 0 \qquad (2.9)$$

For the α=0 case the channel Hamiltonian $\tilde{H}_0$, does not differ from the asymptotic Hamiltonian H_0. Thus

$$\tilde{H}_0 f_0 = (\tilde{p}^2 + \tilde{q}^2)\ f_0 \in h_0 \quad . \qquad (2.10)$$

We then introduce a single Hilbert space to describe all these possible asymptotic motions of the three-body system. This space, denoted by $\hat{h}$, must clearly be the following product space

$$\hat{h} = h_0 \oplus h_1 \oplus h_2 \oplus h_3 \qquad (2.11)$$

The inner product of $\hat{h}$ will be $(\; , \;)_{\wedge}$, its identity will be $\hat{E}$. This inner product is given in terms of previous inner products as

$$(f, f')_{\wedge} = \sum_{\alpha=0}^{3} (f_\alpha, f'_\alpha)_\alpha \quad . \tag{2.12}$$

An important remark we have to make here is that for multichannel scattering this Hilbert space describing free asymptotic motion, namely $\hat{h}$, is different from the Hilbert space describing the exact solution, namely h. So, if the channel functions f_α are set in h by writing $f_\alpha \psi_\alpha$ then the channels are not orthogonal viz. $(f_\alpha \psi_\alpha, f'_\beta \psi_\beta) \neq 0 \quad (\alpha, \beta > 0)$.

To conclude this part, we first define a projection operator P_α from h into h by

$$P_\alpha f = f_\alpha \psi_\alpha \in h \qquad \alpha > 0 \tag{2.13}$$

The subspace associated with the range of P_α consists of all separable functions in $\vec{p}_\alpha$ and $\vec{q}_\alpha$ where the function of $\vec{q}_\alpha$ is ψ_α. Secondly we define an operator I_α from h onto h_α by

$$I_\alpha f = f_\alpha \in h_\alpha \quad . \tag{2.14}$$

We now turn to the discussion of the Moller operators $U_\alpha^{(\pm)}$ which are the basic elements of scattering theory. Faddeev's work[3] establishes that $U_\alpha^{(\pm)}$ may be constructed from the solutions of a Fredholm integral equation that contains the same physics as the three-body time-independent Schrödinger equation, with the supplementary advantage that the boundary conditions are built into the structure of the equation.

The $U_\alpha^{(\pm)}$ operators which map h_α into h, have the following three properties:

$$1^\circ. \qquad U_\alpha^{(\pm)\dagger} U_\beta^{(\pm)} = \delta_{\alpha\beta} E_\beta \qquad : h_\beta \rightarrow h_\alpha \tag{2.15}$$

$$2^{o}. \qquad \sum_{\alpha=0}^{3} U_\alpha^{(\pm)} U_\alpha^{(\pm)\dagger} = E - P_d \qquad : h \to h \tag{2.16}$$

$$3^{o}. \qquad H\, U_\alpha^{(\pm)} = U_\alpha^{(\pm)} \widetilde{H}_\alpha \qquad : h_\alpha \to h \tag{2.17}$$

We shall refer to these basic statements as the fundamental theorem. Property 1^{o} is a statement of the channel orthogonality of the exact wavefunction solution, when $\alpha=\beta$ it becomes a statement of probability conservation. Property 2^{o} is the asymptotic completeness of the exact scattering states. P_d is the projection operator onto the subspace spanned by the eigenfunctions of the discrete spectrum of H. Property 3^{o} is the intertwining property and states that the exact wavefunction will have the same energy as the incident wavefunction, i.e., energy conservation. Furthermore the function $<\vec{p}_\alpha \vec{q}_\alpha | U_\alpha^{(\pm)} | \vec{p}\,'_\alpha>$ has the following structure:

$$<\vec{p}_\alpha \vec{q}_\alpha | U_\alpha^{(\pm)} | \vec{p}\,'_\alpha> \; = \; \psi_\alpha(\vec{q}_\alpha)\, \delta(\vec{p}_\alpha - \vec{p}\,'_\alpha) - <\vec{p}_\alpha \vec{q}_\alpha | K_\alpha^{(\pm)} | \vec{p}\,'_\alpha> \tag{2.18}$$

The first term on the right represents the unscattered portion of the wavefunction. The second term is the scattered wave and can be written as

$$<\vec{p}_\alpha \vec{q}_\alpha | K_\alpha^{(\pm)} | \vec{p}\,'_\alpha> = \frac{<\vec{p}_\alpha \vec{q}_\alpha | \mathscr{B}_{0\alpha}^{(\mp)} | \vec{p}\,'_\alpha>}{\tilde{p}^2 + \tilde{q}^2 - \tilde{p}'^2_\alpha + \chi_\alpha^2 \pm i0} \tag{2.19}$$

where

$$<\vec{p}_\alpha \vec{q}_\alpha | \mathscr{B}_{0\alpha}^{(\pm)} | \vec{p}\,'_\alpha> = - \sum_{\gamma=1}^{3} \left[<\vec{p}_\alpha \vec{q}_\alpha | \mathscr{G}_{\gamma\alpha}^{(\pm)} | \vec{p}\,'_\alpha> - \frac{\phi_\gamma(\vec{q}_\gamma) <\vec{p}_\gamma | \mathscr{H}_{\gamma\alpha}^{(\pm)} | \vec{p}\,'_\alpha>}{\tilde{p}_\gamma^2 - \chi_\gamma^2 - \tilde{p}'^2_\alpha + \chi_\alpha^2 \mp i0} \right] . \tag{2.20}$$

Here the functions $<\vec{p}_\alpha \vec{q}_\alpha | \mathscr{G}_{\gamma\alpha}^{(\pm)} | \vec{p}\,'_\alpha>$, $<\vec{p}_\alpha | \mathscr{H}_{\gamma\alpha}^{(\pm)} | \vec{p}\,'_\alpha>$ are the half-on-shell solutions of the well-known Faddeev integral equations[10] viz.

$$<\vec{p}_\gamma | \mathscr{H}_{\gamma\alpha}^{(\pm)} | \vec{p}\,'_\alpha> = \mathscr{H}_{\gamma\alpha}(\vec{p}_\gamma; \vec{p}\,'_\alpha; \tilde{p}'^2_\alpha - \chi_\alpha^2 \pm i0) \tag{2.21}$$

$$<\vec{p}_\gamma \vec{q}_\gamma | \mathscr{G}^{(\pm)}_{\gamma\alpha} | \vec{p}_\alpha'> = \mathscr{G}_{\gamma\alpha}(\vec{p}_\gamma, \vec{q}_\gamma; \vec{p}_\alpha'; \tilde{p}_\alpha'^2 - \chi_\alpha^2 \pm i0) \tag{2.22}$$

The function ϕ_γ is the vertex function defined by $\phi_\gamma(\vec{q}_\gamma) = (\tilde{q}_\gamma^2 + \chi_\gamma^2)\,\psi_\gamma(\vec{q}_\gamma)$. In the same way, the wavefunction for three to three scattering is

$$<\vec{p}_\alpha \vec{q}_\alpha | U_0^{(\pm)} | \vec{p}_\alpha' \vec{q}_\alpha'> = \delta(\vec{q}_\alpha - \vec{q}_\alpha')\,\delta(\vec{p}_\alpha - \vec{p}_\alpha') - <\vec{p}_\alpha \vec{q}_\alpha | K_0^{(\pm)} | \vec{p}_\alpha' \vec{q}_\alpha'> \tag{2.23}$$

where the matrix elements of $K_0^{(\pm)}$ are related to Faddeev's $M_{\alpha\beta}$ operators[3,5]

$$<\vec{p}_\alpha \vec{q}_\alpha | K_0^{(\pm)} | \vec{p}_\alpha' \vec{q}_\alpha'> = \frac{<\vec{p}_\alpha \vec{q}_\alpha | T^{(\mp)} | \vec{p}_\alpha' \vec{q}_\alpha'>}{\tilde{p}_\alpha^2 + \tilde{q}_\alpha^2 - \tilde{p}_\alpha'^2 - \tilde{q}_\alpha'^2 \pm i0} \tag{2.24}$$

$$<\vec{p}_\alpha \vec{q}_\alpha | T^{(\pm)} | \vec{p}_\alpha' \vec{q}_\alpha'> = \sum_{\alpha,\beta} \mathscr{M}_{\alpha\beta}(\vec{p}_\alpha, \vec{q}_\alpha; \vec{p}_\alpha' \vec{q}_\alpha'; \tilde{p}_\alpha'^2 + \tilde{q}_\alpha'^2 \pm i0)\ . \tag{2.25}$$

In concluding this section we recall that Faddeev proves the above described results with the assumption that the two-body potentials satisfy a boundedness property and a Holder continuity requirement. Using these assumptions, e.g., the half-on-shell two-body t-matrix satisfies[11]

$$\left|<\vec{p}\,| t^{(\pm)} | \vec{p}\,>\right| \leq C/(1 + |\vec{p} - \vec{p}\,'|)^{1+\theta} \tag{2.26}$$

$$\left|<\vec{p} + \Delta\vec{p}\,| t^{(\pm)} | \vec{p}\,' + \Delta\vec{p}\,'> - <\vec{p}\,| t^{(\pm)} | \vec{p}\,'>\right| \leq C/(1 + |\vec{p} - \vec{p}\,'|)^{1+\theta}\ \left[|\Delta\vec{p}|^\nu + |\Delta\vec{p}\,'|^\nu\right] \tag{2.27}$$

where $|\Delta\vec{p}| < 1$, $|\Delta\vec{p}\,'| < 1$ and ν may be taken as close to 1/2 as desired. In our time-delay proof we shall have to construct derivatives of the half-on-shell amplitudes with respect to the momentum arguments. It is clear that the estimate (2.27) is not strong enough to claim that $<\vec{p}\,| t^{(\pm)} | \vec{p}\,'>$ is differentiable with respect to p or p'. We have not investigated the necessary modifications needed to ensure differentiability of $t^{(\pm)}$ and the other half-on-shell matrix elements

$\mathscr{H}^{(\pm)}_{\alpha\beta}$, $\mathscr{B}^{(\pm)}_{0\beta}$, $T^{(\pm)}$. However it is likely that the original potential must be differentiable and that this derivative of the potential must also satisfy a Holder continuity requirement.

