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TIME DELAY AND ITS APPLICATION IN STATISTICAL MECHANICS

by

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C O N T E N T S

Chapter I   Introduction to scattering theory

In this introduction we describe the background material necessary in the study of the time delay aspect of scattering theory. Its ultimate application in statistical mechanics would be dealt with in later chapters. Following Faddeev's[1] three body theory, we restrict our study to the quantum non-relativistic scattering of three particles interacting through two body forces only. Unless stated otherwise, the mathematical assumptions used in this thesis are those stated in Faddeev's book.

We shall discuss all scattering in the center of mass system. In the two body case, we have the interacting Hamiltonian $h = h_0 + v$ where h_0 is the free Hamiltonian and v the two body potential. We define the resolvents $r(z) = (h - ze)^{-1}$ and $r_0(z) = (h_0 - ze)^{-1}$ where e is the identity and z a complex number. The usual Moeller operator is defined as

$$\lim_{t \to \pm\infty} e^{-ih_0 t} e^{iht} = \Omega^{(\pm)} \tag{I.1}$$

The scattering S-matrix is defined as

$$S = \Omega^{(+)^{+}} \Omega^{(-)} \tag{I.2}$$

The usual results of scattering theory can be summarized in three simple theorems:

(1) $\Omega^{(\pm)^{+}} \Omega^{(\pm)} = e$ (conservation of probability)

(2) $\Omega^{(\pm)} \Omega^{(\pm)^{+}} = e - P_b$ (asymptotic completeness)

(3) $\varphi(h)\, \Omega^{(\pm)} = \Omega^{(\pm)} \varphi(h_0)$ (conservation of energy)

P_b is the projection operator into the bound state and φ is a function. We also use the T-matrix in our derivations.

$$t = v - v\, r\, v \tag{I.3}$$
$$= v - v\, r_0\, t \tag{I.4}$$

The unitarity equation can be stated as

$$t(z_1) - t(z_2) = (z_2 - z_1)\; t(z_1)\, r_0(z_1)\, r_0(z_2)\; t(z_2) \tag{I.5}$$

We use only the above results to derive all the two body time-delay properties.

The equivalent set of scattering theory results that we need for three body time delay is considerably more extensive. The three body problem is the simplest non-trivial example of many body interaction. It comprises many fundamental N-body properties: break-up, rescattering, rearrangement, off-shell matrix elements, etc. that are noticeably absent in two body scattering. We here outline the Faddeev results to be used in the following chapters.

If $\vec{k}_1, \vec{k}_2, \vec{k}_3$ are the momentum vectors of the three particles then $\vec{K} = \vec{k}_1 + \vec{k}_2 + \vec{k}_3$ is the independent momentum variable of the center of mass. The remaining six momentum coordinates can be expressed in three equivalent sets of Jacobian variables.

$$\vec{p}_1 = \frac{m_1(\vec{k}_2+\vec{k}_3) - (m_2+m_3)\vec{k}_1}{m_1+m_2+m_3}\ , \quad \vec{q}_1 = \frac{m_3\vec{k}_2 - m_2\vec{k}_3}{m_2+m_3}$$

or, $$\vec{p}_2 = \frac{m_2(\vec{k}_3+\vec{k}_1) - (m_3+m_1)\vec{k}_2}{m_1+m_2+m_3}\ , \quad \vec{q}_2 = \frac{m_1\vec{k}_3 - m_3\vec{k}_1}{m_3+m_1}$$

or, $$\vec{p}_3 = \frac{m_3(\vec{k}_1+\vec{k}_2) - (m_1+m_2)\vec{k}_3}{m_1+m_2+m_3}\ , \quad \vec{q}_3 = \frac{m_2\vec{k}_1 - m_1\vec{k}_2}{m_1+m_2} \tag{I.6}$$

$\vec{p}_\alpha$ and $\vec{q}_\alpha$ are conjugate momenta to the spatial coordinates $\vec{x}_\alpha$ and $\vec{y}_\alpha$ respectively. $\vec{x}_\alpha$ is the spatial separation of particle

α from the center of mass of the remaining pair β and γ , together called the α cluster. y_α gives the spatial separation of the α cluster itself, i.e. between particles β and γ .

In these coordinates the free Hamiltonian is simply expressed as $H_0(p,q) = \frac{1}{2\mu_1} q_1^2 + \frac{1}{2n_1} p_1^2 = \frac{1}{2\mu_2} q_2^2 + \frac{1}{2n_2} p_2^2 = \frac{1}{2\mu_3} q_3^2 + \frac{1}{2n_3} p_3^2$

where $\mu_\alpha = \dfrac{m_\beta m_\gamma}{m_\beta + m_\gamma}$, $n_\alpha = \dfrac{m_\alpha (m_\beta + m_\gamma)}{m_\alpha + m_\beta + m_\gamma}$; $\alpha, \beta, \gamma \in (1,2,3)$.

For convenience we define special coordinates $\tilde{p}_\alpha$ and $\tilde{q}_\alpha$, such that $\tilde{q}_\alpha^2 \equiv q_\alpha^2 / 2\mu_\alpha$, $\tilde{p}_\alpha^2 \equiv p_\alpha^2 / 2n_\alpha$.

Hence, $$H_0(p,q) = \tilde{q}_\alpha^2 + \tilde{p}_\alpha^2 \quad , \alpha = 1, 2, 3 . \qquad (I.7)$$

To discuss the three body S-matrix, Moeller operators and their related fundamental theorems, we must firstly describe the Hilbert space structure in which these operators act. Here lies the channel property that characterizes the three body problem.

The complete Hamiltonian is obtained by adding all the possible two body interactions to the free Hamiltonian H_0 .

$$H = H_0 + \sum_{\alpha=1}^{3} V_\alpha \qquad (I.8)$$

V_α is the potential of the α cluster. Both H and H_0 act in $\mathcal{H}$ which is a six dimensional Hilbert space of square integrable functions, denoted as $L^2(\vec{p},\vec{q})$. The inner product related to $\mathcal{H}$ is $(,)$ and the identity operator on $\mathcal{H}$ is E . Acting in $\mathcal{H}$, H and H_0 are both self-adjoint operators.

The channel structure is a manifestation of the possible asymptotic behaviour. There are one channel ($\alpha = 0$) with all three particles free and three channels ($\alpha = 1, 2, 3$) with the α particle free while the α cluster is bounded. Hence the scattering system can come in four different channels and can also go out in four different channels. A system in any cluster channel ($\alpha = 1,2,3$) must be described by a wave function of the form $f(\vec{p}_\alpha)\varphi_\alpha(q_\alpha)$ where $\varphi_\alpha(q_\alpha)$ is the normalized bound state wave function of the α cluster. $f(\vec{p}_\alpha)$ describe the free particle and must be in $\mathcal{H}_\alpha$, a three dimensional Hilbert space of square integrable function, $L^2(\vec{p}_\alpha)$. The Hilbert space related to the free channel ($\alpha = 0$) is $\mathcal{H}_0$ which is a six dimensional Hilbert space of square integrable functions $L^2(p,q)$ and is mathematically identical with $\mathcal{H}$.

To describe together all these possible asymptotic motion of the three body system, we introduce a single Hilbert space $\hat{\mathcal{H}} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3$. A function $\hat{f}$ in $\hat{\mathcal{H}}$ necessarily has four components, i.e. $\hat{f} = f_0 \oplus f_1 \oplus f_2 \oplus f_3$.
It is clear that $\hat{\mathcal{H}}$ is different from $\mathcal{H}$.

$$(\hat{f}, \hat{f}')_\wedge = \sum_{\alpha=0}^{3} (f_\alpha, f'_\alpha)_\alpha \qquad (I.9)$$

To complete the description of these Hilbert spaces, we introduce the operators P_α and I_α . For $f \in \mathcal{H}$,

$$P_\alpha f = f_\alpha \psi_\alpha \quad , \quad \mathcal{H} \longrightarrow \mathcal{H} \qquad (I.10)$$

$$I_\alpha f = f_\alpha \quad , \quad \mathcal{H} \longrightarrow \mathcal{H}_\alpha \qquad (I.11)$$

where ψ_α is the α bound state wave function and

$$f_\alpha(\vec{p}_\alpha) = \int d\vec{q}_\alpha \; f(\vec{p}_\alpha, \vec{q}_\alpha)\, \psi_\alpha^*(q_\alpha) \qquad (I.12)$$

For illustration we list here all the Hamiltonians that are associated with each of the spaces discussed above.

In $\mathcal{H}$, $f(\vec{p},\vec{q}) \in \mathcal{H}$, $H_0 f(\vec{p},\vec{q}) = (\vec{p}_\alpha^{\,2} + \vec{q}_\alpha^{\,2})\, f(\vec{p},\vec{q})$, $\alpha = 1, 2, 3.$

In $\mathcal{H}$, $f_\alpha(\vec{p}_\alpha)\psi_\alpha(\vec{q}_\alpha) \in \mathcal{H}$, $H_\alpha f_\alpha(\vec{p}_\alpha)\psi_\alpha(\vec{q}_\alpha) = (\vec{p}_\alpha^{\,2} - \chi_\alpha^2)\, f_\alpha(\vec{p}_\alpha)\psi_\alpha(\vec{q}_\alpha)$

In $\mathcal{H}_0$, $f_0(\vec{p},\vec{q}) \in \mathcal{H}_0$, $\widetilde{H}_0\, f_0(\vec{p},\vec{q}) = (\tilde{p}^2+\tilde{q}^2)\, f_0(\vec{p},\vec{q})$

In $\mathcal{H}_\alpha$, $f_\alpha(\vec{p}_\alpha) \in \mathcal{H}_\alpha$, $\widetilde{H}_\alpha\, f_\alpha(\vec{p}_\alpha) = (\tilde{p}_\alpha^2 - \chi_\alpha^2)\, f_\alpha(\vec{p}_\alpha)$

The Hamiltonians with the tilda ($\widetilde{H}_0$, $\widetilde{H}_0$, $\widetilde{H}_1$ and $\widetilde{H}_2$) are called channel Hamiltonians. Of course $\widetilde{H}_0$ and H_0 are mathematically identitical.

In terms of these Hilbert spaces, $\mathcal{H}_0$, $\mathcal{H}_1$, $\mathcal{H}_2$, $\mathcal{H}_3$ and $\hat{\mathcal{H}}$ we can now describe the S-matrix and Moeller operators.

$$U_\alpha^{(\pm)} = \lim_{t\to\pm\infty} e^{-iHt}\, e^{iH_\alpha t}\, I_\alpha^\dagger \quad : \quad \mathcal{H}_\alpha \longrightarrow \mathcal{H} \qquad (I.13)$$

$$S_{\beta\alpha} = U_\beta^{(+)\dagger}\, U_\alpha^{(-)} \quad : \quad \mathcal{H}_\alpha \to \mathcal{H}_\beta \qquad (I.14)$$

If we write $[S]_{\beta\alpha} = S_{\beta\alpha}$, the S-matrix would now act in $\hat{\mathcal{H}}$, e.g. $\hat{f}' = S\hat{f} \quad : \hat{\mathcal{H}} \to \hat{\mathcal{H}}$

Unitarity in $\hat{\mathcal{H}}$ is simply $S^\dagger S = SS^\dagger = \hat{E}$ while in $\mathcal{H}_\beta$ it is $\sum_{\gamma=0}^{3} S_{\gamma\alpha}^\dagger S_{\gamma\beta} = E_\beta\, \delta_{\alpha\beta}$.

The three fundamental theorems runs parallel to those of the two body case.

(1) $U_\alpha^{(\pm)\dagger}\, U_\beta^{(\pm)} = \delta_{\alpha\beta}\, E_\beta \quad : \quad \mathcal{H}_\beta \longrightarrow \mathcal{H}_\alpha$

(2) $\sum_{\alpha=0}^{3} U_\alpha^{(\pm)}\, U_\alpha^{(\pm)\dagger} = E - P_B \quad : \quad \mathcal{H} \to \mathcal{H}$

(3) $H\, U_\alpha^{(\pm)} = U_\alpha^{(\pm)}\, \widetilde{H}_\alpha \quad : \quad \mathcal{H}_\alpha \to \mathcal{H}$

The singularity structure of $U_\alpha^{(\pm)}$ has been well studied by Faddeev. For $\alpha = 1,2,3$, $\langle \vec{p}_\alpha \vec{q}_\alpha |\, U_\alpha^{(\pm)} | \vec{p}_\alpha{}' \rangle = \psi_\alpha(\vec{q}_\alpha)\, \delta(\vec{p}_\alpha - \vec{p}_\alpha{}') -$ $\langle \vec{p}_\alpha \vec{q}_\alpha |\, K_\alpha^{(\pm)} | \vec{p}_\alpha{}' \rangle$

where
$$\langle \vec{p}_\alpha \vec{q}_\alpha |\, K_\alpha^{(\pm)} | \vec{p}_\alpha{}' \rangle = \frac{\langle \vec{p}_\alpha \vec{q}_\alpha |\, B_{0\alpha}^{(\mp)} | \vec{p}_\alpha{}' \rangle}{E_0 - E_\alpha' \pm i0} \ , \quad \begin{array}{l} E_0 = \tilde{p}_\alpha^2 + \tilde{q}_\alpha^2 \\ E_\alpha' = \tilde{p}_\alpha^{2\prime} - \chi_\alpha^2 \end{array} \qquad (I.15)$$

$$\begin{aligned} \langle \vec{p}_\alpha \vec{q}_\alpha |\, B_{0\alpha}^{(\pm)} | \vec{p}_\alpha{}' \rangle &= B_{0\alpha}(\vec{p}_\alpha \vec{q}_\alpha ; \vec{p}_\alpha{}' ; E_\alpha' \pm i0) \\ &= -\sum_{\gamma=1}^{3} \Big(G_{\gamma\alpha}(\vec{p}_\gamma \vec{q}_\gamma ; \vec{p}_\alpha{}' ; E_\alpha' \pm i0) \\ &\qquad - \frac{\phi_\gamma(\vec{q}_\gamma)}{E_\gamma - E_\alpha' \pm i0}\, H_{\gamma\alpha}(\vec{p}_\gamma ; \vec{p}_\alpha{}' ; E_\alpha' \pm i0) \Big) \end{aligned} \qquad (I.16)$$

The vertex function $\phi_\gamma(\vec{q}_\gamma)$ is given by $\phi_\gamma(\vec{q}_\gamma) = (\vec{q}_\gamma^{\,2} + \chi_\gamma^2)\,\psi_\gamma(\vec{q}_\gamma)$.

For the 3-3 channel, we have the following,

$$\langle \vec{p}\vec{q} \,|\, U_0^{(\pm)} \,|\, \vec{p}'\vec{q}' \rangle = \delta(\vec{p}_\alpha - \vec{p}_\alpha')\,\delta(\vec{q}_\alpha - \vec{q}_\alpha') - \langle \vec{p}\ \vec{q} \,|\, K_0^{(\pm)} \,|\, \vec{p}'\vec{q}' \rangle$$

where $$\langle \vec{p}\vec{q} \,|\, K_0^{(\pm)} \,|\, \vec{p}'\vec{q}' \rangle = \frac{\langle \vec{p}\vec{q} \,|\, T^{(\mp)} \,|\, \vec{p}'\vec{q}' \rangle}{E_0 - E_0' \pm i0}$$

$$\langle \vec{p}\vec{q} \,|\, T^{(\pm)} \,|\, \vec{p}'\vec{q}' \rangle = \sum_{\alpha,\beta=1}^{3} M_{\alpha\beta}(\vec{p}\vec{q}\,;\vec{p}'\vec{q}'\,;E_0' \pm i0)$$

$$\begin{aligned} M_{\alpha\beta}(\vec{p}\vec{q}\,;\vec{p}'\vec{q}'\,;z) = {} & \delta_{\alpha\beta}\,\delta(\vec{p}_\alpha - \vec{p}_\alpha')\left[\frac{\varphi_\alpha(\vec{q}_\alpha)\,\varphi_\alpha^*(\vec{q}_\alpha')}{z - E_\alpha} + \hat{t}_\alpha(\vec{q}_\alpha, \vec{q}_\alpha', z - \vec{p}_\alpha^{\,2})\right] \\ & + F_{\alpha\beta}(\vec{p}\vec{q}\,;\vec{p}'\vec{q}'\,;z) + \frac{\varphi_\alpha(\vec{q}_\alpha)}{z - E_\alpha}\,\tilde{G}_{\alpha\beta}(\vec{p}_\alpha\,;\vec{p}'\vec{q}'\,;z) \\ & + G_{\alpha\beta}(\vec{p}\vec{q}\,;\vec{p}_\beta'\,;z)\,\frac{\varphi_\beta^*(\vec{q}_\beta')}{z - E_\beta'} \\ & + \frac{\varphi_\alpha(\vec{q}_\alpha)}{z - E_\alpha}\,H_{\alpha\beta}(\vec{p}_\alpha\,;\vec{p}_\beta'\,;z)\,\frac{\varphi_\beta^*(\vec{q}_\beta')}{z - E_\beta'} \quad . \qquad (I.17) \end{aligned}$$

We should note here that $B_{0\alpha}^{(\pm)}$, $H_{\alpha\beta}^{(\pm)}$ and $T^{(\pm)}$ are the physical scattering amplitudes of the α to 0 channel, β to α channel and 0 to 0 channel respectively.[42]

Chapter II Spectral property of time delay

This chapter discusses the spectral property of time delay. If one considers the scattering by a potential v, then the spectral property is the statement that the trace of the time-delay operator is proportional to the change in state density produced by the interaction v. We give a new and elementary proof of this result.

II.1 Introduction

As a preface to our discussion of the spectral property of time delay, we shall describe the known results for two-body time delay. The general abstract definition of time delay first proposed by Goldberger and Watson[2)] is

$$(f, Qf) = \lim_{R\to\infty} \int_{-\infty}^{\infty} [(\psi(t), P(R)\psi(t)) - (\phi(t), P(R)\phi(t))]\, dt \qquad \text{(II.1.1)}$$

Here $\psi(t)$ is the exact time-dependent wave function which asymptotically behaves as the freely evolving wave packet $\phi(t)$ and $P(R)$ is a spatial projection operator which is one inside the sphere of radius R. The function f specifies the initial scattering state through

$$\phi(t) = e^{-iH_0 t} f \qquad \text{(II.1.2)}$$

and $\psi(t)$ is given by the usual formula

$$\psi(t) = e^{-iHt}\Omega^{(+)} f \qquad \text{(II.1.3)}$$

It is obvious from equation (II.1.1) that before the limit

$R \to \infty$ is taken that the right hand side represents the time difference that the exact wave $\Psi(t)$ and the free wave $\phi(t)$ spend inside the sphere of radius R. Then (f, Qf) is the time difference computed over all space. The problem is then one of evaluating (f, Qf). Jauch and Marchand[3] solved this problem. Their result may be stated through the following equations. Associate with (f, Qf) the momentum space kernel $\langle \vec{p} | Q | \vec{p}' \rangle$,

$$(f, Qf) = \int f^*(\vec{p}) \langle \vec{p} | Q | \vec{p}' \rangle f(\vec{p}') \, d\vec{p} \, d\vec{p}' \qquad \text{(II.1.4)}$$

then Q conserves energy and may be written

$$\langle \vec{p} | Q | \vec{p}' \rangle = \frac{\delta(E - E')}{\mu p} \langle \hat{p} | q(E) | \hat{p}' \rangle \qquad \text{(II.1.5)}$$

where we may think of $q(E)$ as an operator on a two-dimensional Hilbert space $L^2(\hat{p})$. The quantity $\hat{p}$ is of course the unit verctor in the direction of $\vec{p}$. The energies are $E = p^2/2\mu$ and $E' = p'^2/2\mu$ for reduced mass μ. We associate with the momentum space S-matrix elements a similar reduced operator $s(E)$ defined by

$$\langle \vec{p} | S | \vec{p}' \rangle = \frac{\delta(E - E')}{\mu p} \langle \hat{p} | s(E) | \hat{p}' \rangle \qquad \text{(II.1.6)}$$

Then the solution of this problem is given by the operator relation on $L^2(\hat{p})$:

$$q(E) = -i s^{\dagger}(E) \frac{d}{dE} s(E) \, . \qquad \text{(II.1.7)}$$

The unitarity of $s(E)$ implies that the $q(E)$ is hermitian on $L^2(\hat{p})$ for each E.

In the following section we prove that the time delay has another physical meaning, besides the one given by its definition equation (II.1.4). This result was first obtained in an elaborate paper by Jauch, Sinha and Misra.[4)] The purpose of the next section is to show that the statement of the spectral property may be obtained by a simple argument utilizing only a few elementary identites in scattering theory. Jauch, Sinha and Misra take great care in analyzing the most general case, where there may exist bound states in the scattering continuum. We take the physicist's view that such states will not occur in any reasonable physical scattering problem. So we explicitly prohibit by assumption bound states in the continuum.

II.2 The derivation

In this section we give an elementary proof of the spectral property of two-body time delay. The proof rests on two well-known general features of scattering theory, viz.:

$$r(z) = r_0(z) - r_0(z)\, t(z)\, r_0(z) \qquad \text{(II.2.1)}$$

$$t(z_1) - t(z_2) = (z_2 - z_1)\, t(z_1)\, r_0(z_1)\, r_0(z_2)\, t(z_2) \qquad \text{(II.2.2)}$$

Each of these statements is associated with a physical feature of scattering theory: (II.2.1) is the definition of the T-matrix operator; (II.2.2) is the operator form of off-shell unitarity. Our proof also employs the weak restriction that the off-shell T-matrix is differentiable in $|\vec{p}|$ and $|\vec{p}\,'|$. The Hamiltonians h_0 and h that appear in the resolvents $r_0(z)$ and $r(z)$ are naturally assumed to be hermitian, having a continuous spectrum devoid of discrete eigenvalues.

Our task is to compute the imaginary part of the trace of the resolvent difference $r(z) - r_0(z)$. We first rewrite this expression, I, as

$$I = 2i \, \mathrm{Im} \, \mathrm{tr}\,[r(z) - r_0(z)] = \mathrm{tr}\,[r(z) - r(z^*) - r_0(z) + r_0(z^*)]$$

$$= \mathrm{tr}\,[r_0^2(z^*) t(z^*) - r_0^2(z) t(z)] \tag{II.2.4}$$

In the above equation, we have used $r_0(z^*) = r_0^{\dagger}(z)$ and the trace property to rearrange the order of operators. Equation (II.2.4) is equivalent to

$$I = \frac{1}{2} \mathrm{tr}\left\{[r_0^2(z^*) - r_0^2(z)][t(z^*) + t(z)] + [r_0^2(z^*) + r_0^2(z)][t(z^*) - t(z)]\right\} \tag{II.2.5}$$

Now we observe that the definition of the resolvent $r_0(z) = (h_0 - z)^{-1}$ implies

$$\frac{d}{d\lambda}[(z^* - z) r_0(z) r_0(z^*)] = r_0^2(z^*) - r_0^2(z) \tag{II.2.6}$$

where we set $z = \lambda + i\mu$.

This last identity permits us to write I as the sum of three terms,

$$I = I_1 + I_2 + I_3 = I_1 + 2i \, \mathrm{Im} \, I_2 \tag{II.2.7}$$

where

$$I_1 = \frac{1}{2} \mathrm{tr}\left\{\frac{d}{d\lambda}[(z^* - z) r_0(z) r_0(z^*)]\right\}[t(z^*) + t(z)] \tag{II.2.8}$$

$$I_2 = \frac{1}{2} \mathrm{tr} \, r_0^2(z^*) [t(z^*) - t(z)] \tag{II.2.9}$$

$$I_3 = \frac{1}{2} \mathrm{tr} \, r_0^2(z) [t(z^*) - t(z)] \tag{II.2.10}$$

If one takes the complex conjugate of I_3 then we see that it is the negative of I_2. So as the last form of equation (II.2.7) indicates it suffices to compute I_1 and $\mathrm{Im}\, I_2$.

The next step is to introduce the reduced representation of all the operators. The operator $\tau(E,E';z)$ will be that associated with $t(z)$. The kernel of $\tau(E,E';z)$ gives its precise definition. Specifically

$$\langle\hat{p}|\tau(E,E';z)|\hat{p}'\rangle = j(E)\langle\vec{p}\,|t(z)|\vec{p}'\rangle j(E') \qquad \text{(II.2.11)}$$

where the jacobian factor is

$$j(E) = (2\mu^3 E)^{\frac{1}{4}} \quad , \quad E = p^2/2\mu \qquad \text{(II.2.12)}$$

The reduced operators act on the two-dimensional Hilbert space of $L^2(\hat{p})$. On this space we denote the trace by $\hat{tr}$. For future reference we note that the matrix element of τ is zero when either $E=0$ or $E'=0$.

First we evaluate I_1 in the limit $\mu \to +0$. From equation (II.2.8) we have

$$I_1 = \hat{tr}\int_0^\infty dE\left[\frac{d}{d\lambda}(-2\pi i)\,\delta(E-\lambda)\right] Re\ \tau(E,E;\lambda-i0) \qquad \text{(II.2.13)}$$

This expression becomes after one integrates by parts and observes that the surface term vanishes

$$I_1 = -2\pi i\ \hat{tr}\frac{\partial}{\partial E} Re\ \tau(E,E;\lambda-i0)\Big|_{E=\lambda} . \qquad \text{(II.2.14)}$$

Turning to I_2 we introduce the off-shell unitarity relation (II.2.2) two times to obtain,

$$\begin{aligned} I_2 &= \tfrac{1}{2}\,tr\ \Lambda_0^2(z^*)(z-z^*)\,t(z^*)\Lambda_0(z^*)\Lambda_0(z)\,t(z) \\ &= \tfrac{1}{2}\,tr\ \Lambda_0^2(z^*)(z-z^*)\,t(z^*)\Lambda_0(z^*)\Lambda_0(z)\ \times \\ &\qquad \times\left[t(z^*) + (z^*-z)\ t(z)\Lambda_0(z)\Lambda_0(z^*)\,t(z^*)\right] \end{aligned} \qquad \text{(II.2.15)}$$

Off-shell unitarity also implies

$$\frac{d}{dz}t(z) = -t(z)\Lambda_0^2(z)\,t(z) \qquad \text{(II.2.16)}$$

Thus I_2 may be stated

$$I_2 = \frac{1}{2}\, tr\, \frac{d}{dz^*} t(z^*) \quad (z^*-z)\, \rho_0(z^*)\, \rho_0(z)$$
$$+ \frac{1}{2}\, tr\, \frac{d\, t(z^*)}{dz^*} (z^*-z)\, \rho_0(z^*) \rho_0(z)\, t(z)\, (z^*-z)\, \rho_0(z)\, \rho_0(z^*) \tag{II.2.17}$$

In the limit $\mu \to +0$ this becomes in the reduced language

$$I_2 = \frac{1}{2}\, \hat{tr} \int_0^\infty dE\, (-2\pi i)\, \delta(E-\lambda)\, \frac{d}{d\lambda}\, \tau(E,E;\lambda-i0)$$
$$+ \frac{1}{2}\, \hat{tr} \int_0^\infty dE \int_0^\infty dE' \Big\{ \Big[\frac{\partial}{\partial\lambda} \tau(E,E';\lambda-i0) \Big]^* \times (-2\pi i)^2 \delta(E'-\lambda)\, \tau(E',E;\lambda+i0)\, \delta(E-\lambda) \Big\} \tag{II.2.18}$$

Take the imaginary part of this,

$$2i\, \mathrm{Im}\, I_2 = -2\pi i\, \hat{tr}\, \mathrm{Re}\, \frac{\partial}{\partial\lambda} \tau(E,E,\lambda-i0) \Big|_{E=\lambda}$$
$$+ i(2\pi i)^2 \hat{tr}\, \mathrm{Im} \Big[\frac{\partial}{\partial\lambda} \tau(E,E;\lambda-i0) \Big]_{E=\lambda} \tau(\lambda,\lambda,\lambda+i0). \tag{II.2.19}$$

Equation (II.2.19) may be also expressed as

$$2i\, \mathrm{Im}\, I_2 = -2\pi i\, \hat{tr}\, \mathrm{Re}\, \frac{\partial}{\partial\lambda} \tau(E,E,\lambda-i0) \Big|_{E=\lambda}$$
$$+ i(2\pi i)^2 \hat{tr}\, \mathrm{Im} \Big\{ \Big[\frac{d}{d\lambda} \tau(\lambda,\lambda,\lambda-i0) \Big] \tau(\lambda,\lambda,\lambda+i0) \Big\} \tag{II.2.20}$$

Here the change in the second term is the result of the identity

$$0 = \hat{tr}\, \mathrm{Im} \Big(\frac{\partial}{\partial E} \tau(E,E;\lambda-i0) \Big|_{E=\lambda} \Big) \tau(\lambda,\lambda,\lambda+i0). \tag{II.2.21}$$

This equation can be obtained from the unitarity equation in the reduced space language.

$$\tau(E,E';z_1) - \tau(E,E';z_2) = (z_2-z_1) \int dE'' \frac{\tau(E,E'';z_1)\, \tau(E'',E',z_2)}{(E''-z_1)\,(E''-z_2)} \tag{II.2.22}$$

Let $z_1 = \lambda + i\mu$, $z_2 = \lambda - i\mu$, $\mu \to 0^+$ and take the trace.

$$\hat{tr}\left(\tau(E,E';\lambda+i0)-\tau(E,E';\lambda-i0)\right) = \lim_{\mu\to 0^+}(-2i\mu)\int dE''\,\hat{tr}\,\frac{\tau(E,E'';\lambda+i\mu)\,\tau(E'',E';\lambda-i\mu)}{(E''-\lambda)^2+\mu^2}$$
$$= -2\pi i\,\hat{tr}\,\tau(E,\lambda;\lambda+i0)\,\tau(\lambda,E';\lambda-i0)$$
(II.2.23)

Take partial derivatives with respect to E' .

$$\hat{tr}\left(\frac{\partial}{\partial E'}\tau(E,E';\lambda+i0)-\frac{\partial}{\partial E'}\tau(E,E';\lambda-i0)\right) = (-2\pi i)\,\hat{tr}\,\tau(E,\lambda;\lambda+i0)\frac{\partial}{\partial E'}\tau(\lambda,E';\lambda-i0)$$
(II.2.24)

Similarly, we can obtain another expression starting with

$$\tau(E,E';z_1)-\tau(E,E';z_2) = (z_2-z_1)\int_0^\infty dE''\,\frac{\tau(E,E'';z_2)\,\tau(E'',E';z_1)}{(E''-z_2)(E''-z_1)}$$
(II.2.25)

and let $z_1=\lambda-i\mu$, $z_2=\lambda+i\mu$ and $\mu\to 0^+$.

$$\hat{tr}\,\frac{\partial}{\partial E}\left(\tau(E,E';\lambda-i0)-\tau(E,E',\lambda+i0)\right)$$
$$= 2\pi i\,\hat{tr}\,\frac{\partial}{\partial E}\tau(E,\lambda;\lambda-i0)\,\tau(\lambda,E',\lambda+i0)$$
(II.2.26)

Now set both E and E' equal to λ for both equations (II.2.24 and 26), and then subtract one from the other.

$$\hat{tr}\,\frac{\partial}{\partial E}\left(\tau(E,E;\lambda+i0)-\tau(E,E;\lambda-i0)\right)_{E=\lambda}$$
$$= -2\pi i\,\hat{tr}\left[\frac{\partial}{\partial E}\tau(E,E;\lambda-i0)\right]_{E=\lambda}\tau(\lambda,\lambda,\lambda+i0)$$
(II.2.27)

Since $t^+(z)=t(z^*)$, the left hand side is an imaginary number. Hence, the real part of the right hand side must vanish. This produces equation (II.2.21).

Let us return to the basic argument. Combining equations (II.2.20, 14 and 7) we obtain

$$2i\,\mathrm{Im}\,tr\left[R(\lambda+i0)-R_0(\lambda+i0)\right] = -2\pi i\,\hat{tr}\,\frac{d}{d\lambda}\,\mathrm{Re}\,\tau(\lambda,\lambda;\lambda-i0)$$
$$+\,i(2\pi i)^2\,\hat{tr}\,\mathrm{Im}\left\{\left[\frac{d\tau(\lambda,\lambda;\lambda-i0)}{d\lambda}\right]\tau(\lambda,\lambda;\lambda+i0)\right\}$$
(II.2.28)

The right hand side of (II.2.28) is related to the time delay by noting that $q(\lambda) = q^{\dagger}(\lambda)$, so $\hat{tr}\, q(\lambda) = \hat{tr}\, \mathrm{Re}\, q^{\dagger}(\lambda)$. Using the S-matrix representation of $q(\lambda)$ and the representation of $s(\lambda)$ in terms of the T-matrix,

$$s(\lambda) = 1 - 2\pi i\, \tau(\lambda,\lambda;\lambda+i0) \tag{II.2.29}$$

we have

$$\hat{tr}\, q(\lambda) = -2\pi\, \hat{tr}\, \frac{d}{d\lambda} \mathrm{Re}\, \tau(\lambda,\lambda;\lambda-i0) - (2\pi)^2\, \hat{tr}\, \mathrm{Im}\left[\frac{d\tau(\lambda,\lambda;\lambda-i0)}{d\lambda} \right] \tau(\lambda,\lambda;\lambda+i0) \tag{II.2.30}$$

Version (II.2.30) of $\hat{t}\, q(\lambda)$ together with equation (II.2.4) allows us to conclude that

$$2\, \mathrm{Im}\, tr\left[r(\lambda+i0) - r_0(\lambda+i0) \right] = \hat{tr}\, q(\lambda) \tag{II.2.31}$$

This is the spectral property of time delay.

II.3 The physical interpretation

It is appropriate to give an explicit physical interpretation to the spectral property found above. Following Birman and Krein[5] we introduce the spectral shift function $\Delta(\lambda)$. The exact and free Hamiltonians have a spectral representation[6] given by

$$h = \int \lambda\, de(\lambda), \qquad h_0 = \int \lambda\, de_0(\lambda) \tag{II.3.1}$$

Here $e(\lambda)$ and $e_0(\lambda)$ denote the spectral projection operators for h and h_0. In the continuum, i.e. $\lambda \geq 0$ we define $\Delta(\lambda)$ as

$$\Delta(\lambda) = tr\left[e(\lambda) - e_0(\lambda) \right] \tag{II.3.2}$$

The spectral shift has a simple physical interpretation. Suppose for purposes of discussion that we were considering a quantum problem with box normalization and boundary conditions. In these circumstances the continuum is absent and $\mathrm{tr}\, e(\lambda)$ is a finite positive intrger that is equal to the number of eigenstates with energy less than λ . Here $\mathrm{tr}[e(\lambda)-e_0(\lambda)]$ is the excess number of eigenstates created when the perturbation $v = h - h_0$ is turned on. So, $\Delta(\lambda)$ is a definition of this excess number of states and the definition remains meaningful even when we remove the box normalization and the continuous spectrum is present. For the continuous spectrum case, of course $\mathrm{tr}\, e_0(\lambda)$ and $\mathrm{tr}\, e(\lambda)$ are both infinite. Thus if we form the derivative $\frac{d\Delta(\lambda)}{d\lambda}$ it has the meaning of the change of state density at energy λ due to the interaction v . For the resolvents $r(z)$ and $r_0(z)$ equation (II.3.1) allows the representation

$$r(z) = \int (\lambda'-z)^{-1}\, de(\lambda')\,, \qquad \mathrm{Im}\, z \neq 0 \qquad \text{(II.3.3)}$$

$$r_0(z) = \int (\lambda'-z)^{-1}\, de_0(\lambda')\,, \qquad \mathrm{Im}\, z \neq 0 \qquad \text{(II.3.4)}$$

For any state ϕ in the $L^2(\vec{p})$ Hilbert space one has

$$(\phi, \mathrm{Im}[r(\lambda+i\mu) - r_0(\lambda+i\mu)]\phi)$$

$$= \int \mathrm{Im}\left[\frac{1}{\lambda'-\lambda-i\mu}\right] \frac{d(\phi,[e(\lambda')-e_0(\lambda')]\phi)}{d\lambda'}\, d\lambda' \qquad \text{(II.3.5)}$$

Taking $\mu \to 0^+$, give us

$$(\phi, \mathrm{Im}[r(\lambda+i0) - r_0(\lambda+i0)]\phi) = \pi \frac{d}{d\lambda}(\phi, [e(\lambda)-e_0(\lambda)]\phi). \qquad \text{(II.3.6)}$$

Suppose now $\{\phi_n\}$ is a complete orthonormal set in $L^2(\vec{p})$, then if we sum equation (II.3.6) over n for each ϕ_n we have

$$\operatorname{tr} \operatorname{Im}\left[r(\lambda+i0) - r_0(\lambda+i0)\right] = \pi \frac{d}{d\lambda} \Delta(\lambda) \tag{II.3.7}$$

Thus, from (II.2.31) we deduce

$$\hat{\operatorname{tr}}\, q(\lambda) = 2\pi \frac{d\,\Delta(\lambda)}{d\lambda} \tag{II.3.8}$$

From a physical perspective this means that $\hat{\operatorname{tr}}\, q(\lambda)$ is a remarkable object. As indicated in the opening discussion it is known that $\langle\hat{p}|q(\lambda)|\hat{p}\rangle$ gives the physical time delay for an incident plane wave. Equation (II.3.8) shows us that $q(\lambda)$ has a second, very different, physical meaning - namely the change of state density due to the perturbation. For example, it is because of the state density of $q(\lambda)$ meaning that it enters the theory of statistical mechanics and the computation of virial coefficients for dilute gases.

From the spectral property of $q(\lambda)$ it is a short step to the time delay version of Levinson's theorem. For a spherically symmetrical potential, we can project $q(\lambda)$ onto a angular momentum subspace as $q_\ell(\lambda)$. The spectral property in this subspace bears the same form as (II.2.31)

$$2 \operatorname{Im} \operatorname{tr}\left[r(\lambda+i0) - r_0(\lambda+i0)\right]_\ell = q_\ell(\lambda) \tag{II.3.9}$$

The function $\operatorname{tr}\left[r(\lambda+i\mu) - r_0(\lambda+i\mu)\right]_\ell$ is an analytic function of z in the cut plane excluding the positive real axis. This function has simple poles at the bound state energies of h. We apply Cauchy's theorem to a contour which is a circle of radius R centered about the origin of z and running along the real axis so as to exclude the branch cut lying along the positive real axis. The contour has separate small circles about each simple pole of $\operatorname{tr}[\Lambda(z)-\Lambda_0(z)]_\ell$. Then

$$\int_{C(R)} \operatorname{tr}[\Lambda(z)-\Lambda_0(z)]_\ell \, dz = 0 \qquad \text{(II.3.10)}$$

It is easy to show that

$$|z| \left| \operatorname{tr}[\Lambda(z)-\Lambda_0(z)]_\ell \right| \longrightarrow 0 \qquad \text{(II.3.11)}$$

uniformly as $|z| \to \infty$. So when $R \to \infty$ the contour at infinity vanishes, thus (II.3.10) gives us

$$\int_0^\infty 2i \operatorname{Im} \operatorname{tr}[\Lambda(\lambda+io)-\Lambda_0(\lambda+io)]_\ell \, d\lambda + 2\pi i N_\ell = 0 \qquad \text{(II.3.12)}$$

where N_ℓ is the number of bound states of angular momentum ℓ , including degeneracy.

By applying the spectral property (II.3.9) one then has

$$\int_0^\infty q_\ell(\lambda) \, d\lambda = -2\pi N_\ell \qquad \text{(II.3.13)}$$

This is the time-delay variant of Levinson's theorem. A substitution of $q_\ell(\lambda) = \frac{d\delta_\ell(E)}{dE}$ in terms of the phase shift $\delta_\ell(E)$ one recovers the familiar form of Levinson's theorem.

$$\delta_\ell(0) - \delta_\ell(\infty) = 2\pi N_\ell \qquad \text{(II.3.14)}$$

An attractive aspect of this statement of Levinson's theorem is that we may understand the theorem as a relation between two observable quantities - time delay on one hand and the number of bound states on the other. Note also that equation (II.3.13) predicts some striking general results concerning time delay. Consider the case when at some energy $E = E_R$ there is a long lived resonance. In the energy region around E_R , $q_\ell(\lambda)$ is very large and positive. In order for (II.3.13) to remain valid, what must happen is that in other energy regions away from E_R there will be an increased time advance.

In the situation where the potential has only a finite number of partial waves, one could sum over all the angular momentum states and arrive at a Levinson's theorem for the entire space,

$$\int_0^\infty \hat{\mathrm{tr}}\, q(\lambda)\, d\lambda = -2\pi N \tag{II.3.15}$$

where $N = \sum_{\ell=1}^{M} N_\ell$ and M is finite.

For a general potential however, the Levinson's theorem[41] must be modified.

$$\int_0^\infty \left[\hat{\mathrm{tr}}\, q(\lambda) + \frac{2}{\pi}\left(\frac{\mu}{2}\right)^{3/2} \frac{\tilde{v}}{\sqrt{\lambda}} \right] d\lambda = -2\pi N \tag{II.3.16}$$

where $\tilde{v} = \int d\vec{x}\; v(\vec{x})$. Mathematically, the difficulty lies in the vanishing of (II.3.11) as $|z| \to \infty$. An infinite sum of partial waves would not vanish, i.e.

$$\begin{aligned} &\lim_{|z|\to\infty} \sum_{\ell=1}^{M} |z| \left| \mathrm{tr}[\lambda(z) - \lambda_0(z)]_\ell \right| \\ &= \sum_{\ell=1}^{M} \lim_{|z|\to\infty} |z| \left| \mathrm{tr}[\lambda(z) - \lambda_0(z)]_\ell \right| = 0 \end{aligned} \tag{II.3.17}$$

However,

$$\begin{aligned} &\lim_{|z|\to\infty} \sum_{\ell=1}^{\infty} |z| \left| \mathrm{tr}[\lambda(z) - \lambda_0(z)]_\ell \right| \\ &\neq \sum_{\ell=1}^{\infty} \lim_{|z|\to\infty} |z| \left| \mathrm{tr}[\lambda(z) - \lambda_0(z)]_\ell \right| \end{aligned} \tag{II.3.18}$$

and hence, would not vanish. This necessitate the modification in (II.3.16).

Chapter III U and W functions and binary kernels

In this chapter we give a summary of the methods employed by Kahn and Uhlenbeck[7] in investigating the quantum virial coefficients. This will serve as an historical background to illustrate the character of our derivation in the coming chapters. Since the bulk of this thesis is concerned with the three body problem, one must necessarily project onto the N-body problem ($N > 3$) from the three body solution. The method of Kahn and Uhlenbeck provides a proper basis for such a projection. In particular, one can perceive why the problem of disconnectedness is absent in the two body case but present in the three body case, and also how it can be handled for $N > 3$ cases.

Even though the Kahn and Uhlenbeck method are exact, they are not very useful for actual numerical calculations. Many workers seek approximations from the theory in order to calculate even the third virial coefficient. The binary kernel method by Lee and Yang[8], which we shall illustrate, is a well known systematic method of approximation. Otherwise, the theory of virial coefficients has not progressed much and are generally taken as complete.