III. REDUCED S-MATRIX ELEMENTS

In this section we describe the essential features of the S-matrix and introduce the reduced S-matrix elements needed in our derivation. The S-matrix is defined to be a mapping between the initial experimentally determined wavepacket f_α and the observed post-scattering wavepackets f'_β. We know[3] that, in terms of the Moller wave operators, this mapping looks like

$$f'_\beta = U_\beta^{(+)\dagger} U_\alpha^{(-)} f_\alpha \tag{3.1}$$

So

$$S_{\beta\alpha} = U_\beta^{(+)\dagger} U_\alpha^{(-)} \qquad : \mathscr{h}_\alpha \rightarrow \mathscr{h}_\beta \tag{3.2}$$

This S-matrix is even simpler when written down as an operator on the asymptotic channel space $\hat{\mathscr{h}}$. In this case the information in Eq. (3.1) can be expressed as

$$\hat{f}' = S\hat{f} \qquad : \hat{\mathscr{h}} \rightarrow \hat{\mathscr{h}} \tag{3.3}$$

Let us now recall the basic properties of the S-matrix because it will turn out that the time-delay operator has properties which parallel those of the S-matrix. The first basic property of the S-matrix is that it is a unitary operator when acting on the channel space $\hat{\mathscr{h}}$ viz.

$$S^\dagger S = SS^\dagger = \hat{E} \quad . \tag{3.4}$$

In component form the equivalent of Eq. (3.4) is

$$\sum_{\gamma=0}^{3} S^\dagger_{\gamma\alpha} S_{\gamma\beta} = E_\beta \delta_{\alpha\beta} \quad . \tag{3.5}$$

This unitarity is an immediate consequence of the statements 1^o and 2^o in the fundamental theorem.

The second basic property of S we want to stress is the intertwining property with the channel Hamiltonians $\widetilde{H}_\alpha$,

$$S_{\alpha\beta}\widetilde{H}_\beta = \widetilde{H}_\alpha S_{\alpha\beta} \quad . \tag{3.6}$$

This intertwining feature is the direct consequence of statement 3^o in the fundamental theorem.

We now shall turn to the definition of the reduced matrix elements of S. In order to carry out this definition we first require the known[4, 5] representations of the kernels of S in terms of $T^{(+)}$, $\mathscr{B}^{(+)}_{0\beta}$ and $\mathscr{H}^{(+)}_{\alpha\beta}$ introduced in Section II. For a rearrangement scattering process one has,

$$S_{\alpha\beta}(\vec{p}_\alpha;\vec{p}^{\,\prime}_\beta) = \delta_{\alpha\beta}\,\delta(\vec{p}_\alpha-\vec{p}^{\,\prime}_\beta) - 2\pi i\,\delta(\widetilde{p}^{2}_\alpha-\chi^2_\alpha-\widetilde{p}^{\prime 2}_\beta+\chi^2_\beta)\langle\vec{p}_\alpha\,|\mathscr{H}^{(+)}_{\alpha\beta}\,|\,\vec{p}^{\,\prime}_\beta\rangle \,. \tag{3.7}$$

The S matrices involving three free particles in either the initial or final state are given by

$$S_{0\beta}(\vec{p},\vec{q};\vec{p}^{\,\prime}_\beta) = -2\pi i\;\delta(\widetilde{p}^2+\widetilde{q}^2-\widetilde{p}^{\prime 2}_\beta+\chi^2_\beta)\langle\vec{p}\,\vec{q}\,|\,\mathscr{B}^{(+)}_{0\beta}\,|\,\vec{p}^{\,\prime}_\beta\rangle \;, \tag{3.8}$$

and

$$S_{\alpha 0}(\vec{p}_\alpha;\vec{p}^{\,\prime},\vec{q}^{\,\prime}) = -2\pi i\;\delta(\widetilde{p}^2_\alpha-\chi^2_\alpha-\widetilde{p}^{\prime 2}-\widetilde{q}^{\prime 2})\;\langle\vec{p}_\alpha\,|\,\mathscr{B}^{(+)}_{\alpha 0}\,|\,\vec{p}^{\,\prime}\vec{q}^{\,\prime}\rangle \quad . \tag{3.9}$$

The amplitude $\mathscr{B}^{(+)}_{\alpha 0}$ is related to $\mathscr{B}^{(-)}_{0\alpha}$ by

$$\langle\vec{p}_\alpha\,|\,\mathscr{B}^{(+)}_{\alpha 0}\,|\,\vec{p}^{\,\prime}\vec{q}^{\,\prime}\rangle = \langle\vec{p}^{\,\prime}\vec{q}^{\,\prime}\,|\,\mathscr{B}^{(-)}_{0\alpha}\,|\,\vec{p}_\alpha\rangle^* \quad . \tag{3.10}$$

The * indicates complex conjugation. Finally the three-to-three S-matrix is

$$S_{00}(\vec{p},\vec{q};\vec{p}^{\,\prime}\vec{q}^{\,\prime}) = \delta(\vec{p}-\vec{p}^{\,\prime})\;\delta(\vec{q}-\vec{q}^{\,\prime}) - 2\pi i\;\delta(\widetilde{p}^2+\widetilde{q}^2-\widetilde{p}^{\prime 2}-\widetilde{q}^{\prime 2})\langle\vec{p}\,\vec{q}\,|\,T^{(+)}\,|\,\vec{p}^{\,\prime}\vec{q}^{\,\prime}\rangle \tag{3.11}$$

We want to construct S matrices related to the expression above but with the energy delta function removed. We will use a lower case s to denote these new S matrices. Consider, in the first instance, $S_{\alpha\beta}$. Defining $E = \widetilde{p}^2_\alpha - \chi^2_\alpha$ and

$E' = p'^2_\beta - \chi^2_\beta$ and employing the relation,

$$\delta_{\alpha\beta}\,\delta(\vec{p}_\alpha - \vec{p}'_\beta) = \delta_{\alpha\beta}\,\frac{\delta(E-E')\,\delta(\hat{p}_\alpha - \hat{p}'_\beta)}{(n_\alpha p_\alpha\, n_\beta p'_\beta)^{1/2}} \tag{3.12}$$

we may write Eq. (3.7) in the form

$$S_{\alpha\beta}(\vec{p}_\alpha;\vec{p}'_\beta) = \frac{\delta(E-E')}{(n_\alpha p_\alpha\, n_\beta p'_\beta)^{1/2}}\left[\delta_{\alpha\beta}\,\delta(\hat{p}_\alpha - \hat{p}'_\beta) - 2\pi i\,(n_\alpha p_\alpha n_\beta p'_\beta)^{1/2} <\vec{p}_\alpha|\mathscr{H}^{(+)}_{\alpha\beta}|\vec{p}'_\beta>\right] \tag{3.13}$$

In these expressions $\hat{p}$ indicates the unit direction vector associated with $\vec{p}$. Thus we are lead to define $s_{\alpha\beta}(E)$ by

$$<\hat{p}_\alpha|s_{\alpha\beta}(E)|\hat{p}'_\beta> \equiv \delta_{\alpha\beta}\,\delta(\hat{p}_\alpha - \hat{p}'_\beta) - 2\pi i\,(n_\alpha p_\alpha\, n_\beta p'_\beta)^{1/2} <\vec{p}_\alpha|\mathscr{H}^{(+)}_{\alpha\beta}|\vec{p}'_\beta> \tag{3.14}$$

The energy dependence E appears on the right-hand side of Eq. (3.14) by virtue of the fact that $p_\alpha = \left[2n_\alpha(E+\chi^2_\alpha)\right]^{1/2}$ and $p'_\beta = \left[2n_\beta(E+\chi^2_\beta)\right]^{1/2}$. The kernel $<\hat{p}_\alpha|s_{\alpha\beta}(E)|\hat{p}'_\beta>$ represents an operator that will map square integrable functions with respect to the measure $d\Omega_{\hat{p}'_\beta}$, i.e., $L^2(\hat{p}'_\beta)$, into $L^2(\hat{p}_\alpha)$. When $\alpha=\beta$ the leading factor on the right of Eq. (3.14) is the identity operator on the space $L^2(\hat{p}_\alpha)$. The energy dependence indicated on the left of Eq. (3.14) means that for each $S_{\alpha\beta}$ operator we have a one-parameter family of operators $s_{\alpha\beta}(E)$.

We consider next S matrices involving three free particles in the initial or final state. The kinematic relation $E = \tilde{p}^2_\alpha + \tilde{q}^2_\alpha$ suggests we define the angle ω_α such that

$$\tilde{p}_\alpha = \sqrt{E}\cos\omega_\alpha\,,\qquad \tilde{q}_\alpha = \sqrt{E}\sin\omega_\alpha\,,\qquad 0 \leq \omega_\alpha \leq \frac{\pi}{2} \tag{3.15}$$

Using this convention the six-dimension delta function appearing in (3.11) may be written

$$\delta(\vec{p}_\alpha - \vec{p}'_\alpha)\,\delta(\vec{q}_\alpha - \vec{q}'_\alpha) = \frac{\delta(E-E')\,\delta(\omega_\alpha - \omega'_\alpha)\,\delta(\hat{p}_\alpha - \hat{p}'_\alpha)\,\delta(\hat{q}_\alpha - \hat{q}'_\alpha)}{p_\alpha q_\alpha p'_\alpha q'_\alpha(\mu_\alpha n_\alpha)^{1/2}} \tag{3.16}$$

Using then Eq. (3.11) we find that the reduced matrix operator $s_{00}(E)$ is

$$<\omega_\alpha \hat{p}_\alpha \hat{q}_\alpha | s_{00}(E) | \omega'_\alpha \hat{p}'_\alpha \hat{q}'_\alpha> \equiv \delta(\omega_\alpha - \omega'_\alpha)\ \delta(\hat{p}_\alpha - \hat{p}'_\alpha)\ \delta(\hat{q}_\alpha - \hat{q}'_\alpha)$$

$$- 2\pi i (\mu_\alpha n_\alpha)^{\frac{1}{2}} p_\alpha q_\alpha p'_\alpha q'_\alpha <\vec{p}_\alpha \vec{q}_\alpha | T^{(+)} | \vec{p}'_\alpha \vec{q}'_\alpha > \tag{3.17}$$

Here the operator $s_{00}(E)$ takes a function from $L^2(\omega'_\alpha, \hat{q}'_\alpha, \hat{p}'_\alpha)$ into $L^2(\omega_\alpha, \hat{q}_\alpha, \hat{p}_\alpha)$. In this case the Hilbert space is defined relative to the measure $\frac{1}{2}(2\mu_\alpha 2n_\alpha)^{3/2} \cos^2 \omega_\alpha \sin^2 \omega_\alpha\, d\omega_\alpha\, d\hat{p}_\alpha d\hat{q}_\alpha$. This measure is independent of α. From now on, we will denote this space by L_0^2 and L_α^2 will indicate the space $L^2(\hat{p}_\alpha)$.