In terms of time delay, we have found a new theory for virial coefficients. We shall establish in chapter IV, on a rigorous operator level, the simple functional dependence of virial coefficients upon time delay. In the next chapter, through the Cayley transform method we verify the calculation using kernels and integrations. We illustrate the internal structure of these virial coefficients from which we hope, one can make new, and may be better, approximations.

To be consistent with the rest of the thesis, we only illustrate the simple case of Boltzmann statistics. Bose or Fermi statistics can be treated accordingly but the complication only tend to confound rather than to illuminate the physics of time delay.

We follow the standard treatment and introduce the W_N and U_N operator functions.

$$W_N \equiv exp. -\beta H_N \qquad (III.1)$$

where H_N is the full N particle Hamiltonian. The partition function is simply $Q_N = Tr\ W_N$. To obtain the logarithm of the grand partition function $\mathcal{L}$ in a simple form, we follow a procedure first introduced by Ursell[9] and by Mayer[10] for classical statistical mechanics and by Kahn and Uhlenbeck for quantum statistical mechanics.

One defines U_N functions by

$$\langle 1' | W_1 | 1 \rangle \equiv \langle 1' | U_1 | 1 \rangle$$

$$\langle 1', 2' | W_2 | 1, 2 \rangle \equiv \langle 1' | U_1 | 1 \rangle \langle 2' | U_1 | 2 \rangle + \langle 1', 2' | U_2 | 1, 2 \rangle$$

$$\begin{aligned} \langle 1', 2', 3' | W_3 | 1, 2, 3 \rangle \equiv\ & \langle 1' | U_1 | 1 \rangle \langle 2' | U_1 | 2 \rangle \langle 3' | U_1 | 3 \rangle \\ & + \langle 1' | U_1 | 1 \rangle \ \langle 2', 3' | U_2 | 2, 3 \rangle \\ & + \langle 2' | U_1 | 2 \rangle \ \langle 1', 3' | U_2 | 1, 3 \rangle \\ & + \langle 3' | U_1 | 3 \rangle \ \langle 1', 2' | U_2 | 1, 2 \rangle \\ & + \langle 1', 2', 3' | U_3 | 1, 2, 3 \rangle \qquad (III.2) \end{aligned}$$

... etc.

The numbers 1,2,3... in the bra and ket vectors denote the complete set of coordinates of particle number 1 and of particle number 2, etc. The subscript N in W_N and U_N denotes the total number of particles involved. We can already see the significant difference between W_N and U_N. U_N is the part of W_N which is <u>not</u> (a) contributed by the free Hamiltonian alone, i.e. $\underbrace{\langle 1'|U_1|1\rangle \langle 2'|U_1|2\rangle \cdots \langle N'|U_1|N\rangle}_{N \text{ terms}}$

which is $\langle 1',2',\cdots N'|W_N|1,2,\cdots N\rangle$ if the potential vanishes and $H_N = H_N^{\circ}$; (b) disconnected by having one group of particles interacting within the group only, e.g. $\langle 1'|U_1|1\rangle \langle 2',3'|U_2|2,3\rangle$ where particle number 1 never interact with 2 or 3. Following standard treatment, one arrives at

$$\begin{aligned} \ln \mathcal{Z} &\equiv \ln \sum_{N=0}^{\infty} \frac{1}{N!} Q_N z^N \\ &= \sum_{\ell=1}^{\infty} z^\ell b_\ell = \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell!} \operatorname{Tr} U_\ell \end{aligned} \qquad (\text{II}.3)$$

where the virial coefficients b_ℓ is expressed directly in terms of U_ℓ .

We pause here to state that we have not dealt with the theorems of Lee and Yang concerning the volume dependence of b_ℓ. Our studies involve macroscopic finite volume large enough for the cluster integrals to be essentially the same as those computed at $V \to \infty$. Specifically, any macroscopic R will make $P(R)$ close enough to unity for our calculations in the following chapter.

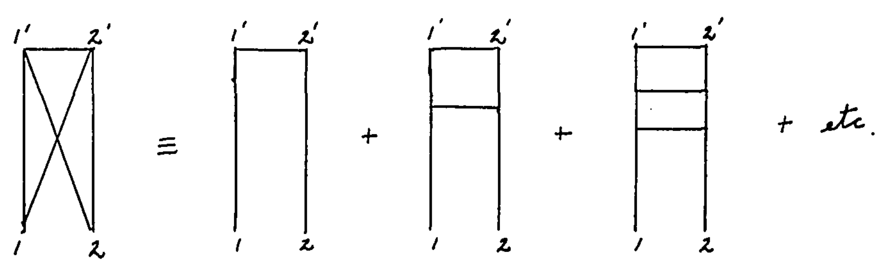
To further our discussion, we introduce the diagrammatic method of Lee and Yang and their binary kernel expansion.

The operator function $W_N = exp.-\beta H_N$, $H_N = H_N^\circ + V_N$ can be expanded in terms of $W_N^\circ = exp.-\beta H_N^\circ$ and V_N .

$$W_N(\beta) = W_N^\circ(\beta) + \int_0^\beta W_N^\circ(\beta-\beta')(-V_N)\, W_N^\circ(\beta')\, d\beta'$$
$$+ \int_0^\beta d\beta' \int_0^{\beta'} d\beta''\ W_N^\circ(\beta-\beta')(-V_N)\, W_N^\circ(\beta'-\beta'')(-V_N)\, W_N^\circ(\beta'')$$
$$+ \ \cdot \ \cdot \ \cdot \qquad (\text{III}.4)$$

We represent the first few $W_N(\beta)$ in figure III-1, diagrammatically. The horizontal lines represent $(-V_N)$ and each vertical line represent one particle. The length along the vertical lines represent β and the integration variables β', β'', β''' ...etc.

In these diagrams, the contribution from the free Hamiltonian are the diagrams without horizontal lines (i.e. no $-V_N$). Disconnectedness is rather self-explanatory. It describes diagrams where at least two groups of vertical lines are not joint to each otherby any horizontal line. e.g. the 2nd, 3rd, 4th and 5th diagram of $W_3(\beta)$. In terms of these potential diagrams, the U_N's have a simple meaning. U_N is the sum of all "connected diagrams" with N vertical lines each of length β . We can now introduce the binary kernel as a particular way of summing these connected diagrams.

$B(\beta;1,2) \equiv$ 

A new set of binary kernel diagrams can be drawn to represent

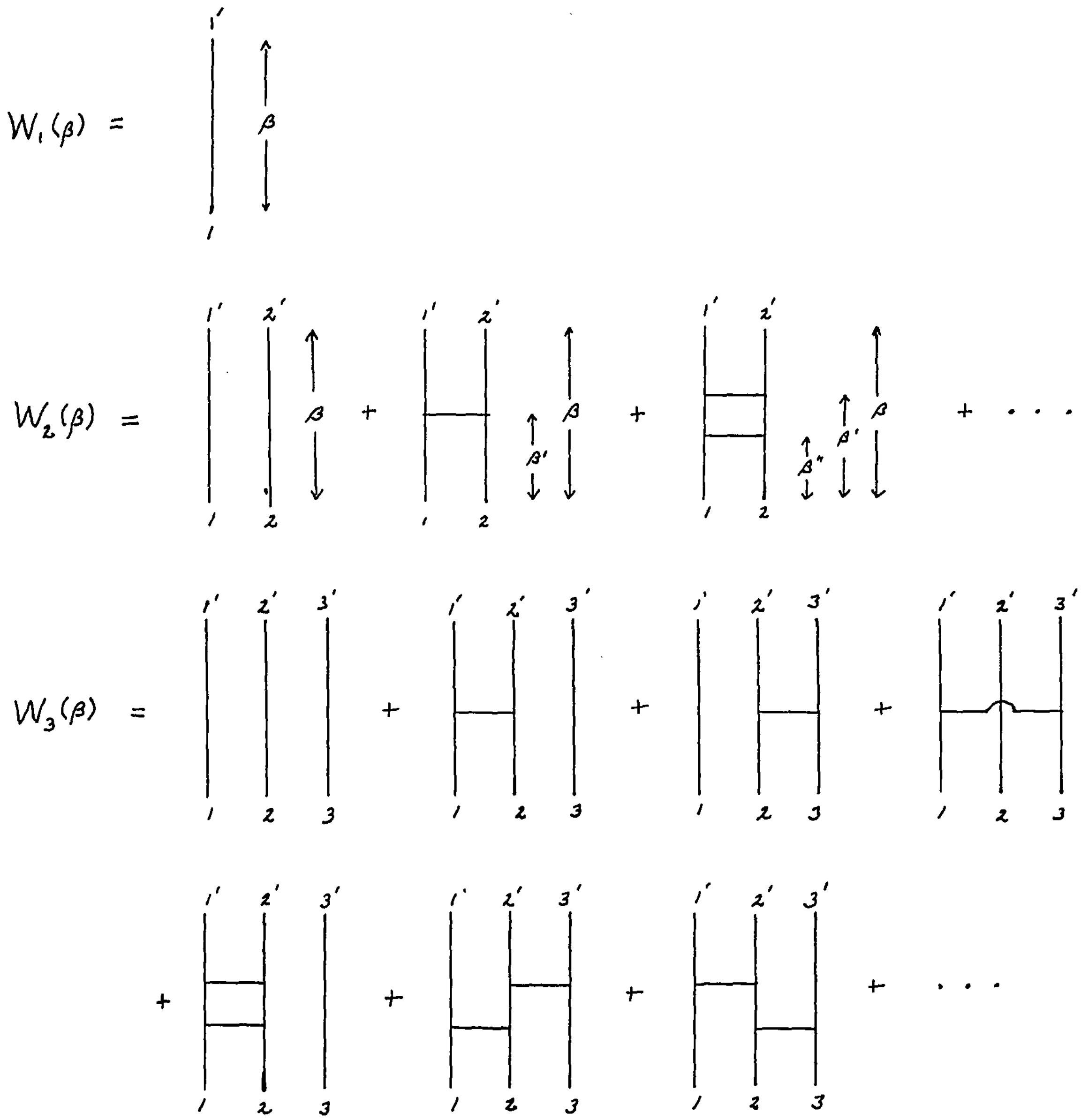


Figure III-1   Potential diagrams

U_N as in figure III-2.

We can also define the binary kernel as

$$\mathcal{B}(\beta; 1,2) \equiv -V_{12} W_2(\beta) = -V_{12} \exp. -\beta H_2$$

The binary kernel $\mathcal{B}(\beta;1,2)$ could be solved from the two body problem and will therefore, provide a way of approximating all virial coefficients in powers of $\mathcal{B}$. For example,

$$U_2(\beta) = \int_0^\beta d\beta' \, W_1(\beta-\beta'; 1) \, W_1(\beta-\beta'; 2) \, \mathcal{B}(\beta'; 1, 2) \qquad (\text{III}.5)$$

$$U_3(\beta) = \int_0^\beta d\beta' \int_0^{\beta'} d\beta'' \, W_1(\beta-\beta''; 1) \, W_1(\beta-\beta'; 2) \, W_1(\beta-\beta'; 3) \times$$
$$\mathcal{B}(\beta'-\beta''; 2,3) \, \mathcal{B}(\beta''; 1, 2) \, W_1(\beta''; 3)$$

$$+ \int_0^\beta d\beta' \int_0^{\beta'} d\beta'' \, W_1(\beta-\beta'; 1) \, W_1(\beta-\beta'; 2) \, W_1(\beta-\beta''; 3) \times$$
$$\mathcal{B}(\beta'-\beta''; 1,2) \, \mathcal{B}(\beta''; 2, 3) \, W_1(\beta''; 1)$$

+ four other terms of order $\mathcal{B}^2$

+ terms of higher orders in $\mathcal{B}$. $\qquad (\text{III}.6)$

In concluding this chapter, we must state explicitly the couple of physical aspects that this theory does not provide for. While it deals adequately with the obvious problem of spectator particle (disconnectedness), it cannot allow for the possibility of bound states and hence, channel structure in the various virial coefficients. It also bypasses the problem of rescattering singularity. Both of these problems are solved in the time delay theory of virial coefficients in the following chapters.

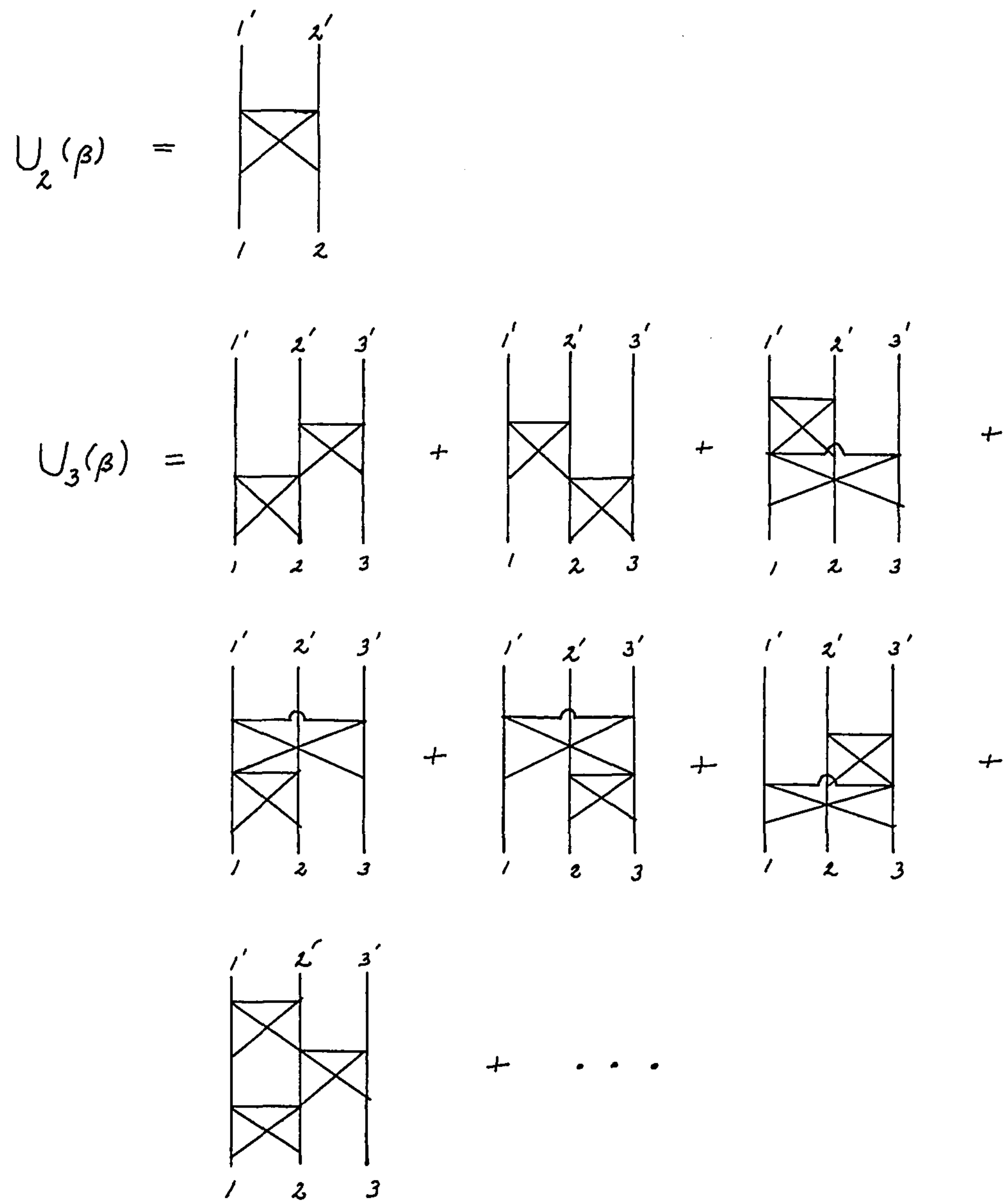


Figure III-2 Binary Kernel diagrams

Chapter IV Quantum theory of virial coefficients

This chapter presents a general quantum theory of the higher virial coefficients. The objective is to derive from first principles the equilibrium statistical behaviour of an interacting N-particle quantum gas. A brief summary and physical picture of our problem is helpful. We shall not impose any restrictions on the strength of the interactions, if attractive enough, are free to form two, three or n-particle bound states. The formation of these stable clusters is the creation by the interaction of species types in the gas. The equation of state for such a system is one such that there are collisions between elementary constituents and clusters. These scatterings will involve pickup, rearrangement, breakup and elastic scattering. For equilibrium these various possible outcome of the scattering process occur at rates such that the fractional amounts of the various species types remain constant.

The system we consider is N ($\cong 10^{23}$) distinguishable particles having identical mass m. We restrict the statistical character of this system to that of Boltzmann statistics. Consequently effects arising from the symmetry of the N-particle wave function, such as exchange phenomena, are omitted from this analysis. While we believe this restriction to Boltzmann statistics can be relaxed, we impose it because our basic aim is to find which aspects of the physical scattering process control the thermodynamic behavior of the system.

Our study employs modern few-particle scattering theory. This theory does not yet exist for long-range Coulomb forces. For this reason we must confine our treatment to forces that fall off faster than the Coulomb force. Aside from this one physical restriction, our interaction may be quite general. For example, the theory remains valid for interactions that do no obey time reversal invariance or conserve angular momentum.

IV.1 Introcuction

Let us outline the basic investigatory tools we will utilize. Assume that V is the volume and T the temperature of our system. For $\beta = \frac{1}{kT}$ the grand partition function is defined in terms of the fugacity z by

$$\mathcal{Z}(V,T,z) = \sum_{N=1}^{\infty} \frac{z^N}{N!} \, Tr \, e^{-\beta H_N} \qquad \text{(IV.1.1)}$$

where H_N is the exact Hamiltonian for a N-particle system. The trace is taken over the entire N-particle Hilbert space without the imposition of any symmetry restrictions. It is the absence of symmetry requirements that identifies this system as one governed by Boltzmann statistics. Of course, k is the Boltzmann constant.

Ursell[11] developed a cluster expansion for this system which leads to a second form for the grand partition function given by

$$\mathcal{Z}(V,T,z) = exp. \left\{ V \sum_{\ell=1}^{\infty} b_\ell z^\ell \right\} \qquad \text{(IV.1.2)}$$

The key quantity in this representation is the coefficients

b_ℓ - the ℓth cluster integral. If one expands both forms of $\mathcal{L}$ and equates the coefficients of the different powers of z then simple trace definitions of b_ℓ results. For example,

$$b_1 = \frac{1}{V} Tr\, e^{-\beta H_1} = \lambda^{-3} \tag{IV.1.3}$$

where $\lambda = (\hbar^2 2\pi/mkT)^{\frac{1}{2}}$. The quantity λ is the thermal wavelength of the particle mass m. We shall be especially interested in the cluster integral for two and three particle systems. Equations (IV.1.1 and 2) imply

$$b_2 = \frac{2^{3/2}}{2!\lambda^3} Tr\left(e^{-\beta h} - e^{-\beta h_0}\right) \tag{IV.1.4}$$

In this formula the center-of-mass motion has been extracted leading to the factor of $2^{\frac{3}{2}}\lambda^{-3}$. So the trace ranges over just the relative motion degrees of freedom of this system. If we denote the interaction by v then h_0 is the free two particle Hamiltonian and h is the fully interacting Hamiltonian $h = h_0 + v$. The temperature dependence of b_2 will not be exhibited. The formula for third cluster integral is also found from equations (IV.1.1 and 2). We have

$$b_3 = \frac{3^{\frac{3}{2}}}{3!\lambda^3} Tr\left[e^{-\beta H} - e^{-\beta H_0} - \sum_{\alpha=1}^{3}\left(e^{-\beta H_\alpha} - e^{-\beta H_0}\right)\right] \tag{IV.1.5}$$

The quantities H, H_α and H_0 in this formula are three-body Hamiltonians.

In this formalism, once we have an explicit form for the cluster integral b_ℓ then the grand partition function and the other thermodynamic properties of the system are determined. For example the equation of state is

$$PV = NkT \sum_{i=1}^{\infty} a_i \rho^{i-1} \tag{IV.1.6}$$

where ρ is the particle space density N/V and the a_i 's are the virial coefficients which are determined in a known way by the cluster integrals, i.e. $a_1 = 1$, $a_2 = -b_2 b_1^{-2}$, $a_3 = 4a_2^2 - 2b_3 b_1^{-3}$, etc. A systematic feature of these Ursell cluster representations is that the n^{th} cluster integral or n^{th} virial coefficient involves only n and fewer particle effects.

All studies of higher virial coefficients begin with these Ursell formulae. The task confronting successful theory is to evaluate these cluster integrals b_ℓ , in terms of scattering quantities, The analysis given here relies on the time dependent form of few particle scattering theory found in Faddeev's[1] work. More specificially, we shall base our solution on the properties of the theory of few particle time delay. The key feature of time delay phenomena will turn out to be the spectral property of time delay.[12] Illustrative of a successful determination of the quantum virial coefficients is the solution for the second cluster integral found in 1936 by Beth and Uhlenbeck[13] and independently by Gropper.[14] These authors find a closed form expression for this virial coefficient in terms of the phase shifts for two body scattering. Our goal in this paper is to find closed form expressions for the higher cluster integrals.

There exists a large literature on this problem and the approach outlined above has its antecedents. First Smith[15] and later Bedeaux[16] have used the time delay approach to attempt to solve the virial coefficient problem. The reason the work of these authors must be considered incomplete is that they do not treat the few- body problem realistically. Not considered by these authors are the new physical phenomena occuring in the three and N particle scattering problem that have no parallell in two-particle scattering. These phenomena are - the existence of stable subclusters, disconnected scattering processes, pickup, rearrangement, and breakup collisions, and rescattering singularities in the on-shell three-to-three S-matrix. Only the modern scattering formulism of the type developed by Faddeev treats these features adequately.

A parallel to this one is also developed in the literature. A direct attempt to evaluate the virial coefficients in terms of n-particle phase-shifts or S-matrices has been carried out by Dashen and collaborators,[17] by Larsen and Mascheroni,[18] and by Buslaev and Merkuriev.[19] Where appropriate we discuss where these two separate approaches coalesce. We should also point out several other prior attempts to introduce Faddeev's equations into the problem of determining the higher virial coefficients. A beginning in this direction was attempted by Reiner,[20] Baumgartl[21] and Gibson.[22] None of these authors had the theory of few particle time delay available to them, and partly for this reason their results are largely inconclusive.

IV.2 Second virial coefficient

This section gives a determination of the second virial coefficient. Although the physics of this case is well understood it is nevertheless constructive to present our approach for this limited problem first. Here one can clearly see the pattern of the derivation in a context simpler than for the n-particle case. Here it is easy to identify the sensitive mathematical features of the derivation. Finally, it is instructive to compare the two- and few-body solutions. We shall show that knowledge of the spectral property of time delay at once leads to an evaluation of the second cluster integral. Thus the central result of this section is a direct proof of the spectral property. In contrast to the method used in chapter II, the calculation here offers a generalization to the three body problem.

Through out this and the next section, we shall adapt the scattering theory notation used by Faddeev. We shall need more details than appeared in chapter II. The Moeller wave operators, $U^{(\pm)}$ represent the exact solutions of the Lippmann-Schwinger equation. The wave operators are isometries on the Hilbert space $L^2(\mathbb{R}^3)$. The coordinate occuring in the square integrable functions of this space is the interparticle separation vector. The identity on $L^2(\mathbb{R}^3)$ we denote as e. Then the Moeller wave operators and their adjoints satisfy the three fundamental identities:

$$U^{(\pm)+} U^{(\pm)} = e \tag{IV.2.1}$$

$$U^{(\pm)} U^{(\pm)+} + P_b = e \tag{IV.2.2}$$

$$h U^{(\pm)} = U^{(\pm)} h_o \tag{IV.2.3}$$

The (-) superscript demotes the solution with outgoing radiation boundary condition satisfied. The (+) indicates an incoming wave condition. The first statement implies wave-function probability is conserved in the scattering process. The next statement provides that either $U^{(+)}$ or $U^{(-)}$ are a complete set of scattering states. The last statement tell us that the exact scattered wave $U^{(-)}$ has the same energy as the incident plane wave. The validity of these three identities has been studied for a wide variety of assumptions on the two body potential.[23] We shall not be interested in studying the broadest possible class of potential for which our results remain valid. On the other hand we want to establish the spectral property for a class of potentials that are not felt to exclude any physically interesting cases. To this end we assume the potential

$$v \varepsilon L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3) \tag{IV.2.4}$$

With this assumption then Kato[24] proved equations (IV.2.1-3). It is at this point that Coulomb potentials are excluded from our study. The physical limitations that condition (IV.2.4) imposes on the potential are that local and infinity behavior are controlled. Thus $v \varepsilon L^1$ requires that $v(\vec{x})$ vanishes faster than $|\vec{x}|^{-3-\delta}$ at infinity, for some $\delta > 0$. The membership of v in L^2 confines the local singularity to be like $|\vec{x}|^{-\frac{3}{2}+\delta}$. The form in which we state two-body scattering theory also presumes that the constituent aprticles are spinless. Including spin involves only an extension of our notation. We have chosen to impose this restriction in order that the presentation of the analysis be simplified. Finally, we note that we will not assume that our interaction v satisfy either time reversal invariance nor that it conserves angular momentum. Of course it is necessary that v be hermitian.

Now let us recall the definition of time delay. We consider the time evolution of two related states of the system. Associated with each $f \varepsilon L^2(R^3)$ we have a 'freely' evolving system given by $\phi(t) = exp.(-ih_0 t) f$. This state $\phi(t)$ does not feel the effect of the interaction v between the particles. Related to $\phi(t)$ is $\Psi(t) = e^{-iht} U^{(-)} f$. The state $\Psi(t)$ is the exact scattering state that coincides with $\phi(t)$ for times long before the scattering, viz.

$$\lim_{t \to -\infty} \| \Psi(t) - \phi(t) \| = 0 \qquad \text{(IV.2.5)}$$

Next one introduces a projection operator P(R) that is related to the spatial separation of the two particles. Choosing $\vec{x}$ to denote the vector separation of the two particles then $P(R) f(\vec{x})$ is equal to zero if $|\vec{x}| > R$ and equal $f(\vec{x})$ otherwise. Thus $P(R)$ defines the projection onto a sphere of radius R centered about the center-of-mass vector for the two particle system. For each of our evolving states $\phi(t)$ and $\Psi(t)$ there is a quantum mechanical transit time. The probability of having $\Psi(t)$ inside the sphere is $(\Psi(t), P(R)\Psi(t))$. Thus the transit time of $\Psi(t)$ is $\int_{-\infty}^{\infty} (\Psi(t), P(R)\Psi(t)\, dt$. The corresponding transit time of the free wave is $\int_{-\infty}^{\infty} (\phi(t), P(R)\phi(t))\, dt$. The difference of these two real numbers is the definition of time delay for the incident state specified by the function f.

This time delay is in principle an observable feature of the scattering process. The remaining task of our definition is to specify the hermitian operator that must be associated with this observable. This task is traight forward. As given above, the time delay for sphere R and wave packet f is given by the expression

$$\int_{-\infty}^{\infty} [(\Psi(t), P(R)\Psi(t)) - (\phi(t), P(R)\phi(t))]\, dt \tag{IV.2.6}$$

If the intertwining property (IV.2.3) is used, then all the time dependence in inner products may be written in terms of $e^{-ih_0 t}$. Thus expression (IV.2.6) can also be stated as

$$(f, Q(R)f) = \int_{-\infty}^{\infty} (f, e^{ih_0 t}[U^{(-)^+} P(R) U^{(-)} - P(R)]\, e^{-ih_0 t} f)\, dt \tag{IV.2.7}$$

where $Q(R)$ is the operator whose diagonal matrix elements gives the value of the observed time delay. By doing the time integration we obtain a delta function in energy. Thus we are led to a useful kernel representation of $Q(R)$,

$$(f, Q(R)f) = \int f^*(\vec{p}\,') \frac{\delta(E-E')}{\mu p} \langle \hat{p}'| q(E,R) |\hat{p}\rangle f(\vec{p})\, d\vec{p}\, d\vec{p}\,' \tag{IV.2.8}$$

where $q(E,R)$ is an operator acting on $L^2(\hat{p})$ and is determined by

$$\langle \hat{p}'| q(E,R) |\hat{p}\rangle = 2\pi\mu p \langle \vec{p}| U^{(-)^+} P(R) U^{(-)} - P(R) |\vec{p}\,'\rangle \tag{IV.2.9}$$

In both of the equations above, energy and momenta are restricted by the on-shell condition $E = p^2/2\mu$. The symbol μ stands for the reduced mass of the system. Eventually we shall need the time delay for all of space. This is obtained from equation (IV.2.8) by letting $R \to \infty$. We shall denote the kernel associated with this limit by $\langle \hat{p}'| q(E) |\hat{p}\rangle$. It is given by

$$\lim_{R\to\infty} (f, Q(R)f) = \int f^*(\vec{p}\,') \frac{\delta(E-E')}{\mu p} \langle \hat{p}'| q(E) |\hat{p}\rangle f(\vec{p})\, d\vec{p}\, d\vec{p}\,' \tag{IV.2.10}$$

For most of our purposes we shall only need the definitions stated in equations (IV.2.7-10) More extensive discussion of time delay in the two-particle case are found in references [25-30].

With these scattering theory preliminaries complete let us return to the basic problem of evaluating the second cluster integral. We need to compute $Tr(e^{-\beta h} - e^{-\beta h_0})$. Both Hamiltonians h and h_0 define resolvents for complex energies z by $r(z) = (h-z)^{-1}$ and $r_0(z) = (h_0 - z)^{-1}$. The resolvent $r(z)$ is connected to the statistical operator $e^{-\beta h}$ by the Watson transform[31] which tells us that,

$$e^{-\beta h} = -\frac{1}{2\pi i}\oint_C e^{-\beta z} r(z)\, dz \qquad \text{(IV.2.11)}$$

where C is any positively oriented contour in the complex plane that encircles the spectrum of h. An identical formula holds for h_0 and $r_0(z)$. The spectrum of h is restricted to the real axis of the z plane consisting of all the positive values and isolated negative values where h has eigenfunctions. The spectrum of h_0 includes the positive real axis. Thus the cluster integral has the form

$$b_2 = -\frac{2^{\frac{3}{2}}}{2!\,\lambda^3}\frac{1}{2\pi i}\oint_C e^{-\beta z}\, Tr\big(r(z) - r_0(z)\big)\, dz \qquad \text{(IV.2.12)}$$

If we let the contour approach the real axis the integrand becomes $2\, Im\, Tr\big(r(E+i0) - r_0(E+i0)\big)$. So the determination of this later quantity becomes equivalent to the solution of cluster integral problem.

The spectral property of two-body time-delay theory is the statement that

$$2\,\mathrm{Im}\,\mathrm{Tr}\left[R(E+i0) - R_0(E+i0)\right] = \hat{\mathrm{tr}}\,q(E) \qquad \text{(IV.2.13)}$$

for positive E. The trace of $q(E)$ is that appropriate for the Hilbert space $q(E)$ acts on, namely $L^2(\hat{p})$. It is easy to show that the left hand side of this equation has the interpretation as the change of state density in the scattering system produced by the interaction $v = h - h_0$. Thus equation 13 tells us that this state density change at energy E equals the total time delay for that same energy. Clearly, establishing the spectral property is equivalent to solving the cluster integral problem. Several proofs of equation 13 exist[32,33] which employ the S-matrix. Here we intend to establish 13 directly without reference to the S-matrix and in such a manner that the analysis is also successful for the few body spectral property. We shall assume only that the hermitian potential v obey condition 4. The demonstration of equation 13 will rest on the scattering theory structure, equations 1-3, and on elementary properties of the trace and the continuity of of the projection operator $P(R)$ in the variable R.

To begin we note the definition of the trace of an operator.[34] Let $\{\phi_i\}_1^\infty$ be any complete orthonormal set. Then a bounded operator A is trace class if and only if the sum

$$\sum_i (\phi_i, |A|\,\phi_i) < \infty \qquad \text{(IV.2.14)}$$

Here $|A|$ is the absolute value operator related to A by $A = (A^\dagger A)^{1/2}$. When A is trace class the trace is defined by

$$Tr\, A = \sum_i (\phi_i , A\, \phi_i) \tag{IV.2.15}$$

The sums in both equations 14 and 15 are independent of the choice of the set $\{\phi_i\}$.

Consider the operator $P(R)$ used in the definition of time delay. This operator is a projection which means

$$P(R) = P^2(R) = P^{+}(R) \tag{IV.2.16}$$

This operator converges strongly to the identity e as $R \rightarrow \infty$. We establish in Appendis A that it is a general feature of any trace class operator A that the trace $Tr\, P(R) A$ is uniformly convergent in R so that it is justified to write

$$Tr A = Tr \lim_{R\to\infty} P(R) A = \lim_{R\to\infty} Tr\, P(R) A \tag{IV.2.17}$$

We shall use the right member of the above equation to calculate the trace of our resolvent difference.

Let us find the trace of the resolvent difference occuring in left hand part of equation 13. Appendix A shows us that when v satisfies condition (IV.2.4) then the operator C defined by

$$C = \mathcal{R}(z) - \mathcal{R}^{+}(z) - \mathcal{R}_0(z) + \mathcal{R}_0^{+}(z) \tag{IV.2.18}$$

is trace class. Thus we may employ equation 17 to calculate the trace of C . In particular we note that $P(R)\left(\mathcal{R}_0(z) - \mathcal{R}_0^{+}(z)\right)$ and $P(R)\left[\mathcal{R}(z) - \mathcal{R}^{+}(z)\right]$ are both trace class for $R < \infty$ and $\Im m\, z > 0$. This fact is also established in Appendix A.

So we may write

$$\mathrm{Tr}\, P(R)\, C = \mathrm{Tr}\, P(R)\left[\Lambda(z) - \Lambda^{\dagger}(z)\right] + \mathrm{Tr}\, P(R)\left[\Lambda_0(z) - \Lambda_0^{\dagger}(z)\right] \tag{IV.2.19}$$

Consider the trace on the right hand side of the above equation, using the Hilbert identity

$$\Lambda(z) - \Lambda^{\dagger}(z) = (z - z^{*})\, \Lambda(z)\, \Lambda^{\dagger}(z) \tag{IV.2.20}$$

we may write this trace (without the factor $z - z^{*}$)

$$\mathrm{Tr}\, P(R)\left[\Lambda(z)\, \Lambda^{\dagger}(z)\right] P(R) = \mathrm{Tr}\, \Lambda^{\dagger}(z)\, P(R)\, \Lambda(z) \tag{IV.2.21}$$

The last form has utilized the cyclical invariance property of the trace and the idempotent property of $P(R)$. Now insert the form of the identity e that appears in the asymptotic completeness statement equation 2

$$\mathrm{Tr}\, \Lambda^{\dagger}(z)\, P(R)\, \Lambda(z) = \mathrm{Tr}\left[U^{(-)} U^{(-)\dagger} + P_b\right] \Lambda^{\dagger}(z)\, P(R)\, \Lambda(z) \tag{IV.2.22}$$

$$\mathrm{Tr}\, U^{(-)} U^{(-)\dagger} \Lambda(z)\, P(R)\, \Lambda(z) = \mathrm{Tr}\, \Lambda_0^{\dagger}(z)\, U^{(-)} P(R)\, U^{(-)} \Lambda_0(z) \tag{IV.2.23}$$

Equation 23 relies on the intertwining feature of $U^{(-)}$. The remaining term containing the projection operator P_b can be explicitly computed. The general form of this bound state projection operator is

$$P_b = \sum_{i=1}^{N_2} \psi_i \otimes \psi_i^{*} \tag{IV.2.24}$$

where $\{\psi_i\}$ are the N_2 bound-state eigenfunctions of h with eigenvalue $-\chi_i^2$, viz.

$$h\, \psi_i = -\chi_i^2\, \psi_i \,, \quad i = 1, 2, \ldots, N_2 \tag{IV.2.25}$$

Consequently,

$$\mathrm{Tr}\; P_b\, \mathcal{R}^{\dagger}(z)\, P(R)\, \mathcal{R}(z) \;=\; \sum_{i=1}^{N_\lambda} \frac{(\Psi_i\,,\, P(R)\,\Psi_i)}{|\chi_i^2 + z|^2} \tag{IV.2.26}$$

Collecting the results of equations 18, 19,23and 26 leads us to

$$2i\, \mathrm{Im}\, \mathrm{Tr}\left(\mathcal{R}(z) - \mathcal{R}_0(z)\right) = 2i\, \mathrm{Im}\, z \sum_{i=1}^{N_\lambda} \left(|\chi_i^2 + z|^2\right)^{-1}$$
$$+ \lim_{R\to\infty} \mathrm{Tr}\; 2i\,\mathrm{Im}\,z\; |\mathcal{R}_0(z)|^2 \left[U^{(-)\dagger} P(R)\, U^{(-)} - P(R)\right] \tag{IV.2.27}$$

where $|\mathcal{R}_0(z)|^2 = \mathcal{R}_0^{\dagger}(z)\mathcal{R}_0(z)$.

The diagonal integral form for the trace may now be introduced. This form of the trace is allowed since the two operators in the right member of equation 27 are both of the form $A^{\dagger}A$ where A is a Schmidt operator (see equation A.4 of the Appendix). Specifically A is either $P(R)\mathcal{R}_0(z)$ or $P(R)U^{(-)}\mathcal{R}_0(z)$. As discussed in the Appendix it is easy to show the first of this operators is Schmidt-class. That the second shares this property is the consequence of $P(R)\,U^{(-)}\mathcal{R}_0(z) = P(R)\mathcal{R}(z)\,U^{(-)}$. Again $P(R)\,\mathcal{R}(z)$ is Schmidt-class and the isometry $U^{(-)}$ is by definition a bounded operator. Thus (cf. property iv in Appendix) we have that $P(R)\,U^{(-)}\mathcal{R}_0(z)$ is Schmidt-class. So for the last term on the right of equation 27 we may write

$$\lim_{R\to\infty} \int_0^{\infty} \frac{2i\eta}{(\xi - \vec{p}'^2/2\mu)^2 + \eta^2} \langle \vec{p}'\,|\, U^{(-)\dagger} P(R)\, U^{(-)} - P(R)\,|\,\vec{p}'\rangle\, d\vec{p}'$$

$$= \lim_{R\to\infty} \int_0^{\infty} \frac{2i\eta}{(\xi - E')^2 + \eta^2}\; \frac{1}{2\pi}\, \hat{\mathrm{tr}}\, q(E', R)\, dE \tag{IV.2.28}$$

Here we have set $z = \xi + i\eta$. A change of variables with $E' = \vec{p}'^2/2\mu$ and the use of representation (IV.2.9) for the time delay operator in sphere R gives 28. The definition of in equation 10 permits us to express equation 27 in the form

$$2i\, \mathrm{Im}\, \mathrm{Tr}\left[r(E+i\eta) - r_0(E+i\eta) \right]$$
$$= \sum_{i=1}^{N_2} \frac{2i\eta}{|\chi_i^2 + E + i\eta|^2} + \int_0^\infty \frac{2i\eta}{(E-E')^2+\eta^2} \frac{1}{2\pi} \hat{t}\, q(E')\, dE' \qquad \text{(IV.2.29)}$$

The last step is to take the limit $\eta \to 0$. In this case the first term on the right hand side vanishes for $E \geq 0$ and the η dependent part of the E' integrand becomes a delta function giving us equation 13. This completes the demonstration of the spectral property.

As claimed we have proved the spectral property without reference to the S-matrix. The derivation above only employs the fundamental scattering theory structure, equation 1-3 and the definition of time delay stated in equations 7-10. The spectral property is seen to require neither angular momentum conservation nor time reversal invariance for its validity. Now that equation 13 is established we may combine it with expression 12 to give us the time-delay form of the second cluster integral

$$b_2 = \frac{2^{\frac{3}{2}}}{2!\,\lambda^3} \left\{ \sum_{i=1}^{N_2} e^{\beta \chi_i^2} + \frac{1}{2\pi} \int_0^\infty e^{-\beta E} \hat{t}\, q(E)\, dE \right\} \qquad \text{(IV.2.30)}$$

This formula manisfestly tells us that the scattering contribution to the second virial coefficient is entirely dependent on the timedelay. All other independent information about the two particle collision process does not affect b_2.

The above formula also provides us with a precise understanding of the physics of the virial representation of the equation of state. Following an argument of Bar-Gadda, we write the virial equation of state (neglecting the boundstate terms for the moment)

$$PV = NkT\left\{1 - \left(\frac{\sqrt{2}}{2\pi}\int_0^\infty e^{-\beta E}\,\hat{tr}\,q(E)\,dE\right)\lambda^3\rho + \cdots\right\} \qquad \text{(IV.2.31)}$$

Assume that V and T are held fixed. Equation 31 tells us if $\hat{tr}\,q(E) > 0$ then the pressure is decreased relative to the ideal gas law. This makes good physical sense since $\hat{tr}\,q(E) > 0$ describes the situation where the two particles scattering at energy E may stay together longer than could free particles of the same incident energy. Thus the interaction is effectively creating extra space for the particles to exist in relation to free-particle dynamics. Stated another way, we can say that an increase in time delay will result in a decreased flux of particles striking the container wall, thus decreasing the pressure. This interpretation is valid independent of whether the underlying dynamics are classical or quantum mechanics. In fact, by studying time delay in a classical collision Bar-Gadda[35)] was able to find the classical approximation to equation 30.

Consider now the role of the S-matrix in this problem. It is well know[25,26,29,30)] that $q(E)$ may be expressed in terms of the on-shell S-matrix $\mathcal{S}(E)$. The energy dependent operators $\mathcal{S}(E)$ act on the same $L^2(\hat{p})$ Hilbert space as $q(E)$ and are defined by

$$\langle \vec{p}'|S|\vec{p}\rangle = \frac{\delta(E-E')}{\mu p}\,\langle \hat{p}'|\mathcal{S}(E)|\hat{p}\rangle \qquad \text{(IV.2.32)}$$

where $$\mathcal{S} = U^{(+)^{+}} U^{(-)} \tag{IV.2.33}$$

Capital $\mathcal{S}$ is the standard energy independent S-matrix. Equation 32 defines in terms of $\mathcal{S}$ the kernels $\langle \hat{p}' | \mathcal{A}(E) | \hat{p} \rangle$. This in turn defines the operators $\mathcal{A}(E)$. The S-matrix expression for $q(E)$ is

$$q(E) = -i\, \mathcal{A}^{+}(E) \frac{d}{dE} \mathcal{A}(E) \tag{IV.2.34}$$

We can, at this point, insert representation (IV.2.34) into form (IV.2.30) for the second cluster integral and obtain an expression which employs the on-shell S-matrix. This form of the cluster integral representation is the one sought by Dashen and collaborators.[17] There the point of view is taken that the S-matrix contains all of the physically available information about the collision process, and consequently the second and higher virial coefficients must have representations containing only the S-matrix. The time delay solution is, of course, consistent with this requirement. However, this time delay solution has the added advantage of explaining the physical mechanism of how the non-ideal gas law behavior occurs. From the point of view of convenience we concede that at the present time the easiest way to compute is to use the S-matrix form. In fact if we impose rotational invariance on the interaction V then $\mathcal{A}(E)$ acquires the familiar partial-wave form,

$$\langle \hat{p}' | \mathcal{A}(E) | \hat{p} \rangle = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi}\, e^{2i\delta_\ell(E)}\, P_\ell(\hat{p}'\cdot\hat{p}) \tag{IV.2.35}$$

where $\delta_\ell(E)$ is the ℓ^{th} partial wave phase shift. This then implies that

$$\hat{\mathrm{tr}}\, q(E) = 2 \sum_{\ell=0}^{\infty} (2\ell+1) \frac{d}{dE} \delta_\ell(E) \qquad \text{(IV.2.36)}$$

The phase-shift representation of $\hat{\mathrm{tr}}\, q(E)$ may be inserted in equation 30. This gives us the Beth-Uhlenbeck[13] solution,

$$b_2 = \frac{\sqrt{2}}{\lambda^3} \left\{ \sum_{i=1}^{N_2} e^{\beta \chi_i^2} + \frac{1}{\pi} \int_0^{\infty} e^{-\beta E} \sum_\ell (2\ell+1) \frac{d\delta_\ell(E)}{dE}\, dE \right\} \qquad \text{(IV.2.37)}$$

One feature of our solution equation 30 is that it remains defined even when angular momentum is not conserved and the phase shift is indefined. This later feature becomes important in the third cluster integral where for three-body breakup amplitudes no phase shift representation is known to exist.