The reduced S-operator related to $S_{0\beta}$ and $S_{\alpha 0}$ are defined in the same way, e.g.,

$$S_{0\beta}(\vec{p}_\alpha, \vec{q}_\alpha; \vec{p}'_\beta) \equiv \delta(E-E') \frac{<\omega_\alpha \hat{p}_\alpha \hat{q}_\alpha | s_{0\beta}(E) | \hat{p}'_\beta>}{(\mu_\alpha n_\alpha)^{1/4} p_\alpha q_\alpha (n_\beta p'_\beta)^{1/2}} \tag{3.18}$$

and, using Eq. (3.8)

$$<\omega_\gamma \hat{p}_\gamma \hat{q}_\gamma | s_{0\beta}(E) | \hat{p}'_\beta> = -2\pi\, i (\mu_\gamma n_\gamma)^{1/4}\ p_\gamma q_\gamma (n_\beta p'_\beta)^{1/2} <\vec{p}_\gamma \vec{q}_\gamma | \mathscr{B}^{(+)}_{0\beta} | \vec{p}'_\beta > \tag{3.19}$$

where p_α and q_α are the momenta determined by E.

The momentum and reduced mass factors are chosen such that the operator relations S obeys on $\hat{h}$ are also valid for s(E) on a reduced space. To illustrate this consider the kernel form of the unitarity Eq. (3.5) for $\alpha, \beta > 0$

$$\delta^3(\vec{p}_\alpha - \vec{p}'_\beta)\, \delta_{\alpha\beta} = \sum_{\gamma=1}^{3} \int S_{\gamma\alpha}(\vec{p}''_\gamma, \vec{p}_\alpha)^* S_{\gamma\beta}(\vec{p}''_\gamma, \vec{p}'_\beta)\, d\vec{p}''_\gamma$$

$$+ \int S_{0\alpha}(\vec{p}''_\alpha, \vec{q}''_\alpha; \vec{p}_\alpha)^* S_{0\beta}(\vec{p}''_\alpha \vec{q}''_\alpha; \vec{p}'_\beta)\, d\vec{p}''_\alpha\, d\vec{q}''_\alpha \tag{3.20}$$

If we now use

$$d\vec{p}''_\alpha\, d\vec{q}''_\alpha = (n_\alpha \mu_\alpha)^{1/2}\ p''^2_\alpha q''^2_\alpha dE' d\omega''_\alpha\, d\hat{p}''_\alpha d\hat{q}''_\alpha \tag{3.21}$$

together with Eq. (3.12) and we equate the coefficient of $\delta(E-E')$ appearing on both sides we obtain for Eq. (3.20)

$$\delta_{\alpha\beta}\,\delta(\hat{p}_\alpha-\hat{p}'_\beta) = \sum_{\gamma=1}^{3}\int \langle\hat{p}''_\gamma|s_{\gamma\alpha}(E)|\hat{p}_\alpha\rangle^* \langle\hat{p}''_\gamma|s_{\gamma\beta}(E)|\hat{p}'_\beta\rangle\, d\hat{p}''_\gamma$$

$$+\int \langle\omega''_\alpha\hat{p}''_\alpha\hat{q}''_\alpha|s_{0\alpha}(E)|\hat{p}_\alpha\rangle^* \langle\omega''_\alpha\hat{p}''_\alpha\hat{q}''_\alpha|s_{0\beta}(E)|\hat{p}'_\beta\rangle\, d\omega''_\alpha\, d\hat{p}''_\alpha\, d\hat{q}''_\alpha \qquad (3.22)$$

This result is the kernel form of the operator equation

$$\delta_{\alpha\beta}1_\alpha = \sum_{\gamma=0}^{3} s^\dagger_{\gamma\alpha}(E)\, s_{\gamma\beta}(E) \quad . \qquad (3.23)$$

A similar demonstration shows that this equation is valid for all values of α and β. The operator 1_α stands for the identity operator on the space L^2_α, 1_0 is the identity operator on L^2_0.

Note that we can introduce a reduced channel space defined by

$$\hat{h}_r \equiv L^2_0 \oplus L^2_1 \oplus L^2_2 \oplus L^2_3 \quad . \qquad (3.24)$$

Acting on this space, the Eq. (3.23) is the component form of the first part of

$$\hat{1}_r = s^\dagger(E)\, s(E) = s(E)\, s^\dagger(E) \quad . \qquad (3.25)$$

where 1_r is the identity on $\hat{h}_r$. The second equality here is obtained in the same way as the first. Clearly Eq. (3.25) is a one parameter family of operator relations on $\hat{h}_r$ which are equivalent to the relation (3.4) on the channel space $\hat{h}$. It shall turn out that the three-body time-delay operator will also have two forms—one on $\hat{h}$ and one on $\hat{h}_r$.

IV. DEFINITION OF TIME DELAY AND STATEMENT OF THE PROBLEM

Let us now describe the definition of the time–delay operator. Consider the exact wavepacket given by

$$\Psi_\alpha(t) = e^{-iHt}\, U_\alpha^{(-)} f_\alpha \qquad f_\alpha \in \mathscr{h}_\alpha, \qquad \Psi_\alpha(t) \in \mathscr{h} \tag{4.1}$$

This is the wavepacket that evolves from the asymptotic channel wavepacket f_α. Likewise consider

$$\Psi'_\beta(t) = e^{-iHt}\, U_\beta^{(-)} f'_\beta \qquad f'_\beta \in \mathscr{h}_\beta, \qquad \Psi'_\beta(t) \in \mathscr{h}$$

If we recall that $\tilde{\rho} = (\tilde{x}_\alpha^2 + \tilde{y}_\alpha^2)^{1/2}$ is independent of α=1, 2, 3 then we can use the distance $\tilde{\rho}$ to define the radius of a sphere in the six-dimensional space $\vec{x}_\alpha, \vec{y}_\alpha$. We will associate a projection operator $\bar{\mathscr{P}}(R)$ on $\mathscr{h}$ with this sphere,

$$\begin{aligned} \bar{\mathscr{P}}(R)\, f(\vec{x}_\alpha, \vec{y}_\alpha) &= f(\vec{x}_\alpha, \vec{y}_\alpha) \qquad && \text{if } \ |\tilde{x}_\alpha^2 + \tilde{y}_\alpha^2|^{1/2} \leq R \\ &= 0 && \text{if } \ |\tilde{x}_\alpha^2 + \tilde{y}_\alpha^2|^{1/2} > R \end{aligned} \tag{4.2}$$

The inner product $(\Psi_\alpha(t), \bar{\mathscr{P}}(R)\Psi_\alpha(t))$ is the likelihood of finding the state Ψ_α inside the sphere of radius R at time t. Now if we form the integral

$$\int_{-t_0}^{t_0} (\Psi_\alpha(t), \bar{\mathscr{P}}(R)\, \Psi_\alpha(t))\, dt \tag{4.3}$$

its physical interpretation is the fraction of time between $-t_0$ and t_0 that the state Ψ_α spends inside the sphere of radius R. If we perform the limit $t_0 \to \infty$ then the integral represents the total time Ψ_α spends inside the sphere. In association with the integral above we can form the more general integral which gives the overlap within the sphere of two distinct states Ψ_α and Ψ'_β. We define

$$T^E_{\alpha\beta}(R, t_0) \equiv \int_{-t_0}^{t_0} (\Psi_\alpha(t),\ \bar{\mathscr{P}}(R)\ \Psi'_\beta(t))\, dt \tag{4.4}$$

In the notation for the complex number $T^E_{\alpha\beta}$ we have indicated some but not all the factors that it depends on. For example the value of $T^E_{\alpha\beta}$ will depend on f_α and f'_β as well as R and t_0. In the circumstance $\alpha=\beta$ and $f_\alpha = f'_\alpha$ then $T^E_{\alpha\beta}$ is real and has the interpretation we have given for the expression (4.3). Our notation for $T^E_{\alpha\beta}$ carries a superscript E in order to specify that the times associated with $T^E_{\alpha\beta}$ relate to the exact wavefunctions $\Psi(t)$.

We may also write down similar definitions that pertain to the evolution of the asymptotic solutions in the absence of the intercluster potentials. For example these wavepackets are given by

$$\Phi_\alpha(t) = e^{-iH_\alpha t} I^\dagger_\alpha f_\alpha \qquad f_\alpha \in \mathscr{h}_\alpha, \quad \Phi_\alpha(t) \in \mathscr{h} \tag{4.5}$$

$$\Phi'_\beta(t) = e^{-iH_\beta t} I^\dagger_\beta f'_\beta \qquad f'_\beta \in \mathscr{h}_\beta, \quad \Phi'_\beta(t) \in \mathscr{h} \tag{4.6}$$

The absence of the intercluster potentials means that the corresponding evolution may be thought of as 'free' since the interaction between the target and the incident wave has no effect on the evolution of the wavepacket. The 'free' equivalent of the integral (4.3) is

$$\int_{-t_0}^{t_0} (\Phi_\alpha(t), \bar{\mathscr{P}}(R)\, \Phi_\alpha(t))\, dt \tag{4.7}$$

This gives the fraction of the time interval $(-t_0, t_0)$ that the 'free' system spends in the sphere. The numerical value of the 'free' integral will differ from that of the integral for the exact wavepacket. This time difference is entirely due to the effect of the intercluster interaction on the evolution of the wavepacket. As above we write down a general matrix element that has the form (4.7) as its diagonal element.

$$T^F_{\alpha\beta}(R, t_0) \equiv \delta_{\alpha\beta} \int_{-t_0}^{t_0} (\Phi_\alpha(t), \bar{\mathscr{P}}(R)\, \Phi'_\beta(t))\, dt \tag{4.8}$$

The Kronecker delta function appears in the definition (4.8) of the free transit time for the following reason. In the α channel free scattering there is no interaction between the target cluster and the incident particle. Thus any scattering which begins in the α-channel must remain in the α-channel. Since the asymptotic forms $\Phi_\alpha(t)$ and $\Phi'_\beta(t)$ are not orthogonal, the Kronecker delta is necessary to preserve the diagonality of the free scattering. Taking the difference of $T^E_{\alpha\beta}$ and $T^F_{\alpha\beta}$ gives us the time-delay for the time interval $(-t_0, t_0)$ and a sphere of radius R.