IV.3. Third cluster integral

The aim of this section is to explicitly evaluate the third cluster integral in terms of the three-body time delay. The central result and idea of the previous section that the two-body time delay controls the second virial coefficient entirely is of limited use in statistical mechanics unless this idea has a valid extension for all the higher virial coefficients. The difficulties in finding a solution for the third and higher cluster integral are substantially larger than for the two-particle case because the problem of the few-particle collision has a richer physical structure. In particular, the full multi-channel structure of composite scattering processes is now present. We have pickup, rearrangement, breakup and elastic scatterings. New technical features also arise such as disconnected processes, off-shell T-matrix and the rescattering singularity. A valid analysis must acknowledge and cope with all these features.

The solution we give here parallels that presented in section IV.2. The central device is the statement and proof of the three-body spectral property. As in the two-body case we define here a three-body time delay valid for multichannel scattering. In a broad sense the trace of this time delay equals the change of state density produced by all the non-asymptotic interactions. We shall presume that each two-body interaction is such that it produces only one bound state. This assumption is trivial to relax but affords us considerable notational simplification.

The first preliminary is to recount those features of time dependent three-body scattering theory that our proof utilizes. By in large our notation, except formomenta, exactly follows Faddeev[1]. We shall use Jacobi variables $\vec{x}_\alpha$, $\vec{y}_\alpha$ to describe the spatial coordinates of the three-particle system. These six degrees of freedom completely specify the orientation of the three particles relative to the three body center of mass position. The variable $\vec{x}_\alpha$ is the vector separation of particle α from the center of mass of the (β , γ) cluster. The remaining independent coordinate 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 $\vec{p}_\alpha$ specifies the relative motion of particle α and cluster α. Let m_α be the masses of our three particles, then $n_\alpha = m_\alpha(m_\beta+m_\gamma)/(m_1+m_2+m_3)$ represents the reduced mass of particle α and cluster α. Thus the kinetic energy of this relative motion is $p_\alpha^2/2n_\alpha$. The internal momentum of the fragments of cluster α is just $\vec{q}_\alpha$. Cluster α has reduced mass $\mu_\alpha = m_\beta m_\gamma / m_\beta + m_\gamma$ and a kinetic energy given by $q_\alpha^2/2\mu_\alpha$. With this notation the free three particle kinetic energy Hamiltonian is

$$H_0 = \frac{p_\alpha^2}{2n_\alpha} + \frac{q_\alpha^2}{2\mu_\alpha} = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{p_3^2}{2m_3} \qquad \text{(IV.3.1)}$$

Clearly H_0 is an invariant independent of which of the three Jacobi systems we choose to express it in. Associated with H_0 is a coordinate space metric invariant ρ_0 given by

$$\rho_0^2 = \frac{1}{2m_0}\left(2n_\alpha x_\alpha^2 + 2\mu_\alpha y_\alpha^2\right) = \frac{1}{2m_0}\left(2m_1 r_1^2 + 2m_2 r_2^2 + 2m_3 r_3^2\right) \qquad \text{(IV.3.2)}$$

where $\vec{r}_1$, $\vec{r}_2$ and $\vec{r}_3$ are the individual position vectors of particles 1, 2 and 3 in the center of mass system, and $m_0 = (m_1 m_2 m_3 / m_1 + m_2 + m_3)^{\frac{1}{2}}$.

The motion of the three particle state is governed by the various Hamiltonians the admits. Let V_α represent the potential acting between particles β and γ. So, in coordinate space we have

$$V_\alpha(\vec{x}_\alpha, \vec{y}_\alpha) = v_\alpha(\vec{y}_\alpha) \qquad \text{(IV.3.3)}$$

Thus we may define the Hamiltonians

$$H_\alpha = H_0 + V_\alpha \quad , \alpha = 1, 2, 3. \qquad \text{(IV.3.4)}$$

$$H = H_0 + \sum_{\alpha=1}^{3} V_\alpha \qquad \text{(IV.3.5)}$$

We denote by $\mathcal{H}$ the space of square integrable functions over the six coordinate degrees of freedom - either $\vec{p}_\alpha$, $\vec{q}_\alpha$ or $\vec{x}_\alpha$, $\vec{y}_\alpha$. The identity on $\mathcal{H}$ will be E . The L^2 space over $\vec{x}_\alpha$ we denote by $\mathcal{H}_\alpha$. Its associated identity is given by E_α . Likewise the L^2 space over $\vec{y}_\alpha$ is indicated by h_α and its identity by e_α . So in this notation $E = e_\alpha \otimes E_\alpha$, $\alpha = 1, 2, 3$.

Contained within the three particle problem are three distinct two particle problems. We have stated above that each two body interaction is capable of supporting only one bound state. We shall represent this state as $\psi_\alpha(\vec{q}_\alpha)$. It is the eigenfunction that satisfies

$$(q_\alpha^2/2\mu_\alpha + v_\alpha)\ \psi_\alpha = -\chi_\alpha^2\ \psi_\alpha\ , \quad \alpha = 1, 2, 3. \qquad \text{(IV.3.6)}$$

where ψ_α is unit normalized in h_α . Free channel motion is characterized by a function like $f_\alpha(\vec{p}_\alpha)\psi_\alpha(\vec{q}_\alpha)$. Since ψ_α is known, the non-trival wave packet information is given by $f_\alpha \in \mathcal{H}_\alpha$. The total energy available for asymptotic motion in channel α is determined by H_α . Related to H_α is $\widetilde{H}_\alpha$.

$$H_\alpha\ f_\alpha(\vec{p}_\alpha)\,\psi_\alpha(\vec{q}_\alpha) = \psi_\alpha(\vec{q}_\alpha)\,\widetilde{H}_\alpha\ f_\alpha \ , \quad \alpha > 0 \qquad \text{(IV.3.7)}$$

This equation defines a channel Hamiltonian acting on the space $\mathcal{H}_\alpha$ given by

$$\widetilde{H}_\alpha = (p_\alpha^2/2n_\alpha - \chi_\alpha^2)\ , \quad \widetilde{H}_0 = H_0 \qquad \text{(IV.3.8)}$$

Frequently one must extract from a function in $\mathcal{H}$ its channel component in $\mathcal{H}_\alpha$. This is accomplished by the operator I_α

$$f_\alpha = I_\alpha f \ ; \ f \in \mathcal{H}\ , \ f_\alpha \in \mathcal{H}_\alpha\ , \quad \alpha > 0$$

$$f_\alpha(\vec{p}_\alpha) = \int \psi_\alpha^*(\vec{q}_\alpha)\, f\,(\vec{p}_\alpha, \vec{q}_\alpha)\, d\vec{q}_\alpha \qquad \text{(IV.3.9)}$$

The adjoint of I_α is clearly an injection operator specified by

$$I_\alpha^\dagger f_\alpha = \psi_\alpha^* \otimes f_\alpha \quad \varepsilon\ \mathcal{H} \quad . \tag{IV.3.10}$$

The exact scattering solutions for this system are obtained from knowledge of the multichannel Moeller operators defined by

$$\tilde{U}_\alpha^{(\pm)} = \lim_{t \to \pm\infty} e^{iHt} e^{-iH_\alpha t} P_\alpha \tag{IV.3.11}$$

$$\tilde{U}_0^{(\pm)} = \lim_{t \to \pm\infty} e^{iHt} e^{-iH_0 t} \tag{IV.3.12}$$

where $P_\alpha = I_\alpha^\dagger I_\alpha$. The operator P_α is a projection operator on $\mathcal{H}$ associated with the subspace of α channel motion and has a kernel representation given by

$$\langle \vec{p}_\alpha \vec{q}_\alpha | P_\alpha | \vec{p}_\alpha' \vec{q}_\alpha' \rangle = \psi_\alpha(\vec{q}_\alpha)\, \psi_\alpha^*(\vec{q}_\alpha')\, \delta(\vec{p}_\alpha - \vec{p}_\alpha') \tag{IV.3.13}$$

Faddeev's analysis expresses $\tilde{U}_0^{(\pm)}$, $\tilde{U}_\alpha^{(\pm)}$ in terms of a closely related set $U_0^{(\pm)}$, $U_\alpha^{(\pm)}$ which may in turn be uniquely constructed from the time independent Fredholm integral equation that Faddeev discovered. Basically the place wave matrix elements $\langle \vec{p}\vec{q} | U_0^{(\pm)} | \vec{p}'\vec{q}' \rangle$ and $\langle \vec{p}\vec{q} | U_\alpha^{(\pm)} | \vec{p}'\vec{q}' \rangle$ are the exact wave function solutions to the Schroedinger equations with the (−) indicating the outgoing solution, (+) indicating the incoming solution. Thus

$$\tilde{U}_0^{(\pm)} = U_0^{(\pm)} \quad , \quad \tilde{U}_\alpha^{(\pm)} = U_\alpha^{(\pm)} I_\alpha \quad , \quad \alpha > 0. \tag{IV.3.14}$$

These Moeller operators obey the fundamental equations

(i)
$$U_\alpha^{(\pm)\dagger} U_\beta^{(\pm)} = \delta_{\alpha\beta} E_\beta \quad : \quad \mathcal{H}_\beta \to \mathcal{H}_\alpha \tag{IV.3.15}$$

$$\tilde{U}_\alpha^{(\pm)\dagger} \tilde{U}_\beta^{(\pm)} = \delta_{\alpha\beta} P_\beta \quad : \quad \mathcal{H} \to \mathcal{H} \tag{IV.3.15'}$$

(ii) $$\sum_{\alpha=0}^{3} U_\alpha^{(\pm)} U_\alpha^{(\pm)\dagger} + B_0 = E \qquad \text{(IV.3.16)}$$

$$\sum_{\alpha=0}^{3} \tilde{U}_\alpha^{(\pm)} \tilde{U}_\alpha^{(\pm)\dagger} + B_0 = E \qquad \text{(IV.3.16')}$$

(iii) $$H\, U_\alpha^{(\pm)} = U_\alpha^{(\pm)} \tilde{H}_\alpha \;:\; \mathcal{H}_\alpha \to \mathcal{H} \qquad \text{(IV.3.17)}$$

$$H\, \tilde{U}_\alpha^{(\pm)} = \tilde{U}_\alpha^{(\pm)} H_\alpha \;:\; \mathcal{H} \to \mathcal{H} \qquad \text{(IV.3.17')}$$

The two versions of these results depend on whether we use $\tilde{U}_\alpha^{(\pm)}$ or $U_\alpha^{(\pm)}$. The definition in equation 14 lets one obtain the primed version from the unprimed version of these equations. We shall use both forms in our derivation. The operator B_0 denotes the projection onto the bound state subspace of $\mathcal{H}$ spanned by the N_3 eigenfunctions Ψ_i of $\mathcal{H}$, i.e.

$$H\, \Psi_i = -\chi_i^2\, \Psi_i \;, \quad i = 1, 2, \ldots N_3 \qquad \text{(IV.3.18)}$$

$$B_0 = \sum_{i=1}^{N_3} \Psi_i \otimes \overline{\Psi}_i \qquad \text{(IV.3.19)}$$

Of course statement (i) is channel orthogonality; (ii) is asymptotic completeness; (iii) is the intertwining property.

The results above reflect the contemporary two Hilbert space treatment of the multi-channel scattering problem. In this treatment the structure above has a generalization for the N-particle scattering problem.[36)] In the three body case, these equations were first given a proof by Faddeev[1)] under some what different assumptions than condition (IV.2.4). Recently, Thomas[37)] has provided new proofs valid when the potential does obey (IV.2.4).

To the scattering theory given above, we must add the description of the three body system which evolves exclusively by H_α. Such a system is really a two body system with a third particle that is a non-interacting spectator. Thus we must restate the content of equations (IV.2.1-3), but now set in the space of $\mathcal{H}$. To do this, define

$$W_\alpha^{(\pm)} = e_\alpha \otimes U^{(\pm)}(\alpha) \tag{IV.3.20}$$

and

$$\mathcal{B}_\alpha = e_\alpha \otimes P_b(\alpha) \tag{IV.3.21}$$

$$P_b(\alpha) = \Psi_\alpha \otimes \overline{\Psi}_\alpha \tag{IV.3.22}$$

The projection operator $\mathcal{B}_\alpha$ is the sub-space in $\mathcal{H}$ spanned by all moving bound clusters Ψ_α. We have three of these systems $\alpha = 1, 2, 3$ and each satisfies

(i) $$W_\alpha^{(\pm)\dagger} W_\alpha^{(\pm)} = E \tag{IV.3.23}$$

(ii) $$W_\alpha^{(\pm)} W_\alpha^{(\pm)\dagger} = E - \mathcal{B}_\alpha \tag{IV.3.24}$$

(iii) $$H_\alpha W_\alpha^{(\pm)} = W_\alpha^{(\pm)} H_0 \tag{IV.3.25}$$

We now have in place the necessary scattering theory to solve our problem. Our first task is to define the multi-channel time delay valid in a three body collision. Consider any of the channels with a stable cluster as a target, i.e. $\alpha > 0$. The incident state is completely determined by a wave packet $f_\alpha \in \mathcal{H}_\alpha$. The time dependent non-interacting asymptotic state is

$$\Phi_\alpha(t) = e^{-iH_\alpha t} I_\alpha^\dagger f_\alpha = I_\alpha^\dagger e^{-i\widehat{H}_\alpha t} f_\alpha \tag{IV.3.26}$$

Associated with this "freely" evolving state is an exact state

$\Psi_\alpha(t)$ evolving by the full Hamiltonian H. This exact wave packet is defined by the boundary condition

$$\lim_{t\to-\infty} \| \Psi_\alpha(t) - \Phi_\alpha(t) \| = 0 \tag{IV.3.27}$$

and given in terms of the Moeller operator by

$$\Psi_\alpha(t) = e^{-iHt} U_\alpha^{(-)} f_\alpha = U_\alpha^{(-)} e^{-i\tilde{H}_\alpha t} f_\alpha \tag{IV.3.28}$$

The intertwining property is used to obtain the last form on the right from the previous member.

As in the two body case, we need a sphere that will define quantum transit times. This sphere is centered about the total three body center of mass coordinate. We denote the projection operator in $\mathcal{H}$ associated with this sphere by $\mathcal{P}(\rho)$, viz.

$$\begin{aligned} \mathcal{P}(\rho)\, f(\vec{x},\vec{y}) &= f(\vec{x},\vec{y}) \quad \text{if } \rho_0 < \rho \\ &= 0 \quad \text{otherwise.} \end{aligned} \tag{IV.3.29}$$

where ρ_0 is that given in equation 2. The integrals

$$\int_{-\infty}^{\infty} (\Phi_\alpha(t), \mathcal{P}(\rho)\, \Phi_\alpha(t))\, dt \tag{IV.3.30}$$

$$\int_{-\infty}^{\infty} (\Psi_\alpha(t), \mathcal{P}(\rho)\, \Psi_\alpha(t))\, dt \tag{IV.3.31}$$

are the "free" and exact transit times for the state specified by f_α. This difference in transit times we shall denote as $(f_\alpha, Q_{\alpha\alpha}(\rho) f_\alpha)$. By employing equation 15 - 17, an hermitian operator form of $Q_{\alpha\alpha}$ is given by the expression,

$$(f_\alpha, Q_{\alpha\alpha}(\rho) f_\alpha) = \int_{-\infty}^{\infty} (f_\alpha, e^{-i\tilde{H}_\alpha t} [U_\alpha^{(-)\dagger} \mathcal{P}(\rho) U_\alpha^{(-)} - \mathcal{P}_\alpha(\rho)] e^{-i\tilde{H}_\alpha t} f_\alpha)\, dt \tag{IV.3.32}$$

In this integrand $\mathcal{P}_\alpha(\rho)$ is now a new operator given by

$$\mathcal{P}_\alpha(\rho) = I_\alpha \mathcal{P}(\rho) I_\alpha^\dagger \quad : \quad \mathcal{H}_\alpha \to \mathcal{H}_\alpha \tag{IV.3.33}$$

This is obviously a restriction of $\mathcal{P}(\rho)$ to the single channel space $\mathcal{H}_\alpha$. In $\mathcal{H}_\alpha$, $\mathcal{P}_\alpha(\rho)$ is a multiplication operator given by

$$\mathcal{P}_\alpha(\rho, \vec{x}_\alpha) = \int |\Psi_\alpha(\vec{y}_\alpha)|^2 \, \Theta(\rho - \rho_0(\vec{x}_\alpha, \vec{y}_\alpha)) \, d\vec{y}_\alpha \tag{IV.3.34}$$

where Θ is the theta function and Ψ_α is given in equation 6.

Carrying out the time integration leads us to the time independent form of our defifition. We have

$$(f_\alpha, Q_{\alpha\alpha}(\rho) f_\alpha) = \int f_\alpha^*(\vec{p}_\alpha') \frac{\delta(E'-E)}{n_\alpha p_\alpha} \langle \hat{p}_\alpha' | q_{\alpha\alpha}(E,\rho) | \hat{p}_\alpha \rangle f_\alpha(\vec{p}_\alpha) \, d\vec{p}_\alpha \, d\vec{p}_\alpha' \tag{IV.3.35}$$

Here the energy arguments of the delta function E' and E are $\frac{p_\alpha'^2}{2n_\alpha} - \chi_\alpha^2$ and $\frac{p_\alpha^2}{2n_\alpha} - \chi_\alpha^2$ respectively. The kernel in the integrand of equation 35 defines a reduced operator acting on $L^2(\hat{p})$ by the expression,

$$\langle \hat{p}_\alpha' | q_{\alpha\alpha}(E,\rho) | \hat{p}_\alpha \rangle = 2\pi n_\alpha p_\alpha \langle \vec{p}_\alpha' | U_\alpha^{(-)\dagger} \mathcal{P}(\rho) U_\alpha^{(-)} - \mathcal{P}_\alpha(\rho) | \vec{p}_\alpha \rangle \tag{IV.3.36}$$

The momenta appearing in the right of the above equation are restricted to be the on-shell momenta specified by energy E. One obtains from equation 35 and 36 a time delay independent of the sphere by taking the limit $\rho \to \infty$ in equation 35. This process defines $q_{\alpha\alpha}(E)$, viz.

$$\lim_{\rho\to\infty} (f_\alpha, Q_{\alpha\alpha}(\rho) f_\alpha)$$
$$= \int f_\alpha^*(\vec{p}_\alpha') \frac{\delta(E-E')}{n_\alpha p_\alpha} \langle \hat{p}_\alpha' | q_{\alpha\alpha}(E) | \hat{p}_\alpha \rangle f_\alpha(\vec{p}_\alpha) \, d\vec{p}_\alpha \, d\vec{p}_\alpha' \tag{IV.3.37}$$

For the most part, our derivations will employ only this definition of multichannel time delay. Extended discussion of the properties and physics of this concept may be found in references [12] and [38].

There remains one case of time delay we have not discussed. This case is three to three scattering. Here both the initial and final state are composed of three asymptotically free particles. The initial wave packet can be any function $f_0 \varepsilon \mathcal{H}_0 = L^2(\vec{p},\vec{q})$. The freely evolving state is

$$\Phi_0(t) = e^{-iH_0t} f_0 \qquad \text{(IV.3.38)}$$

We shall indicate by $\Psi_0(t)$ the exact state. It is determined by the boundary condition (IV.3.27) with $\alpha = 0$. The resulting form for $\Psi_0(t)$ in terms of the Moeller operator $U_0^{(-)}$ is

$$\Psi_0(t) = e^{-iHt} U_0^{(-)} f_0 \qquad \text{(IV.3.39)}$$

The physics of the definition and content of the current case is not entirely analogous to the cases with $\alpha > 0$. Here, for example, in $\mathcal{H}_0$ there exist f_0 that are wave packets describing a remote spectator particle that remains unaltered as the remaining two particles collide. This is not a true three-particle collision. By way of contrast for $\alpha > 0$ all the collisions possible for any $f_\alpha \varepsilon \mathcal{H}_\alpha$ involve the collision of all three particles. Thus our definition of three to three time delay must remove the effects of these spurious two-particle collisions that sit in the three particle Hilbert space. This is easy to accomplish. From the difference

$$\int_{-\infty}^{\infty} \Big[\big(\Psi_0(t), \mathcal{P}(\rho)\, \Psi_0(t) \big) - \big(\Phi_0(t), \mathcal{P}(\rho)\, \Phi_0(t) \big) \Big]\, dt \qquad \text{(IV.3.40)}$$

we must subtract the difference

$$\sum_{\alpha>0}\int_{-\infty}^{\infty}\left[\left(\Psi_0^\alpha(t),\mathcal{P}(\rho)\Psi_0^\alpha(t)\right)-\left(\Phi_0(t),\mathcal{P}(\rho)\Phi_0(t)\right)\right]dt \tag{IV.3.41}$$

where $\Psi_0^\alpha(t)$ is defined by

$$\lim_{t\to-\infty}\|\Psi_0^\alpha(t)-\Phi_0(t)\| = 0 \tag{IV.3.42}$$

Clearly $\Psi_0^\alpha(t)$ is the exact solution that evolves according to H_α, from $\Phi_0(t)$. So

$$\Psi_0^\alpha(t) = e^{-iH_\alpha t}\,W_\alpha^{(-)}f_0 \tag{IV.3.43}$$

and $W_\alpha^{(-)}$ is the Moeller operator given in equation 20. Combined, expressions 40 and 41, provide us with a connected three to three time delay.

$$(f_0,Q_{00}(\rho)f_0) = \int_{-\infty}^{\infty}\Big(f_0,\,e^{iH_0t}\Big\{\left[U_0^{(-)\dagger}\mathcal{P}(\rho)U_0^{(-)}-\mathcal{P}(\rho)\right] - \sum_{\alpha>0}\left[W_\alpha^{(-)\dagger}\mathcal{P}(\rho)W_\alpha^{(-)}-\mathcal{P}(\rho)\right]\Big\}e^{-iH_0t}f_0\Big) \tag{IV.3.44}$$

As in the $\alpha>0$ situation we carry out the time integration. This introduces the delta function in energy in the integral representation of $Q_{00}(\rho)$. Thus we define an energy dependent reduced operator $q_{00}(E,\rho)$ given by

$$\langle\hat{p}_0'|q_{00}(E,\rho)|\hat{p}_0\rangle = 2\pi m_0 p_0^4\,\langle\vec{p}_0'|\left[U_0^{(-)\dagger}\mathcal{P}(\rho)U_0^{(-)}-\mathcal{P}(\rho)\right] - \sum_{\alpha>0}\left[W_\alpha^{(-)\dagger}\mathcal{P}(\rho)W_\alpha^{(-)}-\mathcal{P}(\rho)\right]|\vec{p}_0\rangle \tag{IV.3.45}$$

The momentum representation used here is appropriate to the six dimensional space $L^2(\vec{p}_\alpha,\vec{q}_\alpha)$. In detail one defines

$$\frac{p_0^2}{2m_0} = \frac{p_\alpha^2}{2n_\alpha}+\frac{q_\alpha^2}{2\mu_\alpha} \tag{IV.3.46}$$

The vector $\vec{p}_0$ specifies the six dimensional point $(\vec{p}_\alpha,\vec{q}_\alpha)$

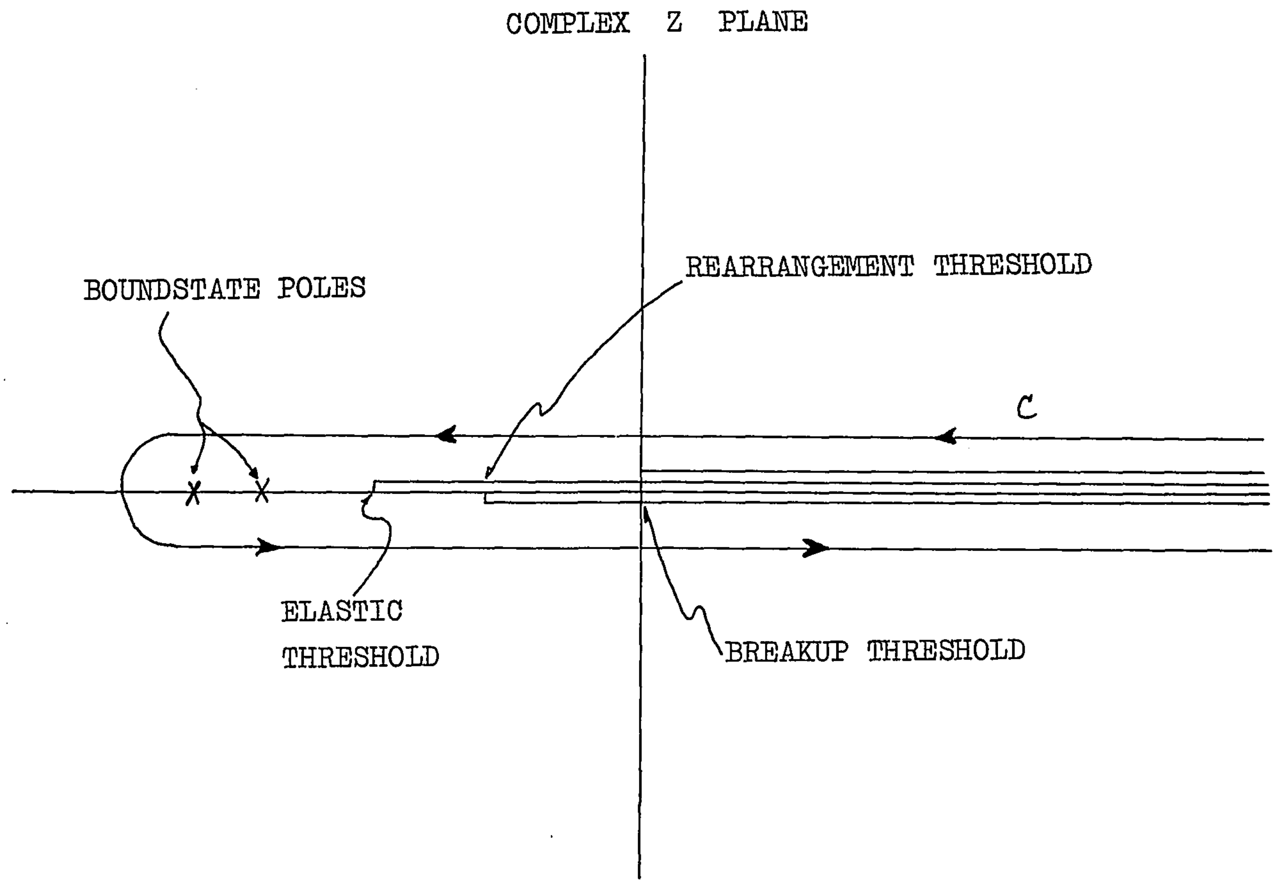


Figure IV.1 The Spectrum of $R(z)$, and the Contour $\mathcal{C}$.

and (ρ_o , $\hat{P}_o$) is the spherical coordinate description of $\vec{P}_o$ where $\hat{P}_o$ is the six dimensional unit vector in the direction of $\vec{P}_o$. The energy dependence enters the right hand side of equation 43 by the on-shell requirement that $E = \frac{P_o^2}{2m_o} = \frac{P_o'^2}{2m_o}$. Finally a time delay that is independent of ρ is given by

$$\lim_{\rho \to \infty} (f_o, Q_{oo} f_o) = \int f_o^*(\vec{p}_o') \frac{\delta(E'-E)}{m_o p_o^4} \langle \hat{p}_o' | q_{oo}(E) | \hat{p}_o \rangle f_o(\vec{p}_o) \, d\vec{p}_o \, d\vec{p}_o' \tag{IV.3.47}$$

With equation 47 we have completed the account of the scattering theory structures and the time delay formula that the ensuing derivation requires.

We turn our attention at this point to the evaluation of the third cluster integral. We must compute the trace appearing in equation (IV.1.5). The first step is to use the Watson[31)] transform for the statistical operator $e^{-\beta H}$. For an appropriate contour this transform is

$$e^{-\beta H} = \frac{i}{2\pi} \oint_C e^{-\beta z} R(z) \, dz \tag{IV.3.48}$$

The suitable contour C is illustrated in Figure IV-1. It encircles the entire spectrum of H . With this same contour equation 46 remains valid when the pair of operators H , $R(z)$ are replaced by the pairs H_α , $R_\alpha(z)$ and H_o , $R_o(z)$. Here the three body resolvents are defined by $R(z) = (H - z)^{-1}$, $R_\alpha(z) = (H_\alpha - z)^{-1}$ and $R_o(z) = (H_o - z)^{-1}$. The problem of finding b_3 is by equation 48 and its companions turned into evaluating,

$$b_3 = \frac{3^{\frac{3}{2}}}{3!\,\lambda^3} \frac{i}{2\pi} \oint_C e^{-\beta z} \, Tr \, R_c(z) \, dz \tag{IV.3.49}$$

where $R_c(z)$ denotes the connected resolvent structure

$$R_c(z) = R(z) - R_0(z) - \sum_{\alpha=1}^{3} \left(R_\alpha(z) - R_0(z) \right) \tag{IV.3.50}$$

Since the contour C is symmetric about the real axis and $R_c(z^*) = R_c^+(z)$ we must know

$$2i \, \mathrm{Im} \, \mathrm{Tr} \, R_c(z) = \mathrm{Tr} \left(R_c(z) - R_c^+(z) \right) \tag{IV.3.51}$$

as $\mathrm{Im}\, z \to 0$. The three body version of the spectral property of time delay provides us with the identity

$$2 \, \mathrm{Im} \, \mathrm{Tr} \, R_c(E + i0) = \sum_{\alpha=0}^{3} \hat{\mathrm{tr}}_\alpha \, q_{\alpha\alpha}(E) \tag{IV.3.52}$$

The four traces on the right of this formula are those appropriate for the Hilbert spaces that the time-delay operators act on. For all α, $\hat{\mathrm{tr}}_\alpha$ is the trace on $L^2(\hat{p}_\alpha)$. Thus for $\alpha=0$, $\hat{\mathrm{tr}}_0$ acts on a five dimensional space. For $\alpha>0$, it acts on a two dimensional space. The physical content of this equation is analogous to that in the two body case. The left side is the generalized change of state density at energy E produced by the interactions V_α. The right hand side is the sum over the total time delay at energy E of each possible asymptotic channel. Clearly, knowing equation 52 effects the solution of the third cluster integral.

The three body spectral property not only provides us with a solution of the third cluster integral b_3 but has the virtue that each side of the equality in equation 52 has its own distinct physical interpretation. As briefly alluded to in the outset of this section the term $\mathrm{Im}\, \mathrm{Tr}\, R_c(\xi + i0)$ is proportional to the change of state density at energy ξ effected by the scattering - which is here of a composite multichannel character. We pause to give a brief demonstration of this important fact. Suppose $E(\xi)$ is the family of spectral projection operators related to H acting on $\mathcal{H}$. Then $E(\xi)$ is the projection onto all states of the three body system with energy less than ξ. The spectral representation of H is

$$H = \int \xi \, dE(\xi) \tag{IV.3.53}$$

In this notation the associated resolvent $R(z)$ has the form,

$$R(z) = \int \frac{1}{\xi - z} \, dE(\xi) \tag{IV.3.54}$$

If $E_\alpha(\xi)$ is the spectral family generated by H_α then it is obvious that equations 53 and 54 are fulfilled by each of the sets $\left\{ H_\alpha , R_\alpha(z) , E_\alpha(\xi) \right\}$.

For the purposes of this discussion let Q be the projection onto an arbitrary finite demensional subspace of $\mathcal{H}$. We note that $\mathrm{Tr}\, Q E(\xi)$ is the number of eigenstates (discrete and continuous) of energy less than ξ in the subspace $Q\mathcal{H}$. Likewise $\mathrm{Tr}\, Q E_\alpha(\xi)$, $\alpha = 0,1,2,3$ is the number of states of H_α with energy less than ξ in $Q\mathcal{H}_\alpha$. Define now the connected spectral operator

$$E_c(\xi) = E(\xi) - E_0(\xi) - \sum_{\alpha > 0} \left(E_\alpha(\xi) - E_0(\xi) \right) \tag{IV.3.55}$$

$\mathrm{Tr}\, Q \left[E_c(\xi_2) - E_c(\xi_1) \right]$ is the composite excess or deficit of states in $Q\mathcal{H}$ due to all the interactions between the energies ξ_2 and ξ_1, $\xi_2 > \xi_1$. Consequently $\frac{d}{d\xi} \mathrm{Tr}\, Q E_c(\xi)$ has the meaning of the change of state density at energy in the subspace

$Q\mathcal{H}$ produced by all the scatterings.

The relationship of these observations to the connected resolvent diffęerence $R_c(z)$ is easily established from equation 54. From $R(z)$ subtract $R^{+}(z)$, take the inner product of this sum with respect to any $f \varepsilon Q\mathcal{H}$. One has at once

$$(f, [R(\xi+i\eta) - R^{+}(\xi+i\eta)] f) = \int \frac{2i\eta}{(\xi-\xi')^2+\eta^2} (f, \frac{dE(\xi)}{d\xi} f) \, d\xi \tag{IV.3.56}$$

Taking $\eta \to +0$, and summing over an orthogonal set of f's that span $Q\mathcal{H}$ gives

$$Tr\, Q[R(\xi+i0) - R^{+}(\xi+i0)] = 2i\pi \frac{d}{d\xi} Tr\, Q\, E(\xi) \tag{IV.3.57}$$

Naturally this relation is also valid for the replacements of $\{H, R(z), E(\xi)\}$ by $\{H_\alpha, R_\alpha(z), E_\alpha(\xi)\}$, $\alpha = 0, 1, 2, 3$. Thus we may sum these statements with the relative signs given by equation 55 to find

$$2i\, \mathrm{Im}\, Tr\, Q R_c(\xi+i0) = 2i\pi \frac{d}{d\xi} Tr\, Q\, E_c(\xi) \tag{IV.3.58}$$

Since $Q\mathcal{H}$ is an arbitrary subspace of $\mathcal{H}$, equation 58 is the statement that $\pi^{-1} \mathrm{Im}\, Tr\, R_c(\xi+i0)$ is proportional to the change of three body state density.

We shall now give a proof of the spectral property. Our proof will allow us to establish the property directly, and without any reference to the S-matrix. We employ in the proof only the scattering theory structure outlined above and certain convenient mathematical properties of the trace. We shall specifically rely on the assumptions used by Faddeev plus one additional technical restriction, equation (B.3). As noted in the two particle case this means the spectral property is established even when time reversal invariance and angular momentum are not respected in the three body problem.

The form of the proof to be given depends on the general idea of the analysis presented in the two body case. The structure of the derivation is modified by the multichannel character of the scattering and by technical features peculiar to the three body problem. One technical fact relevant to our proof is that the operator $R_c(z)$ is not by itself trace-class. However, it can be shown (cf. Appendix B) that

$$A(z) = \frac{dR_c(z)}{dz} = R^2(z) - R_0^2(z) - \sum_{\alpha=1}^{3}\left(R_\alpha^2(z) - R_0^2(z)\right) \tag{IV.3.59}$$

is trace-class for all z not on the spectrum of H. Let Π_δ denote all points in the z plane that are a distance $\delta > 0$ or greater from the spectrum of H. Then $Tr\, A(z)$ is an analytic function which is a uniformly convergent series of analytic functions in any bounded sector of the set Π_δ. The distance δ may be as small as we desire. Thus, in Π_δ the operations of complex integration or differentiation may be passed through the trace. A consequence of this is that if one integrates $Tr\, A(z)$ from z_1 to z_2, and notes $\frac{d}{dz}R(z) = R^2(z)$, etc. it follows that $Tr\left[R_c(z_2) - R_c(z_1)\right]$ is trace-class.

The second technical feature, relevant for us, is that the products $\mathcal{P}(\rho)\, R_0(z)$, $\mathcal{P}(\rho)\, R_\alpha(z)$ and $\mathcal{P}(\rho)\, R(z)$ are not Schmidt-class in $\mathcal{H}$. This result is in contrast to that for the two body problem and comes about for a simple reason. The change of dimension of the L^2 space from three to six degrees of freedom alters the relation between the inner product measure and energy. In the two particle case the measure in momentum space is proportional to $E^{\frac{1}{2}}dE$. But for the three particle six dimensional space the L^2 measure becomes $E^2 dE$. However, in both situations the resolvents are proportional to E^{-1}. So the Schmidt norm of $P(R)R_0(z)$ is finite, but that for $\mathcal{P}(\rho)R_0(z)$ is unbounded. What one can prove is that $\mathcal{P}(\rho)R_0^2(z)$, $\mathcal{P}(\rho)R_\alpha^2(z)$ and $\mathcal{P}(\rho)R^2(z)$ are all Schmidt class for $\rho<\infty$ and $\mathrm{Im}\, z\neq 0$. (cf. Appendix B). For these reasons we shall not prove the spectral property directly, but rather will prove that the second derivative with respect to energy of the relation is valid. Then integrating twice will recover equation 52 for us.

We begin by expressing the trace of $\frac{d^2}{d\xi}R_c(\xi+i\eta)$ in terms of the limit $\rho\to\infty$,

$$\mathrm{Tr}\,\frac{d^2}{d\xi^2}\left[R_c(\xi+i\eta)-R_c(\xi-i\eta)\right] = \lim_{\rho\to\infty}\mathrm{Tr}\,\mathcal{P}(\rho)\,\frac{d^2}{d\xi^2}\left[R_c(\xi+i\eta)-R_c(\xi-i\eta)\right] \qquad \text{(IV.3.60)}$$

An essential observation is that $\mathcal{P}(\rho)\frac{d^2}{d\xi^2}\left[R_c(\xi+i\eta)-R_c(\xi-i\eta)\right]$ may be written as the sum of five separate trace-class operators, viz.

$$\mathcal{P}(\rho)\frac{d^2}{d\xi^2}\left[R(\xi+i\eta)-R(\xi-i\eta)\right]\mathcal{P}(\rho) = 2i\eta\,\mathcal{P}(\rho)\,\frac{d^2}{d\xi^2}\left|R(\xi+i\eta)\right|^2\mathcal{P}(\rho) \qquad \text{(IV.3.61)}$$

$$\mathcal{P}(\rho)\,\frac{d^2}{d\xi^2}\left[R_\alpha(\xi+i\eta)-R_\alpha(\xi-i\eta)\right]\mathcal{P}(\rho) = 2i\eta\,\mathcal{P}(\rho)\,\frac{d^2}{d\xi^2}\left|R_\alpha(\xi+i\eta)\right|^2\mathcal{P}(\rho) \qquad \text{(IV.3.62)}$$

where $\alpha=0,1,2,3$. The equations above depend on the Hilbert identity (IV.2.20) which all the resolvents satisfy. Because the right hand side always involves the product of four resolvents after the derivative is taken it is the product of two Schmidt operators. Thus the left hand sides are individually trace class. Consider first the $\mathcal{H}$ -trace of the operator in equation 61

$$\mathrm{Tr}\, \frac{d^2}{d\xi^2} |R(\xi+i\eta)|^2 \mathcal{P}(\rho) = \mathrm{Tr}\, \frac{d^2}{d\xi^2} \Big[\sum_{\alpha=0}^{3} \tilde{U}_\alpha^{(-)} \tilde{U}_\alpha^{(-)\dagger} + B_0 \Big] |R(\xi+i\eta)|^2 \mathcal{P}(\rho)$$

$$= \sum_{\alpha=0}^{3} \mathrm{Tr}\, \frac{d^2}{d\xi^2} |R(\xi+i\eta)|^2 \tilde{U}_\alpha^{(-)\dagger} \mathcal{P}(\rho) \tilde{U}_\alpha^{(-)} + \mathrm{Tr}\, \frac{d^2}{d\xi^2} B_0 |R(\xi+i\eta)|^2 \mathcal{P}(\rho)$$

$$= \sum_{\alpha=0}^{3} \mathrm{Tr}_\alpha \frac{d^2}{d\xi^2} |\tilde{R}_\alpha(\xi+i\eta)|^2 U_\alpha^{(-)\dagger} \mathcal{P}(\rho) U_\alpha^{(-)} + \sum_{i=1}^{N_3} \frac{d^2}{d\xi^2} \frac{(\Psi_i, \mathcal{P}(\rho)\Psi_i)}{|X_i^2+\xi+i\eta|^2} \tag{IV.3.63}$$

The first form of the trace uses the cyclical invariance property of the trace and the idempotency of $\mathcal{P}(\rho)$; the second employs the asymptotic completeness relations equation 16'; the third relies on the intertwining property, equation 17'; the last equation is a consequence of the definition of I_α and the relation equation 14. We have introduced Tr_α as the trace on the space $\mathcal{H}_\alpha$. The resolvent $\tilde{R}_\alpha(z) = (\tilde{H}_\alpha - z)^{-1}$ also acts on this same space.

Focus now on the second set of operators given by equation 62 with $\alpha > 0$. We successively modify the trace of the first form in a manner parallel to that just carried out

$$\mathrm{Tr}\, \frac{d^2}{d\xi^2} |R_\alpha(\xi+i\eta)|^2 \mathcal{P}(\rho) = \mathrm{Tr}\, \frac{d^2}{d\xi^2} \Big[W_\alpha^{(-)} W_\alpha^{(-)\dagger} + P_b(\alpha) \Big] |R_\alpha(\xi+i\eta)|^2 \mathcal{P}(\rho)$$

$$= \mathrm{Tr}\, \frac{d^2}{d\xi^2} |R_0(\xi+i\eta)|^2 W_\alpha^{(-)\dagger} \mathcal{P}(\rho) W_\alpha^{(-)} + \mathrm{Tr}\, \frac{d^2}{d\xi^2} |R_\alpha(\xi+i\eta)|^2 \mathcal{B}_\alpha^{(\rho)} \tag{IV.3.62}$$

Above we have relied on the elementary properties of the spectator scattering system stated in equations 20 - 25. Now combine equation 63 and 64 together with the trace equation 62 for $\alpha = 0$, to obtain

$$\mathrm{Tr}\,\frac{d^2}{d\varsigma^2}\mathcal{P}(\rho)\left[R_c(\varsigma+i\eta)-R_c(\varsigma-i\eta)\right] = 2i\eta\sum_{i=1}^{N_3}\frac{d^2}{d\varsigma^2}\frac{(\Psi_i,\mathcal{P}(\rho)\Psi_i)}{|X_i^2+\varsigma+i\eta|^2}$$
$$+\,2i\eta\,\mathrm{Tr}\,\frac{d^2}{d\varsigma^2}|R_0(\varsigma+i\eta)|^2\left\{U_0^{(-)+}\mathcal{P}(\rho)U_0^{(-)}-\mathcal{P}(\rho)-\sum_{\alpha=1}^{3}\left[W_\alpha^{(-)+}\mathcal{P}(\rho)W_\alpha^{(-)}-\mathcal{P}(\rho)\right]\right\}$$
$$+\,2i\eta\sum_{\alpha=1}^{3}\mathrm{Tr}_\alpha\,\frac{d^2}{d\varsigma^2}|\tilde{R}_\alpha(\varsigma+i\eta)|^2\left\{U_\alpha^{(-)+}\mathcal{P}(\rho)U_\alpha^{(-)}-\mathcal{P}_\alpha(\rho)\right\}.$$

(IV.3.65)

Throughout the traces of equation 65 appear the operators that define the various three body time delays. The individual operators found in Tr and Tr_α are always in the form of products of Schmidt operators. So we may evaluate them in the diagonal form (cf. Appendix A)

Take the variable $\rho\to\infty$ on both sides of equation 65. Property (IV.3.60) guarantees that the limit exists and is equal to the trace we seek

$$\mathrm{Tr}\,\frac{d^2}{d\varsigma^2}\left[R_c(\varsigma+i\eta)-R_c(\varsigma-i\eta)\right] = 2i\eta\sum_{i=1}^{N_3}\frac{d^2}{d\varsigma^2}\left|X_i^2+\varsigma+i\eta\right|^{-2}$$
$$+\int\frac{d^2}{d\varsigma^2}\,\frac{2i\eta}{(\varsigma-P_0'^2/2m_0)^2+\eta^2}\,\frac{\langle\hat{P}_0'|\,q_{00}(P_0'^2/2m_0)\,|\hat{P}_0'\rangle}{2\pi\, m_0\, P_0'^4}\,d\vec{P}_0'$$
$$+\sum_{\alpha>0}\int\frac{d^2}{d\varsigma^2}\,\frac{2i\eta}{(\varsigma-P_\alpha'^2/2n_\alpha)^2+\eta^2}\,\frac{\langle\hat{P}_\alpha'|\,q_{\alpha\alpha}(P_\alpha'^2/2n_\alpha-\chi_i^2)\,|\hat{P}_\alpha'\rangle}{2\pi\, n_\alpha\, P_\alpha'}\,d\vec{P}_\alpha'$$

(IV.3.66)

The last step in our proof is to take the limit $\eta\to 0$. If we do this and carry out the change of variables $d\vec{p}_\alpha' = n_\alpha p_\alpha \, d\hat{p}_\alpha' \, d\varepsilon'$ and $d\vec{p}_0' = m_0 p_0'^4 \, d\hat{p}_0' \, d\varepsilon'$, then the integrals in equation 66 become

$$\frac{d^2}{d\varphi^2} \mathrm{Tr}\left[R_c(\varphi+i0) - R_c(\varphi-i0)\right] = 2i \, \frac{d^2}{d\varphi^2} \sum_{\alpha=0}^{3} \hat{\mathrm{tr}}_\alpha \, q_{\alpha\alpha}(\varphi) \tag{IV.3.67}$$

Of course the operators $q_{\alpha\alpha}(\varphi)$ are zero unless the energy φ is greater than one of the channel thresholds, $\varphi > -\max_\alpha \chi_\alpha^2$. Let $\varphi < -\max_\alpha \chi_\alpha^2$ then

$$\int_{\varphi_0}^{E} \frac{d^2}{d\varphi^2} \mathrm{Tr}\left[R_c(\varphi+i0) - R_c(\varphi-i0)\right] d\varphi = \frac{d}{dE} \mathrm{Tr}\left[R_c(E+i0) - R_c(E-i0)\right] \tag{IV.3.68}$$

There is no contribution from the lower limit since the point φ_0 is to the left of the continuous spectrum and can be assumed not to be an isolated spectral point. In this region of energy $R_c(z)$ has no discontinuity across the real axis. A second integration, like that in equation 68, gives us the spectral property of equation 52. This completes our proof.

IV.4 Conclusion

In this section we continue our analysis and write out the forms of the third cluster integral and give the physical interpretation of our solution in the context of the equation of state. Also we contrast our result with several others reported in the literature.

The time delay form for the third virial coefficient is found by substituting the spectral property (IV.3.52) into the Watson transform (IV.3.49)

$$b_3 = \frac{3^{\frac{3}{2}}}{3!\,\lambda^3}\left\{ \sum_{i=1}^{N_3} e^{\beta X_i^2} + \frac{1}{2\pi}\int_{Th}^{\infty} e^{-\beta E} \sum_{\alpha=0}^{3} \hat{t}_{\alpha}\, g_{\alpha\alpha}(E)\, dE \right\}$$

(IV.4.1)

The lower limit of the integral is the negative energy value at which the scattering continuum first appears. This reduction to quadrature of the third cluster integral tells us again that the only aspect of the three particle scattering that affects the cluster integral is the time delay. Of course, the specific form of our solution indicates its validity when stable two particle clusters are present in the gas. The terms $exp.\ \beta X_i^2$ are three body clusters that will take part in the four body scattering processes. The general pattern of our solution reveals why it is successful. Most constructs in statistical mechanics are based on sums over the allowed quantum states of a system. Here the quantity needed is the difference of the number of states in the scattering continuum between a free and an interacting system. The spectral property in both the two and three body problem provide us with the needed difference in terms of traces over the various channel time delays. Nevertheless, we pause to note there is even a more econimical way to obtain equation 1 than that is presented in section IV.3. The trace defining b_3 in equation IV.1.5 is known to be trace class.[19] Further we show in Appendix B that the operators $e^{-\beta H_0}\mathcal{P}(\rho)$, $e^{-\beta H_\alpha}\mathcal{P}(\rho)$ and $e^{-\beta H}\mathcal{P}(\rho)$ are Schmidt class. So one could start from the expression for b_3 in (IV.1.5) and use the techniques for restructuring the trace found in equations (IV.3.60 - 66). The result is again equation 1, one does not have to use the Watson transform or make any reference to resolvents and their analytic properties. The reason we have presented the form of the proof we have is because we believe the spectral property of time delay is physically interesting in its own right. For example, it may be used as a starting point for deriving multichannel Levinson's theorems.

It is instructive to see what the solution above tells us about the equation of state. For purposes of providing this interpretation we shall assume that there are no three body bound states. The third virial coefficient is

$$\begin{aligned} a_3 &= 4a_2^2 - 2\, b_3 b_1^{-3} \\ &= 4a_2^2 - \frac{\lambda^6 3^{\frac{1}{2}}}{2\pi} \int_{Th}^{\infty} e^{-\beta E} \sum_{\alpha=0}^{3} \hat{tr}_\alpha\, q_{\alpha\alpha}(E)\, dE \end{aligned} \tag{IV.4.2}$$

Thus the three body contribution to the equation of state is

$$PV = NkT \left\{ 1 + \cdots - \left(\frac{\lambda^6 \sqrt{3}}{2\pi} \int_{Th}^{\infty} e^{-\beta E} \sum_{\alpha=0}^{3} \hat{tr}_\alpha\, q_{\alpha\alpha}(E)\, dE \right) \rho^2 + \cdots \right\} \tag{IV.4.3}$$

As in the two body case, an increase in any of the $\hat{tr}_\alpha\, q_{\alpha\alpha}(E)$ while the other variables V, N, T and the two body virial coefficient remain constant leads to a decrease in pressure. This decrease is proportional to the density squared. Again the dynamical interaction of the colliding particles at energy E is effectively creating extra space for the particles, thus reducing the pressure. In this description of the effect of scattering on the statistical system, we have chosen to highlight the equation of state. It is trivial to extend our results to give analogous formulae for the internal energy, the specific heat, entropy, etc. Each of these thermodynamic quantities may be stated as functions of two and few body time delay.

As in the two body problem it is interesting to give the S-matrix forms of the solution. In the cases where the three body scattering has a two body bound cluster in the initial or final channel the relation between time delay and the S-matrix is known.[12] One may state the connection in the following way. Let $\mathcal{S}_{\alpha\beta}$ be the channel S-matrix Faddeev defines, i.e.

$$S_{\alpha\beta} = U_\alpha^{(+)\dagger} U_\beta^{(-)} \quad : \quad \mathcal{H}_\alpha \rightarrow \mathcal{H}_\beta \tag{IV.4.4}$$

We shall require the kernels for the reduced energy-dependent S-matrices,

$$\mathcal{S}_{\alpha\beta}(\vec{p}_\alpha ; \vec{p}_\beta{}') = \frac{\delta(E-E')}{(n_\alpha p_\alpha n_\beta p_\beta')^{\frac{1}{2}}} \langle \hat{p}_\alpha | \mathcal{A}_{\alpha\beta}(E) | \hat{p}_\beta' \rangle \tag{IV.4.5}$$

$$S_{o\beta}(\vec{p}_o ; \vec{p}_\beta{}') = \frac{\delta(E-E')}{(m_o p_o^4 n_\beta p_\beta')^{\frac{1}{2}}} \langle \hat{p}_o | \mathcal{A}_{o\beta}(E) | \hat{p}_\beta' \rangle \tag{IV.4.6}$$

Thus the energy dependent family of operators $\mathcal{A}_{\alpha\beta}(E)$ are defined. They are all free of the energy delta function occuring in $\mathcal{S}_{\alpha\beta}$. With these operators it is proved in [12] that

$$q_{\alpha\alpha}(E) = -\sum_{\gamma=0} \mathcal{A}_{\gamma\alpha}^{\dagger}(E) \frac{d}{dE} \mathcal{A}_{\gamma\alpha}(E) \quad , \quad \alpha > 0 \tag{IV.4.7}$$

For this reason the $\alpha > 0$ channel portions of time delay in equation 1 are,

$$\sum_{\alpha=1}^{3} q_{\alpha\alpha}(E) = -i \sum_{\alpha>0} \sum_{\gamma=0}^{3} \mathcal{A}_{\gamma\alpha}^{\dagger}(E) \frac{d}{dE} \mathcal{A}_{\gamma\alpha}(E) \tag{IV.4.8}$$

The formulae for the three to three connected time delay have not yet been worked out. Analogy with equation 7 suggests what the answer is likely to be. Define the disconnected spectator S-matrix by

$$S_\alpha = W_\alpha^{(+)^\dagger} W_\alpha^{(-)} , \qquad \alpha > 0 \tag{IV.4.9}$$

Both S_{oo} and S_α generate reduced S-matrices:

$$S_{oo}(\vec{p}_o ; \vec{p}_o') = \frac{\delta(E-E')}{(m_o p_o^4 \, m_o p_o'^4)^{1/2}} \langle \hat{p}_o | \mathcal{S}_{oo}(E) | \hat{p}_o' \rangle \tag{IV.4.10}$$

$$S_\alpha(\vec{p}_o ; \vec{p}_o') = \frac{\delta(E-E')}{(m_o p_o^4 \, m_o p_o'^4)^{\frac{1}{2}}} \langle \hat{p}_o | \mathcal{S}_\alpha(E) | \hat{p}_o' \rangle \tag{IV.4.11}$$

Thus the expected form for $q_{oo}(E)$ is

$$q_{oo}(E) = -i \left[\mathcal{S}_{oo}^\dagger(E) \frac{d}{dE} \mathcal{S}_{oo}(E) - \sum_{\alpha=1}^{3} \mathcal{S}_\alpha^\dagger(E) \frac{d}{dE} \mathcal{S}_\alpha(E) \right] - i \sum_{\gamma=1}^{3} \mathcal{S}_{\gamma o}^\dagger(E) \frac{d}{dE} \mathcal{S}_{\gamma o}(E) \tag{IV.4.12}$$

We note that this the S-matrix form that Dashen et al[17] and Smith[15] believe to be valid.

If one assumes the interaction is not strong enough to form stable two particle clusters then only the square bracket term in equation 12 remains in formula (IV.4.1) for the third cluster integral. For this restricted problem all the channel structure is absent and only three to three scattering is possible. If one further assumes that angular momentum is conserved then the situation is precisely that studied in detail by Larsen.[18] Using a hyperspherical method Larsen describes this scattering in terms of a phase shift, and obtains a solution paralleling that of Uhlenbeck and Beth.[13]

At this point we have demonstrated that the second and third cluster integral are explicitly determined by time delay. We are confident that this analysis can be extended to four or more particle collisions. Observe that our argument rests on just a few general facts of three particle scattering. Specifically, we required the existence of the Moeller wave operators in order to define the concept of time delay. Secondly, we used the energy conserving (intertwining) and completeness properties of these wave operators. These features must exist for any physically reasonable few body scattering theory.

In closing we remark that in collisions like breakup, where the initial and final state differ by three continous degrees of freedom no phase shift description of scattering exists. By comparing the two particle solution with that for the three body problem we can perceive a general trend. What is happening in our formalism is that the trace of the time delay is replacing the phase shift as the universal descriptor of the scattering process.

Chapter V Cayley Transform method

In this chapter, we verify the results of chapter IV by a different method: Cayley Transform. This method has particular merits in the three body case. It focuses not only on "connectedness" and "channel structure" as in chapter IV, but also bring to light "rescattering singularities". We show how to treat these singularities which has been generally ignored by workers in this area.

V.1 Introduction

An alternative method of expressing the change of state density in terms of time delay is possible through the development of Cayley transform. The time delay here takes the form of the logarithmic derivative of the familiar scattering S-matrix instead of the original Goldberger and Watson[2] form using the range projector.

$$\begin{aligned} q(E) &= -i\, s^{\dagger}(E) \frac{d}{dE} s(E) \\ &= -i \frac{d}{dE} \ln s(E) \end{aligned} \qquad \text{(V.1.1)}$$

The equivalence of the two forms of time delay was proven in the two body case by Jauch and Marchand[3]. Osborn and Bolle[12] established the relationship in the two-bodylike channels of the three body problem, $\alpha = 1, 2, 3$. They propose the operator form of time delay to be

$$q_{\alpha\alpha}(E) = -i \sum_{\beta=0}^{3} \left[s^{\dagger}_{\beta\alpha}(E) \frac{d}{dE} s_{\beta\alpha}(E) \right]_{C}, \quad \alpha = 0, 1, 2, 3. \qquad \text{(V.1.2)}$$

The Cayley transform method differs from the previous chapter in that it deals, not with the operators themselves, but rather with the kernels of the operators, especially their traces in the form of integrals. The outcome on the two-body-like channels effectively verifies what one would have expected using the results of the previous chapter and the calculations of Osborn and Bolle. In the three-to-three channel ($\alpha = 0$), the Cayley transform method reveals a much more complex structure to the trace of three body time delay than one would have proposed from equation 2 above.

Specifically, we have shown here that, even in the absence of two body bound states, the trace of time delay

$$\hat{tr}\, q_{00}(E) = -i\, \hat{tr} \left[\mathcal{S}^{+}_{00}(E) \frac{d}{dE} \mathcal{S}_{00}(E) \right]_{c}$$

cannot be obtained by direct substitution of the known form of the kernel $\mathcal{S}_{00}(E)$,

$$\mathcal{S}_{00}(\hat{p}_0 E, \hat{p}_0' E, E+i0) = \delta(\hat{p}_0 - \hat{p}_0') - 2\pi i \sum_{\alpha,\beta} \mathcal{M}_{\alpha\beta}(\hat{p}_0 E, \hat{p}_0' E, E+i0)$$

The subscript c denotes "connected", meaning that terms with over all delta function in momentum are removed. The diagonal elements of "disconnected" terms are singular as $\delta(0)$. Such substitution only leads to meaningless infinities in the trace of time delay which we have already shown to be finite. While the operator form may well be expressed as in equation 2, the generalized functions in the kernels of the trace must be properly treated, a process known as regulariation in the theory generalized functions.[40] Schematically, the regularized result has the form

$$i\,\widehat{tr}\,q_{00}(E) = \widehat{tr}\left[s_{00}^{+}(E)\,\frac{d}{dE}s_{00}(E) - \chi(E)\right]_c + tr\,\tilde{\chi}(E) \qquad \text{(V.1.3)}$$

where the trace of the function in square brackets no longer has any of the rescattering singularities. The term $tr\,\tilde{\chi}(E)$ contains only two body T-matrices.

This mathematical problem, generally known as rescattering singularity, has received little treatment from authors working in this area (Dashen,[17] Larsen,[18] etc.) We are aware of a similar calculation reported by Buslaev and Merkuriev.[19] However, due to incomplete translation of Russian literature, we are not able to compare with their results. Moreover, their calculations appears to involve findings in mathematical analysis much beyond the scope of this thesis.

V.2 Two body Cayley transform

We would like first to define Cayley transforms and then relate them to resolvent differences. For each Hamiltonian h we associate the function $b_h(z) = (h-z^*)/(h-z)$ as its Cayley transform. z is a complex number, $z = \lambda + i\mu$, λ and μ are both real. $b_{h_0}(z) = (h_0 - z^*)/(h_0 - z)$ is the Cayley transform of the free Hamiltonian h_0. All Cayley transforms are unitary by definition.

$$b_h^{\dagger}(z)\, b_h(z) = \frac{h-z}{h-z^*} \cdot \frac{h-z^*}{h-z} = e = b_h(z)\, b_h^{\dagger}(z) \tag{V.2.1}$$

Cayley transforms can also be expressed in terms of resolvents, $r(z) = (h-z)^{-1}$,

$$b_h(z) = \frac{h-z^*}{h-z} = \frac{h-z+z-z^*}{h-z} = e + 2i\mu\, r(z) \tag{V.2.2}$$

and,

$$b_{h_0}(z) = e + 2i\mu\, r_0(z) \tag{V.2.3}$$

We also define a new unitary operator, as a product of Cayley transforms,

$$a_{h/h_0}(z) = b_h(z)\, b_{h_0}^{\dagger}(z) \tag{V.2.4}$$

This operator can be expressed in terms of resolvents also.

$$\begin{aligned} a_{h/h_0}(z) &= (e + 2i\mu\, r(z))\,(e - 2i\mu\, r_0(z^*)) \\ &= e + 2i\mu\, r(z) - 2i\mu\, r_0(z^*) - (2i\mu)^2\, r(z)\, r_0(z^*) \\ &= e + 2i\mu\left[r_0(z) - r_0(z)\, t(z)\, r_0(z)\right] - 2i\mu\, r_0(z^*) \\ &\quad - (2i\mu)^2\left[r_0(z) - r_0(z)\, t(z)\, r_0(z)\right] r_0(z^*) \end{aligned}$$

$$a_{h/h_0}(z) = e + 2i\mu\left[r_0(z) - r_0(z^*) - 2i\mu\, r_0(z)\, r_0(z^*)\right]$$
$$- 2i\mu\, r_0(z)\, t(z)\, r_0(z) + 2i\mu\, r_0(z)\, t(z)\left[r_0(z) - r_0(z^*)\right]$$
$$= e - 2i\mu\, r_0(z)\, t(z)\, r_0(z^*) \qquad \text{(V.2.5)}$$

where we have used the standard unitarity condition and definition of the T-matrix.

$$r(z) - r(z^*) = 2i\mu\, r(z)\, r(z^*)$$
$$r(z) - r_0(z) = -r_0(z)\, t(z)\, r_0(z)$$

Now we want to express the resolvent difference $\operatorname{Im}\left[r(z) - r_0(z)\right]$ in terms of these Cayley tranforms. Since $r(z) = \frac{\partial}{\partial\lambda} \ln (h-z)^{-1}$ it follows that

$$r(z) - r(z^*) = \frac{\partial}{\partial\lambda} \ln \frac{h - z^*}{h - z} = \frac{\partial}{\partial\lambda} \ln b_h(z) = b_h^\dagger(z) \frac{\partial}{\partial\lambda} b_h(z) \qquad \text{(V.2.6)}$$

$$r_0(z) - r_0(z^*) = b_{h_0}^\dagger(z) \frac{\partial}{\partial\lambda} b_{h_0}(z) \qquad \text{(V.2.7)}$$

To form the difference of the above two equations, we write $b_h(z)$ as $a_{h/h_0}(z)\, b_{h_0}(z)$ and substitute into equation 6.

$$r(z) - r(z^*) = b_h^\dagger(z) \frac{\partial}{\partial\lambda} b_h(z) = \left[a_{h/h_0}(z)\, b_{h_0}(z)\right]^\dagger \frac{\partial}{\partial\lambda}\left[a_{h/h_0}(z)\, b_{h_0}(z)\right]$$
$$= b_{h_0}^\dagger(z)\, a_{h/h_0}^\dagger(z)\left[\left(\frac{\partial}{\partial\lambda} a_{h/h_0}(z)\right) b_{h_0}(z) + a_{h/h_0}(z) \frac{\partial}{\partial\lambda} b_{h_0}(z)\right]$$
$$= b_{h_0}^\dagger(z)\left(a_{h/h_0}^\dagger(z) \frac{\partial}{\partial\lambda} a_{h/h_0}(z)\right) b_{h_0}(z) + b_{h_0}^\dagger(z) \frac{\partial}{\partial\lambda} b_{h_0}(z) \qquad \text{(V.2.8)}$$

Now it is clear what the resolvent difference is.

$$2i \operatorname{Im}\left[r(z) - r_0(z)\right] = r(z) - r(z^*) - r_0(z) + r_0(z^*)$$
$$= b_{h_0}^\dagger(z)\left(a_{h/h_0}^\dagger(z) \frac{\partial}{\partial\lambda} a_{h/h_0}(z)\right) b_{h_0}(z) \qquad \text{(V.2.9)}$$

Because of unitarity, this equation has an alternative form.

$$r(z) - r(z^*) - r_0(z) + r_0(z^*) = - b^+_{k_0}(z)\left(a_{k/k_0}(z)\frac{\partial}{\partial\lambda}a^+_{k/k_0}(z)\right)b_{k_0}(z) \quad (\text{V.2.9}')$$

The change of state density is related to the trace of the operator on the left. The trace is a pure imaginary number which can be evaluated in terms of the free resolvent and the T-matrix through the right hand side of the above equation.

$$\begin{aligned} L &= 2i\,\mathrm{Im}\,\mathrm{tr}\,(r(z) - r_0(z)) \\ &= i\,\mathrm{Im}\,\mathrm{tr}\; b^+_{k_0}(z)\left(a^+_{k/k_0}(z)\frac{\partial}{\partial\lambda}a_{k/k_0}(z)\right)b_{k_0}(z) \\ &= i\,\mathrm{Im}\,\mathrm{tr}\; a^+_{k/k_0}(z)\frac{\partial}{\partial\lambda}a_{k/k_0}(z) \\ &= i\,\mathrm{Im}\,\mathrm{tr}\left[e + 2i\mu\, r_0(z)\, t(z^*)\, r_0(z^*)\right] \\ &\qquad \times \frac{\partial}{\partial\lambda}\left[e - 2i\mu\, r_0(z)\, t(z)\, r_0(z^*)\right] \end{aligned} \quad (\text{V.2.10})$$

This can be further developed as a sum of two terms, a linear term L_1 and a quandratic term L_2. $L = L_1 + L_2$.

$$L_1 = i\,\mathrm{Re}\,\mathrm{tr}\; -2\mu\frac{\partial}{\partial\lambda}\left(r_0(z)\,t(z)\,r_0(z^*)\right) \quad (\text{V.2.11})$$

$$L_2 = i\,\mathrm{Im}\,\mathrm{tr}\;(2\mu)^2 r_0(z)\,t(z^*)\,r_0(z^*)\frac{\partial}{\partial\lambda}\left(r_0(z)\,t(z)\,r_0(z^*)\right) \quad (\text{V.2.12})$$

We specifically develop the energy dependence of the trace operation, i.e.

$$\mathrm{tr}\,A(z) = \int_0^\infty dE\;\hat{\mathrm{tr}}\;j(E)\,A(E,E,z)\,j(E) \quad (\text{V.2.13})$$

where $\hat{\mathrm{tr}}$ is the reduced trace in the reduced space, $j^2(E) = n\sqrt{2nE}$ is the Jacobian and $\tau(E,E,z) = j(E)\,t(E,E,z)\,j(E)$ as the reduced T-matrix. The notation here is the same as in chapter II.

In this reduced space notation we can calculate L_1.

$$\begin{aligned} L_1 &= i\,\mathrm{Re}\int_0^\infty dE\; -2\mu\frac{\partial}{\partial\lambda}\frac{1}{E-\lambda-i\mu}\;\hat{\mathrm{tr}}\,\tau(E,E,\lambda+i\mu)\,\frac{1}{E-\lambda+i\mu} \\ &= i\,\mathrm{Re}\int_0^\infty dE\; -2\mu\left\{\left[\frac{\partial}{\partial\lambda}\frac{1}{(E-\lambda)^2+\mu^2}\right]\hat{\mathrm{tr}}\,\tau(E,E,\lambda+i\mu) \;+\right. \end{aligned}$$

$$+ \frac{1}{(E-\lambda)^2+\mu^2} \frac{\partial}{\partial\lambda} \hat{tr}\, \tau(E,E,\lambda+i\mu) \Big\}$$

$$L_1 = i\, Re \Big\{ \frac{2\mu}{(E-\lambda)^2+\mu^2} \hat{tr}\, \tau(E,E,\lambda+i\mu) \Big|_{E=0}^{E=\infty} + \int_0^\infty \frac{d}{dE} \frac{-2\mu}{(E-\lambda)^2+\mu^2} \times$$

$$\times \frac{\partial}{\partial E} \hat{tr}\, \tau(E,E,\lambda+i\mu) + \int_0^\infty dE \frac{-2\mu}{(E_0-\lambda)^2+\mu^2} \frac{\partial}{\partial\lambda} \hat{tr}\, \tau(E,E,\lambda+i\mu) \Big\}$$

(V.2.14)

In the limit $\mu \to 0^+$, $\frac{2\mu}{(E-\lambda)^2+\mu^2} \longrightarrow 2\pi\,\delta(E-\lambda)$. The surface term vanishes because of the structure of $\tau(E,E,\lambda+i\mu)$. Hence,

$$\lim_{\mu\to 0^+} L_1 = i\, Re\, -2\pi \frac{\partial}{\partial\lambda} \hat{tr}\, \tau(\lambda,\lambda,\lambda+i0)$$

(V.2.15)

Next, we want to develop L_2.

$$L_2 = i\, Im\, tr\, (2\mu)^2 \Lambda_0(z)\, t(z^*)\, \Lambda_0(z^*) \frac{\partial}{\partial\lambda} \left[\Lambda_0(z)\, t(z)\, \Lambda_0(z^*) \right]$$

$$= i\, Im\, tr\, 4\mu^2 \Lambda_0(z)\, t(z^*)\, \Lambda_0(z^*) \Lambda_0(z) \left[\frac{\partial}{\partial\lambda} t(z)\right] \Lambda_0(z^*) + R$$

(V.2.16)

where $$R = i\, Im\, tr \Big[4\mu^2 \Lambda_0(z)\, t(z^*)\, \Lambda_0(z^*)\, \Lambda_0^2(z)\, t(z)\, \Lambda_0(z^*)$$

$$+ 4\mu^2 \Lambda_0(z)\, t(z^*)\, \Lambda_0(z^*)\, \Lambda_0(z)\, t(z)\, \Lambda_0^2(z^*) \Big]$$

$$= i\, Im\, tr \Big[2\mu i \big(-2i\mu\, t(z)\, \Lambda_0(z^*)\, \Lambda_0(z)\, t(z^*) \big) \Lambda_0(z^*)\, \Lambda_0^2(z)$$

$$+ 2\mu i \big(-2i\mu\, t(z^*)\, \Lambda_0(z^*)\, \Lambda_0(z)\, t(z) \big)\, \Lambda_0^2(z^*)\, \Lambda_0(z) \Big]$$

$$= i\, Im\, tr\, 2\mu i \big(t(z) - t(z^*) \big) \big(\Lambda_0(z^*)\, \Lambda_0^2(z) + \Lambda_0^2(z^*)\, \Lambda_0(z) \big)$$

$$= 0$$

(V.2.17)

since the above trace is explicitly a real number. Hence,

$$\lim_{\mu\to 0^+} L_2 = i\, Im\, 4\pi^2 \int_0^\infty dE \int_0^\infty dE'\, \delta(E-\lambda)\, \hat{tr}\, \tau(E,E',\lambda-i0)\, \delta(E'-\lambda)\, \tau(E',E,\dot{\lambda}+i0)$$

$$= i\, Im\, 4\pi^2\, \hat{tr}\, \tau(\lambda,\lambda,\lambda-i0)\, \tau(\lambda,\lambda,\dot{\lambda}+i0)$$

(V.2.18)

where we introduce the notation

$$\tau(E,E,\dot{\lambda}+io) = \frac{\partial}{\partial\lambda}\tau(E,E,\lambda+io)$$

Next we want to show the following unitarity identity:

$$0 = \mathrm{Im}\,\hat{tr}\,\tau(\lambda,\lambda,\lambda-io)\,\tau(\dot{\lambda},\dot{\lambda},\lambda+io) \qquad (V.2.19)$$

such that

$$L_2 = 4i\pi^2\,\mathrm{Im}\,\hat{tr}\,\tau(\lambda,\lambda,\lambda-io)\frac{d}{d\lambda}\tau(\lambda,\lambda,\lambda+io) \qquad (V.2.20)$$

The unitarity equation in reduced space takes the following forms,

$$\tau(E,E',\lambda-io)-\tau(E,E',\lambda+io) = -2\pi i\,\tau(E,\lambda,\lambda-io)\,\tau(\lambda,E',\lambda+io) \qquad (V.2.21)$$

$$= -2\pi i\,\tau(E,\lambda,\lambda+io)\,\tau(\lambda,E',\lambda-io) \qquad (V.2.21')$$

We then take energy derivatives $\partial/\partial E'$ with respect to equation 21 and $\partial/\partial E$ with respect to 21'. Next we put $E = E' = \lambda$ in both equations. Taking the trace of both resulting equations and add, we obtain:

$$\hat{tr}\left(\tau(\lambda,\dot{\lambda},\lambda-io)-\tau(\lambda,\dot{\lambda},\lambda+io)\right) + \hat{tr}\left(\tau(\dot{\lambda},\lambda,\lambda-io)-\tau(\dot{\lambda},\lambda,\lambda+io)\right)$$

$$= -2\pi i\left(\hat{tr}\,\tau(\lambda,\lambda,\lambda-io)\,\tau(\lambda,\dot{\lambda},\lambda+io) + \hat{tr}\,\tau(\dot{\lambda},\lambda,\lambda+io)\,\tau(\lambda,\lambda,\lambda-io)\right)$$

$$(V.2.22)$$

Or, $\hat{tr}\left(\tau(\dot{\lambda},\dot{\lambda},\lambda-io)-\tau(\dot{\lambda},\dot{\lambda},\lambda+io)\right)$

$$= -2\pi i\left(\hat{tr}\,\tau(\lambda,\lambda,\lambda-io)\,\tau(\lambda,\dot{\lambda},\lambda+io) + \hat{tr}\,\tau(\lambda,\lambda,\lambda-io)\,\tau(\dot{\lambda},\lambda,\lambda+io)\right)$$

$$= -2\pi i\,\hat{tr}\,\tau(\lambda,\lambda,\lambda-io)\,\tau(\dot{\lambda},\dot{\lambda},\lambda+io)$$

$$(V.2.23)$$

Since the left side is explicitly pure imaginary, the real part of right side must be zero. Hence, we obtain equation (V.2.19).

Gathering all the results in equations 15 and 20, we have

$$
\begin{aligned}
\lim_{\mu\to 0^+} L &= -2\pi i \, \mathrm{Re} \frac{\partial}{\partial\lambda} \hat{tr}\, \tau(\lambda,\lambda,\lambda+i0) \\
&\quad + (2\pi)^2 i \, \mathrm{Im} \, \hat{tr}\, \tau(\lambda,\lambda,\lambda-i0) \frac{d}{d\lambda} \tau(\lambda,\lambda,\lambda+i0) \\
&= i \, \mathrm{Im} \, \hat{tr}\, s^{\dagger}(\lambda) \frac{\partial}{\partial\lambda} s(\lambda) \\
&= i \, \hat{tr}\, s^{+}(\lambda) \frac{d}{d\lambda} s(\lambda) \qquad (V.2.24)
\end{aligned}
$$

where we have used $s(\lambda) = e - 2\pi i \, \tau(\lambda,\lambda,\lambda+i0)$.

Using the form of time delay in (V.1.1) we recovers (II.2.31).

$$2 \, \mathrm{Im} \, tr\left[R(\lambda+i0) - R_0(\lambda+i0)\right] = \hat{tr}\, q(\lambda)$$

We have arrived at the spectral property of time delay for the two body problem using Cayley transform.

We note here the prominent features of this derivation. They will appear again in the three body case together with many other new features. Firstly, we note the mathematical procedure involved in forming the energy conserving delta functions, i.e. $\frac{\mu}{(E-\lambda)^2+\mu^2} \longrightarrow \pi\delta(E-\lambda)$ as $\mu \to 0^+$. The energy conserving delta function must be present for the formation of time delay which is fully on-shell. Secondly, we want to note the necessity of the unitarity equation (V.2.19) in forming the total derivative in L_2. This is not needed in L_1 , which is a total derivative. It is useful to bear these points in mind when studying the next section on three body Cayley Transform. This will help to identify the new features as one goes from two body to three body problem.

V.3 Three body Cayley transform

Because of the length of this section, we would introduce subsections to help clarify the material. All equations in this section will be labelled without reference to the chapter. "Disconnectedness" is treated in the context of Cayley transform in the first subsection. To develop the channel structure, the resulting Cayley transform is evaluated by dividing the volume of integration in the trace and internal states into five disjoint subsets. In the three to three channel, we encounter a new mathematical problem of regularization in the rescattering terms. The two-bodylike channels are treated in about the same fashion as the last section with the two body problem. The double poles that develop here are cancelled by similar poles in the unitarity equation in the following subsection. The three body unitarity equation also contains the same channel structure as the Cayley transform itself. It is also evaluated in five disjoint subsets.

V.3.1. Connectedness

In generalizing the Cayley transform method to the three body problem, the first noticeable difference we encounter is the existence of disconnected terms in the scattering amplitude. This type of singularity exists even in the absence of two body bound state channels. It is an inherent three body scattering characteristic. Of course, disconnectedness persists in all N-body scattering for $N \geqq 3$.

One first come across with this singularity when examining the structure of the three body scattering amplitude $M_{\alpha\beta}(z)$. The mathematical signiture of disconnectedness is the presence of a delta function in the momentum vector. The delta function is singular in the forward scattering direction, i.e. with zero momentum transfer. Faddeev determined that $M_{\alpha\beta}(z) = \delta_{\alpha\beta} T_\alpha(z) + W_{\alpha\beta}(z)$ where $W_{\alpha\beta}(z)$ is free of delta functions. The kernel of this equation is

$$M_{\alpha\beta}(\vec{p}_\alpha \vec{q}_\alpha ; \vec{p}_\beta' \vec{q}_\beta' ; z) = \delta_{\alpha\beta} T_\alpha(\vec{p}\vec{q} ; \vec{p}'\vec{q}' ; z) + W_{\alpha\beta}(\vec{p}_\alpha \vec{q}_\alpha ; \vec{p}_\alpha' \vec{q}_\alpha' ; z) \qquad (3.1.1)$$

The first term is disconnected.

$$T_\alpha(\vec{p}\vec{q} ; \vec{p}'\vec{q}' ; z) = \delta(\vec{p}_\alpha - \vec{p}_\alpha') \, t_\alpha(\vec{q}_\alpha ; \vec{q}_\alpha' ; z - \tilde{p}_\alpha^2) \qquad (3.1.2)$$

The energy of the α-pair is $z - \tilde{p}_\alpha^2$, i. e. less by the amount of kinetic energy of the spectator particle $\tilde{p}_\alpha^2$.

In this representation, it is easy to interpret the physics of disconnectedness. It describe the possible scattering where particles β and γ (i.e. α pair) scatters while the α particle does not interact with either one of them. It acts merely as a spectator whose presence makes the otherwise two body scattering into a three body event.

Before we derive the Cayley tranform results, we want to point out that while disconnectedness exists in the absence of two body bound states, it is not separable from the bound state channels. That is, it is present in all four channels, $\alpha = 0, 1, 2, 3$. In the presence of two body bound state the $T_\alpha(z)$ we have just examined takes on a more complicated kernel.

$$T_\alpha(\vec{p}\vec{q}\,;\vec{p}'\vec{q}'\,;z) = \delta(\vec{p}_\alpha - \vec{p}_\alpha')\left[\frac{\varphi_\alpha(\vec{q}_\alpha)\,\varphi_\alpha(\vec{q}_\alpha')}{(z-\tilde{p}_\alpha^2)-(\vec{q}_\alpha^2-\varkappa_\alpha^2)} + \hat{t}_\alpha(\vec{q}_\alpha,\vec{q}_\alpha',z-\tilde{p}_\alpha^2)\right] \quad (3.1.3)$$

where $\hat{t}_\alpha(\vec{q}_\alpha,\vec{q}_\alpha',z-\tilde{p}_\alpha^2)$ is a smooth function. The first term has both delta function and channel singularity. We shall see that this particular structure plays a significant role in the following derivation. It provides for the linear term for the $\alpha = 1, 2, 3$. channels from the quadratic term. The linear term from the three body Cayley transform, as we shall see, provides for only the $\alpha = 0$ channel.

Now we shall start deriving the three body Cayley transform. If one repeats the two body derivation of equation (V.2.9) using three body operators instead, one arrives at similar results. The only input in the making of (V.2.9) are the definitions of resolvents and Cayley transform and the unitarity equation which are basic to both two and three body scattering theory. Specifically, if one use $R(z)$, $R_0(z)$ and $T(z)$ instead of $r(z)$, $r_0(z)$ and $t(z)$ respectively, one arrives at

$$\left[R(z) - R(z^*)\right] - \left[R_0(z) - R_0(z^*)\right] = B^{+}_{H_0}(z)\left[A^{+}_{H/H_0}(z)\,\frac{\partial}{\partial\lambda}\,A_{H/H_0}(z)\right]B_{H_0}(z) \quad (3.1.4)$$

where $B_{H_0}(z) = E + 2i\mu\, R_0(z)$

$A_{H/H_0}(z) = E - 2i\mu\, R_0(z)\, T(z)\, R_0(z^*)$

If one uses $R_\alpha(z)$, $R_0(z)$ and $T_\alpha(z)$ instead of $r(z)$, $r_0(z)$ and $t(z)$ respectively, one arrives at

$$\left[R_\alpha(z) - R_\alpha(z^*)\right] - \left[R_0(z) - R_0(z^*)\right] = B^{\dagger}_{H_0}(z)\left[A^{\dagger}_{H_\alpha/H_0}(z)\,\frac{\partial}{\partial\lambda}\,A_{H_\alpha/H_0}(z)\right]B_{H_0}(z) \qquad (3.1.5)$$

where $A_{H_\alpha/H_0}(z) = E - 2i\mu\, R_0(z)\, T_\alpha(z)\, R_0(z^*)$.

Both $R_0(z)$ and E conserve 6-momentum ($\vec{p}_\alpha$, $\vec{q}_\alpha$) so that $B_{H_0}(z)$ also conserves ($\vec{p}$, $\vec{q}$). $T_\alpha(z)$ conserves only the momentum of the α particle $\vec{p}_\alpha$ and hence $A_{H_\alpha/H_0}(z)$ conserves $\vec{p}_\alpha$. Each of the kernel of the four operators on the right of (3.1.5) conserves $\vec{p}_\alpha$, so that equation 5 has a overall delta function $\delta(\vec{p}_\alpha - \vec{p}_\alpha')$ and hence is disconnected.

(3.1.4) also contains some disconnected terms since $T(z)$ contains $T_\alpha(z)$. However, if we substract (3.1.5)from (3.1.4) we can arrive at an equation free of disconnectedness.

$$\left[R(z) - R(z^*)\right] - \left[R_0(z) - R_0(\bar{z})\right] - \sum_{\alpha=1}^{3}\left\{\left[R_\alpha(z) - R_\alpha(z^*)\right] - \left[R_0(z) - R_0(z^*)\right]\right\}$$

$$= B^{\dagger}_{H_0}(z)\left[A^{\dagger}_{H/H_0}(z)\,\frac{\partial}{\partial\lambda}\,A_{H/H_0}(z) - \sum_{\alpha=1}^{3} A^{\dagger}_{H_\alpha/H_0}(z)\,\frac{\partial}{\partial\lambda}\,A_{H_\alpha/H_0}(z)\right]B_{H_0}(z) \qquad (3.1.6)$$

To develop further, one must put in the value of the A 's in terms of resolvents and T-matrices.

$$\left[A^{\dagger}_{H/H_0}(z)\,\frac{\partial}{\partial\lambda}\,A_{H/H_0}(z) - \sum_{\alpha=1}^{3} A^{\dagger}_{H_\alpha/H_0}(z)\,\frac{\partial}{\partial\lambda}\,A_{H_\alpha/H_0}(z)\right]$$

$$= \left[E - 2i\mu\, R_0(z)\, T(z)\, R_0(z^*)\right]^{\dagger}\frac{\partial}{\partial\lambda}\left[-2i\mu\, R_0(z)\, T(z)\, R_0(z^*)\right]$$

$$- \sum_{\alpha=1}^{3}\left[E - 2i\mu\, R_0(z)\, T_\alpha(z)\, R_0(z^*)\right]^{\dagger}\frac{\partial}{\partial\lambda}\left[-2i\mu\, R_0(z)\, T_\alpha(z)\, R_0(z^*)\right]$$

$$= \frac{\partial}{\partial\lambda}\left[-2i\mu\, R_0(z)\left(T(z) - \sum_{\alpha=1}^{3} T_\alpha(z)\right)R_0(z^*)\right]$$

$$+ (2\mu)^2\, R_0(z)\left(W(z^*) + \sum_{\alpha=1}^{3} T_\alpha(z^*)\right)R_0(z^*)\,\frac{\partial}{\partial\lambda}\left[R_0(z)\left(W(z) + \sum_{\alpha=1}^{3} T_\alpha(z)\right)R_0(z^*)\right]$$

$$- \sum_{\alpha=1}^{3}(2\mu)^2\, R_0(z)\, T_\alpha(z^*)\, R_0(z^*)\,\frac{\partial}{\partial\lambda}\left[R_0(z)\, T_\alpha(z)\, R_0(z^*)\right]$$

$$
\begin{aligned}
= \; & -2i\mu \frac{\partial}{\partial\lambda} R_o(z)\, W(z)\, R_o(z^*) \\
& + (2\mu)^2 R_o(z)\, W(z^*)\, R_o(z^*) \frac{\partial}{\partial\lambda} R_o(z)\, W(z)\, R_o(z^*) \\
& + (2\mu)^2 R_o(z) \sum_{\alpha=1}^{3} T_\alpha(z^*)\, R_o(z^*) \frac{\partial}{\partial\lambda} R_o(z)\, W(z)\, R_o(z^*) \\
& + (2\mu)^2 R_o(z)\, W(z^*)\, R_o(z^*) \frac{\partial}{\partial\lambda} R_o(z) \sum_{\alpha=1}^{3} T_\alpha(z)\, R_o(z^*) \\
& + \sum_{\alpha\neq\beta} (2\mu)^2 R_o(z)\, T_\alpha(z^*)\, R_o(z^*) \frac{\partial}{\partial\lambda} R_o(z)\, T_\beta(z)\, R_o(z^*)
\end{aligned}
\qquad (3.1.7)
$$

where we have used $T(z) = \sum_{\alpha=1}^{3} T_\alpha(z) + W(z)$, $W(z) = \sum_{\alpha,\beta} W_{\alpha\beta}(z)$.