Now we would like to construct an operator whose expectation value gives us the time-difference described above. We define

$$(f_\alpha, Q_{\alpha\beta}(R, t_0)\, f'_\beta) \equiv T^E_{\alpha\beta}(R, t_0) - T^F_{\alpha\beta}(R, t_0) \tag{4.9}$$

For each f_α and f'_β the quantities $T^E_{\alpha\beta}$ and $T^F_{\alpha\beta}$ have unique values so that $Q_{\alpha\beta}(R, t_0)$ is defined by Eq. (4.9). It is useful to have an explicit form for $Q_{\alpha\beta}$. This may be obtained as follows. One can write $T^F_{\alpha\beta}$ as

$$\begin{aligned} T^F_{\alpha\beta}(R, t_0) &= \delta_{\alpha\beta} \int_{-t_0}^{t_0} \left(e^{-iH_\alpha t}\, I^\dagger_\alpha f_\alpha,\ \bar{\mathscr{P}}(R)\, e^{-iH_\beta t}\, I^\dagger_\beta f'_\beta\right) dt \\ &= \delta_{\alpha\beta} \int_{-t_0}^{t_0} \left(I^\dagger_\alpha\, e^{-i\tilde{H}_\alpha t} f_\alpha,\ \bar{\mathscr{P}}(R)\, I^\dagger_\beta\, e^{-i\tilde{H}_\beta t} f'_\beta\right) dt \qquad (4.10) \\ &= \delta_{\alpha\beta} \int_{-t_0}^{t_0} \left(f_\alpha,\ e^{i\tilde{H}_\alpha t}\, \bar{\mathscr{P}}_\alpha(R)\, e^{-i\tilde{H}_\beta t} f'_\beta\right) dt \end{aligned}$$

where the operator $\bar{\mathscr{P}}_\alpha(R)$ is

$$\bar{\mathscr{P}}_\alpha(R) = I_\alpha\, \bar{\mathscr{P}}(R)\, I^\dagger_\alpha \qquad : \mathscr{h}_\alpha \to \mathscr{h}_\alpha \tag{4.11}$$

From the definition (4.11) it at once follows that $\bar{\mathscr{P}}_\alpha(R)$ is a bounded self-adjoint operator. It is however not a projection operator since the idempotent property is not valid. This is seen from

$$\begin{aligned} \bar{\mathscr{P}}^2_\alpha(R) &= I_\alpha \bar{\mathscr{P}}(R)\, I^\dagger_\alpha I_\alpha\, \bar{\mathscr{P}}(R)\, I^\dagger_\alpha \qquad : \mathscr{h}_\alpha \to \mathscr{h}_\alpha \\ &= I_\alpha \bar{\mathscr{P}}(R)\, P_\alpha \bar{\mathscr{P}}(R)\, I^\dagger_\alpha \quad . \end{aligned} \tag{4.12}$$

where we have used $I^\dagger_\alpha I_\alpha = P_\alpha$ which follows from the definition of I_α, Eq. (2.14). However in the limit $R \to \infty$ then $\bar{\mathscr{P}}^2_\alpha(R)$ becomes the identity operator E_α since $\bar{\mathscr{P}}(R) \to E$ and

$$I_\alpha E P_\alpha E I^\dagger_\alpha = I_\alpha P_\alpha I^\dagger_\alpha = I_\alpha I^\dagger_\alpha = E_\alpha \quad . \tag{4.13}$$

The last equality again follows from the definition (2.14).

We continue with the explicit construction of $Q_{\alpha\beta}$ by treating $T^E_{\alpha\beta}$ in a fashion parallel to that of $T^F_{\alpha\beta}$. The term $T^E_{\alpha\beta}$ can be written as follows

$$\begin{aligned} T^E_{\alpha\beta}(R, t_0) &= \int_{-t_0}^{t_0} \left(e^{-iHt}\, U^{(-)}_\alpha f_\alpha, \bar{\mathscr{P}}(R)\, e^{-iHt}\, U^{(-)}_\beta f'_\beta\right) dt \\ &= \int_{-t_0}^{t_0} \left(U^{(-)}_\alpha\, e^{-i\tilde{H}_\alpha t} f_\alpha, \bar{\mathscr{P}}(R)\, U^{(-)}_\beta\, e^{-i\tilde{H}_\beta t} f'_\beta\right) dt \\ &= \int_{-t_0}^{t_0} \left(f_\alpha, e^{+i\tilde{H}_\alpha t}\, U^{(-)\dagger}_\alpha\, \bar{\mathscr{P}}(R)\, U^{(-)}_\beta\, e^{-i\tilde{H}_\beta t} f'_\beta\right)_\alpha dt \end{aligned} \tag{4.14}$$

In the second version of (4.14) we have employed the intertwinning relation 2°. In the third version we have employed the adjoint operation. The difference of Eq. (4.10) and Eq. (4.14) is

$$(f_\alpha, Q_{\alpha\beta}(R, t_0)\, f'_\beta) = \int_{-t_0}^{t_0} \left(f_\alpha, e^{i\tilde{H}_\alpha t}\left[U^{(-)\dagger}_\alpha \bar{\mathscr{P}}(R)\, U^{(-)}_\beta - \delta_{\alpha\beta}\, \bar{\mathscr{P}}_\alpha(R)\right] e^{-i\tilde{H}_\beta t} f'_\beta\right) dt \tag{4.15}$$

This defines the operator $Q_{\alpha\beta}(R, t_0)$. The expression above is defined for all $f_\alpha \in h_\alpha$ and $f'_\beta \in h_\beta$ since all the operators in the inner product on the right are bounded and the integral is over a finite time interval. So the operator $Q_{\alpha\beta}(R, t_0)$ given by

$$Q_{\alpha\beta}(R, t_0) = \int_{-t_0}^{t_0} e^{i\widetilde{H}_\alpha t} \left[U_\alpha^{(-)\dagger} \bar{\mathscr{P}}(R)\, U_\beta^{(-)} - \delta_{\alpha\beta}\, \bar{\mathscr{P}}_\alpha(R)\right] e^{-i\widetilde{H}_\beta t}\, dt \qquad (4.16)$$

is a bounded operator for finite R, t_0.

Eventually to obtain the physical time-delay we will take the limit $t_0 \to \infty$ and follow it by the limit $R \to \infty$. However, some of the interesting properties of the time-delay operator are already present in form (4.16). First, we see that $Q_{\alpha\beta}$ is the component form of an operator on the channel space $\hat{h}$. Its channel structure is identical to that of the S-matrix. The next property is that

$$Q_{\alpha\beta}(R, t_0) = Q^\dagger_{\beta\alpha}(R, t_0) \qquad (4.17)$$

This follows directly from the structure of (4.16). In fact Eq. (4.17) is just the component form of the self-adjoint property for operators on $\hat{h}$. Thus for any $\hat{f} \in \hat{h}$ which describes the state of the three-body system in terms of the asymptotic channel wavefunctions the time-delay operator Q will have real matrix elements. Since Q represents an observable this must be the case. However off-diagonal component forms of Q, i.e., $Q_{\alpha\beta}$, will not generally be real.

It is desirable to take the limits $t_0 \to \infty$ and $R \to \infty$ in the definition of our operator $Q_{\alpha\beta}(R, t_0)$. In the following section we shall construct an operator $Q_{\alpha\beta}$ defined by a kernel composed of generalized functions such that

$$(f_\alpha, Q_{\alpha\beta}\, f'_\beta)_\alpha = \lim_{R \to \infty}\ \lim_{t_0 \to \infty}\ (f_\alpha, Q_{\alpha\beta}(R, t_0)\, f'_\beta)_\alpha \quad . \qquad (4.18)$$

The functions f_α and f'_β need to be smooth enough so that the generalized functions appearing in the representation of $Q_{\alpha\beta}$ are well-defined. This restricted set of functions, defined in Appendix A, for which Eq. (4.18) is valid are dense in the space $\hat{h}$.

One effect of taking the limit $t_0 \to \infty$ in the representation (4.16) is that the $Q_{\alpha\beta}$ operators will now intertwine with the channel Hamiltonians. By changing the variable of integration in Eq. (4.16) it easily follows that

$$e^{i\tilde{H}_\alpha t} Q_{\alpha\beta}(R,\infty) = Q_{\alpha\beta}(R,\infty)\, e^{i\tilde{H}_\beta t} \tag{4.19}$$

or equivalently,

$$\tilde{H}_\alpha Q_{\alpha\beta}(R,\infty) = Q_{\alpha\beta}(R,\infty)\, \tilde{H}_\beta \quad . \tag{4.20}$$

This property mirrors the intertwining relation (3.6) valid for the S-matrix $S_{\alpha\beta}$.

Before proceeding further we pause to contrast our definition of the time-delay operator with those that exist in the current literature. The main novelty of Eq. (4.16) and the limit process in Eq. (4.18) is of course its multichannel character. However the type of limit in Eq. (4.18) is simpler than that previously introduced by Smith[12] and also adopted by Jauch and Marchand[6] and others.[7] These papers employ an average over R before the $R \to \infty$ limit is taken. This average is used to get rid of oscillatory terms in R. Here we shall find that treating the behavior of the projection operators $\bar{\mathscr{P}}_\beta(R)$ and $\bar{\mathscr{P}}(R)$ carefully enough shows that these oscillating terms all vanish when evaluated between appropriately smooth wavepackets f_α and f'_β.