All of the terms are connected. Now we are able to sum over all the diagonal elements of the operator equation above. An inspection of the trace of the left hand side of equation 7 shows that it is explicitly a pure imaginary number. Hence, the real part of the right hand side must vanish. To evaluate the resulting Cayley transform we rearrange the terms as follows:

$$
2i \,\mathrm{Im}\, \mathrm{Tr}\Big[R(z) - R_o(z) - \sum_{\alpha>0}\big(R_\alpha(z) - R_o(z)\big)\Big] = A + B + C + D + F \qquad (3.1.8)
$$

where $A = \mathrm{Tr} \frac{\partial}{\partial\lambda} -2i\mu\, R_o(z)\, W(z)\, R_o(z^*)$

$$
\begin{aligned}
B = \mathrm{Tr} \Big\{ & 4\mu^2 R_o(z)\, W(z^*)\, R_o(z^*) \Big[\Big(\frac{\partial}{\partial\lambda} R_o(z)\Big) W(z)\, R_o(z^*) + R_o(z)\, W(z) \frac{\partial}{\partial\lambda} R_o(z^*)\Big] \\
& + 4\mu^2 R_o(z) \sum_\alpha T_\alpha(z^*)\, R_o(z^*) \Big[\Big(\frac{\partial}{\partial\lambda} R_o(z)\Big) W(z)\, R_o(z^*) + R_o(z)\, W(z) \frac{\partial}{\partial\lambda} R_o(z^*)\Big] \\
& + 4\mu^2 R_o(z)\, W(z^*)\, R_o(z^*) \Big[\Big(\frac{\partial}{\partial\lambda} R_o(z)\Big) \sum_\alpha T_\alpha(z)\, R_o(z^*) + R_o(z) \sum_\alpha T_\alpha(z) \frac{\partial}{\partial\lambda} R_o(z^*)\Big] \\
& + \sum_{\alpha\neq\beta} 4\mu^2 R_o(z)\, T_\alpha(z^*)\, R_o(z^*) \Big[\Big(\frac{\partial}{\partial\lambda} R_o(z)\Big) T_\beta(z)\, R_o(z^*) + R_o(z)\, T_\beta(z) \frac{\partial}{\partial\lambda} R_o(z^*)\Big] \Big\}
\end{aligned}
$$

$$
C = \mathrm{Tr}\; 4\mu^2 R_o(z)\, W(z^*)\, R_o(z^*)\, R_o(z) \Big(\frac{\partial}{\partial\lambda} W(z)\Big) R_o(z^*)
$$

$$
D = \mathrm{Tr}\; 4\mu^2 R_o(z) \Big(\sum_\alpha T_\alpha(z^*)\Big) R_o(z^*)\, R_o(z) \Big(\frac{\partial}{\partial\lambda} W(z)\Big) R_o(z^*)
$$

$$
E = \mathrm{Tr}\; 4\mu^2 R_o(z)\, W(z^*)\, R_o(z^*)\, R_o(z) \Big(\frac{\partial}{\partial\lambda} \sum_\alpha T_\alpha(z)\Big) R_o(z^*)
$$

$$
F = \mathrm{Tr}\; 4\mu^2 \sum_{\alpha\neq\beta} R_o(z)\, T_\alpha(z^*)\, R_o(z^*)\, R_o(z) \frac{\partial T_\beta(z)}{\partial\lambda} R_o(z^*)
$$

V.3.2 Channel singularities

There are two different types of resolvents in Cayley transform. $R_o(z)$ and its complex conjugate $R_o(z^*)$ signify the free 0-channel. $\tilde{R}_\alpha(z) = (\tilde{H}_\alpha - z)^{-1}$ and $\tilde{R}_\alpha(z^*)$ denotes the presence of the two body-like channels 1, 2 and 3. $R_o(z)$ are found explicitly in the definition of Cayley tranform and also in the kernel of $W(z)$. $\tilde{R}_\alpha(z)$ is found only in the kernel of $T_\alpha(z)$ and $W(z)$. In the limit $\mu \to 0^+$ these resolvents may be singular if $\lambda = E_o$ or $\lambda = E_\alpha$ ($\alpha = 1,2,3$)

In the linear term A , there is a six dimensional integration $\int d\vec{p}\, d\vec{q}$ from the trace. For a fixed λ , the volume of integration does contain the points $\lambda = E_o$, E_1 , E_2, E_3 . We define arbitrarily small neighbourhoods θ_o , θ_1 , θ_2 and θ_3 around the points $\lambda = E_o$, E_1 , E_2 and E_3 respectively. We call the remaining volume of integration Θ , i.e.

$$\Theta \cup \theta_1 \cup \theta_2 \cup \theta_3 \cup \theta_o = \text{volume of integration} \qquad (3.2.1)$$

In Θ all resolvents are finite and well defined. In the limit $\mu \to 0^+$, A vanishes in Θ linearly as μ . In θ_o , only R_o may contribute. $\tilde{R}_\alpha$ is finite in θ_o and can be ignored. Similarly, in θ_α , only $\tilde{R}_\alpha$ may contribute.

In a quadratic term, there are two six-dimensional integrations: $\int d\vec{p}\, d\vec{q}$ for the trace and $\int d\vec{p}'\, d\vec{q}'$ from the integration over the internal states. For these terms we have two sets of neighbourhoods θ_o , θ_1 , θ_2 , θ_3 and θ_o' , θ_1' , θ_2' , θ_3' . In either Θ or Θ' , the quadratic terms vanish quadratically as $\mu^2 \to 0^+$.

To evaluate the Cayley transform one only need to find contributions from the neighbourhoods θ_0 , θ_1 , θ_2 and θ_3 in the linear term A and $\sum_{\alpha,\beta} \theta_\alpha \cup \theta'_\beta$ (α , β $= 1, 2, 3$) in the quadratic terms. We choose to evaluate θ_0 and $\theta_0 \cup \theta'_0$ contribution first. They contain the only contribution if two body bound states do not exist. Moreover, they are richer in structure. They contain rescattering structure which needs special attention.

V.3.3 Term β

Before we begin we would like to eliminate the term β. It is similar to the remainder R in (V.2.17) in the two body case. It is a real number though a close scrutiny of β does show that the operators are in the wrong order. We shall simplify β so that it would be explicitly real.

To begin, we start with the connected unitarity equation.

$$T(z) - T(z^*) - \sum_{\alpha=1}^{3}\left(T_\alpha(z) - T_\alpha(z^*)\right)$$
$$= (\bar{z}-z)\left\{ T(z)\, R_0(z^*)\, R_0(z)\, T(z^*) - \sum_{\alpha=1}^{3} T_\alpha(z)\, R_0(z^*)\, R_0(z)\, T_\alpha(z^*)\right\} \tag{3.3.1}$$

Pre-multiply by $\frac{\partial}{\partial\lambda}R_0(z)$ and post-multiply by $R_0(z^*)$. Then we rearrange in terms of $T_\alpha(z)$ and $W(z)$ only.

$$\left(\frac{\partial}{\partial\lambda}R_0(z)\right)\left(W(z) - W(z^*)\right) R_0(z^*)$$
$$= (\bar{z}-z)\left(\frac{\partial}{\partial\lambda}R_0(z)\right)\Big\{ W(z)\, R_0(z^*) R_0(z)\, W(z^*) + \sum_\alpha T_\alpha(z)\, R_0(z^*) R_0(z)\, T_\alpha(z^*)$$
$$+ W(z)\, R_0(z^*) R_0(z) \sum_\alpha T_\alpha(z^*) + \sum_{\alpha\neq\beta} T_\alpha(z)\, R_0(z^*)\, R_0(z)\, T_\beta(z^*)\Big\} \tag{3.3.2}$$

The trace of the right hand side is equal to one half of β after three cyclic permutations.

$$\mathrm{Tr}\; R_0(z^*)\left(\frac{\partial}{\partial\lambda}R_0(z)\right)\left(W(z) - W(z^*)\right)$$
$$= (\bar{z}-z)\;\mathrm{Tr}\Big\{ R_0(z)\; W(z^*)\, R_0(z^*)\left(\frac{\partial}{\partial\lambda}R_0(z)\right) W(z)\; R_0(z^*) +$$
$$+ R_0(z) \sum_\alpha T_\alpha(z^*) R_0(z^*)\left(\frac{\partial}{\partial\lambda}R_0(z)\right) W(z)\, R_0(z^*) + R_0(z)\, W(z^*)\, R_0(z^*)\left(\frac{\partial}{\partial\lambda}R_0(z)\right)\sum_\alpha T_\alpha(z)\, R_0(z^*)$$
$$+ \sum_{\alpha\neq\beta} R_0(z)\, T_\alpha(z^*)\, R_0(z^*)\left(\frac{\partial}{\partial\lambda}R_0(z)\right) T_\beta(z)\, R_0(z^*) \tag{3.3.3}$$

To arrive at the other half of β, one must start with the other form of the unitarity equation, where the order of $T(z^*)$ and $T(z)$ is interchanged in the quadratic term.

$$T(z) - T(z^*) - \sum_\alpha \left[T_\alpha(z) - T_\alpha(z^*) \right]$$
$$= (z^* - z)\left\{ T(z^*) R_o(z^*) R_o(z) T(z) - \sum_\alpha T_\alpha(z^*) R_o(z^*) R_o(z) T_\alpha(z) \right\} \tag{3.3.4}$$

Pre-multiply by $R_o(z)$ and post-multiply by $\frac{\partial}{\partial\lambda} R_o(z^*)$. Then we following the preceeding procedure to arrive at

$$T_\lambda \left(\frac{\partial}{\partial\lambda} R_o(z^*) \right) R_o(z) \Big(W(z) - W(z^*) \Big)$$
$$= (z^* - z)\, T_\lambda \Big\{ R_o(z)\, W(z^*)\, R_o(z^*)\, R_o(z)\, W(z) \frac{\partial}{\partial\lambda} R_o(z^*) \; +$$
$$+ R_o(z) \sum_\alpha T_\alpha(z^*) R_o(z^*) R_o(z) W(z) \frac{\partial}{\partial\lambda} R_o(z^*) + R_o(z) W(z^*) R_o(z^*) R_o(z) \sum_\alpha T_\alpha(z) \frac{\partial}{\partial\lambda} R_o(z^*)$$
$$+ \sum_{\alpha\neq\beta} R_o(z)\, T_\alpha(z^*)\, R_o(z^*)\, R_o(z)\, T_\beta(z) \frac{\partial}{\partial\lambda} R_o(z^*) \Big\} \tag{3.3.5}$$

Combining equation 3 and 5, we have the entire term B on the right hand side.

$$T_\lambda\, (z^* - z)\, \frac{\partial}{\partial\lambda}\Big(R_o(z^*) R_o(z) \Big) \Big(W(z) - W(z^*) \Big) = B \tag{3.3.6}$$

Now we have a compact form of B which is explicitly real.

V.3.4 Contribution from $\theta_0 \cup \theta_0'$

In the neighbourhoods $\theta_0 \cup \theta_0'$, we expect to find all the three-to-three channel contributions. As we have noted many times before, this particular channel provides the most mathematical challenge to investigate. First of all, it does contain the "normal" contributions one would come to expect as a projection from the two body case. The resolvents do in some terms form simple energy conserving delta functions. However, in the rescattering terms other resolvents get on the same energy shell as those forming the delta function. Together they form generalized functions that are no longer simple delta functions. The seeking of meaningful generalized functions from these new resolvent groups is called regularization.

Before we start to diverge to the lengthy process of regularization, we should calculate the contributions from the "normal" terms first. The reason why these are consider normal while others are to be regularized will be clear later when we define rescattering. We here now list and calculate the terms in (V.3.1.8) in the neighbourhood $\theta_0 \cup \theta_0'$, less all rescattering terms. The subscript oo denotes the neighbourhood and primed letters denote the absence of rescattering terms.

Introduce the notation $\widetilde{W}(z)$ used by Faddeev,

$$W(z) = \sum_{\alpha \neq \beta} Q^{(1)}_{\alpha\beta}(z) + \widetilde{W}(z) \tag{3.4.1}$$

where

$$Q^{(1)}_{\alpha\beta}(z) = - T_\alpha(z) R_0(z) T_\beta(z) \tag{3.4.2}$$

$$A_0' = Tr \frac{\partial}{\partial\lambda}(-2i\mu)\, R_0(z)\, \tilde{W}(z)\, R_0(z^*)$$

$$C_{00}' = Tr\, 4\mu^2 R_0(z)\left[\sum_{\alpha\neq\beta} Q^{(1)}_{\alpha\beta}(z^*) + \tilde{W}(z^*)\right] R_0(z^*) R_0(z) \times$$

$$\times \frac{\partial}{\partial\lambda}\left[\sum_{\gamma\neq\delta} Q^{(1)}_{\gamma\delta}(z) + \tilde{W}(z)\right] R_0(z^*)$$

with the stipulation that either $\alpha \neq \delta$ or $\beta \neq \gamma$.

$$D_{00}' = Tr\, 4\mu^2 \sum_\alpha R_0(z)\, T_\alpha(z^*) R_0(z^*) R_0(z) \frac{\partial}{\partial\lambda}\left[\sum_{\gamma\neq\delta} Q^{(1)}_{\gamma\delta}(z) + \tilde{W}(z)\right] R_0(z^*)$$

with $\alpha \neq \gamma$ and $\alpha \neq \delta$.

(i.e. for $T_1(z^*)$ we have only $Q^{(1)}_{23}(z)$ and $Q^{(1)}_{32}(z)$.)

$$E_{00}' = Tr\, 4\mu^2 R_0(z)\left[\sum_{\gamma\neq\delta} Q^{(1)}_{\gamma\delta}(z^*) + \tilde{W}(z^*)\right] R_0(z^*) R_0(z)\left[\frac{\partial}{\partial\lambda} T_\beta(z)\right] R_0(z^*)$$

with $\beta \neq \gamma$ and $\beta \neq \delta$ again. (3.4.3)

The term B is already shown to vanish and F is a rescattering term.

The limit $\mu \to 0^+$ can now be taken trivially turning $\mu R_0(z) R_0(z^*)$ into $\pi\delta(H_0-\lambda)$.

$$A_0' = \int_{\theta_0} d\vec{p}\, d\vec{q}\, \frac{\partial}{\partial\lambda} - 2\pi i\, \delta(E_0-\lambda)\, \tilde{W}(\vec{p}\vec{q}\,;\vec{p}\vec{q}\,;\lambda+i0)$$

$$= -2\pi i \frac{\partial}{\partial\lambda} \hat{tr}_0\, \tilde{\mathcal{W}}(\lambda,\lambda,\lambda+i0)$$

$$C_{00}' = \int_{\theta_0} d\vec{p}\, d\vec{q} \int_{\theta_0'} d\vec{p}\,'\, d\vec{q}\,'\; 4\pi^2\, \delta(E_0-\lambda)\left[\sum_{\alpha\neq\beta} Q^{(1)}_{\alpha\beta}(\vec{p}\vec{q}\,;\vec{p}\,'\vec{q}\,';\lambda-i0) + \right.$$

$$\left.\tilde{W}(\vec{p}\vec{q}\,;\vec{p}\,'\vec{q}\,';\lambda-i0)\right] \times \delta(E_0'-\lambda)\left[\sum_{\gamma\neq\delta} Q^{(1)}_{\gamma\delta}(\vec{p}\,'\vec{q}\,';\vec{p}\vec{q}\,;\dot{\lambda}+i0) + \right.$$

$$\left.\tilde{W}(\vec{p}\,'\vec{q}\,';\vec{p}\vec{q}\,;\dot{\lambda}+i0)\right]$$

$$= 4\pi^2\, \hat{tr}_0\left[\sum_{\alpha\neq\beta} \mathcal{Q}^{(1)*}_{\beta\alpha}(\lambda,\lambda,\lambda+i0) + \tilde{\mathcal{W}}^*(\lambda,\lambda,\lambda+i0)\right] \times$$

$$\times \left[\sum_{\gamma\neq\delta} \mathcal{Q}^{(1)}_{\gamma\delta}(\lambda,\lambda,\dot{\lambda}+i0) + \tilde{\mathcal{W}}(\lambda,\lambda,\dot{\lambda}+i0)\right]$$

with $\alpha \neq \delta$ or $\beta \neq \gamma$.

$$D'_{oo} = \int_{\theta_o} d\vec{p}\, d\vec{q} \int_{\theta'_o} d\vec{p}'\, d\vec{q}'\ 4\pi^2\ \delta(E_o-\lambda)\ \sum_\alpha T_\alpha(\vec{p}\vec{q};\vec{p}'\vec{q}';\lambda-io)$$

$$\times\ \delta(E'_o-\lambda)\left[\sum_{\gamma\neq\delta} Q^{(I)}_{\gamma\delta}(\vec{p}'\vec{q}';\vec{p}\vec{q};\dot{\lambda}+io) + \widetilde{W}(\vec{p}'\vec{q}';\vec{p}\vec{q};\dot{\lambda}+io)\right]$$

$$= 4\pi^2\ \hat{tr}_o\ \sum_\alpha \mathcal{T}^*_\alpha(\lambda,\lambda,\lambda+io)\left[\sum_{\gamma\neq\delta} \mathcal{Q}^{(I)}_{\gamma\delta}(\lambda,\lambda,\dot{\lambda}+io) + \right.$$

$$\left. +\ \widetilde{\mathcal{W}}(\lambda,\lambda,\dot{\lambda}+io)\right]$$

with $\alpha\neq\gamma$ and $\alpha\neq\delta$.

$$E'_{oo} = 4\pi^2\ \hat{tr}_o\left[\sum_{\gamma\neq\delta}\mathcal{Q}^{(I)*}_{\gamma\delta}(\lambda,\lambda,\lambda+io) + \widetilde{\mathcal{W}}^*(\lambda,\lambda,\lambda+io)\right]\times$$

$$\times\ \sum_\alpha \mathcal{T}_\alpha(\lambda,\lambda,\dot{\lambda}+io)$$

with $\alpha\neq\gamma$ and $\alpha\neq\delta$. (3.4.4)

For notational convenience the momentum delta functions $\delta(\vec{p}_\alpha-\vec{p}_\alpha')$ in $T_\alpha(\vec{p}\vec{q};\vec{p}'\vec{q}';\lambda+io)$ or $\mathcal{T}_\alpha(\lambda,\lambda,\lambda+io)$ have been left unintegrated.

Having dispose of the "normal" terms, we can now work on the rescattering terms. By rescattering we mean terms with only one T_α and one T_β and a number of resolvents in between and around them. Because of the unitarity condition,

$$2i\,\mathcal{I}m\,T_\alpha(z) = T_\alpha(z) - T_\alpha(z^*) = (z^*-z)\ T_\alpha(z)\,R_o(z)\,R_o(z^*)\,T_\alpha(z^*)$$

two T_α 's appearing as on the right may act as only one T_α . The diagonal element of a rescattering term has all its resolvents on the same energy shell. The integration over internal states between T_α and T_β is done trivially by the momentum delta functions $\delta(\vec{p}_\alpha-\vec{p}_\alpha')\,\delta(\vec{p}_\beta-\vec{p}_\beta')$,

i.e. $\int d\vec{p}'d\vec{q}'\ \delta(\vec{p}_\alpha-\vec{p}_\alpha')\,\delta(\vec{p}_\beta-\vec{p}_\beta')\,f(\vec{p}\vec{q};\vec{p}'\vec{q}';z) = f(\vec{p}\vec{q};\vec{p}\vec{q};z)$.

To be specific during the course of this thesis, by rescattering terms we mean the following list of terms. Together with (3.4.3) they form the entire contribution of (3.1.8) in $\theta_0 \cup \theta_0'$.

$$A_0'' = \mathrm{Im} \sum_{\alpha \neq \beta} Tr_{\theta_0} \frac{\partial}{\partial \lambda} (-2i\mu)\, R_0(z) \left[- T_\alpha(z) R_0(z) T_\beta(z) \right] R_0(z^*)$$

$$C_{00}'' = \mathrm{Im} \sum_{\alpha \neq \beta} Tr_{\theta_0} 4\mu^2 \, R_0(z) \left[- T_\alpha(z^*) R_0(z^*) T_\beta(z^*) \right] R_0(z^*)\, R_0(z) \times$$
$$\times \left[- T_\beta(z) R_0(z)\, T_\alpha(z) \right] R_0(z^*)$$

$$D_{00}'' = \mathrm{Im} \sum_{\alpha \neq \beta} Tr_{\theta_0} 4\mu^2 \, R_0(z)\, T_\alpha(z^*)\, R_0(z^*)\, R_0(z)\, \frac{\partial}{\partial \lambda} \left[- T_\alpha(z) R_0(z) T_\beta(z) \right.$$
$$\left. - T_\beta(z) R_0(z) T_\alpha(z) \right] R_0(\bar{z})$$

$$E_{00}'' = \mathrm{Im} \sum_{\alpha \neq \beta} Tr_{\theta_0} 4\mu^2 \, R_0(z) \left[- T_\alpha(z^*) R_0(z^*) T_\beta(z^*) - T_\beta(z^*) R_0(z^*) T_\alpha(z^*) \right] \times$$
$$\times R_0(z^*) R_0(z) \left[\frac{\partial}{\partial \lambda} T_\beta(z) \right] R_0(z^*)$$

$$F_{00}'' = \mathrm{Im} \sum_{\alpha \neq \beta} Tr_{\theta_0} 4\mu^2 \, R_0(z)\, T_\alpha(z^*)\, R_0(z^*) R_0(z) \left[\frac{\partial}{\partial \lambda} T_\beta(z) \right] R_0(z^*)$$
$$= F \tag{3.4.5}$$

To facilitate the calculation we have explicitly stated that we will only work with the imaginary part of (3.1.8) since we have shown that it is pure imaginary. This is only one of the many important steps we have taken to shorten the otherwise laborious derivation. We list here all the meaningful generalized functions that we shall use and some short hand notations.

(a) $\pi \delta_\mu(x) = \dfrac{\mu}{x^2+\mu^2}$, such that $\lim\limits_{\mu \to 0^+} \pi \delta_\mu(x) = \pi \delta(x)$

(b) $\dfrac{P_\mu}{x} = \dfrac{x}{x^2+\mu^2}$, such that $\lim\limits_{\mu \to 0^+} \dfrac{P_\mu}{x} = \dfrac{P}{x}$ the principle value function.

and $\frac{1}{x \pm i\mu} = \frac{x \mp i\mu}{x^2+\mu^2} = \frac{P_\mu}{x} \mp i\pi\delta_\mu(x)$.

(c) $\pi\delta_\mu'(x) = \pi\frac{\partial}{\partial x}\delta_\mu(x) = -\frac{(-2\mu x)}{(x^2+\mu^2)^2}$

(d) $\frac{P_\mu}{x^2} = -\frac{\partial}{\partial x}\frac{P_\mu}{x} = -\frac{\partial}{\partial x}\frac{x}{x^2+\mu^2} = \frac{x^2-\mu^2}{(x^2+\mu^2)^2}$

and $\frac{1}{(x\pm i\mu)^2} = \frac{P_\mu}{x^2} \pm i\pi\delta_\mu'(x)$

(e) $\pi\delta_\mu''(x) = \pi\frac{\partial^2}{\partial x^2}\delta_\mu(x) = \frac{2\mu(3x^2-\mu^2)}{(x^2+\mu^2)^3}$

Define

$$t_\alpha \equiv t_\alpha(\vec{q}_\alpha, \vec{q}_\alpha, \lambda+i\mu-\hat{p}_\alpha^2)$$

$$\begin{aligned}\delta(\vec{p}_\alpha-\vec{p}_\alpha')\, s_\alpha(\vec{q}_\alpha, \vec{q}_\alpha', \lambda+i\mu-\hat{p}_\alpha^2) &\equiv \langle \vec{p}\vec{q}|\, \mu\, T_\alpha(z^*) R_0(z) R_0(z^*) \frac{\partial}{\partial\lambda} T_\alpha(z) |\vec{p}'\vec{q}'\rangle \\ &= \int d\vec{p}_\alpha'' d\vec{q}_\alpha''\, \pi\delta_\mu(E_0''-\lambda)\, \delta(\vec{p}_\alpha-\vec{p}_\alpha'')\, t_\alpha(\vec{q}_\alpha, \vec{q}_\alpha'', \lambda-i\mu-\hat{p}_\alpha^2) \\ &\quad\times \frac{\partial}{\partial\lambda}\delta(\vec{p}_\alpha''-\vec{p}_\alpha')\, t_\alpha(\vec{q}_\alpha'', \vec{q}_\alpha', \lambda+i\mu-\hat{p}_\alpha'^2) \\ &= \delta(\vec{p}_\alpha-\vec{p}_\alpha') \int d\vec{q}_\alpha''\, \pi\delta_\mu(\hat{p}_\alpha^2+\hat{q}_\alpha''^2-\lambda)\, t_\alpha(\vec{q}_\alpha, \vec{q}_\alpha'', \lambda-i\mu-\hat{p}_\alpha^2) \\ &\quad\times \frac{\partial}{\partial\lambda} t_\alpha(\vec{q}_\alpha'', \vec{q}_\alpha', \lambda+i\mu-\hat{p}_\alpha^2)\end{aligned}$$

$$s_\alpha \equiv s_\alpha(\vec{q}_\alpha, \vec{q}_\alpha, \lambda+i\mu-\hat{p}_\alpha^2)$$

Similarly, we associate $\bar{s}_\alpha$ for the elements of $\mu\left(\frac{\partial T_\alpha}{\partial\lambda}\right) R_0 R_0^+ T_\alpha^+$. s_α and $\bar{s}_\alpha$ will eventually yield the same result. At this stage of the calculation one should keep in mind the difference in the ordering of the operators $\mu T_\alpha(z^*) R_0(z) R_0(z^*) \frac{\partial}{\partial\lambda} T_\alpha(z)$ and $\mu\left(\frac{\partial}{\partial\lambda} T_\alpha(z)\right) R_0(z) R_0(z^*)\; T_\alpha(z^*)$.

In this new notation we are able to proceed with the calculation. We pay most attention to the behaviour of the resolvents.

$$A_0'' = \operatorname{Im} \sum_{\alpha\neq\beta} \operatorname{Tr}_{\theta_0} \frac{\partial}{\partial\lambda}\, 2i\mu\, R_0(z)\, T_\alpha(z)\, R_0(z)\, T_\beta(z)\, R_0(z^*)$$

$$= \mathcal{I}m \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q} \int_{\theta_0'} d\vec{p}'\, d\vec{q}' \frac{\partial}{\partial\lambda} \frac{2i\mu}{E_0-\lambda-i\mu} \delta(\vec{p}_\alpha - \vec{p}_\alpha') \, t_\alpha(\vec{q}_\alpha, \vec{q}_\alpha', \lambda+i\mu-\vec{p}_\alpha'^2)$$

$$\times \frac{1}{E_0'-\lambda-i\mu} \delta(\vec{p}_\beta-\vec{p}_\beta') \, t_\beta(\vec{q}_\beta', \vec{q}_\beta, \lambda+i\mu-\vec{p}_\beta^2) \frac{1}{E_0-\lambda+i\mu}$$

$$= \mathcal{I}m \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q} \frac{\partial}{\partial\lambda} \frac{-2i\mu}{E_0-\lambda-i\mu} \, t_\alpha(\vec{q}_\alpha, \vec{q}_\alpha, \lambda+i\mu-\vec{p}_\alpha^2)$$

$$\times \frac{1}{E_0-\lambda-i\mu} \, t_\beta(\vec{q}_\beta, \vec{q}_\beta, \lambda+i\mu-\vec{p}_\beta^2) \frac{1}{E_0-\lambda+i\mu}$$

$$= \mathcal{I}m \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q} \frac{\partial}{\partial\lambda} \, 2i \, t_\alpha \, t_\beta \, \pi\delta_\mu(E_0-\lambda) \frac{1}{E_0-\lambda-i\mu}$$

$$= \mathcal{A}_1 + \mathcal{A}_2 \tag{3.4.6}$$

where

$$\mathcal{A}_1 = \mathcal{I}m \sum_{\alpha\neq\beta} \frac{\partial}{\partial\lambda} \int_{\theta_0} d\vec{p}\, d\vec{q} \; 2i \, t_\alpha \, t_\beta \, \pi\delta_\mu(E_0-\lambda) \frac{P_\mu}{E_0-\lambda}$$

$$= \sum_{\alpha\neq\beta} \frac{\partial}{\partial\lambda} \int_{\theta_0} d\vec{p}\, d\vec{q} \; 2i \left(\mathcal{R}e \, t_\alpha t_\beta\right) \left(-\frac{\pi}{2}\right) \delta_\mu'(E_0-\lambda) \tag{3.4.7}$$

since $\pi\delta_\mu(E_0-\lambda) \frac{P_\mu}{E_0-\lambda} = \frac{\mu}{(E_0-\lambda)^2+\mu} \times \frac{(E_0-\lambda)}{(E_0-\lambda)^2+\mu^2} = \frac{\mu(E_0-\lambda)}{[(E_0-\lambda)^2+\mu^2]^2}$,

$$= -\frac{\pi}{2} \delta_\mu'(E_0-\lambda) \, ,$$

$$\mathcal{A}_2 = \mathcal{I}m \sum_{\alpha\neq\beta} \frac{\partial}{\partial\lambda} \int_{\theta_0} d\vec{p}\, d\vec{q} \; 2i \, t_\alpha \, t_\beta \, \pi\delta_\mu(E_0-\lambda) \, i\,\pi\delta_\mu(E_0-\lambda)$$

$$= \sum_{\alpha\neq\beta} \frac{\partial}{\partial\lambda} \int_{\theta_0} d\vec{p}\, d\vec{q} \; 2i \left(i\,\mathcal{I}m \, t_\alpha t_\beta\right) i\,\pi^2 \delta_\mu(E_0-\lambda)\delta_\mu(E_0-\lambda)$$

$$= \sum_{\alpha\neq\beta} \frac{\partial}{\partial\lambda} \int_{\theta_0} d\vec{p}\, d\vec{q} \; (-4i) \, \mathcal{I}m\, t_\alpha \, \mathcal{R}e\, t_\beta \left[\pi\delta_\mu(E_0-\lambda)\right]^2$$

$$= \mathcal{A}_{2,1} + \mathcal{A}_{2,2} \tag{3.4.8}$$

with $\mathcal{A}_{2,1} = \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q} \; (8i) \; \mathcal{I}m\, t_\alpha \, \mathcal{R}e\, t_\beta \; \pi\delta_\mu(E_0-\lambda)\, \pi\delta_\mu'(E_0-\lambda)$ (3.4.9)

$$\mathcal{A}_{2,2} = \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q} \; (-4i) \left[\pi\delta_\mu(E_0-\lambda)\right]^2 \frac{\partial}{\partial\lambda}\left(\mathcal{I}m\, t_\alpha \, \mathcal{R}e\, t_\beta\right) . \tag{3.4.10}$$

In evaluating $\mathcal{A}_{2,1}$ we used the fact

$$\frac{\partial}{\partial\lambda}\delta_\mu(E_0-\lambda) = -\delta'(E_0-\lambda) .$$

From now on the standard step of integrating the delta functions will be done implicitly. Separation of real and imaginary parts would also be a standard step for most terms. We now go on with the rest of the terms.

In both C''_{00} and $\mathcal{D}''_{00}$, the λ derivative acts on a product of three operators. Each will contribute three terms, each with a different operator derivative by using the chain rule.

$$C''_{00} = \mathcal{C}_1 + \mathcal{C}_2 + \mathcal{C}_3 \qquad (3.4.11)$$

with
$$\mathcal{C}_1 = \mathrm{Im}\, \mathrm{Tr}_{\theta_0} 4\mu^2 \sum_{\alpha\neq\beta} R_0(z)\, T_\alpha(z^*) R_0(z^*) \left[T_\beta(z^*) R_0(z^*) R_0(z) \frac{\partial}{\partial\lambda} T_\beta(z)\right] R_0(z)\, T_\alpha(z)\, R_0(z^*)$$

$$= \mathrm{Im}\, \mathrm{Tr}_{\theta_0} 4\mu^2 \sum_{\alpha\neq\beta} \left[T_\alpha(z) R_0(z^*) R_0(z)\, T_\alpha(z^*)\right] R_0(z^*) \left[T_\beta(z^*) R_0(z^*) R_0(z) \frac{\partial}{\partial\lambda} T_\beta(z)\right] R_0(z)$$

$$= \mathrm{Im} \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\; (-4)\; \mathrm{Im}\, t_\alpha \frac{1}{E_0-\lambda+i\mu}\; \Delta_\beta \frac{1}{E_0-\lambda-i\mu} \qquad (3.4.12)$$

$$\mathcal{C}_2 = \mathrm{Im}\, \mathrm{Tr}_{\theta_0} 4\mu^2 \sum_{\alpha\neq\beta} R_0(z)\, T_\alpha(z^*) R_0(z^*) \left[T_\beta(z^*) R_0(z^*) R_0(z)\, T_\beta(z)\right] R_0^2(z)\; T_\alpha(z) R_0(z^*)$$

$$= \mathrm{Im} \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\;\; 4\;\; \mathrm{Im}\, t_\alpha \frac{1}{E_0-\lambda+i\mu}\;\; \mathrm{Im}\, t_\beta \frac{1}{(E_0-\lambda-i\mu)^2}$$

$$= \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\;\; 4i\;\; \mathrm{Im}\, t_\alpha\, \mathrm{Im}\, t_\beta\;\; \pi\delta_\mu(E_0-\lambda) \frac{1}{(E_0-\lambda)^2+\mu^2} \qquad (3.4.13)$$

$$\mathcal{C}_3 = \mathrm{Im}\, \mathrm{Tr}_{\theta_0} 4\mu^2 \sum_{\alpha\neq\beta} R_0(z)\, T_\alpha(z^*) R_0(z) \left[T_\beta(z^*) R_0(z^*) R_0(z)\, T_\beta(z)\right] R_0(z) \left(\frac{\partial T_\alpha(z)}{\partial\lambda}\right) R_0(z^*)$$

$$= \mathrm{Im} \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\, (-4)\, \bar{\Delta}_\alpha \frac{1}{E_0-\lambda+i\mu}\;\; \mathrm{Im}\, t_\beta \frac{1}{E_0-\lambda-i\mu} \qquad (3.4.14)$$

We note that $\mathcal{C}_1$ and $\mathcal{C}_3$ are the same except for the difference between Δ_α and $\bar{\Delta}_\alpha$.

Next, $D''_{oo} = \mathcal{D}_1 + \mathcal{D}_2 + \mathcal{D}_3$ (3.4.15)

where
$$\mathcal{D}_1 = \mathrm{Im}\ Tr_{\theta_0} - 4\mu^2 \sum_{\alpha\neq\beta} \Big\{ R_0(z) \Big[T_\alpha(z^*) R_0(z^*) R_0(z) \frac{\partial}{\partial\lambda} T_\alpha(z)\Big] R_0(z) T_\beta(z) R_0(z^*)$$
$$+ R_0(z) T_\alpha(z^*) R_0(z^*) R_0(z) T_\beta(z) R_0(z) \Big(\frac{\partial}{\partial\lambda} T_\alpha(z)\Big) R_0(z^*)\Big\}$$

$$= \mathrm{Im} \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\ -4\pi\delta_\mu(E_0-\lambda)\ (s_\alpha + \bar{s}_\alpha)\frac{1}{E_0-\lambda-i\mu}\ t_\beta$$ (3.4.16)

$$\mathcal{D}_2 = \mathrm{Im}\ Tr_{\theta_0} - 4\mu^2 \sum_{\alpha\neq\beta} \Big\{ R_0(z)\ T_\alpha(z^*)\ R_0(z^*) R_0(z)\ T_\alpha(z)\ R_0^2(z)\ T_\beta(z)\ R_0(z^*)$$
$$+ R_0(z)\ T_\alpha(z^*)\ R_0(z^*)\ R_0(z)\ T_\beta(z)\ R_0^2(z)\ T_\alpha(z)\ R_0(z^*)\Big\}$$

$$= \mathrm{Im} \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\ \ 8\pi\ \delta_\mu(E_0-\lambda)\ \mathrm{Im}\, t_\alpha\ \frac{1}{(E_0-\lambda-i\mu)^2}\ t_\beta$$

$$= \mathcal{D}_{2,1} + \mathcal{D}_{2,2}$$ (3.4.17)

with
$$\mathcal{D}_{2,1} = \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\ \ 8\pi\ \delta_\mu(E_0-\lambda)\ \mathrm{Im}\, t_\alpha\ \frac{P_\mu}{(E_0-\lambda)^2}\ i\ \mathrm{Im}\, t_\beta$$ (3.4.18)

$$\mathcal{D}_{2,2} = \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\ \ 8\pi\ \delta_\mu(E_0-\lambda)\ \mathrm{Im}\, t_\alpha\ \ (-i\pi)\,\delta'_\mu(E_0-\lambda)\ \mathrm{Re}\, t_\beta$$ (3.4.19)

$$\mathcal{D}_3 = \mathrm{Im}\ Tr_{\theta_0} - 4\mu^2 \sum_{\alpha\neq\beta} \Big\{ R_0^{(z)}\Big[T_\alpha(z^*) R_0(z^*)\ R_0(z) T_\alpha(z)\Big]\ R_0(z)\ \Big(\frac{\partial}{\partial\lambda} T_\beta(z)\Big) R_0(z^*)$$
$$+ R_0(z)\ T_\alpha(z^*)\ R_0(z^*)\ R_0(z) \Big(\frac{\partial}{\partial\lambda} T_\beta(z)\Big)\ R_0(z)\ T_\alpha(z)\ R_0(z^*)\Big\}$$

$$= \mathrm{Im} \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\ \ 8\pi\ \delta_\mu(E_0-\lambda)\ \mathrm{Im}\, t_\alpha\ \frac{1}{E_0-\lambda-i\mu}\ \ \frac{\partial t_\beta}{\partial\lambda}$$

$$= \mathcal{D}_{3,1} + \mathcal{D}_{3,2}$$ (3.4.20)

With
$$\mathcal{D}_{3,1} = \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\ \ 8\pi\ \delta_\mu(E_0-\lambda)\ \ \mathrm{Im}\, t_\alpha \frac{P_\mu}{E_0-\lambda}\ \ i\ \frac{\partial}{\partial\lambda}\mathrm{Im}\, t_\beta$$

$$= \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\,(-4i)\ \pi\ \delta'_\mu(E_0-\lambda)\ \ \mathrm{Im}\, t_\alpha\ \frac{\partial}{\partial\lambda}\mathrm{Im}\, t_\beta$$ (3.4.21)

$$\mathcal{D}_{3,2} = \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\ \ 8i\,\big[\pi\,\delta_\mu(E_0-\lambda)\big]^2\ \mathrm{Im}\, t_\alpha\ \frac{\partial}{\partial\lambda}\mathrm{Re}\, t_\beta$$ (3.4.22)

Here we see that $\mathcal{D}_{3,1}$ has the same generalized function as $\mathcal{A}_1$ and is regular while $\mathcal{D}_{3,2}$ behaves as $\mathcal{A}_2$ which has the irregular generalized function $[\pi\delta_\mu(E_0-\lambda)]^2$. The latter must be combined with other terms later.

Next,

$$E''_{00} = \mathrm{Im}\, Tr_{\theta_0} \sum_{\alpha\neq\beta} -4\mu^2 \left[T_\alpha(z^*) R_0(z^*) T_\beta(z^*) + T_\beta(z^*) R_0(z^*) T_\alpha(z^*) \right] R_0(z^*) \times$$
$$R_0(z) \left(\frac{\partial}{\partial\lambda} T_\beta(z) \right) R_0(z^*) R_0(z)$$
$$= \mathrm{Im} \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\, (-4)\ \pi\delta_\mu(E_0-\lambda)\ t^*_\alpha \frac{1}{E_0-\lambda+i\mu} (\Delta_\beta + \bar{\Delta}_\beta)$$

(3.4.23)

$$F''_{00} = \mathrm{Im}\, Tr_{\theta_0} 4\mu^2 \sum_{\alpha\neq\beta} R_0(z^*) R_0(z) T_\alpha(z^*) R_0(z^*) R_0(z) \frac{\partial}{\partial\lambda} T_\beta(z)$$
$$= \mathrm{Im} \int_{\theta_0} d\vec{p}\, d\vec{q} \sum_{\alpha\neq\beta} 4 \left[\pi\delta_\mu(E_0-\lambda)\right]^2\ t^*_\alpha \frac{\partial}{\partial\lambda} t_\beta$$
$$= \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\ i4 \left[\pi\delta_\mu(E_0-\lambda)\right]^2 \left[\mathrm{Re}\, t_\alpha \frac{\partial}{\partial\lambda} \mathrm{Im}\, t_\beta - \mathrm{Im}\, t_\alpha \frac{\partial}{\partial\lambda} \mathrm{Re}\, t_\beta \right]$$

(3.4.24)

In the second stage of regularization, we rearrange and regroup all these various terms to come up with meaningful generalized functions.

First, we want to show two groups to be vanishing.

$$\mathcal{A}_{2,2} + F''_{00} + \mathcal{D}_{3,2} = 0 \tag{3.4.25}$$

$$\mathcal{A}_{2,2} + F''_{00} + \mathcal{D}_{3,2} = \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\ 4i \left[\pi\delta_\mu(E_0-\lambda)\right]^2 \times \left\{ -\frac{\partial}{\partial\lambda}(\mathrm{Im}\, t_\alpha\, \mathrm{Re}\, t_\beta) + \right.$$
$$\left. + \mathrm{Re}\, t_\alpha \frac{\partial}{\partial\lambda} \mathrm{Im}\, t_\beta - \mathrm{Im}\, t_\alpha \frac{\partial}{\partial\lambda} \mathrm{Re}\, t_\beta + 2\, \mathrm{Im}\, t_\alpha \frac{\partial}{\partial\lambda} \mathrm{Re}\, t_\beta \right\}$$
$$= 0$$

We have used the fact

$$\sum_{\alpha\neq\beta} \mathrm{Re}\, t_\alpha \frac{\partial}{\partial\lambda} \mathrm{Im}\, t_\beta = \sum_{\alpha\neq\beta} \left(\frac{\partial}{\partial\lambda} \mathrm{Im}\, t_\alpha \right) \mathrm{Re}\, t_\beta \ .$$

$$\mathcal{A}_{2,1} + \mathcal{D}_{2,2} = 0 \tag{3.4.26}$$

$$\mathcal{A}_{2,1} + \mathcal{D}_{2,2} = \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\;\; 8i \;\, \mathrm{Im}\, t_\alpha \; \mathrm{Re}\, t_\beta \;\, \pi\delta_\mu(E_0-\lambda)\; \pi\delta_\mu'(E_0-\lambda)$$

$$+ \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\;\; 8 \;\; \mathrm{Im}\, t_\alpha \; (-i\pi)\, \delta_\mu'(E_0-\lambda)\; \mathrm{Re}\, t_\beta \;\, \pi\delta_\mu(E_0-\lambda)$$

$$= 0$$

Next we gather all the terms with the coefficient $\mathrm{Im}\, t_\alpha \mathrm{Im}\, t_\beta$.

$$\mathcal{D}_{2,1} + \mathcal{C}_2 = \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\;\; 4i \Big[2\pi\delta_\mu(E_0-\lambda)\; \mathrm{Im}\, t_\alpha \frac{P_\mu}{(E_0-\lambda)^2} \; \mathrm{Im}\, t_\beta \; +$$

$$+ \mathrm{Im}\, t_\alpha \; \mathrm{Im}\, t_\beta \; \frac{1}{(E_0-\lambda)^2+\mu^2}\; \pi\delta_\mu(E_0-\lambda) \Big]$$

The generalized function can be simplified.

$$2\pi\,\delta_\mu(x)\, \frac{P_\mu}{x^2} + \frac{\pi\,\delta_\mu(x)}{x^2+\mu^2}$$

$$= \frac{2\mu}{x^2+\mu^2}\;\frac{x^2-\mu^2}{(x^2+\mu^2)^2} + \frac{\mu}{(x^2+\mu^2)^2}$$

$$= \frac{\mu(2x^2-2\mu^2+x^2+\mu^2)}{(x^2+\mu^2)^3}$$

$$= \frac{\mu(3x^2-\mu^2)}{(x^2+\mu^2)^3}$$

$$= \frac{1}{2}\,\pi\,\delta_\mu''(x) \tag{3.4.27}$$

Hence,

$$\mathcal{D}_{2,1} + \mathcal{C}_2 = \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\;\; 2i\,\pi\,\delta_\mu''(E_0-\lambda)\; \mathrm{Im}\, t_\alpha \; \mathrm{Im}\, t_\beta \tag{3.4.28}$$

Add $\mathcal{D}_{3,1}$ to the above.

$$\mathcal{D}_{2,1} + \mathcal{C}_2 + \mathcal{D}_{3,1} = \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\; \Big[2i\,\pi\,\delta_\mu''(E_0-\lambda)\; \mathrm{Im}\, t_\alpha \; \mathrm{Im}\, t_\beta$$

$$- 4i\,\pi\,\delta_\mu'(E_0-\lambda)\; \mathrm{Im}\, t_\alpha \; \frac{\partial}{\partial\lambda}\, t_\beta \Big]$$

$$= \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q} \Big[-2i\pi\, \delta_\mu'(E_0-\lambda) \frac{\partial}{\partial\lambda} (\mathrm{Im}\, t_\alpha\, \mathrm{Im}\, t_\beta) - 2i \Big(\frac{\partial}{\partial\lambda} \pi\delta_\mu'(E_0-\lambda) \Big) \mathrm{Im}\, t_\alpha\, \mathrm{Im}\, t_\beta \Big]$$

$$= \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\, (-2i) \frac{\partial}{\partial\lambda} \Big[\pi\delta_\mu'(E_0-\lambda)\, \mathrm{Im}\, t_\alpha\, \mathrm{Im}\, t_\beta \Big] \tag{3.4.29}$$

Add $\mathcal{A}_1$ to the above.

$$\mathcal{D}_{2,1} + \mathcal{B}_2 + \mathcal{D}_{3,1} + \mathcal{A}_1 = \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q} \Big\{ (-2i) \frac{\partial}{\partial\lambda} \pi\delta_\mu'(E_0-\lambda)\, \mathrm{Im}\, t_\alpha\, \mathrm{Im}\, t_\beta + (-i) \frac{\partial}{\partial\lambda} \pi\delta_\mu'(E_0-\lambda) (\mathrm{Re}\, t_\alpha\, \mathrm{Re}\, t_\beta - \mathrm{Im}\, t_\alpha\, \mathrm{Im}\, t_\beta) \Big\}$$

$$= \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\; -i \frac{\partial}{\partial\lambda} \Big[\pi\delta_\mu'(E_0-\lambda) (\mathrm{Re}\, t_\alpha\, \mathrm{Re}\, t_\beta + \mathrm{Im}\, t_\alpha\, \mathrm{Im}\, t_\beta) \Big] \tag{3.4.30}$$

The remaining terms all contain $\mathcal{S}_\alpha$ or $\bar{\mathcal{S}}_\alpha$.

$$\mathcal{B}_1 + \mathcal{B}_3 + \mathcal{D}_1 + E_{00}''$$

$$= \mathrm{Im} \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\; -4 \Big\{ \mathrm{Im}\, t_\alpha\, (\mathcal{S}_\beta + \bar{\mathcal{S}}_\beta) \frac{1}{(E_0-\lambda)^2+\mu^2} + t_\alpha\, (\mathcal{S}_\beta + \bar{\mathcal{S}}_\beta) \frac{\pi\delta_\mu(E_0-\lambda)}{E_0-\lambda-i\mu} + t_\alpha^*\, (\mathcal{S}_\beta + \bar{\mathcal{S}}_\beta) \frac{\pi\delta_\mu(E_0-\lambda)}{E_0-\lambda+i\mu} \Big\}$$

$$= \mathrm{Im} \sum_{\alpha\neq\beta} \int_{\theta_0} d\vec{p}\, d\vec{q}\, (-4) \Big\{ (\mathcal{S}_\beta + \bar{\mathcal{S}}_\beta) \Big[\mathrm{Re}\, t_\alpha \Big(\frac{\pi\delta_\mu(E_0-\lambda)}{E_0-\lambda-i\mu} + \frac{\pi\delta_\mu(E_0-\lambda)}{E_0-\lambda+i\mu} \Big) + \mathrm{Im}\, t_\alpha \Big(\frac{1}{(E_0-\lambda)^2+\mu^2} + \frac{i\pi\delta_\mu(E_0-\lambda)}{E_0-\lambda-i\mu} - \frac{i\pi\delta_\mu(E_0-\lambda)}{E_0-\lambda+i\mu} \Big) \Big] \Big\} \tag{3.4.31}$$

We can simplify the groups of generalized functions.

$$\pi\delta_\mu(E_0-\lambda) \Big(\frac{1}{E_0-\lambda-i\mu} + \frac{1}{E_0-\lambda+i\mu} \Big)$$

$$= \pi\, \delta_\mu(E_0-\lambda) \frac{2P_\mu}{E_0-\lambda}$$

$$= -\pi\, \delta_\mu'(E_0-\lambda) \tag{3.4.32}$$

$$\frac{1}{(E_0-\lambda)^2+\mu^2} + \frac{i\pi\delta_\mu(E_0-\lambda)}{E_0-\lambda-i\mu} - \frac{i\pi\delta_\mu(E_0-\lambda)}{E_0-\lambda+i\mu}$$

$$= \frac{1}{(E_0-\lambda)^2+\mu^2}\left(1+\frac{i\mu}{E_0-\lambda-i\mu} - \frac{i\mu}{E_0-\lambda+i\mu}\right)$$

$$= \frac{1}{(E_0-\lambda)^2+\mu^2}\ \frac{(E_0-\lambda)^2+\mu^2+i\mu(E_0-\lambda+i\mu)-i\mu(E_0-\lambda-i\mu)}{(E_0-\lambda)^2+\mu^2}$$

$$= \frac{(E_0-\lambda)^2+\mu^2-\mu^2+\mu^2}{[(E_0-\lambda)^2+\mu^2]^2}$$

$$= \frac{P_\mu}{(E_0-\lambda)^2} \qquad (3.4.33)$$

Substituting equations 32 and 33 to 31, we arrive at

$$\mathcal{B}_1+\mathcal{B}_3+\mathcal{D}_1+E'_{00}$$

$$= \mathrm{Im}\sum_{\alpha\neq\beta}\int_{B_0} d\vec{p}\,d\vec{q}\ (-4)(\mathcal{A}_\beta+\bar{\rho}_\beta)\left[\mathrm{Re}\,t_\alpha(-\pi)\delta'_\mu(E_0-\lambda) + \mathrm{Im}\,t_\alpha\frac{P_\mu}{(E_0-\lambda)^2}\right]$$

(3.4.34)

Even though the particular form of equation 34 is quite arbitrary we prefer to express it interms of two body time delay. We do so in two steps. First we express the term in square brackets in time delay and then we express $(\mathcal{A}_\beta+\bar{\rho}_\beta)$ in terms of time delay also.

$$I = \int d\vec{q}_\alpha\left[\mathrm{Re}\,t_\alpha(-\pi)\delta'_\mu(E_0-\lambda) + \mathrm{Im}\,t_\alpha\frac{P_\mu}{(E_0-\lambda)^2}\right]$$

$$= \int d\vec{q}_\alpha\Big[-\pi\delta'_\mu(\tilde{q}_\alpha^2-(\lambda-\tilde{p}_\alpha^2))\,\mathrm{Re}\,t_\alpha(\vec{q}_\alpha,\vec{q}_\alpha,\lambda-\tilde{p}_\alpha^2+i\mu)$$

$$+\ \mathrm{Im}\,t_\alpha(\vec{q}_\alpha,\vec{q}_\alpha,\lambda-\tilde{p}_\alpha^2+i\mu)\frac{P_\mu}{\tilde{q}_\alpha^2-(\lambda-\tilde{p}_\alpha^2)}\Big]$$

$$= \int d\vec{q}_\alpha\ \mathrm{Im}\frac{1}{(\tilde{q}_\alpha^2-(\lambda-\tilde{p}_\alpha^2)-i\mu)^2}\ t_\alpha(\vec{q}_\alpha,\vec{q}_\alpha,\lambda-\tilde{p}_\alpha^2+i\mu)$$

$$= \operatorname{tr} \operatorname{Im} R_0^2(\lambda-\tilde{p}_\alpha^2+i\mu)\, t_\alpha(\lambda-\tilde{p}_\alpha^2+i\mu)$$

$$= \operatorname{tr} \operatorname{Im} R_0(\lambda-\tilde{p}_\alpha^2+i\mu)\, t_\alpha(\lambda-\tilde{p}_\alpha^2+i\mu)\, R_0(\lambda-\tilde{p}_\alpha^2+i\mu) \qquad (3.4.35)$$

Recall the two body spectral property (II.2.31)

$$\hat{\operatorname{tr}}\, g(E) = 2 \operatorname{Im} \operatorname{tr}\left[R(E+i0) - R_0(E+i0)\right]$$

and the identity

$$R(E+i0) - R_0(E+i0) = -R_0(E+i0)\, t(E+i0)\, R_0(E+i0)$$

We have

$$\lim_{\mu\to 0^+} I = -\tfrac{1}{2}\, \hat{\operatorname{tr}}\, g_\alpha(\lambda-\tilde{p}_\alpha^2)$$

$$= -\tfrac{1}{2} \int d\tilde{q}_\alpha^2\, \delta(\lambda-E_0)\, \hat{\operatorname{tr}}\, g_\alpha(\tilde{q}_\alpha^2) \qquad (3.4.36)$$

For notational convenience later, I is expressed in the second form in equation 36. Substituting back into (3.4.34),

$$\wp_1 + \wp_3 + \mathcal{D}_1 + E_{00}''$$

$$= \operatorname{Im} \sum_{\alpha\neq\beta} \int_{D_0} d\vec{q}_\beta \int d\tilde{q}_\alpha^2\, \delta(\lambda-E_0)\, 2(\rho_\beta+\bar{\rho}_\beta)\, \hat{\operatorname{tr}}\, g_\alpha(\tilde{q}_\alpha^2)$$

$$= \sum_{\alpha\neq\beta} \int d\tilde{q}_\beta^2\, d\tilde{q}_\alpha^2\, \delta(\lambda-E_0)\, \hat{\operatorname{tr}}\, g_\alpha(\tilde{q}_\alpha^2)\left[2\int d\hat{q}_\beta \operatorname{Im}(\rho_\beta+\bar{\rho}_\beta)\right] j^2(\tilde{q}_\beta^2) \qquad (3.4.37)$$

We now take the second step and express $\rho_\beta+\bar{\rho}_\beta$ in terms of $g(E)$.

$$\rho_\beta = \rho_\beta(\vec{q}_\beta, \vec{q}_\beta, \lambda+i\mu-\tilde{p}_\beta^2)$$

$$= \int d\vec{q}_\beta''\, \pi\, \delta_\mu(\tilde{p}_\beta^2+\tilde{q}_\beta^{2\prime\prime}-\lambda)\, t_\beta(\vec{q}_\beta, \vec{q}_\beta'', \lambda-i\mu-\tilde{p}_\beta^2)\, t_\beta(\vec{q}_\beta'', \vec{q}_\beta, \lambda+i\mu-\tilde{p}_\beta^2)$$

$$\int d\hat{q}_\beta^2\, j(\tilde{q}_\beta^2) \operatorname{Im}\rho_\beta\, j(\tilde{q}_\beta^2) = \pi \operatorname{Im} \hat{\operatorname{tr}}\, \tau_\beta(\tilde{q}_\beta^2, \tilde{q}_\beta^2, \tilde{q}_\beta^2-i\mu)\, \tau_\beta(\tilde{q}_\beta^2, \tilde{q}_\beta^2, \tilde{q}_\beta^2+i\mu)$$

Add to this the identity (II.2.21)

$$0 = \hat{\operatorname{tr}} \operatorname{Im} \tau(E,E,E-i0)\, \tau(E,E,E+i0)$$

$$\lim_{\mu\to 0^+} \int d^2\tilde{q}_\beta \; j(\tilde{q}_\beta^2) \; \mathrm{Im}\, s_\beta \; j(\tilde{q}_\beta^2)$$

$$= \pi \; \mathrm{Im} \; \hat{\mathrm{tr}} \; \tau_\beta(\tilde{q}_\beta^2, \tilde{q}_\beta^2, \tilde{q}_\beta^2 - io) \; \frac{d}{d\tilde{q}_\beta^2} \; \tau_\beta(\tilde{q}_\beta^2, \tilde{q}_\beta^2, \tilde{q}_\beta^2 + io)$$

Similarly,

$$\lim_{\mu\to 0^+} \int d^2\tilde{q}_\beta \; j(\tilde{q}_\beta^2) \; \mathrm{Im}\, \bar{s}_\beta \; j(\tilde{q}_\beta^2)$$

$$= \pi \; \mathrm{Im} \; \hat{\mathrm{tr}} \; \left[\frac{d}{d\tilde{q}_\beta^2} \tau_\beta(\tilde{q}_\beta^2, \tilde{q}_\beta^2, \tilde{q}_\beta^2 + io)\right] \tau_\beta(\tilde{q}_\beta^2, \tilde{q}_\beta^2, \tilde{q}_\beta^2 - io)$$

Express the above in terms of time delay through (II.2.30)

$$\hat{\mathrm{tr}}\; q(\lambda) = -2\pi \; \hat{\mathrm{tr}} \; \frac{\partial}{\partial\lambda} \mathrm{Re}\, \tau(\lambda, \lambda, \lambda + io) + (2\pi)^2 \; \hat{\mathrm{tr}} \; \mathrm{Im}\, \tau(\lambda, \lambda, \lambda - io) \frac{d}{d\lambda} \tau(\lambda, \lambda, \lambda + io)$$

Hence,

$$\lim_{\mu\to 0^+} \int d^2\tilde{q}_\beta \; j(\tilde{q}_\beta^2) \; \mathrm{Im}\,(s_\beta + \bar{s}_\beta) \; j(\tilde{q}_\beta^2)$$

$$= \frac{1}{2\pi} \; \hat{\mathrm{tr}} \; q_\beta(\tilde{q}_\beta^2) + \hat{\mathrm{tr}} \; \frac{\partial}{\partial\tilde{q}_\beta^2} \mathrm{Re}\, \tau_\beta(\tilde{q}_\beta^2, \tilde{q}_\beta^2, \tilde{q}_\beta^2 + io)$$

Substituting back into (3.4.37),

$$\mathcal{G}_1 + \mathcal{G}_3 + E_{00}'' + \mathcal{A}_1$$

$$= \sum_{\alpha\neq\beta} \int d\tilde{q}_\alpha^2 \, d\tilde{q}_\beta^2 \; \delta(\lambda - E_0) \; \hat{\mathrm{tr}}\; g_\alpha(\tilde{q}_\alpha^2) \quad \left[\frac{1}{\pi} \hat{\mathrm{tr}}\; q_\beta(\tilde{q}_\beta^2) + 2\, \hat{\mathrm{tr}} \frac{\partial}{\partial\tilde{q}_\beta^2} \mathrm{Re}\, \tau_\beta(\tilde{q}_\beta^2, \tilde{q}_\beta^2, \tilde{q}_\beta^2 + io)\right]$$

(3.4.38)

We have now accounted for all the rescattering terms.

In summary, the entire contribution from $\theta_0 \cup \theta_0'$ is

$$= (3.4.4) + (3.4.30) + (3.4.38) \quad .$$

It has been argued [Dashen et al[17]] that the rescattering terms will provide for an excellent approximation for the entire Cayley transform. Since it is so "close" to being singular, when it is regularized it must give "big" contributions. Our findings cannot support such arguement. They may be good approximation only because they are the first terms in the series. It remains to be seen whether numerical calculations would bear this out.

Using Landau's equation Grossman[43] arrives at an approximation having only part of (3.4.30). Baumgartl[21] derives the same results using approximation to the second order of $Re\, t_\alpha$. Buslaev and Merkuriev[19] have also derived the regularization of the Cayley transform. However, we find their solution to be unnecessarily confusing. Our results are complete and simple. In this sense, the above authors' various results are considered insufficient.

V.3.5 Contribution from $\theta_\alpha \cup \theta'_\beta$ ($\alpha, \beta > 0$)

We start again to calculate the entire equation (3.1.8)

$$2i \,\mathrm{Im}\, \mathrm{Tr}\left[R(z) - R_0(z) - \sum_{\alpha=1}^{3} R_\alpha(z) - R_0(z)\right] = A + C + D + E + F$$

in the neighbourhood θ_α for A and $\theta_\alpha \cup \theta'_\beta$ for C, D, E & F. There is no rescattering contribution here since the free resolvent R_0 is finite in these neighbourhoods.

$$\begin{aligned} A_\alpha = \int_{\theta_\alpha} d\vec{p}\, d\vec{q}\; \frac{2}{\partial\lambda}\,(-2i\mu)\frac{1}{(E_0-E_\alpha)^2+\mu^2}\Bigg[& \frac{\varphi_\alpha(\vec{q}_\alpha)}{\lambda+i\mu-E_\alpha}\sum_{\beta>0}\widetilde{G}_{\alpha\beta}(\vec{p}_\alpha;\vec{p}\vec{q};\lambda+i\mu) \\ & + \sum_{\beta>0} G_{\beta\alpha}(\vec{p}\vec{q};\vec{q}_\alpha;\lambda+i\mu)\frac{\varphi^*_\alpha(\vec{q}_\alpha)}{\lambda+i\mu-E_\alpha} + \frac{\varphi_\alpha(\vec{q}_\alpha)}{\lambda+i\mu-E_\alpha} H_{\alpha\alpha}(\vec{p}_\alpha;\vec{p}_\alpha;\lambda+i\mu)\frac{\varphi^*_\alpha(\vec{q}_\alpha)}{\lambda+i\mu-E_\alpha} \\ & + \sum_{\beta\neq\alpha}\left(\frac{\varphi_\alpha(\vec{q}_\alpha)}{\lambda+i\mu-E_\alpha}H_{\alpha\beta}(\vec{p}_\alpha,\vec{p}_\beta,\lambda+i\mu)\frac{\varphi^*_\beta(\vec{q}_\beta)}{\lambda+i\mu-E_\beta} + \frac{\varphi_\beta(\vec{q}_\beta)}{\lambda+i\mu-E_\beta}H_{\beta\alpha}(\vec{p}_\beta,\vec{p}_\alpha,\lambda+i\mu)\frac{\varphi^*_\alpha(\vec{q}_\alpha)}{\lambda+i\mu-E_\alpha}\right)\Bigg] \end{aligned}$$

(3.5.1)

Since $(\lambda+i\mu-E_\alpha)^{-1}$ and $(\lambda+i\mu-E_\alpha)^{-2}$ are both well defined and finite generalized functions, in the limit $\mu\to 0^+$ A_α vanishes linearly as μ . Hence, the linear term A only have contribution in θ_0 not θ_α .

$$\begin{aligned} C_{\alpha\beta} &= \mathrm{Tr}_{\alpha\beta}\; 4\mu^2 R_0(z)\, W(z^*)\, R_0(z) R_0(z^*)\left(\frac{2}{\partial\lambda} W(z)\right) R_0(z) \\ &= 4\mu^2 \int_{\theta_\alpha} d\vec{p}\, d\vec{q} \int_{\theta'_\beta} d\vec{p}'\, d\vec{q}'\; \left[(E_0-E_\alpha)^2+\mu^2\right]^{-1}\left[(E'_0-E'_\beta)^2+\mu^2\right]^{-1} \\ &\quad \times \Bigg\{ \sum_{\alpha,\beta} F_{\alpha\beta}(\vec{p}\vec{q};\vec{p}'\vec{q}';\lambda-i\mu) + \frac{\varphi_\alpha(\vec{q}_\alpha)}{\lambda-i\mu-E_\alpha}\Bigg[\sum_\beta \widetilde{G}_{\alpha\beta}(\vec{p}_\alpha;\vec{p}'\vec{q}';\lambda-i\mu) \\ &\quad + \sum_{\gamma\neq\beta} H_{\alpha\gamma}(\vec{p}_\alpha;\vec{p}'_\gamma;\lambda-i\mu)\frac{\varphi^*_\gamma(\vec{q}'_\gamma)}{\lambda-i\mu-E'_\gamma}\Bigg] + \end{aligned}$$

$$+\Big[\Sigma_\alpha G_{\alpha\beta}(\vec{p}\vec{q};\vec{p}'_\beta;\lambda-i\mu)+\sum_{\gamma\neq\alpha}\frac{\varphi_\gamma(\vec{q}_\gamma)}{\lambda-i\mu-E_\gamma}H_{\gamma\beta}(\vec{p}_\gamma,\vec{p}'_\beta;\lambda-i\mu)\Big]\frac{\varphi^*_\beta(\vec{q}'_\beta)}{\lambda-i\mu-E'_\beta}$$

$$+\frac{\varphi_\alpha(\vec{q}_\alpha)}{\lambda-i\mu-E_\alpha}H_{\alpha\beta}(\vec{p}_\alpha,\vec{p}'_\beta,\lambda-i\mu)\frac{\varphi^*_\beta(\vec{q}'_\beta)}{\lambda-i\mu-E'_\beta}\Big\}\times$$

$$\times\Big\{\sum_{\alpha,\beta}F_{\alpha\beta}(\vec{p}'\vec{q}';\vec{p}\vec{q};\lambda+i\mu)+\frac{\varphi_\beta(\vec{q}'_\beta)}{\lambda+i\mu-E'_\beta}\frac{\partial}{\partial\lambda}\Big[\sum_\gamma\tilde{G}_{\beta\gamma}(\vec{p}'_\beta;\vec{p}\vec{q};\lambda+i\mu)$$

$$+\sum_{\gamma\neq\alpha}H_{\beta\gamma}(\vec{p}'_\beta,\vec{p}_\gamma,\lambda+i\mu)\frac{\varphi^*_\gamma(\vec{q}_\gamma)}{\lambda+i\mu-E_\gamma}\Big]+\frac{\partial}{\partial\lambda}\Big[\sum_\gamma G_{\gamma\alpha}(\vec{p}'\vec{q}';\vec{p}_\alpha;\lambda+i\mu)$$

$$+\sum_{\gamma\neq\beta}\frac{\varphi_\gamma(\vec{q}'_\gamma)}{\lambda+i\mu-E'_\gamma}H_{\gamma\alpha}(\vec{p}'_\gamma,\vec{p}_\alpha,\lambda+i\mu)\Big]\frac{\varphi^*_\alpha(\vec{q}_\alpha)}{\lambda+i\mu-E_\alpha}+$$

$$+\frac{\varphi_\beta(\vec{q}'_\beta)}{\lambda+i\mu-E'_\beta}H_{\beta\alpha}(\vec{p}'_\beta,\vec{p}_\alpha,\lambda+i\mu)\frac{\varphi^*_\alpha(\vec{q}_\alpha)}{\lambda+i\mu-E_\alpha}\Big\}$$

$$+\quad C'_{\alpha\beta}\tag{3.5.2}$$

where $C'_{\alpha\beta}$ contains derivatives of $(\lambda+i\mu-E_\alpha)^{-1}$ and $(\lambda+i\mu-E'_\beta)^{-1}$.

$$C'_{\alpha\beta}=4\mu^2\int_{\theta_\alpha}d\vec{p}\,d\vec{q}\int_{\theta'_\beta}d\vec{p}'\,d\vec{q}'\,\big[(E_0-E_\alpha)^2+\mu^2\big]^{-1}\big[(E'_0-E'_\beta)^2+\mu^2\big]^{-1}\times$$

$$\times W(\vec{p}\vec{q};\vec{p}'\vec{q}';\lambda-i\mu)\Big\{\frac{\varphi_\beta(\vec{q}'_\beta)}{(\lambda+i\mu-E'_\beta)^2}\Big[\sum_\alpha\tilde{G}_{\beta\alpha}(\vec{p}'_\beta;\vec{p}\vec{q};\lambda+i\mu)+$$

$$+\sum_{\gamma=1}^{3}H_{\beta\gamma}(\vec{p}'_\beta,\vec{p}_\gamma,\lambda+i\mu)\frac{\varphi^*_\gamma(\vec{q}_\gamma)}{\lambda+i\mu-E_\gamma}\Big]+\Big[\sum_\beta G_{\beta\alpha}(\vec{p}'\vec{q}';\vec{p}_\alpha;\lambda+i\mu)+$$

$$+\sum_\gamma\frac{\varphi_\gamma(\vec{q}'_\gamma)}{\lambda+i\mu-E'_\gamma}H_{\gamma\alpha}(\vec{p}'_\gamma,\vec{p}_\alpha,\lambda+i\mu)\Big]\frac{\varphi^*_\alpha(\vec{q}_\alpha)}{(\lambda+i\mu-E_\alpha)^2}\Big\}\tag{3.5.3}$$

$C'_{\alpha\beta}$ will be treated with the development of the unitarity equation later.

To evaluate $C_{\alpha\beta}-C'_{\alpha\beta}$ we must carefully study its terms' behaviour as $\mu \to 0^+$. All terms with $F_{\alpha\beta}$ vanish as μ^2 . They only contain finite well defined resolvents $(\lambda \pm i\mu - E_\alpha)^{-1}$ or $(\lambda \pm i\mu - E'_\beta)^{-1}$ or $(\lambda \pm i\mu - E_\alpha)^{-1}(\lambda \pm i\mu - E'_\beta)^{-1}$. Many other terms with these resolvents only also vanish as μ^2 . Terms with either

$$\mu(\lambda - i\mu - E_\alpha)^{-1}(\lambda + i\mu - E_\alpha)^{-1} = \pi\delta_\mu(\lambda - E_\alpha)$$

or

$$\mu(\lambda - i\mu - E'_\beta)^{-1}(\lambda + i\mu - E'_\beta)^{-1} = \pi\delta_\mu(\lambda - E'_\beta)$$

but not both, will vanish linearly as μ . Only the terms with both factors survive.

$$\lim_{\mu \to 0^+} \mu^2 \frac{1}{(\lambda - i\mu - E_\alpha)(\lambda + i\mu - E_\alpha)} \frac{1}{(\lambda - i\mu - E'_\beta)(\lambda + i\mu - E'_\beta)} = \pi^2 \delta(\lambda - E_\alpha)\,\delta(\lambda - E'_\beta)$$

Hence,

$$\begin{aligned} C_{\alpha\beta} - C'_{\alpha\beta} &= \int_{\theta_\alpha} d\vec{p}\, d\vec{q} \int_{\theta'_\beta} d\vec{p}'\, d\vec{q}'\; (2\pi)^2\, \delta(\lambda - E_\alpha)(\lambda - E'_\beta)\,(E_0 - E_\alpha)^{-2}(E'_0 - E'_\beta)^{-2} \\ &\qquad \varphi_\alpha(\vec{q}_\alpha) H_{\alpha\beta}(\vec{p}_\alpha, \vec{p}'_\beta, \lambda - i0)\, \varphi^*_\beta(\vec{q}'_\beta)\; \varphi_\beta(\vec{q}'_\beta) H_{\beta\alpha}(\vec{p}'_\beta, \vec{p}_\alpha, \mathring{\lambda} + i0)\, \varphi^*_\alpha(\vec{q}_\alpha) \\ &= \int d\vec{p}_\alpha \int d\vec{p}'_\beta\; (2\pi)^2\, \delta(\lambda - E_\alpha)\, \delta(\lambda - E'_\beta)\, H_{\alpha\beta}(\vec{p}_\alpha, \vec{p}'_\beta, \lambda - i0)\, H_{\beta\alpha}(\vec{p}'_\beta, \vec{p}_\alpha, \mathring{\lambda} + i0) \\ &= (2\pi)^2\, \hat{tr}_\alpha\, \mathcal{H}_{\alpha\beta}(\lambda, \lambda, \lambda - i0)\, \mathcal{H}_{\beta\alpha}(\lambda, \lambda, \mathring{\lambda} + i0) \end{aligned} \tag{3.5.4}$$

We have used the fact that

$$\int d\vec{q}_\alpha \frac{\varphi_\alpha(\vec{q}_\alpha)\, \varphi^*_\alpha(\vec{q}_\alpha)}{(E_0 - E_\alpha)^2} = \int d\vec{q}_\alpha \frac{\Psi_\alpha(\vec{q}_\alpha)\, \Psi^*_\alpha(\vec{q}_\alpha)\, (\tilde{q}_\alpha^2 + \varkappa_\alpha^2)^2}{(\tilde{p}_\alpha^2 + \tilde{q}_\alpha^2 - \tilde{p}_\alpha^2 + \varkappa_\lambda^2)^2} = 1 .$$

The last form of (3.5.4) is in reduced space notation. It is intended for conversion into time delay format.

$$D_{\alpha\beta} = tr_{\alpha\beta}\; 4\mu^2\, R_0(z) \sum_\alpha T_\alpha(z^*)\, R_0(z^*)\, R_0(z) \left(\frac{\partial}{\partial\lambda} W(z)\right) R_0(z^*)$$

$$
\begin{aligned}
D_{\alpha\beta} = {} & 4\mu^2 \int_{\theta_\alpha} d\vec{p}\, d\vec{q} \int_{\theta'_\beta} d\vec{p}\,' d\vec{q}\,' \left[(E_0-E_\alpha)^2+\mu^2\right]^{-1} \left[(E_0'-E_\beta')^2+\mu^2\right]^{-1} \\
& \times \Big\{ \delta(\vec{p}_\alpha - \vec{p}_\alpha{}') \left[\frac{\varphi_\alpha(\vec{q}_\alpha)\, \varphi_\alpha^*(\vec{q}_\alpha{}')}{\lambda - i\mu - E_\alpha} + \hat{t}_\alpha(\vec{q}_\alpha, \vec{q}_\alpha{}', \lambda - i\mu - \hat{p}_\alpha{}^2) \right] \\
& + \delta(\vec{p}_\beta - \vec{p}_\beta{}') \left[\frac{\varphi_\beta(\vec{q}_\beta)\, \varphi_\beta^*(\vec{q}_\beta{}')}{\lambda - i\mu - E_\beta'} + \hat{t}_\beta(\vec{q}_\beta, \vec{q}_\beta{}', \lambda - i\mu - \hat{p}_\beta{}^2) \right] \\
& + \underset{\gamma\neq\alpha,\, \gamma\neq\beta}{T_\gamma} (\vec{p}, \vec{q}\,; \vec{p}\,'\vec{q}\,'; \lambda - i\mu) \Big\} \times \Big\{ \sum_{\alpha,\beta} F_{\alpha\beta}(\vec{p}\,'\vec{q}\,'; \vec{p}\vec{q}\,; \lambda + i\mu) + \\
& + \frac{\varphi_\beta(\vec{q}_\beta{}')}{\lambda + i\mu - E_\beta'} \frac{\partial}{\partial\lambda} \left[\sum_\gamma \tilde{G}_{\beta\gamma}(\vec{p}_\beta{}'; \vec{p}\vec{q}\,; \lambda + i\mu) + \sum_{\gamma\neq\alpha} H_{\beta\gamma}(\vec{p}_\beta{}', \vec{p}_\gamma, \lambda + i\mu) \frac{\varphi_\gamma^*(\vec{q}_\gamma)}{\lambda + i\mu - E_\gamma} \right] \\
& + \frac{\partial}{\partial\lambda} \left[\sum_\gamma G_{\gamma\alpha}(\vec{p}\,'\vec{q}\,'; \vec{p}_\alpha; \lambda + i\mu) + \sum_{\gamma\neq\beta} \frac{\varphi_\gamma(\vec{q}_\gamma{}')}{\lambda + i\mu - E_\gamma'} H_{\gamma\alpha}(\vec{p}_\gamma{}', \vec{p}_\alpha, \lambda + i\mu) \right] \frac{\varphi_\alpha^*(\vec{q}_\alpha)}{\lambda + i\mu - E_\alpha} \\
& + \frac{\varphi_\beta(\vec{q}_\beta{}')}{\lambda + i\mu - E_\beta'} H_{\beta\alpha}(\vec{p}_\beta{}', \vec{p}_\alpha, \lambda + i\mu) \frac{\varphi_\alpha^*(\vec{q}_\alpha)}{\lambda + i\mu - E_\alpha} \Big\} \\
& + D'_{\alpha\beta}
\end{aligned}
\tag{3.5.5}
$$

where $D'_{\alpha\beta}$ contains derivatives of $(\lambda + i\mu - E_\alpha)^{-1}$ and $(\lambda + i\mu - E_\beta')^{-1}$.

$$
\begin{aligned}
D'_{\alpha\beta} = {} & 4\mu^2 \int_{\theta_\alpha} d\vec{p}\, d\vec{q} \int_{\theta'_\beta} d\vec{p}\,' d\vec{q}\,' \left[(E_0-E_\alpha)^2+\mu^2\right]^{-1} \left[(E_0'-E_\beta')^2+\mu^2\right]^{-1} \\
& \times \sum_\alpha T_\alpha(\vec{p}\vec{q}\,; \vec{p}\,'\vec{q}\,'; \lambda - i\mu) \Big\{ \frac{\varphi_\beta(\vec{q}_\beta{}')}{(\lambda + i\mu - E_\beta')^2} \Big[\sum_\gamma \tilde{G}_{\beta\gamma}(\vec{p}_\beta{}'; \vec{p}\vec{q}\,; \lambda + i\mu) \\
& + \sum_\gamma H_{\beta\gamma}(\vec{p}_\beta{}', \vec{p}_\gamma, \lambda + i\mu) \frac{\varphi_\gamma^*(\vec{q}_\gamma)}{\lambda + i\mu - E_\gamma} \Big] + \Big[\sum_\gamma G_{\gamma\alpha}(\vec{p}\,'\vec{q}\,'; \vec{p}_\alpha; \lambda + i\mu) \\
& + \sum_\gamma \frac{\varphi_\gamma(\vec{q}_\gamma{}')}{\lambda + i\mu - E_\gamma'} H_{\gamma\alpha}(\vec{p}_\gamma{}', \vec{p}_\alpha, \lambda + i\mu) \Big] \frac{\varphi_\alpha(\vec{q}_\alpha)}{(\lambda + i\mu - E_\alpha)^2} \Big\}
\end{aligned}
\tag{3.5.6}
$$

$D'_{\alpha\beta}$ will be treated later in the same way as $C'_{\alpha\beta}$ in the development of the unitarity equation.

The same arguement used in evaluating $C_{\alpha\beta}$ can be used here for $D_{\alpha\beta}$. Almost all terms vanish either as μ or μ^2 . The only possible contribution comes if $\alpha = \beta$, i.e. in $\theta_\alpha \cup \theta'_\alpha$.

$$D_{\alpha\alpha} - D'_{\alpha\alpha} = 4\mu^2 \int_{\theta_\alpha} d\vec{p}\, d\vec{q} \int_{\theta'_\alpha} d\vec{p}'d\vec{q}' \left[(E_0 - E_\alpha)^2 + \mu^2 \right]^{-1} \left[(E_0' - E_\alpha')^2 + \mu^2 \right]^{-1}$$
$$\times\, \delta(\vec{p}_\alpha - \vec{p}_\alpha') \frac{\varphi_\alpha(\vec{q}_\alpha)\varphi^*_\alpha(\vec{q}_\alpha')}{\lambda - i\mu - E_\alpha} \times \frac{\varphi_\alpha(\vec{q}_\alpha')}{\lambda + i\mu - E_\alpha'} H_{\alpha\alpha}(\vec{p}_\alpha', \vec{p}_\alpha, \dot{\lambda} + i\mu) \frac{\varphi^*_\alpha(\vec{q}_\alpha)}{\lambda + i\mu - E_\alpha} \tag{3.5.7}$$

The momentum delta function forces $E_\alpha = E'_\alpha$, thus making all three resolvents on the same energy shell. This is the effect of disconnectedness in the two body-like channels that we referred to earlier in section V.3.1.

$$D_{\alpha\alpha} - D'_{\alpha\alpha} = \int_{\theta_\alpha} d\vec{p}_\alpha \frac{4\mu^2}{(\lambda - i\mu - E_\alpha)(\lambda + i\mu - E_\alpha)^2} H_{\alpha\alpha}(\vec{p}_\alpha, \vec{p}_\alpha, \dot{\lambda} + i\mu) \tag{3.5.8}$$

All the bound state wave functions have been integrated.

In the following identity,

$$\frac{2\mu i}{(x + i\mu)^2} - \frac{2\mu i}{(x - i\mu)(x + i\mu)} = \frac{2\mu i\,(x - i\mu - x - i\mu)}{(x + i\mu)^2(x - i\mu)} = \frac{4\mu^2}{(x - i\mu)(x + i\mu)^2}$$

the first term on the left vanishes as μ , while the second becomes a delta function $-2\pi i\, \delta(x)$ as $\mu \to 0^+$.

Hence,

$$\lim_{\mu \to 0^+} D_{\alpha\alpha} - D'_{\alpha\alpha} = \int d\vec{p}_\alpha\, -2\pi i\, \delta(\lambda - E_\alpha)\, H_{\alpha\alpha}(\vec{p}_\alpha, \vec{p}_\alpha, \dot{\lambda} + i0)$$
$$= \hat{tr}_\alpha\, -2\pi i\, \mathcal{H}_{\alpha\alpha}(\lambda, \lambda, \dot{\lambda} + i0) \tag{3.5.9}$$

The term E cannot contribute in $\theta_\alpha \cup \theta'_\beta$ for $\alpha \neq \beta$.

$$E = 4\mu^2 \, Tr \, R_0(z) \, W(\bar{z}) \, R_0(\bar{z}) \, R_0(z) \left(\frac{1}{\partial\lambda} \sum_{\gamma=1}^{3} T_\gamma(z) \right) R_0(\bar{z})$$

If γ is not equal to either α or β , the only pole in $\theta_\alpha \cup \theta'_\beta$ is in $W(\bar{z})$ which are well defined and finite. Hence the term vanishes as μ^2. If $\gamma = \alpha$ or β , the momentum delta function $\delta(\vec{p}_\alpha - \vec{p}'_\alpha)$ in T_α is inconsistent with the condition $\lambda = E_\alpha = E'_\beta$. The term does not exist in $\theta_\alpha \cup \theta'_\beta$. Hence $E_{\alpha\beta} = 0$ for $\alpha \neq \beta$.

In $\theta_\alpha \cup \theta'_\alpha$,

$$E_{\alpha\alpha} = 4\mu^2 \int_{\theta_\alpha} d\vec{p}\, d\vec{q} \int_{\theta'_\alpha} d\vec{p}'\, d\vec{q}' \left[(E_0 - E_\alpha)^2 + \mu^2 \right]^{-1} \left[(E'_0 - E'_\alpha)^2 + \mu^2 \right]^{-1}$$

$$\times W(\vec{p}\vec{q}\,;\, \vec{p}'\vec{q}'\,;\, \lambda - i\mu) \, \delta(\vec{p}_\alpha - \vec{p}'_\alpha) \left[\frac{\varphi_\alpha(\vec{q}_\alpha) \varphi^*_\alpha(\vec{q}'_\alpha)}{(\lambda - i\mu - E_\alpha)^2} + \hat{t}_\alpha(\vec{q}'_\alpha, \vec{q}_\alpha, \lambda + i\mu - \tilde{p}_\alpha^2) \right]$$

$$= 4\mu^2 \int_{\theta_\alpha} d\vec{p}\, d\vec{q} \int_{\theta'_\alpha} d\vec{p}'\, d\vec{q}' \left[(E_0 - E_\alpha)^2 + \mu^2 \right]^{-1} \left[(E'_0 - E'_\alpha)^2 + \mu^2 \right]^{-1} \times$$

$$\times \Bigg\{ \frac{\varphi_\alpha(\vec{q}_\alpha)}{\lambda - i\mu - E_\alpha} \left(\sum_\beta \tilde{G}_{\alpha\beta}(\vec{p}_\alpha, \vec{p}'\vec{q}'\,;\, \lambda - i\mu) + \sum_{\beta \neq \alpha} H_{\alpha\beta}(\vec{p}_\alpha, \vec{p}'_\beta, \lambda - i\mu) \frac{\varphi^*_\beta(\vec{q}'_\beta)}{\lambda - i\mu - E'_\beta} \right)$$

$$+ \left(\sum_\beta G_{\beta\alpha}(\vec{p}\vec{q}, \vec{p}'_\alpha, \lambda - i\mu) + \sum_{\beta \neq \alpha} \frac{\varphi_\beta(q_\beta)}{\lambda - i\mu - E_\beta} H_{\beta\alpha}(\vec{p}_\beta, \vec{p}'_\alpha, \lambda - i\mu) \right) \frac{\varphi^*_\alpha(\vec{q}'_\alpha)}{\lambda - i\mu - E'_\alpha}$$

$$+ \frac{\varphi_\alpha(\vec{q}_\alpha)}{\lambda - i\mu - E_\alpha} H_{\alpha\alpha}(\vec{p}_\alpha, \vec{p}'_\alpha, \lambda - i\mu) \frac{\varphi_\alpha(\vec{q}'_\alpha)}{\lambda - i\mu - E'_\alpha} \Bigg\} \times$$

$$\times \delta(\vec{p}_\alpha - \vec{p}'_\alpha) \frac{\varphi_\alpha(\vec{q}_\alpha) \varphi^*_\alpha(\vec{q}'_\alpha)}{(\lambda + i\mu - E_\alpha)^2} \qquad (3.5.10)$$

All non-pole terms are dropped. $E_{\alpha\alpha}$ will be treated in later section on unitarity identity.