Let us now resume the development of the problem. At this point we shall utilize the approach found in Jauch and Marchand's[6] treatment of time-delay in the two-body case. Since the inverse of S exists one can find Q by determining SQ. An element of this product takes the form

$$S_{\gamma\alpha}Q_{\alpha\beta}(R,t_0) = \int_{-t_0}^{t_0} S_{\gamma\alpha}\, e^{i\widetilde{H}_\alpha t}\left[U_\alpha^{(-)\dagger}\,\overline{\mathscr{P}}(R)\,U_\beta^{(-)} - \delta_{\alpha\beta}\overline{\mathscr{P}}_\beta(R)\right] e^{-i\widetilde{H}_\beta t}\, dt$$

$$= \int_{-t_0}^{t_0} e^{i\widetilde{H}_\gamma t}\, S_{\gamma\alpha}\left[U_\alpha^{(-)\dagger}\overline{\mathscr{P}}(R)\, U_\beta^{(-)} - \delta_{\alpha\beta}\,\overline{\mathscr{P}}_\beta(R)\right] e^{-i\widetilde{H}_\beta t}\, dt \tag{4.22}$$

The first term in the square brackets may be simplified by noting that

$$\sum_{\alpha=0}^{3} S_{\gamma\alpha}\, U_\alpha^{(-)\dagger} = \sum_{\alpha=0}^{3} U_\gamma^{(+)\dagger}\, U_\alpha^{(-)}\, U_\alpha^{(-)\dagger} = U_\gamma^{(+)\dagger}(1-P_d) = U_\gamma^{(+)\dagger}\ . \tag{4.23}$$

The second equality is the asymptotic completeness of the U's and the third equality follows from orthogonality properties of bound and scattering states. So

$$\sum_{\alpha=0}^{3} S_{\gamma\alpha}Q_{\alpha\beta}(R,t_0) = \int_{-t_0}^{t_0} e^{i\widetilde{H}_\gamma t}\, U_\gamma^{(+)\dagger}\left[\overline{\mathscr{P}}(R)\, U_\beta^{(-)} - U_\beta^{(-)}\,\overline{\mathscr{P}}_\beta(R)\right] e^{-i\widetilde{H}_\beta t}\, dt \tag{4.24}$$

Our problem is now reduced to evaluating the right-hand side Eq. (4.24). Let us take matrix elements of Eq. (4.24) and let the $t_0 \to \infty$. For $\gamma \neq 0$ and $\beta \neq 0$ one has

$$\left(f_\gamma,\ \sum_{\alpha=0}^{3} S_{\gamma\alpha}Q_{\alpha\beta}(R,\infty)\, f'_\beta\right)_\gamma =$$

$$\int_{-\infty}^{\infty}\left(f_\gamma, e^{i\widetilde{H}_\gamma t}\, U_\gamma^{(+)\dagger}\left[\overline{\mathscr{P}}(R)\, U_\beta^{(-)} - U_\beta^{(-)}\,\overline{\mathscr{P}}_\beta(R)\right] e^{-i\widetilde{H}_\beta t}\, f'_\beta\right)_\gamma dt \tag{4.25}$$

We now assume that f_γ and f'_β are well enough behaved so we may interchange the order of integration in Eq. (4.25). Thus we can rewrite our equation in the following form

$$\left(f_\gamma, -\sum_{\alpha=0}^{3} S_{\gamma\alpha} Q_{\alpha\beta}(R,\infty)\, f'_\beta\right)_\gamma = \int f_\gamma(\vec{p}_\gamma)^* \left\{ \int_{-\infty}^{\infty} e^{it(\tilde{p}_\gamma^2 - \chi_\gamma^2 - \tilde{p}_\beta'^2 + \chi_\beta^2)}\, dt \right\}$$

$$< \vec{p}_\gamma | U_\gamma^{(+)\dagger} \left[\bar{\mathscr{P}}(R)\, U_\beta^{(-)} - U_\beta^{(-)} \bar{\mathscr{P}}_\beta(R) \right] | \vec{p}'_\beta > f'_\beta(\vec{p}'_\beta)\, d\vec{p}_\gamma\, d\vec{p}'_\beta \tag{4.26}$$

The integral in the curly brackets is $2\pi\delta(\tilde{p}_\gamma^2 - \chi_\gamma^2 - \tilde{p}_\beta'^2 + \chi_\beta^2)$ and physically enforces energy conservation between an asymptotic state in the β channel and one in the γ channel. Since Eq. (4.26) holds for a dense set of functions f_γ and f'_β we can associate it with the following kernel in momentum space.

$$< \vec{p}_\gamma | \sum_{\alpha=0}^{3} S_{\gamma\alpha} Q_{\alpha\beta}(R,\infty) | \vec{p}'_\beta > =$$

$$= 2\pi\, \delta(\tilde{p}_\gamma^2 - \chi_\gamma^2 - \tilde{p}_\beta'^2 + \chi_\beta^2) < \vec{p}_\gamma | U_\gamma^{(+)\dagger} \left[\bar{\mathscr{P}}(R)\, U_\beta^{(-)} - U_\beta^{(-)} \bar{\mathscr{P}}_\beta(R) \right] | \vec{p}'_\beta >$$

$$\gamma > 0, \quad \beta > 0 \tag{4.27}$$

For values of the indices γ and β where either one or both are zero, one can repeat an evaluation similar to the one above. We find that

$$< \vec{p}\,\vec{q} | \sum_{\alpha=0}^{3} S_{0\alpha} Q_{\alpha\beta}(R,\infty) | \vec{p}'_\beta > =$$

$$= 2\pi\, \delta(\tilde{p}^2 + \tilde{q}^2 - \tilde{p}_\beta'^2 + \chi_\beta^2) < \vec{p}\,\vec{q} | U_0^{(+)\dagger} \left[\bar{\mathscr{P}}(R)\, U_\beta^{(-)} - U_\beta^{(-)} \bar{\mathscr{P}}_\beta(R) \right] | \vec{p}'_\beta >$$

$$\beta > 0 \tag{4.28}$$

$$< \vec{p}\,\vec{q} | \sum_{\alpha=0}^{3} S_{0\alpha} Q_{\alpha 0}(R,\infty) | \vec{p}'\vec{q}' > =$$

$$= 2\pi\, \delta(\tilde{p}^2 + \tilde{q}^2 - \tilde{p}'^2 - \tilde{q}'^2) < \vec{p}\,\vec{q} | U_0^{(+)\dagger} \left[\bar{\mathscr{P}}(R)\, U_0^{(-)} - U_0^{(-)} \bar{\mathscr{P}}(R) \right] | \vec{p}'\vec{q}' > \tag{4.29}$$

The remaining portions of the paper are concerned with evaluating the matrix elements appearing in these last three equations.

V. DERIVATION OF THE TIME-DELAY RELATION

The previous section has demonstrated that if we can evaluate the matrix element $U_\gamma^{(+)\dagger}\left[\bar{\mathscr{P}}(R)\, U_\beta^{(-)} - U_\beta^{(-)}\bar{\mathscr{P}}_\beta(R)\right]$, then we know the product SQ. This is equivalent to knowing Q since S^{-1} exists. We now shall compute the <u>on-shell</u> values of the above matrix element. Let us define

$$X_\beta(R) \equiv \bar{\mathscr{P}}(R)\, U_\beta^{(-)} - U_\beta^{(-)}\bar{\mathscr{P}}_\beta(R) \qquad : \mathscr{h}_\beta \rightarrow \mathscr{h} \tag{5.1}$$

We note that the operator form of Eq. (2.18) may be written

$$U_\gamma^{(\pm)} = I_\gamma^\dagger - K_\gamma^{(\pm)} \tag{5.2}$$

The kernel associated with K_γ is that given by Eq. (2.19). Physically K_γ contains all features of the wavefunction related to the scattered parts of the wavefunction. We note that Eq. (5.1) can be expanded as the sum of two terms, which we may treat separately.

$$X_\beta(R) = \bar{\mathscr{P}}(R)\, (I_\beta^\dagger - K_\beta^{(-)}) - (I_\beta^\dagger - K_\beta^{(-)})\,\bar{\mathscr{P}}_\beta(R) \tag{5.3}$$

$$= \left[\bar{\mathscr{P}}(R) - P_\beta\bar{\mathscr{P}}(R)\right] I_\beta^\dagger + \left[K_\beta^{(-)}\bar{\mathscr{P}}_\beta(R) - \bar{\mathscr{P}}(R)\, K_\beta^{(-)}\right] \tag{5.4}$$

Here we have used $I_\beta^\dagger I_\beta = P_\beta$. Now we observe that the first term in expression (5.4) for $X_\beta(R)$ vanishes strongly as $R \rightarrow \infty$. That this is so may be seen as follows.

Let f_β be any function in $\mathscr{h}_\beta$. Then

$$\|\left[\bar{\mathscr{P}}(R) - P_\beta\bar{\mathscr{P}}(R)\right] I_\beta^\dagger f_\beta\| = \|\left[\bar{\mathscr{P}}(R) - P_\beta(\bar{\mathscr{P}}(R) - E) - P_\beta E\right] I_\beta^\dagger f_\beta\|$$

$$\leq \|(\bar{\mathscr{P}}(R) - P_\beta) I_\beta^\dagger f_\beta\| + \|P_\beta(\bar{\mathscr{P}}(R) - E) I_\beta^\dagger f_\beta\| \quad . \tag{5.5}$$

using $P_\beta I_\beta^\dagger = I_\beta^\dagger$ and $\|P_\beta\| = 1$ our inequality becomes

$$\leq 2\, \|(\bar{\mathscr{P}}(R) - E) I_\beta^\dagger f_\beta\| \quad . \tag{5.6}$$

This last expression goes to zero since $\bar{\mathscr{P}}(R)$ strongly converges to unity. Thus we need only compute the value of $U_\gamma^{(+)\dagger} Y_\beta(R)$, where $Y_\beta(R)$ is defined as

$$Y_\beta(R) \equiv K_\beta^{(-)} \bar{\mathscr{P}}_\beta(R) - \bar{\mathscr{P}}(R) K_\beta^{(-)} \quad . \tag{5.7}$$

A lengthly and detailed analysis is needed to evaluate the expectation values of $U_\gamma^{(+)\dagger} Y_\beta(R)$. Most of the terms entering the computation turn out to be zero. We shall deal with this complexity by placing in the appendices the evaluation of the zero terms. Thus the detail exhibited in this section is somewhat more important since it leads directly to the desired matrix element values. For example we show in Appendix C that $K_\gamma^{(+)\dagger} Y_\beta(R) \to 0$ in the $R \to \infty$ limit. Thus our problem is simplified to computing

$$\lim_{R\to\infty} \langle \vec{p}_\gamma | U_\gamma^{(+)\dagger} \left[\bar{\mathscr{P}}(R)\, U_\beta^{(-)} - U_\beta^{(-)} \bar{\mathscr{P}}_\beta(R) \right] | \vec{p}_\beta^{\,\prime} \rangle = \lim_{R\to\infty} \langle \vec{p}_\gamma | I_\gamma Y_\beta(R) | \vec{p}_\beta^{\,\prime} \rangle \tag{5.8}$$