In any neighbourhood F is a rescattering term. It should be treated as a linear term since the internal integration is trivially done by the two momentum delta functions.

$$\begin{aligned} F_\alpha &= \sum_{\alpha \neq \beta} 4\mu^2 \, tr_\alpha \, R_0(z) \, T_\alpha(z^*) R_0(z^*) \, R_0(z) \left(\frac{2}{\partial \lambda} T_\beta(z) \right) R_0(z^*) \\ &= 4\mu^2 \sum_{\alpha \neq \beta} \int_{\theta_\alpha} d\vec{p} \, d\vec{q} \left[(E_0 - E_\alpha)^2 + \mu^2 \right]^{-2} t_\alpha(\vec{q}_\alpha, \vec{q}_\alpha{}', \lambda - \tilde{p}_\alpha^2 - i\mu) \, t_\beta(\vec{q}_\beta{}', \vec{q}_\beta, \dot{\lambda} - \tilde{p}_\beta^2 + i\mu) \end{aligned} \tag{3.5.11}$$

Since $\alpha \neq \beta$, the primary poles of t_α and t_β will never be the same. Hence in θ_α, each term of F_α contains only one of $(\lambda \pm i\mu - E_\alpha)^{-1}$ or $(\lambda + i\mu - E_\alpha)^{-2}$, each of which are finite and well defined as $\mu \to 0^+$. Hence F vanishes as μ^2.

We have accounted for all contributions in $\theta_\alpha \cup \theta'_\beta$.

V.3.6 Contributions from $\theta_\alpha \cup \theta_0'$ and $\theta_0 \cup \theta_\beta'$

In view of what we have already learned about the calculations with resolvents in all the other neighbourhoods, these remaining contributions are particularly simple. In $\theta_\alpha \cup \theta_0'$ we form the simple delta functions $\delta(\lambda - E_\lambda)$ and $\delta(\lambda - E_0')$. There is no special terms at all. The same goes for $\theta_0 \cup \theta_\beta'$. We here outline the contributions indexed to show the neighbourhoods where they come from. There are no linear term possible and hence A and F are absent. We also simplify the expressions by writing only those with the singular resolvents.

$$C_{\alpha 0} = 4\mu^2 \int_{\theta_\alpha} d\vec{p}\, d\vec{q} \int_{\theta_0'} d\vec{p}'\, d\vec{q}' \left[(E_0 - E_\lambda)^2 + \mu^2\right]^{-1} \left[(E_0' - \lambda)^2 + \mu^2\right]^{-1}$$

$$\times \frac{\varphi_\alpha(\vec{q}_\alpha)}{\lambda - i\mu - E_\alpha} \overset{(\sim)}{B}_{\alpha 0}(\vec{p}_\alpha; \vec{p}'\vec{q}'; \lambda - i\mu) \overset{(\sim)}{B}_{0\alpha}(\vec{p}'\vec{q}'; \vec{p}_\alpha; \lambda + i\mu) \frac{\varphi_\alpha^*(\vec{q}_\alpha)}{\lambda + i\mu - E_\alpha}$$

$$+ C_{\alpha 0}' \tag{3.6.1}$$

where $\overset{(\sim)}{B}_{\alpha 0}(\vec{p}_\alpha, \vec{p}'\vec{q}', \lambda - i\mu) = \sum_\gamma G_{\alpha\gamma}(\vec{p}_\alpha; \vec{p}'\vec{q}'; \lambda - i\mu) + H_{\alpha\gamma}(\vec{p}_\alpha, \vec{p}_\gamma', \lambda - i\mu) \dfrac{\varphi_\gamma(\vec{q}_\gamma')}{\lambda - i\mu - E_\gamma'}$

and
$$C_{\alpha 0}' = 4\mu^2 \int_{\theta_\alpha} d\vec{p}\, d\vec{q} \int_{\theta_0'} d\vec{p}'\, d\vec{q}' \left[(E_0 - E_\alpha)^2 + \mu^2\right]^{-1} \left[(E_0' - \lambda)^2 + \mu^2\right]^{-1}$$

$$\times \frac{\varphi_\alpha(\vec{q}_\alpha)}{\lambda - i\mu - E_\alpha} B_{\alpha 0}(\vec{p}_\alpha; \vec{p}'\vec{q}'; \lambda - i\mu) B_{0\alpha}(\vec{p}'\vec{q}'; \vec{p}_\alpha; \lambda + i\mu) \frac{\varphi_\alpha^*(\vec{q}_\alpha)}{(\lambda + i\mu - E_\alpha)^2} \tag{3.6.2}$$

$$\lim_{\mu \to 0^+} C_{\alpha 0} - C_{\alpha 0}' = \int d\vec{p}_\alpha \int d\vec{p}'\, d\vec{q}'\, (2\pi)^2\, \delta(E_\alpha - \lambda)\, \delta(E_0' - \lambda)\, B_{\alpha 0}(\vec{p}_\alpha; \vec{p}'\vec{q}'; \lambda - i0)$$
$$\times B_{0\alpha}(\vec{p}'\vec{q}'; \vec{p}_\alpha; \lambda + i0)$$

$$= \hat{\mathrm{tr}}_\alpha\, (2\pi)^2\, \mathcal{B}_{\alpha 0}(\lambda, \lambda, \lambda - i0)\, \mathcal{B}_{0\alpha}(\lambda, \lambda, \lambda + i0) \tag{3.6.3}$$

Similarly,

$$C_{o\beta} = \hat{t}_o (2\pi)^2 \mathcal{B}_{o\beta}(\lambda,\lambda,\lambda-io)\, \mathcal{B}_{\beta o}(\lambda,\lambda,\dot{\lambda}+io) + C'_{o\beta}$$

(3.6.4)

$$C'_{o\beta} = 4\mu^2 \int_{\theta_o} d\vec{p}\, d\vec{q} \int_{\theta'_\beta} d\vec{p}'\, d\vec{q}' \left[(E_o-\lambda)^2+\mu^2\right]^{-1} \left[(E'_o-E'_\beta)^2+\mu^2\right]^{-1}$$

$$(\leftarrow)\mathcal{B}_{o\beta}(\vec{p}\vec{q};\vec{p}'_\beta;\lambda-i\mu)\, \frac{\varphi^*_\beta(\vec{q}'_\beta)}{\lambda-i\mu-E'_\beta} \times \frac{\varphi_\beta(\vec{q}'_\beta)}{(\lambda+i\mu-E'_\beta)^2}\, (\rightarrow)\, \mathcal{B}_{\beta o}(\vec{p}'_\beta;\vec{p}\vec{q};\lambda+i\mu)$$

(3.6.5)

Of course $C'_{\alpha o}$ and $C'_{o\beta}$ are to be treated in the unitarity equation later.

$$\mathcal{D}_{\alpha o} = 4\mu^2 \int_{\theta_\alpha} d\vec{p}\, d\vec{q} \int_{\theta'_o} d\vec{p}'\, d\vec{q}' \left[(E_o-E_\alpha)^2+\mu^2\right]^{-1} \left[(E'_o-\lambda)^2+\mu^2\right]^{-1}$$

$$\sum_{\gamma=1}^{3} T_\gamma(\vec{p}\vec{q};\vec{p}'\vec{q}';\lambda-i\mu) \quad W(\vec{p}'\vec{q}';\vec{p}\vec{q};\dot{\lambda}+i\mu)$$

(3.6.6)

If $\gamma \neq \alpha$, all terms vanish as μ^2 since only $(\lambda+i\mu-E_\alpha)^{-1}$ and $(\lambda+i\mu-E_\alpha)^{-2}$ exist in $W(\vec{p}'\vec{q}';\vec{p}\vec{q};\dot{\lambda}+i\mu)$. For $\gamma = \alpha$, the delta function $\delta(\vec{p}_\alpha-\vec{p}'_\alpha)$ forces $E_\alpha = E'_\alpha$ which implies that this term does not exist in $\theta_\alpha \cup \theta'_o$. The condition ($\lambda = E_\alpha$ and $\lambda = E'_o$) is incompatible with ($E_\alpha = E'_\alpha$). Hence $\mathcal{D}_{\alpha o} = 0$. Similarly, $\mathcal{D}_{o\alpha}$ also vanishes. For exactly the same reason $E_{\alpha o}$ and $E_{o\alpha}$ also vanish.

This completes the contributions of (3.1.8) in all the neighbourhoods. It only remains to derive the necessary unitarity equation in the next section.

V.3.7 Unitarity Identity

As in the case of the two body Cayley transform, the final results must be complimented by a unitarity identity, like (V.2.19). In the two body case, it provides for the other two partial derivatives to form a total derivative (i.e.

$$\frac{d}{d\lambda}\tau(\lambda,\lambda,\lambda+i0) = \underline{\tau(\dot{\lambda},\dot{\lambda},\lambda+i0)} + \tau(\lambda,\lambda,\dot{\lambda}+i0)$$

.)

In the three body case, the unitarity identity fulfils firstly this function and it also contains the double poles terms $(\lambda+i\mu-E_\alpha)^{-2}$ necessary to cancel those present in the Cayley tranform. Individually, each double pole term (derived from derivatives of the original simple primary pole) is singular as a generalized function. The unitarity identity, thus also regularize the three body Cayley transform.

To evaluate the trace of the three body unitarity equation we adopt the same method used for the three body Cayley transform itself. We devide the six dimensional volume of integration into five regions Θ, θ_0, θ_1, θ_2 & θ_3 for the trace, and five regions Θ', θ_0', θ_1', θ_2' & θ_3' for the internal state integration. Θ and Θ' contibute nothing. In $\theta_0 \cup \theta_0'$ we have to regularize the rescattering terms. In all the other neighbourhoods, the free resolvents and primary poles form simple delta functions in energy. The unitarity equation appears to have quadratic terms only. However, special attention must be paid to the disconnected pole term $\delta(\vec{p}_\alpha-\vec{p}_\alpha{}')\frac{\varphi_\alpha(\vec{q}_\alpha)\varphi_\alpha^*(\vec{q}_\alpha{}')}{\lambda+i\mu-E_\alpha}$. This special structure produces the linear terms in $q_{\alpha\alpha}^{(1)}$.

To adopt the unitarity method to the three body unitarity equation, one must do a preliminary step. One must first subtract all disconnected terms. The connected unitarity equation is:

$$W(z) - W(z^*) = -2i\mu \Big\{ \sum_{\alpha \neq \beta} T_\alpha(z) R_0(z) R_0(z^*) T_\beta(z^*) +$$

$$+ \sum_\alpha \Big[T_\alpha(z) R_0(z) R_0(z^*) W(z^*) + W(z) R_0(z) R_0(z^*) T_\alpha(z^*) \Big]$$

$$+ W(z) R_0(z) R_0(z^*) W(z^*) \Big\} \tag{3.7.1}$$

Contributions in $\theta_0 \cup \theta_0'$

The next step is to rearrange the right hand side of (3.7.1) so that it would be regular in $\theta_0 \cup \theta_0'$. In any other neighbourhood such a step is not necessary.

We start with the first three terms in the series.

$$A = \sum_{\alpha \neq \beta} -2i\mu\, T_\alpha(z) R_0(z) R_0(z^*) T_\beta(z^*)$$

$$= \sum_{\alpha \neq \beta} -2\pi i\, T_\alpha(z)\, \delta_\mu(H_0 - \lambda)\, T_\beta^{\dagger}(z)$$

$$= \sum_{\alpha \neq \beta} -2\pi i \Big[\mathrm{Re}\, T_\alpha(z)\, \delta_\mu(H_0-\lambda)\, \mathrm{Re}\, T_\beta(z) + \mathrm{Im}\, T_\alpha(z)\, \delta_\mu(H_0-\lambda)\, \mathrm{Im}\, T_\alpha(z) \Big]$$

$$+ 2\pi \Big[-\mathrm{Re}\, T_\alpha(z)\, \delta_\mu(H_0-\lambda)\, \mathrm{Im}\, T_\beta(z) + \mathrm{Im}\, T_\alpha(z)\, \delta_\mu(H_0-\lambda)\, \mathrm{Re}\, T_\beta(z) \Big] \tag{3.7.2}$$

$$B = \sum_{\alpha \neq \beta} +2i\mu\, T_\alpha(z) R_0(z) R_0(z^*) \big[T_\alpha(z^*) R_0(z^*) T_\beta(z^*) \big]$$

$$= \sum_{\alpha \neq \beta} -2i\, \mathrm{Im}\, T_\alpha(z)\, R_0(z^*)\, T_\beta(z^*)$$

$$= \sum_{\alpha \neq \beta} -2i\, \mathrm{Im}\, T_\alpha(z) \Big[\frac{P_\mu}{H_0 - \lambda} - i\pi\, \delta_\mu(H_0-\lambda) \Big] \Big[\mathrm{Re}\, T_\beta(z) - i\, \mathrm{Im}\, T_\beta(z) \Big]$$

$$= \sum_{\alpha \neq \beta} -2\pi\, \mathrm{Im}\, T_\alpha(z)\, \delta_\mu(H_0-\lambda)\, \mathrm{Re}\, T_\beta(z) - 2\, \mathrm{Im}\, T_\alpha(z) \frac{P_\mu}{H_0 - \lambda} \mathrm{Im}\, T_\beta(z)$$

$$-2i\,\mathcal{I}m\,T_\alpha(z)\frac{P_\mu}{H_0-\lambda}\,Re\,T_\beta(z) \quad + \quad 2i\,\mathcal{I}m\,T_\alpha(z)\,\pi\,\delta_\mu(H_0-\lambda)\,\mathcal{I}m\,T_\beta(z)$$

(3.7.3)

$$C = \sum_{\alpha\neq\beta} +2i\mu\left[T_\alpha(z)\,R_0(z)\,T_\beta(z)\right]\,R_0(z)\,R_0(z^*)\;T_\beta(z^*)$$

$$= \sum_{\alpha\neq\beta} -2i\;T_\alpha(z)\;R_0(z)\;\mathcal{I}m\,T_\beta(z)$$

$$= \sum_{\alpha\neq\beta} 2\;Re\,T_\alpha(z)\,\pi\,\delta_\mu(H_0-\lambda)\;\mathcal{I}m\,T_\beta(z) \quad + \quad 2\,\mathcal{I}m\,T_\alpha(z)\frac{P_\mu}{H_0-\lambda}\,\mathcal{I}m\,T_\beta(z)$$

$$-2i\;Re\,T_\alpha(z)\frac{P_\mu}{H_0-\lambda}\;\mathcal{I}m\,T_\beta(z) \;+\; 2i\;\mathcal{I}m\,T_\alpha(z)\,\pi\,\delta_\mu(H_0-\lambda)\;\mathcal{I}m\,T_\beta(z)$$

(3.7.4)

Add them together,

$$A + B + C = \sum_{\alpha\neq\beta} -2\pi i\;Re\,T_\alpha(z)\,\delta_\mu(H_0-\lambda)\,Re\,T_\beta(z) \;+\; 2\pi i\;\mathcal{I}m\,T_\alpha(z)\,\delta_\mu(H_0-\lambda)\;\mathcal{I}m\,T_\beta(z)$$

$$-2i\;\mathcal{I}m\,T_\alpha(z)\;\frac{P_\mu}{H_0-\lambda}\,Re\;T_\beta(z) \;-\; 2i\;Re\,T_\alpha(z)\;\frac{P_\mu}{H_0-\lambda}\;\mathcal{I}m\,T_\beta(z)$$

$$= \sum_{\alpha\neq\beta} -2i\;\mathcal{I}m\left(T_\alpha(z)\;R_0(z)\;T_\beta(z)\right)$$

(3.7.5)

The next three terms also need to be rearranged.

$$D = \sum_{\alpha\neq\beta} +2i\mu\;\;T_\alpha(z)\,R_0(z)\,R_0(z^*)\left[T_\beta(z^*)\;R_0(z^*)\;T_\alpha(z^*)\right]$$

$$= \sum_{\alpha\neq\beta} 2\pi i\;\;T_\alpha(z)\left[\delta_\mu(H_0-\lambda)\;\;T_\beta(z^*)\;\;R_0(z^*)\right]\;T_\alpha(z^*)$$

$$= \sum_{\alpha\neq\beta} T_\alpha(z)\Big[\;2\pi i\;\delta_\mu(H_0-\lambda)\;\;Re\;T_\beta(z)\;\frac{P_\mu}{H_0-\lambda} \;-\; 2\pi i\,\delta_\mu(H_0-\lambda)\;\mathcal{I}m\,T_\beta(z)\,\pi\,\delta_\mu(H_0-\lambda)$$

$$2\pi\,\delta_\mu(H_0-\lambda)\;Re\;T_\beta(z)\,\pi\,\delta_\mu(H_0-\lambda) \;+\; 2\pi\,\delta_\mu(H_0-\lambda)\;\mathcal{I}m\,T_\beta(z)\frac{P_\mu}{H_0-\lambda}\Big]\;T_\alpha(z^*)$$

(3.7.6)

$$E = \sum_{\alpha\neq\beta} +2i\mu\left[T_\alpha(z)\;R_0(z)\;T_\beta(z)\right]\;R_0(z)\,R_0(z^*)\;\;T_\alpha(z^*)$$

$$= \sum_{\alpha\neq\beta} 2\pi i\;\;T_\alpha(z)\;R_0(z)\;\;T_\beta(z)\;\delta_\mu(H_0-\lambda)\;\;T_\alpha^{\dagger}(z)$$

$$= \sum_{\alpha\neq\beta} T_\alpha(z)\Big[\, 2i\,\frac{P_\mu}{H_0-\lambda}\,\mathrm{Re}\,T_\beta(z)\,\pi\delta_\mu(H_0-\lambda) \;-\; 2i\pi\delta_\mu(H_0-\lambda)\,\mathrm{Im}\,T_\beta(z)\,\pi\delta_\mu(H_0-\lambda)$$

$$-\,2\,\frac{P_\mu}{H_0-\lambda}\,\mathrm{Im}\,T_\beta(z)\,\pi\delta_\mu(H_0-\lambda) \;-\; 2\pi\delta_\mu(H_0-\lambda)\,\mathrm{Re}\,T_\beta(z)\,\pi\delta_\mu(H_0-\lambda)\Big]\, T_\alpha(z^*) \tag{3.7.7}$$

$$F = -2i\mu \sum_{\alpha\neq\beta}\big[T_\alpha(z)R_0(z)T_\beta(z)\big]R_0(z)R_0(z^*)\big[T_\beta(z^*)R_0(z^*)T_\alpha(z^*)\big]$$

$$= \sum_{\alpha\neq\beta} T_\alpha(z)\big[R_0(z)\;2i\,\mathrm{Im}\,T_\beta(z)\;R_0(z^*)\big]T_\alpha(z^*)$$

$$= \sum_{\alpha\neq\beta} T_\alpha(z)\Big[\,2i\,\frac{P_\mu}{H_0-\lambda}\,\mathrm{Im}\,T_\beta(z)\,\frac{P_\mu}{H_0-\lambda} \;+\; 2i\pi\delta_\mu(H_0-\lambda)\,\mathrm{Im}\,T_\beta(z)\,\pi\delta_\mu(H_0-\lambda)$$

$$+\,2\,\frac{P_\mu}{H_0-\lambda}\,\mathrm{Im}\,T_\beta(z)\,\pi\delta_\mu(H_0-\lambda) \;-\; 2\pi\delta_\mu(H_0-\lambda)\,\mathrm{Im}\,T_\beta(z)\,\frac{P_\mu}{H_0-\lambda}\Big]\,T_\alpha(z^*) \tag{3.7.8}$$

Adding,

$$D + E + F = \sum_{\alpha\neq\beta} T_\alpha(z)\Big[\,2i\,\frac{P_\mu}{H_0-\lambda}\,\mathrm{Im}\,T_\beta(z)\,\frac{P_\mu}{H_0-\lambda} \;-\; 2i\pi\delta_\mu(H_0-\lambda)\,\mathrm{Im}\,T_\beta(z)\,\pi\delta_\mu(H_0-\lambda)$$

$$+\,2i\pi\delta_\mu(H_0-\lambda)\,\mathrm{Re}\,T_\beta(z)\,\frac{P_\mu}{H_0-\lambda} \;+\; 2i\,\frac{P_\mu}{H_0-\lambda}\,\mathrm{Re}\,T_\beta(z)\,\pi\delta_\mu(H_0-\lambda)\Big]\,T_\alpha(z^*)$$

$$= \sum_{\alpha\neq\beta} 2i\; T_\alpha(z)\Big[\mathrm{Im}\big(R_0(z)\,T_\beta(z)\,R_0(z)\big)\Big]\,T_\alpha(z^*) \tag{3.7.9}$$

Putting this back into the unitarity equation we have a connected and regularized equation.

$$W(\lambda+i\mu) - W(\lambda-i\mu) = \sum_{\alpha\neq\beta}\Big[-2i\,\mathrm{Im}\big(T_\alpha(z)\,R_0(z)\,T_\beta(z)\big)$$

$$+\,2i\;T_\alpha(z^*)\,\mathrm{Im}\big(R_0(z)\,T_\beta(z)\,R_0(z)\big)\,T_\alpha(z)\Big]$$

$$+\Big[\sum_{\alpha\neq\beta} Q^{(1)}_{\alpha\beta}(\lambda-i\mu) + \tilde{W}(z^*)\Big]\big(-2\pi i\,\delta_\mu(H_0-\lambda)\big)\times$$

$$\times\Big[\sum_{\gamma\neq\delta} Q^{(1)}_{\gamma\delta}(\lambda+i\mu) + \tilde{W}(z)\Big] \qquad \alpha\neq\delta,\ \beta\neq\gamma$$

$$+\Big[\sum_{\alpha} T_\alpha(z^*)\Big]\Big(-2\pi i\,\delta_\mu(H_0-\lambda)\Big)\Big[\sum_{\gamma\neq\delta} Q^{(1)}_{\gamma\delta}(z) + \widetilde{W}(z)\Big]_{\alpha\neq\gamma\,,\ \alpha\neq\delta}$$

$$+\Big[\sum_{\gamma\neq\delta} Q^{(1)}_{\gamma\delta}(z^*) + \widetilde{W}(z^*)\Big]\Big(-2\pi i\,\delta_\mu(H_0-\lambda)\Big)\Big[\sum_{\alpha} T_\alpha(z)\Big]_{\alpha\neq\gamma,\ \alpha\neq\delta} \tag{3.7.10}$$

For notational convinience we define the following:

$$X(z) \equiv \sum_{\alpha\neq\beta} -2i\ \mathrm{Im}\Big[T_\alpha(z)\,R_0(z)\,T_\beta(z)\Big] \tag{3.7.11}$$

$$Y(z) \equiv \sum_{\alpha\neq\beta} 2i\ T_\alpha(z^*)\ \mathrm{Im}\Big[R_0(z)\,T_\beta(z)\,R_0(z)\Big]\,T_\alpha(z) \tag{3.7.12}$$

These rescattering terms will be separated out while we deal with the "normal" terms first. They will vanish and not contribute to the unitarity identity. This we prove later. To proceed we must put (3.7.10) into reduced form.

$$\mathcal{W}(E_0',E,z) - \mathcal{W}(E_0',E,z^*) - \mathcal{X}(E_0',E_0,z) - \mathcal{Y}(E_0',E_0,z)$$

$$= \int_{\theta_0''} dE_0''\,(-2\pi i)\,\delta_\mu(E_0''-\lambda)\Big\{\Big[\sum_{\alpha\neq\beta}\mathcal{L}^{(1)}_{\alpha\beta}(E_0',E_0'',z^*) + \widetilde{\mathcal{W}}(E_0',E_0'',z^*)\Big]\times$$

$$\times\Big[\sum_{\gamma\neq\delta}\mathcal{L}^{(1)}_{\gamma\delta}(E_0'',E_0,z) + \widetilde{\mathcal{W}}(E_0'',E_0,z)\Big]_{\alpha\neq\delta\,,\ \beta\neq\gamma} +$$

$$+ \sum_{\alpha}\mathcal{T}_\alpha(E_0',E_0'',z^*)\times\Big[\sum_{\gamma\neq\delta}\mathcal{L}^{(1)}_{\gamma\delta}(E_0'',E_0,z) + \widetilde{\mathcal{W}}(E_0'',E_0,z)\Big]_{\alpha\neq\gamma,\ \alpha\neq\delta}$$

$$+\Big[\sum_{\gamma\neq\delta}\mathcal{L}^{(1)}_{\gamma\delta}(E_0',E_0'',z^*) + \widetilde{\mathcal{W}}(E_0',E_0'',z^*)\Big]\times\sum_{\alpha}\mathcal{T}_\alpha(E_0'',E_0,z)_{\ \alpha\neq\gamma,\ \alpha\neq\delta}\Big\} \tag{3.7.13}$$

Next we follow the procedure used in deriving (V.2.19) to establish our unitarity identity in $\theta_0 \cup \theta_0'$. For clarity and comparison we list here all the necessary steps:

[1] Differentiate with respect to E_0 , $\partial/\partial E_0$.

[2] Set on diagonal, i.e. $E_0 = E_0'$.

[3] Multiply by $2\pi \ \delta_\mu(E_0-\lambda)$.

[4] Integrate in the neighbourhood $\theta_0 \cup \theta_0'$, $\int_{\theta_0} dE_0 \, \hat{tr}_0$.

[5] Repeat steps [1] to [4] with an alternative form of (3.7.13).

[6] Add both results and take the real part.

The first four steps can be done together rather trivially. The notation has been designed to make such steps simple.

$$\int_{\theta_0} dE_0 \ 2\pi \ \delta_\mu(E_0-\lambda) \ \hat{tr}_0 \Big[\mathcal{W}(E_0, \dot{E}_0, \lambda+i\mu) - \mathcal{W}(E_0, \dot{E}_0, \lambda-i\mu)$$

$$- \mathcal{X}(E_0, \dot{E}_0, \lambda+i\mu) - \mathcal{Y}(E_0, \dot{E}_0, \lambda+i\mu) \Big]$$

$$= \int_{\theta_0} dE_0 \ 2\pi \delta_\mu(E_0-\lambda) \int_{\theta_0'} dE_0' \, {-2\pi i} \delta_\mu(E_0'-\lambda) \ \times$$

$$\times \ \hat{tr}_0 \Big\{ \Big[\sum_{\alpha\neq\beta} \mathcal{L}^{(1)}_{\alpha\beta}(E_0, E_0', \lambda-i\mu) + \tilde{\mathcal{W}}(E_0, E_0', \lambda-i\mu) \Big] \times$$

$$\times \Big[\sum_{\gamma\neq\delta} \mathcal{L}^{(1)}_{\gamma\delta}(E_0', \dot{E}_0, \lambda+i\mu) + \tilde{\mathcal{W}}(E_0', \dot{E}_0, \lambda+i\mu) \Big]_{\alpha\neq\delta, \ \beta\neq\gamma.}$$

$$+ \sum_\alpha \mathcal{J}_\alpha(E_0, E_0', \lambda-i\mu) \Big[\sum_{\gamma\neq\delta} \mathcal{L}^{(1)}_{\gamma\delta}(E_0', \dot{E}_0, \lambda+i\mu) + \tilde{\mathcal{W}}(E_0', \dot{E}_0, \lambda+i\mu) \Big]_{\alpha\neq\gamma, \ \alpha\neq\delta}$$

$$+ \Big[\sum_{\gamma\neq\delta} \mathcal{L}^{(1)}_{\gamma\delta}(E_0, E_0', \lambda-i\mu) + \tilde{\mathcal{W}}(E_0, E_0', \lambda-i\mu) \Big] \sum_\alpha \mathcal{J}_\alpha(E_0', \dot{E}_0, \lambda+i\mu)_{\alpha\neq\gamma, \ \alpha\neq\delta} \Big\} \quad (3.7.14)$$

The next natural step is to take the limit $\mu \to 0^+$, and also integrate the resulting energy delta functions. The result assumes the simple form of reduced space operator trace.

$$2\pi \quad \hat{t}r_0 \left[\mathcal{W}(\lambda, \dot{\lambda}, \lambda+i0) - \mathcal{W}(\lambda, \dot{\lambda}, \lambda-i0) - \mathcal{X}(\lambda, \dot{\lambda}, \lambda+i0) - \mathcal{Y}(\lambda, \dot{\lambda}, \lambda+i0) \right]$$

$$= -4\pi^2 i\, \hat{t}r_0 \left\{ \left[\sum_{\alpha\neq\beta} \mathcal{L}^{(1)}_{\alpha\beta}(\lambda, \lambda, \lambda-i0) + \tilde{\mathcal{W}}(\lambda, \lambda, \lambda-i0) \right] \right.$$

$$\times \left[\sum_{\gamma\neq\delta} \mathcal{L}^{(1)}_{\gamma\delta}(\lambda, \dot{\lambda}, \lambda+i0) + \tilde{\mathcal{W}}(\lambda, \dot{\lambda}, \lambda+i0) \right]_{\alpha\neq\delta\ ,\ \beta\neq\gamma}$$

$$+ \sum_{\alpha} \mathcal{J}_{\alpha}(\lambda, \lambda, \lambda-i0) \left[\sum_{\gamma\neq\delta} \mathcal{L}^{(1)}_{\gamma\delta}(\lambda, \dot{\lambda}, \lambda+i0) + \tilde{\mathcal{W}}(\lambda, \dot{\lambda}, \lambda+i0) \right]_{\alpha\neq\gamma,\ \alpha\neq\delta}$$

$$\left. + \left[\sum_{\alpha\neq\beta} \mathcal{L}^{(1)}_{\alpha\beta}(\lambda, \lambda, \lambda-i0) + \tilde{\mathcal{W}}(\lambda, \lambda, \lambda-i0) \right] \sum_{\alpha} \mathcal{J}_{\alpha}(\lambda, \dot{\lambda}, \lambda+i0)_{\alpha\neq\gamma,\ \alpha\neq\delta} \right\}$$

(3.7.15)

In order to carry out step [5] we must write down the alternate unitarity equation to replace(3.7.13).

$$\mathcal{W}(E_0, E_0', z) - \mathcal{W}(E_0, E_0', z^*) - \mathcal{X}(E_0, E_0', z) - \tilde{\mathcal{Y}}(E_0, E_0', z)$$

$$= \int_{\theta_0''} dE_0'' \,(-2\pi i)\, \delta_\mu(E_0''-\lambda) \left\{ \left[\sum_{\gamma\neq\delta} \mathcal{L}^{(1)}_{\gamma\delta}(E_0, E_0'', z) + \tilde{\mathcal{W}}(E_0, E_0'', z) \right] \right.$$

$$\times \left[\sum_{\alpha\neq\beta} \mathcal{L}^{(1)}_{\alpha\beta}(E_0'', E_0', z^*) + \tilde{\mathcal{W}}(E_0'', E_0', z^*) \right]_{\alpha\neq\delta\ ,\ \beta\neq\gamma}$$

$$+ \sum_{\alpha} \mathcal{J}_{\alpha}(E_0, E_0'', z) \left[\sum_{\gamma\neq\delta} \mathcal{L}^{(1)}_{\gamma\delta}(E_0'', E_0', z^*) + \tilde{\mathcal{W}}(E_0'', E_0', z^*) \right]_{\alpha\neq\delta,\ \alpha\neq\gamma}$$

$$\left. + \left[\sum_{\gamma\neq\delta} \mathcal{L}^{(1)}_{\gamma\delta}(E_0, E_0'', z) + \tilde{\mathcal{W}}(E_0, E_0'', z) \right] \sum_{\alpha} \mathcal{J}_{\alpha}(E_0'', E_0', z^*)_{\alpha\neq\delta,\ \alpha\neq\gamma} \right\}$$

(3.7.16)

where $\tilde{Y}$ is the new rescattering term given by

$$\tilde{Y}(z) \equiv \sum_{\alpha\neq\beta} 2i \; T_\alpha(z)\, \mathcal{I}m\left[R_0(z)\, T_\beta(z)\, R_0(z)\right] T_\alpha(\overset{*}{z}) \tag{3.7.17}$$

The results of step [5] closely resemble (3.7.15)

$$2\pi \cdot \hat{\mathcal{t}r}_0\left[\mathcal{W}(\dot{\lambda},\lambda,\lambda+io) - \mathcal{W}(\dot{\lambda},\lambda,\lambda-io) - \mathcal{X}(\dot{\lambda},\lambda,\lambda+io) - \tilde{\mathcal{Y}}(\dot{\lambda},\lambda,\lambda+io)\right]$$

$$= -4\pi^2 i\, \hat{\mathcal{t}r}_0\Big\{\Big[\sum_{\gamma\neq\delta} \mathcal{L}^{(1)}_{\gamma\delta}(\dot{\lambda},\lambda,\lambda+io) + \tilde{\mathcal{W}}(\dot{\lambda},\lambda,\lambda+io)\Big]$$

$$\times\Big[\sum_{\alpha\neq\beta} \mathcal{L}^{(1)}_{\alpha\beta}(\lambda,\lambda,\lambda-io) + \tilde{\mathcal{W}}(\lambda,\lambda,\lambda-io)\Big]_{\alpha\neq\delta,\ \beta\neq\gamma}$$

$$+ \sum_\alpha \mathcal{J}_\alpha(\dot{\lambda},\lambda,\lambda+io)\Big[\sum_{\gamma\neq\delta} \mathcal{L}^{(1)}_{\gamma\delta}(\lambda,\lambda,\lambda-io) + \tilde{\mathcal{W}}(\lambda,\lambda,\lambda-io)\Big]_{\alpha\neq\delta,\ \alpha\neq\gamma}$$

$$+\Big[\sum_{\gamma\neq\delta} \mathcal{L}^{(1)}_{\gamma\delta}(\dot{\lambda},\lambda,\lambda+io) + \tilde{\mathcal{W}}(\dot{\lambda},\lambda,\lambda+io)\Big] \sum_\alpha \mathcal{J}_\alpha(\lambda,\lambda,\lambda-io)_{\alpha\neq\delta,\ \alpha\neq\gamma}\Big\} \tag{3.7.18}$$

Adding equations 15 and 18 together, the real part will give the required unitarity identity.

$$0 = \mathcal{I}m\, \hat{\mathcal{t}r}_0\Big\{\Big[\sum_{\alpha\neq\beta} \mathcal{L}^{(1)}_{\alpha\beta}(\lambda,\lambda,\lambda-io) + \tilde{\mathcal{W}}(\lambda,\lambda,\lambda-io)\Big]$$

$$\times\Big[\sum_{\gamma\neq\delta} \mathcal{L}^{(1)}_{\gamma\delta}(\dot{\lambda},\dot{\lambda},\lambda+io) + \tilde{\mathcal{W}}(\dot{\lambda},\dot{\lambda},\lambda+io)\Big]_{\alpha\neq\delta,\ \beta\neq\gamma}$$

$$+ \sum_\alpha \mathcal{J}_\alpha(\lambda,\lambda,\lambda-io)\Big[\sum_{\gamma\neq\delta} \mathcal{L}^{(1)}_{\gamma\delta}(\dot{\lambda},\dot{\lambda},\lambda+io) + \tilde{\mathcal{W}}(\dot{\lambda},\dot{\lambda},\lambda+io)\Big]_{\alpha\neq\delta,\ \alpha\neq\gamma}$$

$$+\Big[\sum_{\gamma\neq\delta} \mathcal{L}^{(1)}_{\gamma\delta}(\lambda,\lambda,\lambda-io) + \tilde{\mathcal{W}}(\lambda,\lambda,\lambda-io)\Big] \sum_\alpha \mathcal{J}_\alpha(\dot{\lambda},\dot{\lambda},\lambda+io)_{\alpha\neq\delta,\ \alpha\neq\gamma}\Big\} \tag{3.7.19}$$

It remains to be shown that the left hand side is zero.

The first two terms of the left hand side is explicitly imaginary so that its real part is zero. The same is true of the third term.

$$\text{L.H.S.} = 2\pi \hat{h}_0 \Big[\mathcal{W}(\dot{\lambda},\dot{\lambda},\lambda+i0) - \mathcal{W}(\dot{\lambda},\dot{\lambda},\lambda-i0) - \mathcal{X}(\dot{\lambda},\dot{\lambda},\lambda+i0) - \mathcal{Y}(\lambda,\dot{\lambda},\lambda+i0) - \tilde{\mathcal{Y}}(\dot{\lambda},\lambda,\lambda+i0) \Big]$$

If Υ and $\check{\Upsilon}$ are equal, the last two terms will be pure imaginary also.

V.3.8 Contributions in $\theta_0 \cup \theta_\beta'$ and $\theta_\beta \cup \theta_0'$

In any neighbourhood other than $\theta_0 \cup \theta_0'$, there is no rescattering singularities. The unitarity equation (3.7.1) must be developed to show primary singularities rather than rearranged as in (3.7.10). We must simplify (3.7.1) by introducing the subscript notation of "connectedness".

$$W(z) - W(z^*) = -2i\mu\left[M(z)\,R_0(z)\,R_0(z^*)\,M(z^*)\right]_C \tag{3.8.1}$$

where the right hand side denotes the same as in (3.7.1). In kernel form we have:

$$W(\vec{p}'\vec{q}'; \vec{p}\vec{q}; z) - W(\vec{p}'\vec{q}'; \vec{p}\vec{q}; z^*)$$
$$= \int d\vec{p}''d\vec{q}'' \frac{-2i\mu}{(E_0''-\lambda)^2+\mu^2}\left[M(\vec{p}'\vec{q}'; \vec{p}''\vec{q}''; z^*)\;\; M(\vec{p}''\vec{q}''; \vec{p}\vec{q}; z)\right]_C \tag{3.8.2}$$

It is not necessary to expand the full primary pole structure of $M(z)$. It suffices to write down only the coefficients of the particular pole that is singular in the neighbourhood involved. For contributions in $\theta_0 \cup \theta_\beta'$, $\beta = 1,2,3,$ we write (3.8.2) as:

$$W(\vec{p}'\vec{q}'; \vec{p}\vec{q}; z) - W(\vec{p}'\vec{q}'; \vec{p}\vec{q}; z^*)$$
$$= \int_{\theta_\beta''} d\vec{p}''d\vec{q}'' \frac{-2i\mu}{(E_0''-E_\beta'')^2+\mu^2}\left[\delta(\vec{p}_\beta'-\vec{p}_\beta'')\,\varphi_\beta^*(\vec{q}_\beta') + (-)\,B_{0\beta}(\vec{p}'\vec{q}'; \vec{p}_\beta''; z^*)\right]$$
$$\times \frac{\varphi_\beta(\vec{q}_\beta^\circ)\,\varphi_\beta^*(\vec{q}_\beta^\circ)}{(\lambda-i\mu-E_\beta'')(\lambda+i\mu-E_\beta'')}\left[\delta(\vec{p}_\beta''-\vec{p}_\beta)\,\varphi_\beta(\vec{q}_\beta) + (-)\,B_{\beta 0}(\vec{p}_\beta''; \vec{p}\vec{q}; z)\right]_C \tag{3.8.3}$$

+ remainder

The remainder contains no poles in θ''_β , i.e. no coefficient of $(\lambda \pm i\mu - E''_\beta)^{-1}$. The disconnected pole term cannot contribute because $\delta(\vec{P}'_\beta - \vec{P}''_\beta)$ would require $E'_\beta = E''_\beta$ which is inconsistent with $\lambda = E'_0 = E''_\beta$ in $\theta_0 \cup \theta'_\beta$. We rewrite (3.8.3) in reduced space notation after some simplification.

$$\mathcal{W}(E'_0, E_0, \lambda+i\mu) - \mathcal{W}(E'_0, E_0, \lambda-i\mu)$$
$$= \int_{\theta''_\beta} dE''_\beta \left[\int d\vec{q}''_\beta \frac{\varphi_\beta(\vec{q}''_\beta)\,\varphi^*_\beta(\vec{q}''_\beta)}{(E''_0 - E''_\beta)^2 + \mu^2} \right] -2\pi i\, \delta_\mu(E''_\beta - \lambda)\, \mathcal{B}_{0\beta}(E'_0, E''_\beta, \lambda - i\mu)$$
$$\times\, \mathcal{B}_{\beta 0}(E''_\beta, E_0, \lambda + i\mu) \;+\; \text{remainder} \qquad (3.8.4)$$

Following steps [1] to [4] as in section V.3.7 we have

$$\int_{\theta_0} dE_0\; 2\pi\, \delta_\mu(E_0 - \lambda)\, \hat{tr}_0 \left[\mathcal{W}(E_0, \dot{E}_0, \lambda+i\mu) - \mathcal{W}(E_0, \dot{E}_0, \lambda - i\mu) \right]$$
$$= \int_{\theta_0} dE_0\; 2\pi\, \delta_\mu(E_0 - \lambda) \int_{\theta'_\beta} dE'_\beta \; -2\pi i\, \delta_\mu(E'_\beta - \lambda) \left[\int d\vec{q}'_\beta \frac{\varphi_\beta(\vec{q}'_\beta)\,\varphi^*_\beta(\vec{q}'_\beta)}{(E'_0 - E'_\beta)^2 + \mu^2} \right]$$
$$\times\, \hat{tr}_0\, \mathcal{B}_{0\beta}(E_0, E'_\beta, \lambda - i\mu)\, \mathcal{B}_{\beta 0}(E'_\beta, \dot{E}_0, \lambda + i\mu) \;+\; \text{remainder} \qquad (3.8.5)$$

We take the limit $\mu \to 0^+$, so that $\left[\int d\vec{q}''_\beta \frac{\varphi_\beta(\vec{q}''_\beta)\,\varphi^*_\beta(\vec{q}''_\beta)}{(E''_0 - E''_\beta)^2 + \mu^2} \right] \to 1$ and the remainder vanishes.

$$2\pi\, \hat{tr}_0 \left[\mathcal{W}(\lambda, \dot{\lambda}, \lambda + i0) - \mathcal{W}(\lambda, \dot{\lambda}, \lambda - i0) \right] \Big|_{\theta_0 \cap \theta'_\beta}$$
$$= -4\pi^2 i\, \hat{tr}_0\, \mathcal{B}_{0\beta}(\lambda, \lambda, \lambda - i0)\, \mathcal{B}_{\beta 0}(\lambda, \dot{\lambda}, \lambda + i0) \qquad (3.8.6)$$

The alternative unitarity equation would yield

$$2\pi\ \hat{tr}_0\left[W(\dot{\lambda},\lambda,\lambda+io) - W(\dot{\lambda},\lambda,\lambda-io)\right]\Big|_{\theta_\beta\cap\theta_0'}$$

$$= -4\pi^2 i\ \hat{tr}_0\ \mathcal{B}_{0\beta}(\dot{\lambda},\lambda,\lambda+io)\ \mathcal{B}_{\beta 0}(\lambda,\lambda,\lambda-io) \tag{3.8.7}$$

The real part of thesum of (3.8.6) and (3.8.7) gives

$$0 = \mathrm{Im}\ \hat{tr}_0\ \mathcal{B}_{0\beta}(\lambda,\lambda,\lambda-io)\ \mathcal{B}_{\beta 0}(\lambda,\dot{\lambda},\lambda+io)$$
$$+ \mathrm{Im}\ \hat{tr}_0\ \mathcal{B}_{0\beta}(\dot{\lambda},\lambda,\lambda+io)\ \mathcal{B}_{\beta 0}(\lambda,\lambda,\lambda+io) \tag{3.8.8}$$