Our expression for $Y_\beta(R)$ has two terms. We treat the operator $K_\beta^{(-)} \bar{\mathscr{P}}_\beta(R)$ first. Using the Eqs. (2.19) and (2.20) for $K_\beta^{(-)}$ we may write $K_\beta^{(-)} \bar{\mathscr{P}}_\beta(R)$ as

$$\langle \vec{p}_\gamma \vec{q}_\gamma | K_\beta^{(-)} \bar{\mathscr{P}}_\beta(R) | \vec{p}_\beta^{\,\prime} \rangle$$

$$= \int \sum_{\alpha=1}^{3} \left\{ -\langle \vec{p}_\gamma \vec{q}_\gamma | \mathscr{G}_{\alpha\beta}^{(+)} | \vec{p}_\beta^{\,\prime\prime} \rangle + \frac{\phi_\alpha(\vec{q}_\alpha) \langle \vec{p}_\alpha | \mathscr{H}_{\alpha\beta}^{(+)} | \vec{p}_\beta^{\,\prime\prime} \rangle}{\tilde{p}_\alpha^2 - \chi_\alpha^2 - \tilde{p}_\beta^{\prime\prime 2} + \chi_\beta^2 - i0} \right\} \frac{\langle \vec{p}_\beta^{\,\prime\prime} | \bar{\mathscr{P}}_\beta(R) | \vec{p}_\beta^{\,\prime} \rangle \, d^3 p_\beta^{\prime\prime}}{\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta^{\prime\prime 2} + \chi_\beta^2 - i0} \tag{5.9}$$

We further expand this by expressing the singular denominators in terms of their delta-function and principal-value parts. We shall denote a principal-value integral by writing the denominator terms without the customary $\pm i0$ notation. Our expansion of Eq. (5.9) now reads

$$\langle \vec{p}_\gamma \vec{q}_\gamma | K_\beta^{(-)} \bar{\mathscr{P}}_\beta(R) | \vec{p}_\beta^{\,\prime} \rangle \equiv \langle \vec{p}_\gamma \vec{q}_\gamma | \sum_{i=1}^{6} B_i(R) | \vec{p}_\beta^{\,\prime} \rangle \tag{5.10}$$

where the kernels $B_i(R)$ are given by,

$$<\vec{p}_\gamma \vec{q}_\gamma | B_1(R) | \vec{p}'_\beta> \equiv - \int \sum_{\alpha=1}^{3} <\vec{p}_\gamma \vec{q}_\gamma | \mathscr{G}^{(+)}_{\alpha\beta} | \vec{p}''_\beta> \frac{<\vec{p}''_\beta | \bar{\mathscr{P}}_\beta(R) | \vec{p}'_\beta>}{\tilde{p}^2_\gamma + \tilde{q}^2_\gamma - \tilde{p}''^2_\beta + \chi^2_\beta} d^3p''_\beta \tag{5.11}$$

$$<\vec{p}_\gamma \vec{q}_\gamma | B_2(R) | \vec{p}'_\beta> \equiv \int \sum_{\alpha=1}^{3} \frac{\phi_\alpha(\vec{q}_\alpha) <\vec{p}_\alpha | \mathscr{H}^{(+)}_{\alpha\beta} | \vec{p}''_\beta>}{\tilde{p}^2_\alpha - \chi^2_\alpha - \tilde{p}''^2_\beta + \chi^2_\beta} \frac{<\vec{p}''_\beta | \bar{\mathscr{P}}_\beta(R) | \vec{p}'_\beta>}{\tilde{p}^2_\gamma + \tilde{q}^2_\gamma - \tilde{p}''^2_\beta + \chi^2_\beta} d^3p''_\beta \tag{5.12}$$

$$<\vec{p}_\gamma \vec{q}_\gamma | B_3(R) | \vec{p}'_\beta> \equiv \int \sum_{\alpha=1}^{3} i\pi\, \delta(\tilde{p}^2_\alpha - \chi^2_\alpha - \tilde{p}''^2_\beta + \chi^2_\beta)\, \phi_\alpha(\vec{q}_\alpha) \frac{<\vec{p}_\alpha | \mathscr{H}^{(+)}_{\alpha\beta} | \vec{p}''_\beta> <\vec{p}''_\beta | \bar{\mathscr{P}}_\beta(R) | \vec{p}'_\beta>}{\tilde{p}^2_\gamma + \tilde{q}^2_\gamma - \tilde{p}''^2_\beta + \chi^2_\beta} d^3p''_\beta \tag{5.13}$$

$$<\vec{p}_\gamma \vec{q}_\gamma | B_4(R) | \vec{p}'_\beta> \equiv - \int \sum_{\alpha=1}^{3} <\vec{p}_\gamma \vec{q}_\gamma | \mathscr{G}^{(+)}_{\alpha\beta} | \vec{p}''_\beta>\, i\pi\, \delta(\tilde{p}^2_\gamma + \tilde{q}^2_\gamma - \tilde{p}''^2_\beta + \chi^2_\beta) <\vec{p}''_\beta | \bar{\mathscr{P}}_\beta(R) | \vec{p}'_\beta> d^3p''_\beta \tag{5.14}$$

$$<\vec{p}_\gamma \vec{q}_\gamma | B_5(R) | \vec{p}'_\beta> \equiv \int \sum_{\alpha=1}^{3} \frac{\phi_\alpha(\vec{q}_\alpha) <\vec{p}_\alpha | \mathscr{H}^{(+)}_{\alpha\beta} | \vec{p}''_\beta>}{\tilde{p}^2_\alpha - \chi^2_\alpha - \tilde{p}''^2_\beta + \chi^2_\beta}\, i\pi\, \delta(\tilde{p}^2_\gamma + \tilde{q}^2_\gamma - \tilde{p}''^2_\beta + \chi^2_\beta) <\vec{p}''_\beta | \bar{\mathscr{P}}_\beta(R) | \vec{p}'_\beta> d^3p''_\beta \tag{5.15}$$

$$<\vec{p}_\gamma \vec{q}_\gamma | B_6(R) | \vec{p}'_\beta> \equiv \int \sum_{\alpha=1}^{3} i\pi\, \delta(\tilde{p}^2_\alpha - \chi^2_\alpha - \tilde{p}''^2_\beta + \chi^2_\beta)\, \phi_\alpha(\vec{q}_\alpha) <\vec{p}_\alpha | \mathscr{H}^{(+)}_{\alpha\beta} | \vec{p}''_\beta>\, i\pi\, \delta(\tilde{p}^2_\gamma + \tilde{q}^2_\gamma - \tilde{p}''^2_\beta + \chi^2_\beta) \times$$

$$\times <\vec{p}''_\beta | \bar{\mathscr{P}}_\beta(R) | \vec{p}'_\beta> d^3p''_\beta \tag{5.16}$$

It is now appropriate to examine the operator $\bar{\mathscr{P}}(R)K^{(-)}_\beta$. The kernel representation of $\bar{\mathscr{P}}(R)K^{(-)}_\beta$ is

$$<\vec{p}_\gamma \vec{q}_\gamma | \bar{\mathscr{P}}(R)\, K^{(-)}_\beta | \vec{p}'_\beta>$$

$$= \int \frac{<\vec{p}_\gamma \vec{q}_\gamma | \bar{\mathscr{P}}(R) | \vec{p}''_\gamma \vec{q}''_\gamma>}{\tilde{p}''^2_\gamma + \tilde{q}''^2_\gamma - \tilde{p}'^2_\beta + \chi^2_\beta - i0} \sum_{\alpha=1}^{3} \left\{ - <\vec{p}''_\gamma \vec{q}''_\gamma | \mathscr{G}^{(+)}_{\alpha\beta} | \vec{p}'_\beta> + \frac{\phi_\alpha(\vec{q}''_\alpha) <\vec{p}''_\alpha | \mathscr{H}^{(+)}_{\alpha\beta} | \vec{p}'_\beta>}{\tilde{p}''^2_\alpha - \chi^2_\alpha - \tilde{p}'^2_\beta + \chi^2_\beta - i0} \right\} d^3p''_\gamma d^3q''_\gamma \tag{5.17}$$

As before, we expand this in terms of its principal-value and delta-function parts. We have

$$<\vec{p}_\gamma \vec{q}_\gamma \,|\, \overline{\mathscr{P}}(R)\, K_\beta^{(-)} \,|\, \vec{p}_\beta^{\,\prime}> \equiv <\vec{p}_\gamma \vec{q}_\gamma \,|\, \sum_{i=1}^{6} A_i(R) \,|\, \vec{p}_\beta^{\,\prime}> \tag{5.18}$$

where the operators $A_i(R)$ are given by

$$<\vec{p}_\gamma \vec{q}_\gamma \,|A_1(R)|\, \vec{p}_\beta^{\,\prime}> \equiv -\int \frac{<\vec{p}_\gamma \vec{q}_\gamma |\overline{\mathscr{P}}(R)| \vec{p}_\gamma^{\,\prime\prime} \vec{q}_\gamma^{\,\prime\prime}>}{\tilde{p}_\gamma^{\prime\prime 2} + \tilde{q}_\gamma^{\prime\prime 2} - \tilde{p}_\beta^{\prime 2} + \chi_\beta^2} \sum_{\alpha=1}^{3} <\vec{p}_\gamma^{\,\prime\prime} \vec{q}_\gamma^{\,\prime\prime} \,|\, \mathscr{G}_{\alpha\beta}^{(+)} \,|\, \vec{p}_\beta^{\,\prime}> d^3p_\gamma^{\prime\prime}\, d^3q_\gamma^{\prime\prime} \tag{5.19}$$

$$<\vec{p}_\gamma \vec{q}_\gamma |A_2(R)|\, \vec{p}_\beta^{\,\prime}> \equiv +\int \frac{<\vec{p}_\gamma \vec{q}_\gamma |\overline{\mathscr{P}}(R)| \vec{p}_\gamma^{\,\prime\prime} \vec{q}_\gamma^{\,\prime\prime}>}{\tilde{p}_\gamma^{\prime\prime 2} + \tilde{q}_\gamma^{\prime\prime 2} - \tilde{p}_\beta^{\prime 2} + \chi_\beta^2} \sum_{\alpha=1}^{3} \frac{\phi_\alpha(\vec{q}_\alpha^{\,\prime\prime}) <\vec{p}_\alpha^{\,\prime\prime} |\mathscr{H}_{\alpha\beta}^{(+)}| \vec{p}_\beta^{\,\prime}>}{\tilde{p}_\alpha^{\prime\prime 2} - \chi_\alpha^2 - \tilde{p}_\beta^{\prime 2} + \chi_\beta^2} d^3p_\gamma^{\prime\prime} d^3q_\gamma^{\prime\prime} \tag{5.20}$$

$$<\vec{p}_\gamma \vec{q}_\gamma |A_3(R)|\, \vec{p}_\beta^{\,\prime}> \equiv +\int \frac{<\vec{p}_\gamma \vec{q}_\gamma |\overline{\mathscr{P}}(R)| \vec{p}_\gamma^{\,\prime\prime} \vec{q}_\gamma^{\,\prime\prime}>}{\tilde{p}_\gamma^{\prime\prime 2} + \tilde{q}_\gamma^{\prime\prime 2} - \tilde{p}_\beta^{\prime 2} + \chi_\beta^2}$$

$$\sum_{\alpha=1}^{3} i\pi\, \delta(\tilde{p}_\alpha^{\prime\prime 2} - \chi_\alpha^2 - \tilde{p}_\beta^{\prime 2} + \chi_\beta^2)\, \phi_\alpha(\vec{q}_\alpha^{\,\prime\prime}) <\vec{p}_\alpha^{\,\prime\prime} |\mathscr{H}_{\alpha\beta}^{(+)}| \vec{p}_\beta^{\,\prime}> d^3p_\gamma^{\prime\prime} d^3q_\gamma^{\prime\prime} \tag{5.21}$$

$$<\vec{p}_\gamma \vec{q}_\gamma |A_4(R)|\, \vec{p}_\beta^{\,\prime}> \equiv -\int <\vec{p}_\gamma \vec{q}_\gamma |\overline{\mathscr{P}}(R)| \vec{p}_\gamma^{\,\prime\prime} \vec{q}_\gamma^{\,\prime\prime}> \sum_{\alpha=1}^{3} <\vec{p}_\gamma^{\,\prime\prime} \vec{q}_\gamma^{\,\prime\prime} |\mathscr{G}_{\alpha\beta}^{(+)}| \vec{p}_\beta^{\,\prime}> i\pi\, \delta(\tilde{p}_\gamma^{\prime\prime 2} + \tilde{q}_\gamma^{\prime\prime 2} - \tilde{p}_\beta^{\prime 2} + \chi_\beta^2)\, d^3p_\gamma^{\prime\prime} d^3q_\gamma^{\prime\prime} \tag{5.22}$$

$$<\vec{p}_\gamma \vec{q}_\gamma |A_5(R)|\, \vec{p}_\beta^{\,\prime}> \equiv \int <\vec{p}_\gamma \vec{q}_\gamma |\overline{\mathscr{P}}(R)| \vec{p}_\gamma^{\,\prime\prime} \vec{q}_\gamma^{\,\prime\prime}> \sum_{\alpha=1}^{3} \frac{\phi_\alpha(\vec{q}_\alpha^{\,\prime\prime}) <\vec{p}_\alpha^{\,\prime\prime} |\mathscr{H}_{\alpha\beta}^{(+)}| \vec{p}_\beta^{\,\prime}>}{\tilde{p}_\alpha^{\prime\prime 2} - \chi_\alpha^2 - \tilde{p}_\beta^{\prime 2} + \chi_\beta^2}$$

$$i\pi\, \delta(\tilde{p}_\gamma^{\prime\prime 2} + \tilde{q}_\gamma^{\prime\prime 2} - \tilde{p}_\beta^{\prime 2} + \chi_\beta^2)\, d^3p_\gamma^{\prime\prime} d^3q_\gamma^{\prime\prime} \tag{5.23}$$

$$<\vec{p}_\gamma \vec{q}_\gamma |A_6(R)|\, \vec{p}_\beta^{\,\prime}> \equiv \int <\vec{p}_\gamma \vec{q}_\gamma |\overline{\mathscr{P}}(R)| \vec{p}_\gamma^{\,\prime\prime} \vec{q}_\gamma^{\,\prime\prime}> \sum_{\alpha=1}^{3} i\pi\, \delta(\tilde{p}_\alpha^{\prime\prime 2} - \chi_\alpha^2 - \tilde{p}_\beta^{\prime 2} + \chi_\beta^2)\, \phi_\alpha(\vec{q}_\alpha^{\,\prime\prime})$$

$$<\vec{p}_\alpha^{\,\prime\prime} |\mathscr{H}_{\alpha\beta}^{(+)}| \vec{p}_\beta^{\,\prime}> i\pi\, \delta(\tilde{p}_\gamma^{\prime\prime 2} + \tilde{q}_\gamma^{\prime\prime 2} - \tilde{p}_\beta^{\prime 2} + \chi_\beta^2)\, d^3p_\gamma^{\prime\prime} d^3q_\gamma^{\prime\prime} \tag{5.24}$$

We now proceed to evaluate the matrix element given in Eq. (5.8). We show in Appendix B that

$$\lim_{R\to\infty} \langle \vec{p}_\gamma | I_\gamma (B_i(R) - A_i(R)) | \vec{p}_\beta' \rangle = 0 \qquad \text{all } i \neq 2 \quad . \tag{5.25}$$

When this result is combined with Eq. (5.8) we have

$$\lim_{R\to\infty} \langle \vec{p}_\gamma | U_\gamma^{(+)\dagger} \left[\overline{\mathscr{P}}(R) U_\beta^{(-)} - U_\beta^{(-)} \overline{\mathscr{P}}_\beta(R) \right] | \vec{p}_\beta' \rangle = \lim_{R\to\infty} \langle \vec{p}_\gamma | I_\gamma (B_2(R) - A_2(R)) | \vec{p}_\beta' \rangle \tag{5.26}$$

for $\gamma > 0$. When $\gamma = 0$ this equation becomes

$$\lim_{R\to\infty} \langle \vec{p}_\gamma \vec{q}_\gamma | U_0^{(+)\dagger} \left[\overline{\mathscr{P}}(R)\, U_\beta^{(-)} - U_\beta^{(-)} \overline{\mathscr{P}}_\beta(R) \right] | \vec{p}_\beta' \rangle = \lim_{R\to\infty} \langle \vec{p}_\gamma \vec{q}_\gamma | B_2(R) - A_2(R) | \vec{p}_\beta' \rangle \tag{5.27}$$

At this point we stress that we have to evaluate the above matrix elements only for on-shell values of the momentum arguments. This on-shell requirement is a consequence of the delta function appearing in Eq. (4.27) and Eq. (4.28).

We continue by considering the evaluation of the operator $I_\gamma B_2(R)$. Examining $B_2(R)$ we see that it is the sum of three terms. Defining $B_{2\alpha}(R)$ by

$$\langle \vec{p}_\gamma \vec{q}_\gamma | B_{2\alpha}(R) | \vec{p}_\beta' \rangle \equiv \phi_\alpha(\vec{q}_\alpha) \int \frac{\langle \vec{p}_\alpha | \mathscr{H}_{\alpha\beta}^{(+)} | \vec{p}_\beta'' \rangle \langle \vec{p}_\beta'' | \overline{\mathscr{P}}_\beta(R) | \vec{p}_\beta' \rangle}{(\tilde{p}_\alpha^2 - \chi_\alpha^2 - \tilde{p}_\beta''^2 + \chi_\beta^2)(\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta''^2 + \chi_\beta^2)}\, d^3p_\beta'' \;, \tag{5.28}$$

then

$$B_2(R) = \sum_{\alpha=1}^{3} B_{2\alpha}(R) \quad . \tag{5.29}$$

We shall demonstrate in Appendix B that only the term $I_\gamma B_{2\gamma}$ in the above sum contributes to the nonzero matrix elements. So in this section we examine only

$I_\gamma B_{2\gamma}$. Setting $\alpha=\gamma$ in Eq. (5.28) gives us

$$\langle \vec{p}_\gamma \vec{q}_\gamma | B_{2\gamma}(R) | \vec{p}'_\beta \rangle = 2n_\beta \phi_\gamma(\vec{q}_\gamma) \int \frac{\langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}''_\beta \rangle}{\tilde{p}^2_\gamma + \tilde{q}^2_\gamma - \tilde{p}''^2_\beta + \chi^2_\beta} \frac{\langle \vec{p}''_\beta | \overline{\mathscr{P}}_\beta(R) | \vec{p}'_\beta \rangle}{(p'_\beta + p''_\beta)(p'_\beta - p''_\beta)} d^3 p''_\beta \qquad (5.30)$$

We now use a property of $\overline{\mathscr{P}}_\beta(R)$ established in Appendix A, namely, for $f(\vec{p}_\beta)$ a smooth function in $\hat{p}_\beta$ and differentiable in $|\vec{p}_\beta|$ the following limiting relation is valid.

$$\lim_{R\to\infty} \int \frac{\langle \vec{p}_\beta | \overline{\mathscr{P}}_\beta(R) | \vec{p}''_\beta \rangle f(\vec{p}''_\beta)}{p_\beta - p''_\beta} d^3 p''_\beta = -\frac{d}{dp''_\beta} \left[\frac{p''_\beta}{p_\beta} \quad f(p''_\beta \hat{p}_\beta) \right] \Bigg|_{p''_\beta = p_\beta} \qquad (5.31)$$

In obtaining the form of Eq. (5.30) we have exploited the on-shell condition $\tilde{p}^2_\gamma - \chi^2_\gamma = \tilde{p}'^2_\beta - \chi^2_\beta$ to write the first denominator solely in terms of the β momentum. The distinctive feature of this term which prevents it from cancelling against the corresponding term $I_\gamma A_2(R)$ is the fact that the singular surface occurring at $p_\beta = p''_\beta$ changes the character of the $R\to\infty$ limit. Without such a singularity $\overline{\mathscr{P}}_\beta(R) \to E_\beta$. If this were the case then $B_{2\gamma}(R) - A_{2\gamma}(R)$ would go to zero.

We are permitted to use Eq. (5.31) in evaluating the $R\to\infty$ limit in Eq. (5.30) since the portion of the integrand excluding $\langle \vec{p}''_\beta | \overline{\mathscr{P}}_\beta(R) | \vec{p}'_\beta \rangle / p'_\beta - p''_\beta$ is a smooth function of p''_β. This is a consequence of our assumptions in Section II about the physical amplitude $\langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}''_\beta \rangle$, namely it is differentiable function of its arguments. The remaining ingredient of the integrand in Eq. (5.30) is the denominator $\tilde{p}^2_\gamma + \tilde{q}^2_\gamma - \tilde{p}''^2_\beta + \chi^2_\beta$. We need only estimate its behavior in the neighborhood of $p''^2_\beta = p'^2_\beta$. So one has that

$$\tilde{p}^2_\gamma + \tilde{q}^2_\gamma - \tilde{p}'^2_\beta + \chi^2_\beta = \tilde{q}^2_\gamma + \chi^2_\gamma \geq \chi^2_\gamma \qquad (5.32a)$$

Thus for $|\tilde{p}'^2_\beta - \tilde{p}''^2_\beta| < \chi^2_\gamma$ we have the estimate

$$\tilde{p}^2_\gamma + \tilde{q}^2_\gamma - p''^2_\beta + \chi^2_\beta > 0 \qquad \text{all } \vec{q}_\gamma \, . \qquad (5.32b)$$

Employing Eq. (5.31) in Eq. (5.30) now gives us

$$\lim_{R\to\infty} \langle \vec{p}_\gamma \vec{q}_\gamma | B_{2\gamma}(R) | \vec{p}'_\beta \rangle = -2n_\beta \phi_\gamma(\vec{q}_\gamma) \frac{d}{dp''_\beta} \left[\frac{\langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}''_\beta \rangle\, p''_\beta}{(\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}''^2_\beta + \chi_\beta^2)(p'_\beta + p''_\beta) p'_\beta} \right] \Bigg|_{p''_\beta = p'_\beta} \tag{5.32c}$$

where $\vec{p}''_\beta = p''_\beta \hat{p}'_\beta$. If we use

$$\frac{d}{dp''_\beta} \frac{p''_\beta}{(p'_\beta + p''_\beta) p'_\beta} \Bigg|_{p''_\beta = p'_\beta} = \frac{1}{4p'^2_\beta} \tag{5.33}$$

our expression for the right-hand side of Eq. (5.32c) becomes

$$-\frac{n_\beta}{p'_\beta} \psi_\gamma(\vec{q}_\gamma) \frac{d}{dp''_\beta} \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}''_\beta \rangle \Big|_{p''_\beta = p'_\beta} - \frac{n_\beta}{2p'^2_\beta} \psi_\gamma(\vec{q}_\gamma) \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle - \frac{\psi_\gamma(\vec{q}_\gamma)}{\tilde{q}_\gamma^2 + \chi_\gamma^2} \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle \tag{5.34}$$

In order to find $I_\gamma B_{2\gamma}(R)$ we must integrate this last set of terms with $\int \psi_\gamma(\vec{q}_\gamma)^* \, d^3 q_\gamma$. Since ψ_γ is a unit normalized boundstate wavefunction, one has at once that

$$\lim_{R\to\infty} \langle \vec{p}_\gamma | I_\gamma B_{2\gamma}(R) | \vec{p}'_\beta \rangle$$

$$= -\frac{n_\beta}{p'_\beta} \frac{d}{dp'_\beta} \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle - \frac{n_\beta}{2p'^2_\beta} \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle - \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle \int \frac{|\psi_\gamma(\vec{q}_\gamma)|^2}{\tilde{q}_\gamma^2 + \chi_\gamma^2} \, d^3 q_\gamma \tag{5.35}$$

This completes the evaluation of $I_\gamma B_{2\gamma}(R)$.

Let us now study the companion terms of $I_\gamma B_{2\gamma}(R)$ that occur in Eq. (5.26), namely $I_\gamma A_2(R)$. As in the case of $B_2(R)$ we can decompose $A_2(R)$ into a sum of three terms. From the form (5.20) for $A_2(R)$ we can define

$$A_2(R) = \sum_{\alpha=1}^{3} A_{2\alpha}(R) \tag{5.36}$$

where $A_{2\alpha}(R)$ is given by

$$\langle\vec{p}_\gamma\vec{q}_\gamma|A_{2\alpha}(R)|\vec{p}'_\beta\rangle = \int \frac{\langle\vec{p}_\gamma\vec{q}_\gamma|\bar{\mathscr{P}}(R)|\vec{p}''_\gamma\vec{q}''_\gamma\rangle}{(\tilde{p}''^2_\alpha-\chi^2_\alpha-\tilde{p}'^2_\beta+\chi^2_\beta)} \frac{\phi_\alpha(\vec{q}''_\alpha)\langle\vec{p}''_\alpha|\mathscr{H}^{(+)}_{\alpha\beta}|\vec{p}'_\beta\rangle}{(\tilde{p}''^2_\gamma+\tilde{q}''^2_\gamma-\tilde{p}'^2_\beta+\chi^2_\beta)} d^3p''_\gamma d^3q''_\gamma \tag{5.37}$$

Again we demonstrate in Appendix B that

$$\lim_{R\to\infty} \sum_{\alpha\neq\gamma} \langle\vec{p}_\gamma|I_\gamma(B_{2\alpha}(R)-A_{2\alpha}(R))|\vec{p}'_\beta\rangle = 0 \tag{5.38}$$

So here we need consider only the term $A_{2\gamma}(R)$. Using the on-shell condition $\tilde{p}^2_\gamma-\chi^2_\gamma = \tilde{p}'^2_\beta-\chi^2_\beta$ we may write Eq. (5.37) as

$$\langle\vec{p}_\gamma\vec{q}_\gamma|A_{2\gamma}(R)|\vec{p}'_\beta\rangle = 2n_\gamma \int \frac{\langle\vec{p}_\gamma\vec{q}_\gamma|\bar{\mathscr{P}}(R)|\vec{p}''_\gamma\vec{q}''_\gamma\rangle}{p''_\gamma-p_\gamma} \frac{\phi_\gamma(\vec{q}''_\gamma)\langle\vec{p}''_\gamma|\mathscr{H}^{(+)}_{\gamma\beta}|\vec{p}'_\beta\rangle}{(p''_\gamma+p_\gamma)(\tilde{p}''^2_\gamma+\tilde{q}''^2_\gamma-\tilde{p}^2_\gamma+\chi^2_\gamma)} d^3p''_\gamma d^3q''_\gamma \tag{5.39}$$

We now quote another feature of the operator $\bar{\mathscr{P}}(R)$ demonstrated in Appendix A. For $f \in \hbar_0$ and $f(\vec{p}''_\beta,\vec{q}''_\beta)$ differentiable in the $|\vec{p}''_\beta|$ variable then we have the limiting relation

$$\lim_{R\to\infty}\int \frac{\langle\vec{p}_\beta\vec{q}_\beta|\bar{\mathscr{P}}(R)|\vec{p}''_\beta\vec{q}''_\beta\rangle}{p_\beta-p''_\beta} f(\vec{p}''_\beta,\vec{q}''_\beta)\, d^3p''_\beta d^3q''_\beta = -\frac{d}{dp''_\beta}\left[\frac{p''_\beta}{p_\beta} f(p''_\beta\hat{p}_\beta,\vec{q}_\beta)\right]\Bigg|_{p''_\beta=p_\beta} \tag{5.40}$$

In the neighborhood of $p''_\gamma=p_\gamma$ the last denominator in Eq. (5.39) never vanishes. Thus we are justified in using relation (5.40) to evaluate Eq. (5.39). The limit that Eq. (5.39) takes is

$$\lim_{R\to\infty} \langle\vec{p}_\gamma\vec{q}_\gamma|A_{2\gamma}(R)|\vec{p}'_\beta\rangle = 2n_\gamma\phi_\gamma(\vec{q}_\gamma)\frac{d}{dp''_\gamma}\left[\frac{\langle\vec{p}''_\gamma|\mathscr{H}^{(+)}_{\gamma\beta}|\vec{p}'_\beta\rangle p''_\gamma}{p_\gamma(p''_\gamma+p_\gamma)(\tilde{p}''^2_\gamma-\tilde{p}^2_\gamma+\tilde{q}^2_\gamma+\chi^2_\gamma)}\right]\Bigg|_{p''_\gamma=p_\gamma} \tag{5.41}$$

where $\vec{p}''_\gamma = p''_\gamma \hat{p}_\gamma$. Of course the value of $\vec{p}_\gamma$ is on-shell. If we write out the derivative term and perform the integration with respect to $\int \psi(\vec{q}_\gamma)^* \, d^3q_\gamma$ then Eq. (5.41) becomes

$$\lim_{R\to\infty} \langle \vec{p}_\gamma | I_\gamma A_{2\gamma}(R) | \vec{p}'_\beta \rangle = \frac{n_\gamma}{p_\gamma} \frac{d}{dp_\gamma} \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle + \frac{n_\gamma}{2p_\gamma^2} \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle$$

$$- \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle \int \frac{|\psi_\gamma(\vec{q}_\gamma)|^2}{\tilde{q}_\gamma^2 + \chi_\gamma^2} \, d^3q_\gamma \tag{5.42}$$

By combining Eq. (5.42) with Eq. (5.35) we can determine $I_\gamma\left[B_2(R) - A_2(R)\right]$. We have

$$\lim_{R\to\infty} \langle \vec{p}_\gamma | I_\gamma(B_2(R) - A_2(R)) | \vec{p}'_\beta \rangle = -\frac{n_\gamma}{p_\gamma} \frac{d}{dp_\gamma} \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle$$

$$- \frac{n_\beta}{p'_\beta} \frac{d}{dp'_\beta} \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle - \frac{n_\beta}{2p'^2_\beta} \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle - \frac{n_\gamma}{2p_\gamma^2} \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle . \tag{5.43}$$

The sum of the first two terms is just the total energy derivative since $E = \vec{p}'^2_\beta/2n_\beta - \chi_\beta^2 = \vec{p}_\gamma^2/2n_\gamma - \chi_\gamma^2$. So we can simplify Eq. (5.43) to read

$$\lim_{R\to\infty} \langle \vec{p}_\gamma | I_\gamma(B_2(R) - A_2(R)) | \vec{p}'_\beta \rangle = -\frac{d}{dE} \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle$$

$$- \left[\frac{n_\beta}{2p'^2_\beta} + \frac{n_\gamma}{2p_\gamma^2}\right] \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle \tag{5.44}$$

If we use this result together with Eq. (5.26) and Eq. (4.27) we obtain part of our desired solution

$$\lim_{R\to\infty} \langle \vec{p}_\gamma | \sum_{\alpha=0}^{3} S_{\gamma\alpha} Q_{\alpha\beta}(R,\infty) | \vec{p}'_\beta \rangle \equiv \langle \vec{p}_\gamma | \sum_{\alpha=0}^{3} S_{\gamma\alpha} Q_{\alpha\beta} | \vec{p}'_\beta \rangle$$

$$= 2\pi\, \delta(\tilde{p}_\gamma^2 - \chi_\gamma^2 - \tilde{p}'^2_\beta + \chi_\beta^2) \left\{ -\frac{d}{dE} \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle - \left[\frac{n_\beta}{2p'^2_\beta} + \frac{n_\gamma}{2p_\gamma^2}\right] \langle \vec{p}_\gamma | \mathscr{H}^{(+)}_{\gamma\beta} | \vec{p}'_\beta \rangle \right\} \tag{5.45}$$