We should note here that the two terms on the right belong to different channels since

$$\hat{tr}_0\ \mathcal{B}_{0\beta}(\dot{\lambda},\lambda,\lambda+io)\ \mathcal{B}_{\beta 0}(\lambda,\lambda,\lambda-io)$$
$$= \hat{tr}_\beta\ \mathcal{B}_{\beta 0}(\lambda,\lambda,\lambda-io)\ \mathcal{B}_{0\beta}(\dot{\lambda},\lambda,\lambda+io) \tag{3.8.9}$$

Hence,

$$0 = \mathrm{Im}\ \hat{tr}_0\ \mathcal{B}_{0\beta}(\lambda,\lambda,\lambda-io)\ \mathcal{B}_{\beta 0}(\lambda,\dot{\lambda},\lambda+io)$$
$$+ \mathrm{Im}\ \hat{tr}_\beta\ \mathcal{B}_{\beta 0}(\lambda,\lambda,\lambda-io)\ \mathcal{B}_{0\beta}(\dot{\lambda},\lambda,\lambda+io) \tag{3.8.10}$$

In $\theta_\beta \cup \theta_0'$, $\beta = 1,2,3$ we write (3.8.2) as

$$0 = \int_{\theta_0''} d\vec{p}\,''d\vec{q}\,'' - 2\pi i\ \delta_\mu(E_0''-\lambda)\,\frac{\varphi_\beta^*(\vec{q}_\beta')}{\lambda-i\mu-E_\beta'}\ B_{\beta 0}(\vec{p}_\beta\,';\vec{p}\,''\vec{q}\,'';\lambda-i\mu)$$

$$\times B_{0\beta}(\vec{p}\,''\vec{q}\,'';\vec{p}_\beta;\lambda+i\mu)\,\frac{\varphi_\beta(\vec{q}_\beta)}{\lambda+i\mu-E_\beta} \quad + \text{ remainder} \tag{3.8.11}$$

The remainder contains all non-pole quadratic terms as well as $[W(z) - W(z^*)]$ which contains only simple well defined poles. The reduced space unitarity equation is now:

$$0 = \frac{\varphi_\beta^*(\vec{q}_\beta')}{\lambda - i\mu - E_\beta'} \frac{\varphi_\beta(\vec{q}_\beta)}{\lambda + i\mu - E_\beta} \int_{\theta_0''} dE_0'' - 2\pi i\, \delta_\mu(E_0''-\lambda)\, \mathcal{B}_{\beta 0}(E_\beta', E_0'', \lambda - i\mu)$$

$$\times\ \mathcal{B}_{0\beta}(E_\beta'', E_\beta, \lambda + i\mu) \quad + \quad \text{remainder} \qquad (3.8.12)$$

We follow the same procedure as before except $\partial/\partial E_0$ is replaced by $\partial/\partial E_\beta$ and $2\pi\, \delta_\mu(E_0 - \lambda)$ in θ_β is just $2\mu/(E_0 - E_\beta)^2 + \mu^2$. Integrate in $\theta_\beta \cup \theta_0'$ is $\int_{\theta_\beta} dE_\beta\, \hat{h}_\beta \int d\vec{q}_\beta \int_{\theta_0'} dE_0'$.

$$0 = \left[\int d\vec{q}_\beta \frac{\varphi_\beta^*(\vec{q}_\beta)\, \varphi_\beta(\vec{q}_\beta)}{(E_0 - E_\beta)^2 + \mu^2}\right] \left\{ \int_{\theta_\beta} dE_\beta\ 2\pi\, \delta_\mu(\lambda - E_\beta) \int_{\theta_0'} dE_0' - 2\pi i\, \delta_\mu(\lambda - E_0')\right.$$

$$\times\ \hat{h}_\beta\, \mathcal{B}_{\beta 0}(E_\beta, E_0', \lambda - i\mu)\ \mathcal{B}_{0\beta}(E_0', \dot{E}_\beta, \lambda + i\mu)$$

$$+ \int_{\theta_\beta} dE_\beta \frac{2\mu}{(\lambda - i\mu - E_\beta)(\lambda + i\mu - E_\beta)^2} \int_{\theta_0'} dE_0' - 2\pi i\, \delta_\mu(\lambda - E_0')$$

$$\left. \times\ \hat{h}_\beta\, \mathcal{B}_{\beta 0}(E_\beta, E_0', \lambda - i\mu)\ \mathcal{B}_{0\beta}(E_0', E_\beta, \lambda + i\mu) \right\}$$

$$+ \quad \text{remainder} \qquad (3.8.13)$$

Simplifying and taking the limit $\mu \to 0^+$ we have the usual partial derivative term plus the double pole term that we need to cancel those in the Cayley tranform (Cf. $C_{\alpha 0}'$ in 3.6.2)

$$0 = 4\pi^2\, \hat{h}_\beta\, \mathcal{B}_{\beta 0}(\lambda, \lambda, \lambda - i0)\ \mathcal{B}_{0\beta}(\lambda, \dot{\lambda}, \lambda + i0)$$

$$+ \lim_{\mu \to 0^+} \int_{\theta_\beta} d\vec{p}_\beta \frac{2\mu}{(\lambda - i\mu - E_\beta)(\lambda + i\mu - E_\beta)^2} \int_{\theta_0'} d\vec{p}'d\vec{q}' \frac{2\mu}{(E_0' - \lambda)^2 + \mu^2}$$

$$B_{\beta 0}(\vec{p}_\beta, \vec{p}'\vec{q}', \lambda - i\mu)\ B_{0\beta}(\vec{p}'\vec{q}', \vec{p}_\beta, \lambda + i\mu) \qquad (3.8.14)$$

The alternative unitarity equation would provide another similar expression.

$$0 = 4\pi^2 \hat{t}r_\beta \, \mathcal{B}_{\beta 0}(\dot{\lambda},\lambda,\lambda+io)\, \mathcal{B}_{0\beta}(\lambda,\lambda,\lambda-io)$$

$$+ \lim_{\mu\to 0^+} \int_{\theta_\beta} d\vec{p}_\beta \frac{2\mu}{(\lambda-i\mu-E_\beta)(\lambda+i\mu-E_\beta)^2} \int_{\theta_0'} d\vec{p}\,' d\vec{q}\,' \frac{2\mu}{(E_0'-\lambda)^2+\mu^2}$$

$$B_{0\beta}(\vec{p}\,'\vec{q}\,';\vec{p}_\beta;\lambda-i\mu)\, B_{\beta 0}(\vec{p}_\beta;\vec{p}\,'\vec{q}\,';\lambda+i\mu)$$

$$= 4\pi^2 \hat{t}r_0 \, \mathcal{B}_{0\beta}(\lambda,\lambda,\lambda-io)\, \mathcal{B}_{\beta 0}(\dot{\lambda},\lambda,\lambda+io)$$

$$+ \lim_{\mu\to 0^+} \int_{\theta_\beta'} d\vec{p}_\beta\,' \frac{2\mu}{(\lambda-i\mu\, E_\beta')(\lambda+i\mu-E_\beta')^2} \int_{\theta_0} d\vec{p}\, d\vec{q} \frac{2\mu}{(E_0-\lambda)^2+\mu^2}$$

$$B_{0\beta}(\vec{p}\vec{q};\vec{p}_\beta\,';\lambda-i\mu)\, B_{\beta 0}(\vec{p}_\beta\,';\vec{p}\vec{q};\lambda+i\mu) \tag{3.8.15}$$

The double pole term is the same as $C_{0\beta}'$ of (3.6.5). Together with (3.8.14) we form the necessary partial derivatives and double pole terms.

$$0 = 4\pi^2 \hat{t}r_0 \, \mathcal{B}_{0\beta}(\lambda,\lambda,\lambda-io)\, \mathcal{B}_{\beta 0}(\dot{\lambda},\lambda,\lambda+io)$$

$$+ 4\pi^2 \hat{t}r_\beta \, \mathcal{B}_{\beta 0}(\lambda,\lambda,\lambda-io)\, \mathcal{B}_{0\beta}(\lambda,\dot{\lambda},\lambda+io)$$

$$+ \lim_{\mu\to 0^+} \left(C_{0\beta}' + C_{\beta 0}' \right) \tag{3.8.16}$$

V.3.9 Contributions in $\theta_\alpha \cup \theta'_\beta$

In $\theta_\alpha \cup \theta'_\beta$,($\alpha,\beta = 1,2,3$) the disconnected pole term will not contribute if $\alpha \neq \beta$. The condition $\lambda = E_\alpha = E'_\beta$ is inconsistent with $\delta(\vec{p}_\alpha - \vec{p}'_\alpha)$. We shall deal with $\theta_\alpha \cup \theta'_\alpha$ later. (3.8.2) is now written as

$$0 = \int_{\theta''_\beta} d\vec{p}''d\vec{q}'' \frac{-2i\mu}{(E''_0 - E''_\beta)^2 + \mu^2} W(\vec{p}'\vec{q}';\vec{p}''\vec{q}'';\lambda - i\mu)\, W(\vec{p}''\vec{q}'';\vec{p}\vec{q};\lambda + i\mu)$$

$$+ \text{ remainder} \qquad (3.9.1)$$

where

$$\text{remainder} = \int_{\theta''_\beta} d\vec{p}''d\vec{q}'' \frac{-2i\mu}{(E''_0 - E''_\beta)^2 + \mu^2} \Big\{ \delta_{\alpha\beta} \Big[T_\alpha(\vec{p}'\vec{q}';\vec{p}''\vec{q}'';\lambda - i\mu)$$

$$\times W(\vec{p}''\vec{q}'';\vec{p}\vec{q};\lambda + i\mu) + W(\vec{p}'\vec{q}';\vec{p}''\vec{q}'';\lambda - i\mu)\, T_\alpha(\vec{p}''\vec{q}'';\vec{p}\vec{q};\lambda + i\mu)\Big]$$

$$+ \text{ non-contributing terms} \Big\} \qquad (3.9.2)$$

The Kronecker delta indicates that the terms in square brackets will contribute only if $\alpha = \beta$.

Since we anticipate the formation of double pole terms, we must exhibit all coefficients of $(\lambda + i\mu - E_\alpha)^{-1}$.

$$0 = \int_{\theta''_\beta} d\vec{p}''d\vec{q}'' \frac{-2i\mu}{(E''_0 - E''_\beta)^2 + \mu^2} j_\alpha(E'_\alpha)\, W(\vec{p}'\vec{q}';\vec{p}''\vec{q}'';\lambda - i\mu) \times$$

$$\times (-) B_{0\alpha}(\vec{p}''\vec{q}'';\vec{p}_\alpha;\lambda + i\mu)\, j_\alpha(E_\alpha) \frac{\varphi^*_\alpha(\vec{q}_\alpha)}{\lambda + i\mu - E_\alpha} + \text{ remainder}$$

$$(3.9.3)$$

[Note: Actually only the coefficient of $(\lambda - i\mu - E'_\alpha)^{-1}$ in $W(\vec{p}'\vec{q}';\vec{p}''\vec{q}'';\lambda - i\mu)$ will contribute. The rest will not yield any singular

function even when multiplied by a double pole $(\lambda - i\mu - E_\alpha)^{-2}$.
We left them in for easy comparison with $c'_{\alpha\beta}$ in (3.5.5)]

The jacobians are put in to make sure that the final result would have the proper reduced space operator form. We now follow the steps similar to those used previously.

[1] Differentiate with respect to E_α , $\partial/\partial E_\alpha$

[2] Set on diagonal, $\vec{p},\vec{q} = \vec{p}\,',\vec{q}\,'$

[3] Multiply by $2\mu/(E_0-E_\alpha)^2+\mu^2$

[4] Integrate in $\theta_\alpha \cup \theta'_\beta$, i.e. $\int_{\theta_\alpha} dE_\alpha \, \hat{tr}_\alpha \int d\vec{q}_\alpha \int_{\theta'_\beta} d\vec{p}\,' d\vec{q}\,'$

$$0 = \int_{\theta_\alpha} dE_\alpha \, \hat{tr}_\alpha \int d\vec{q}_\alpha \int_{\theta'_\beta} d\vec{p}\,' d\vec{q}\,' \frac{2\mu}{(E_0-E_\alpha)^2+\mu^2} \; \frac{-2i\mu}{(E_0''-E_\beta'')^2+\mu^2} \times$$

$$\times \, j_\alpha(E_\alpha)\, W(\vec{p}\vec{q};\vec{p}\,'\vec{q}\,';\lambda-i\mu)\Big[(-)\, B_{0\alpha}(\vec{p}\,'\vec{q}\,';\vec{p}_\alpha;\lambda+i\mu)\, j_\alpha(E_\alpha) \frac{\varphi_\alpha^*(\vec{q}_\alpha)}{(\lambda+i\mu-E_\alpha)^2}$$

$$+ \frac{\partial}{\partial E_\alpha}\Big((-)\, B_{0\alpha}(\vec{p}\,'\vec{q}\,';\vec{p}_\alpha;\lambda+i\mu)\, j_\alpha(E_\alpha)\Big) \frac{\varphi_\alpha^*(\vec{q}_\alpha)}{\lambda+i\mu-E_\alpha} \qquad (3.9.4)$$

The double pole term corresponds to part of $C'_{\alpha\beta}$ in (3.5.3). In the remaining partial derivative term, we must regconize that only coefficients of $\frac{2\mu}{(E_\alpha-\lambda)^2+\mu^2} \times \frac{2\mu}{(E'_\beta-\lambda)^2+\mu^2}$ can survive. All others will vanish as μ or μ^2 in $\theta_\alpha \cup \theta'_\beta$.

$$\lim_{\mu\to 0^+} \int_{\theta_\alpha} dE_\alpha \, \hat{tr}_\alpha \int d\vec{q}_\alpha \int_{\theta'_\beta} d\vec{p}\,' d\vec{q}\,' \frac{2\mu}{(E_0-E_\alpha)^2+\mu^2} \; \frac{-2i\mu}{(E_0'-E_\beta')^2+\mu^2}$$

$$j_\alpha(E_\alpha)\, W(\vec{p}\vec{q};\vec{p}\,'\vec{q}\,';\lambda-i\mu) \frac{\partial}{\partial E_\alpha}\Big((-)\, B_{0\alpha}(\vec{p}\,'\vec{q}\,';\vec{p}_\alpha;\lambda+i\mu)\, j_\alpha(E_\alpha)\Big) \frac{\varphi_\alpha^*(\vec{q}_\alpha)}{\lambda+i\mu-E_\alpha}$$

$$= \lim_{\mu\to 0^+} \int_{\theta_\alpha} dE_\alpha \, \hat{tr}_\alpha \int d\vec{q}_\alpha \int_{\theta'_\beta} d\vec{p}\,' d\vec{q}\,' \frac{2\mu}{(E_0-E_\alpha)^2+\mu^2} \; \frac{-2i\mu}{(E_0'-E_\beta')^2+\mu^2} \times$$

$$j_\alpha(E_\alpha)\frac{\varphi_\alpha(\vec{q}_\alpha)}{\lambda-i\mu-E_\alpha}\;H_{\alpha\beta}(\vec{p}_\alpha;\vec{p}'_\beta;\lambda-i\mu)\frac{\varphi^*_\beta(\vec{q}'_\beta)}{\lambda-i\mu-E'_\beta}$$

$$\times\frac{2}{\partial E_\alpha}\left(\frac{\varphi_\beta(\vec{q}'_\beta)}{\lambda+i\mu-E'_\beta}\;H_{\beta\alpha}(\vec{p}'_\beta;\vec{p}_\alpha;\lambda+i\mu)\,j_\alpha(E_\alpha)\right)\frac{\varphi^*_\alpha(\vec{q}_\alpha)}{\lambda+i\mu-E_\alpha}$$

$$=\lim_{\mu\to0^+}\left[\int d\vec{q}_\alpha\,\frac{\varphi_\alpha(\vec{q}_\alpha)\varphi^*_\alpha(\vec{q}_\alpha)}{(E_0-E_\alpha)^2+\mu^2}\right]\left[\int d\vec{q}'_\beta\,\frac{\varphi_\beta(\vec{q}'_\beta)\;\varphi^*_\beta(\vec{q}'_\beta)}{(E'_0-E'_\beta)^2+\mu^2}\right]\times$$

$$\times\int_{\theta_\alpha}dE_\alpha\;2\pi\,\delta_\mu(E_\alpha-\lambda)\int_{\theta'_\beta}dE'_\beta\;-2\pi i\;\delta_\mu(E'_\beta-\lambda)$$

$$\times\;\hat{tr}_\alpha\;\mathcal{H}_{\alpha\beta}(E_\alpha,E'_\beta,\lambda-i\mu)\;\mathcal{H}_{\beta\alpha}(E'_\beta,\dot{E}_\alpha,\lambda+i\mu)$$

$$=\;-4\pi^2 i\;\hat{tr}_\alpha\;\mathcal{H}_{\alpha\beta}(\lambda,\lambda,\lambda-i0)\;\mathcal{H}_{\beta\alpha}(\lambda,\dot{\lambda},\lambda+i0)\tag{3.9.5}$$

Now, subsituting back to (3.9.3) we have

$$0=\lim_{\mu\to0^+}\int_{\theta_\alpha}d\vec{p}\,d\vec{q}\int_{\theta'_\beta}d\vec{p}'d\vec{q}'\,\frac{2\mu}{(E_0-E_\alpha)^2+\mu^2}\;\frac{-2i\mu}{(E'_0-E'_\beta)^2+\mu^2}\times$$

$$\times\;W(\vec{p}\vec{q};\vec{p}'\vec{q}';\lambda-i\mu)\;(-)\;B_{0\alpha}(\vec{p}'\vec{q}';\vec{p}_\alpha;\lambda+i\mu)\;\frac{\varphi^*_\alpha(\vec{q}_\alpha)}{(\lambda+i\mu-E_\alpha)^2}$$

$$-\;4\pi^2 i\;\hat{tr}_\alpha\;\mathcal{H}_{\alpha\beta}(\lambda,\lambda,\lambda-i0)\;\mathcal{H}_{\beta\alpha}(\lambda,\dot{\lambda},\lambda+i0)\tag{3.9.6}$$

Similarly, the alternative unitarity equation must yield:

$$0=\lim_{\mu\to0^+}\int_{\theta_\alpha}d\vec{p}\,d\vec{q}\int_{\theta'_\beta}d\vec{p}'d\vec{q}'\,\frac{2\mu}{(E_0-E_\alpha)^2+\mu^2}\;\frac{-2i\mu}{(E'_0-E'_\beta)^2+\mu^2}\times$$

$$\times\;\frac{\varphi_\alpha(\vec{q}_\alpha)}{(\lambda+i\mu-E_\alpha)^2}\;(-)\;B_{\alpha0}(\vec{p}_\alpha;\vec{p}'\vec{q}';\lambda+i\mu)\;W(\vec{p}'\vec{q}';\vec{p}\vec{q};\lambda-i\mu)$$

$$-\;4\pi^2 i\;\hat{tr}_\alpha\;\mathcal{H}_{\alpha\beta}(\dot{\lambda},\lambda,\lambda+i0)\;\mathcal{H}_{\beta\alpha}(\lambda,\lambda,\lambda-i0)\tag{3.9.7}$$

For convenience in comparing with other results, we turn (3.9.7) "inside out" and relabel α and β .

$$0 = \lim_{\mu \to 0^+} \int_{\theta'_\alpha} d\vec{p}' d\vec{q}' \int_{\theta_\beta} d\vec{p}\, d\vec{q}\, \frac{2\mu}{(E'_0 - E'_\alpha)^2 + \mu^2} \; \frac{-2i\mu}{(E_0 - E_\beta)^2 + \mu^2} \times$$

$$\times \frac{\varphi_\alpha(\vec{q}'_\alpha)}{(\lambda + i\mu - E'_\alpha)^2} (-) B_{\alpha 0}(\vec{p}'_\alpha ; \vec{p}\vec{q} ; \lambda + i\mu)\, W(\vec{p}\vec{q} ; \vec{p}'\vec{q}' ; \lambda - i\mu)$$

$$- 4\pi^2 i \; \hat{\hbar}_\beta \, \mathcal{J}_{\beta\alpha}(\lambda, \lambda, \lambda - i0)\, \mathcal{H}_{\alpha\beta}(\dot{\lambda}, \lambda, \lambda + i0)$$

$$= \lim_{\mu \to 0^+} \int_{\theta'_\beta} d\vec{p}' d\vec{q}' \int_{\theta_\alpha} d\vec{p}\, d\vec{q}\, \frac{2\mu}{(E'_0 - E'_\beta)^2 + \mu^2} \; \frac{-2i\mu}{(E_0 - E_\alpha)^2 + \mu^2}$$

$$\times \frac{\varphi_\beta(\vec{q}'_\beta)}{(\lambda + i\mu - E'_\beta)^2} (-) B_{\beta 0}(\vec{p}'_\beta ; \vec{p}\vec{q} ; \lambda + i\mu)\, W(\vec{p}\vec{q} ; \vec{p}'\vec{q}' ; \lambda - i\mu)$$

$$- 4\pi^2 i \; \hat{\hbar}_\alpha \, \mathcal{H}_{\alpha\beta}(\lambda, \lambda, \lambda - i0)\, \mathcal{H}_{\beta\alpha}(\dot{\lambda}, \lambda, \lambda + i0) \qquad (3.9.8)$$

Add (3.9.8) to (3.9.5) and compare with $C'_{\alpha\beta}$ in (3.5.3)

$$0 = \lim_{\mu \to 0^+} C'_{\alpha\beta} + 4\pi^2 \hat{\hbar}_\alpha \mathcal{J}_{\alpha\beta}(\lambda, \lambda, \lambda - i0)\, \mathcal{J}_{\beta\alpha}(\dot{\lambda}, \dot{\lambda}, \lambda + i0)$$

$$\text{for} \quad \alpha \neq \beta \qquad (3.9.9)$$

Finally, we have to deal with $\theta_\alpha \cup \theta'_\alpha$ where we know the disconnected pole term will contribute. We expect to have the same contribution as (3.9.9) for the special case of $\alpha = \beta$ plus extra terms from the disconnected poles. In fact if we review from (3.9.1) to (3.9.9) we find nothing that would exclude the case $\alpha = \beta$. The primed and unprimed system are disjoint. Whether or not $\alpha = \beta$ is irrelevant to the calculation. Only when we deal with disconnected pole terms then the delta function $\delta(\vec{p}_\alpha - \vec{p}'_\alpha)$ connects the primed and unprimed systems. It suffices for us to deal with the square bracket terms with the Kronecker delta in (3.9.3) when $\alpha = \beta$.

$$I = \int_{\theta_\alpha''} d\vec{p}''d\vec{q}'' \frac{-2i\mu}{(E_0''-E_\alpha'')^2+\mu^2} \Big[T_\alpha(\vec{p}'\vec{q}';\vec{p}''\vec{q}'';\lambda-i\mu)\, W(\vec{p}''\vec{q}'';\vec{p}\vec{q};\lambda+i\mu)$$

$$+ W(\vec{p}'\vec{q}';\vec{p}''\vec{q}'';\lambda-i\mu)\; T_\alpha(\vec{p}''\vec{q}'';\vec{p}\vec{q};\lambda+i\mu)\Big] \tag{3.9.10}$$

In $\theta_\alpha \cup \theta_\alpha'$ only parts of T_α or W has the singular pole. We can drop the non-pole parts. Because of the complexity of W , we divide I into four parts

$$I = I_1 + I_2 + I_3 + \text{remainder} \tag{3.9.11}$$

The remainder of course is not contributing.

$$I_1 = \int_{\theta_\alpha''} d\vec{p}''d\vec{q}'' \frac{-2i\mu}{(E_0''-E_\alpha'')^2+\mu^2} \quad \frac{\delta(\vec{p}_\alpha'-\vec{p}_\alpha'')\,\varphi_\alpha(\vec{q}_\alpha')\,\varphi_\alpha^*(\vec{q}_\alpha'')}{\lambda-i\mu-E_\alpha'} \times$$

$$\times \left\{ \frac{\varphi_\alpha(\vec{q}_\alpha'')}{\lambda+i\mu-E_\alpha''} \left(\sum_\beta \widetilde{G}_{\alpha\beta}(\vec{p}_\alpha'';\vec{p}\vec{q};\lambda+i\mu) + \sum_{\alpha\neq\beta} H_{\alpha\beta}(\vec{p}_\alpha'';\vec{p}_\beta;\lambda+i\mu)\, \frac{\varphi_\beta^*(\vec{q}_\beta)}{\lambda+i\mu-E_\beta} \right) \right.$$

$$\left. + \left(\sum_\beta G_{\beta\alpha}(\vec{p}''\vec{q}'';\vec{p}_\alpha;\lambda+i\mu) + \sum_{\beta\neq\alpha} \frac{\varphi_\beta(\vec{q}_\beta'')}{\lambda+i\mu-E_\beta''}\, H_{\beta\alpha}(\vec{p}_\beta'';\vec{p}_\alpha;\lambda+i\mu) \right) \frac{\varphi_\alpha^*(\vec{q}_\alpha)}{\lambda+i\mu-E_\alpha} \right\}$$

$$\tag{3.9.12}$$

$$I_2 = \int_{\theta_\alpha''} d\vec{p}''d\vec{q}'' \frac{-2i\mu}{(E_0''-E_\alpha'')^2+\mu^2} \quad \frac{\delta(\vec{p}_\alpha'-\vec{p}_\alpha'')\,\varphi_\alpha(\vec{q}_\alpha')\,\varphi_\alpha^*(\vec{q}_\alpha'')}{\lambda-i\mu-E_\alpha'} \times$$

$$\times \frac{\varphi_\alpha(\vec{q}_\alpha'')}{\lambda+i\mu-E_\alpha''}\; H_{\alpha\alpha}(\vec{p}_\alpha'';\vec{p}_\alpha;\lambda+i\mu)\, \frac{\varphi_\alpha(\vec{q}_\alpha)}{\lambda+i\mu-E_\alpha} \tag{3.9.13}$$

[Note: I_2 bears the same structure as $D_{\alpha\alpha}$ in (3.5.7) and needs special attention.]

$$I_3 = \int_{\theta''_\alpha} d\vec{p}''d\vec{q}'' \frac{-2i\mu}{(E_0''-E_\alpha'')^2+\mu^2} \Bigg\{ \frac{\varphi_\alpha(\vec{q}_\alpha')}{\lambda-i\mu-E_\alpha'} \Bigg(\sum_\beta \widetilde{G}_{\alpha\beta}(\vec{p}_\alpha';\vec{p}''\vec{q}'';\lambda-i\mu) +$$

$$+ \sum_{\beta\neq\alpha} H_{\alpha\beta}(\vec{p}_\alpha';\vec{p}_\beta'';\lambda-i\mu) \frac{\varphi_\beta^*(\vec{q}_\beta'')}{\lambda-i\mu-E_\beta''} \Bigg) + \Bigg(\sum_\beta G_{\beta\alpha}(\vec{p}'\vec{q}';\vec{p}_\alpha'';\lambda-i\mu) +$$

$$+ \sum_{\beta\neq\alpha} \frac{\varphi_\beta(\vec{q}_\beta')}{\lambda-i\mu-E_\beta'} H_{\beta\alpha}(\vec{p}_\beta';\vec{p}_\alpha'';\lambda-i\mu) \Bigg) \frac{\varphi_\alpha^*(\vec{q}_\alpha'')}{\lambda-i\mu-E_\alpha''} +$$

$$+ \frac{\varphi_\alpha(\vec{q}_\alpha')}{\lambda-i\mu-E_\alpha'} H_{\alpha\alpha}(\vec{p}_\alpha';\vec{p}_\alpha'';\lambda-i\mu) \frac{\varphi_\alpha^*(\vec{q}_\alpha'')}{\lambda-i\mu-E_\alpha''} \Bigg\} \delta(\vec{p}_\alpha''-\vec{p}_\alpha) \frac{\varphi_\alpha(\vec{q}_\alpha'')\varphi_\alpha^*(\vec{q}_\alpha)}{\lambda+i\mu-E_\alpha}$$

(3.9.14)

Now we want to develop I_1, I_2 and I_3 individually in accordance with steps [1] to [4]. One must bear in mind that E_α'' will eventually become E_α because of $\delta(\vec{p}_\alpha''-\vec{p}_\alpha)$. In step [3] we multiply I_1 by μ so that I_1 is of order μ^2. Therefore coefficient of $(\lambda-i\mu-E_\alpha)^{-1}(\lambda+i\mu-E_\alpha)^{-1}$ will vanish linearly as μ. Only the double pole term may contribute. I_1 becomes I_1' .

$$I_1' = \int_{\theta_\alpha} d\vec{p}_\alpha\, d\vec{q}_\alpha \int_{\theta_\alpha'} d\vec{p}'d\vec{q}' \frac{2\mu}{(E_0-E_\alpha)^2+\mu^2} \frac{-2i\mu}{(E_0'-E_\alpha')^2+\mu^2} \delta(\vec{p}_\alpha-\vec{p}_\alpha') \frac{\varphi_\alpha(\vec{q}_\alpha)\varphi_\alpha^*(\vec{q}_\alpha')}{\lambda-i\mu-E_\alpha} \times$$

$$\times \Bigg(\sum_\beta G_{\beta\alpha}(\vec{p}'\vec{q}';\vec{p}_\alpha;\lambda+i\mu) + \sum_{\beta\neq\alpha} \frac{\varphi_\beta(\vec{q}_\beta')}{\lambda+i\mu-E_\beta'} H_{\beta\alpha}(\vec{p}_\beta';\vec{p}_\alpha;\lambda+i\mu) \Bigg) \frac{\varphi_\alpha^*(\vec{q}_\alpha)}{(\lambda+i\mu-E_\alpha)^2}$$

(3.9.15)

I_2 will develop a double pole term similar to I_1 and also contribute a partial derivative in $H_{\alpha\alpha}$. I_2 becomes I_2' .

$$I_2' = \int_{\theta_\alpha} d\vec{p}\, d\vec{q} \int_{\theta_\alpha'} d\vec{p}'d\vec{q}' \frac{2\mu}{(E_0-E_\alpha)^2+\mu^2} \frac{-2i\mu}{(E_0'-E_\alpha')^2+\mu^2} \delta(\vec{p}_\alpha-\vec{p}_\alpha') \frac{\varphi_\alpha(\vec{q}_\alpha)\varphi_\alpha^*(\vec{q}_\alpha')}{\lambda-i\mu-E_\alpha} \times$$

$$\times \frac{\varphi_\alpha(\vec{q}_\alpha')}{\lambda+i\mu-E_\alpha'} H_{\alpha\alpha}(\vec{p}_\alpha';\vec{p}_\alpha;\lambda+i\mu) \frac{\varphi_\alpha^*(\vec{q}_\alpha)}{(\lambda+i\mu-E_\alpha)^2} + I_2'' \tag{3.9.16}$$

where

$$I_2'' = \int_{\theta_\alpha} dE_\alpha \, \hat{t}r_\alpha \int d\vec{q}_\alpha \int_{\theta_\alpha'} d\vec{p}_\alpha' \, d\vec{q}_\alpha' \frac{2\mu}{(E_0-E_\alpha)^2+\mu^2} \frac{-2i\mu}{(E_0'-E_\alpha')^2+\mu^2}$$

$$\times \frac{\delta(\vec{p}_\alpha-\vec{p}_\alpha')\,\varphi_\alpha(\vec{q}_\alpha)\varphi_\alpha^*(\vec{q}_\alpha')}{\lambda-i\mu-E_\alpha} \frac{\varphi_\alpha(\vec{q}_\alpha')}{\lambda+i\mu-E_\alpha'} \mathcal{H}_{\alpha\alpha}(E_\alpha', \dot{E}_\alpha, \lambda+i\mu) \frac{\varphi_\alpha(\vec{q}_\alpha)}{\lambda+i\mu-E_\alpha} \tag{3.9.17}$$

In changing into reduced space notation, both jacobians $j_\alpha^2(E_\alpha) = j_\alpha(E_\alpha)\,j_\alpha(E_\alpha')$ goes to $H_{\alpha\alpha}$.

$$I_2'' = -4i \int_{\theta_\alpha} dE_\alpha \frac{\mu^2}{(\lambda-i\mu-E_\alpha)(\lambda+i\mu-E_\alpha)^2} \hat{t}r_\alpha \mathcal{H}_{\alpha\alpha}(E_\alpha, \dot{E}_\alpha, \lambda+i\mu) \times$$

$$\times \left[\int d\vec{q}_\alpha \frac{\varphi_\alpha(\vec{q}_\alpha)\,\varphi_\alpha^*(\vec{q}_\alpha)}{(E_0-E_\alpha)^2+\mu^2}\right] \left[\int d\vec{q}_\alpha' \frac{\varphi_\alpha(\vec{q}_\alpha')\,\varphi_\alpha^*(\vec{q}_\alpha')}{(E_0'-E_\alpha')^2+\mu^2}\right] \tag{3.9.18}$$

Recall the identity used in (3.5.9).

$$\lim_{\mu\to 0^+} \frac{4\mu^2}{(x-i\mu)(x+i\mu)^2} = -2\pi i\,\delta(x)$$

Hence,

$$\lim_{\mu\to 0^+} I_2'' = -2\pi \int_{\theta_\alpha} dE_\alpha \, \delta(E_\alpha-\lambda) \, \hat{t}r_\alpha \mathcal{H}_{\alpha\alpha}(E_\alpha, \dot{E}_\alpha, \lambda+i0)$$

$$= -2\pi \, \hat{t}r_\alpha \mathcal{H}_{\alpha\alpha}(\lambda, \dot{\lambda}, \lambda+i0) \tag{3.9.19}$$

We can now collect the double pole terms together in I_1' and I_2' and write their sum as

$$\lim_{\mu\to 0^+}\left(I_1'+I_2'\right) = \lim_{\mu\to 0^+}\int_{\theta_\alpha} d\vec{p}\,d\vec{q}\int_{\theta_\alpha'} d\vec{p}_\alpha'\,d\vec{q}_\alpha' \frac{2\mu}{(E_0-E_\alpha)^2+\mu^2}\;\frac{-2i\mu}{(E_0'-E_\alpha')^2+\mu^2}\times$$

$$\times\frac{\delta(\vec{p}_\alpha-\vec{p}_\alpha')\,\varphi_\alpha(\vec{q}_\alpha)\,\varphi_\alpha^*(\vec{q}_\alpha')}{\lambda-i\mu-E_\alpha}\;(-)B_{0\alpha}(\vec{p}\,\vec{q}\,';\vec{p}_\alpha;\lambda+i\mu)\;\frac{\varphi_\alpha^*(\vec{q}_\alpha)}{(\lambda+i\mu-E_\alpha)^2}$$

$$-\,2\pi\,\hat{t}_\alpha\,\mathcal{H}_{\alpha\alpha}(\lambda,\dot{\lambda},\lambda+i0)\tag{3.9.20}$$

From the alternative unitarity equation we will obtain the following:

$$\lim_{\mu\to 0^+}\left(\tilde{I}_1'+\tilde{I}_2'\right) = \lim_{\mu\to 0^+}\int_{\theta_\alpha} d\vec{p}\,d\vec{q}\int_{\theta_\alpha'} d\vec{p}_\alpha'\,d\vec{q}_\alpha' \frac{2\mu}{(E_0-E_\alpha)^2+\mu^2}\;\frac{-2i\mu}{(E_0'-E_\alpha')^2+\mu^2}$$

$$\times\frac{\varphi_\alpha(\vec{q}_\alpha)}{(\lambda+i\mu-E_\alpha)^2}\;(-)B_{\alpha 0}(\vec{p}_\alpha;\vec{p}\,\vec{q}\,';\lambda+i\mu)\;\frac{\delta(\vec{p}_\alpha'-\vec{p}_\alpha)\,\varphi_\alpha(\vec{q}_\alpha')\,\varphi_\alpha^*(\vec{q}_\alpha)}{\lambda-i\mu-E_\alpha}$$

$$-\,2\pi\,\hat{t}_\alpha\,\mathcal{H}_{\alpha\alpha}(\dot{\lambda},\lambda,\lambda+i0)\tag{3.9.21}$$

Next, we must compare these double pole terms to those in the Cayley transform, in particular $D_{\alpha\beta}'$ in (3.5.6). In $D_{\alpha\beta}'$, of the three in $\sum_\alpha T_\alpha(\vec{p}\,\vec{q};\vec{p}\,'\vec{q}\,';\lambda-i\mu)$ one of them has no pole in either θ_α or θ_β'. The remaining two: $T_\alpha(\vec{p}\,\vec{q};\vec{p}\,'\vec{q}\,';\lambda-i\mu)$ and $T_\beta(\vec{p}\,\vec{q};\vec{p}\,'\vec{q}\,';\lambda-i\mu)$ have delta function $\delta(\vec{p}_\alpha-\vec{p}_\alpha')$ or $\delta(\vec{p}_\beta-\vec{p}_\beta')$. This momentum condition is inconsistent with $\lambda = E_\alpha = E_\beta'$ for $\theta_\alpha\cup\theta_\beta'$ unless $\alpha=\beta$. Hence, the non-vanishing element is a lot less than that shown in (3.5.6).

$$\lim_{\mu\to 0^+} D_{\alpha\beta}' = \lim_{\mu\to 0^+}\delta_{\alpha\beta}\,D_{\alpha\alpha}' =$$

$$= \delta_{\alpha\beta} \lim_{\mu\to 0^+} 4\mu^2 \int_{\theta_\alpha} d\vec{p}\, d\vec{q} \int_{\theta'_\alpha} d\vec{p}'d\vec{q}' \left[(E_0-E_\alpha)^2+\mu^2\right]^{-1}\left[(E_0'-E_\alpha')^2+\mu^2\right]^{-1} \times$$

$$\times\ T_\alpha(\vec{p}\vec{q}\,;\vec{p}'\vec{q}'\,;\lambda-i\mu)\left\{ \frac{\varphi_\alpha(\vec{q}_\alpha')}{(\lambda+i\mu-E_\alpha')^2}\,{}^{(-)}B_{\alpha 0}(\vec{p}_\alpha'\,;\vec{p}\vec{q}\,;\lambda+i\mu) \;+\right.$$

$$\left. {}^{(-)}B_{0\alpha}(\vec{p}'\vec{q}'\,;\vec{p}_\alpha\,;\lambda+i\mu)\,\frac{\varphi^*_\alpha(\vec{q}_\alpha)}{(\lambda+i\mu-E_\alpha)^2}\right\} \qquad (3.9.22)$$

Hence,

$$\lim_{\mu\to 0^+}\left(I_1'+I_2'+\tilde{I}_1'+\tilde{I}_2'\right)$$

$$= \lim_{\mu\to 0^+} -i\,D'_{\alpha\alpha} - 2\pi\ \hat{t}r_\alpha\, \mathcal{H}_{\alpha\alpha}(\dot{\lambda},\dot{\lambda},\lambda+i0) \qquad (3.9.23)$$

by subsituting into (3.9.20) and (3.9.21).

It remains to develop I_3 into the only double pole term left in the Cayley transform, $E_{\alpha\alpha}$. Since $\delta(\vec{p}_\alpha-\vec{p}_\alpha') = \dfrac{\delta(E_\alpha-E_\alpha')\,\delta(\hat{p}_\alpha-\hat{p}_\alpha')}{j_\alpha(E_\alpha)\,j_\alpha(E_\alpha')}$ the differentiation in step [1] on I_3 would have an effect on the delta function $\delta(E_\alpha-E_\alpha')$, as well as the primary pole $(\lambda+i\mu-E_\alpha)^{-1}$. The reduced space form of I_3 has the extra jacobians $j_\alpha^2(E_\alpha)$ which turns $\delta(\vec{p}_\alpha-\vec{p}_\alpha'')$ into $\delta(E_\alpha-E_\alpha'')\ \delta(\hat{p}_\alpha-\hat{p}_\alpha'')$.

$$j_\alpha^2(E_\alpha)\,\delta(\vec{p}_\alpha-\vec{p}_\alpha'') = j_\alpha(E_\alpha)\,j_\alpha(E_\alpha'')\,\delta(\vec{p}_\alpha-\vec{p}_\alpha'') = \delta(E_\alpha-E_\alpha'')\,\delta(\hat{p}_\alpha-\hat{p}_\alpha'') \qquad (3.9.24)$$

After steps [1] to [4], I_3 becomes I_3'.

$$I_3' = \int_{\theta_\alpha} dE_\alpha\, d\hat{p}_\alpha \int_{\theta_\alpha'} dE_\alpha'\, d\hat{p}_\alpha'\ d\vec{q}_\alpha\, d\vec{q}_\alpha'\ j_\alpha(E_\alpha)\,j_\alpha(E_\alpha')\,\frac{2\mu}{(E_0-E_\alpha)^2+\mu^2}\times$$

$$\times \frac{-2i\mu}{(E_0'-E_\alpha')^2+\mu^2} \left\{ \frac{\varphi_\alpha(\vec{q}_\alpha)}{\lambda-i\mu-E_\alpha} \left(\sum_\beta \tilde{G}_{\alpha\beta}(\vec{p}_\alpha;\vec{p}'\vec{q}';\lambda-i\mu) \; + \right.\right.$$

$$+ \sum_{\beta\neq\alpha} H_{\alpha\beta}(\vec{p}_\alpha,\vec{p}_\beta',\lambda-i\mu) \frac{\varphi_\beta^*(\vec{q}_\beta')}{\lambda-i\mu-E_\beta'} \Bigg) + \Bigg(\sum_\beta G_{\beta\alpha}(\vec{p}\vec{q};\vec{p}_\alpha';\lambda-i\mu) +$$

$$+ \sum_{\beta\neq\alpha} \frac{\varphi_\beta(\vec{q}_\beta)}{\lambda-i\mu-E_\beta} H_{\beta\alpha}(\vec{p}_\beta,\vec{p}_\alpha',\lambda-i\mu) \Bigg) \frac{\varphi_\alpha^*(\vec{q}_\alpha')}{\lambda-i\mu-E_\alpha'} + \frac{\varphi_\alpha(\vec{q}_\alpha)}{\lambda-i\mu-E_\alpha} \times$$

$$\left. \times H_{\alpha\alpha}(\vec{p}_\alpha,\vec{p}_\alpha',\lambda-i\mu) \frac{\varphi_\alpha^*(\vec{q}_\alpha')}{\lambda-i\mu-E_\alpha'} \right\} \frac{\partial}{\partial E_\alpha} \left[\frac{\delta(E_\alpha-E_\alpha')\,\delta(\hat{p}_\alpha-\hat{p}_\alpha')}{\lambda+i\mu-E_\alpha} \right]$$

(3.9.25)

Since
$$\frac{\partial}{\partial E_\alpha} \left[\frac{\delta(E_\alpha-E_\alpha')\,\delta(\hat{p}_\alpha-\hat{p}_\alpha')}{\lambda+i\mu-E_\alpha} \right]$$

$$= \left(\frac{\partial}{\partial E_\alpha} \delta(E_\alpha-E_\alpha') \right) \frac{\delta(\hat{p}_\alpha-\hat{p}_\alpha')}{\lambda+i\mu-E_\alpha} + \frac{\delta(E_\alpha-E_\alpha')\,\delta(\hat{p}_\alpha-\hat{p}_\alpha')}{(\lambda+i\mu-E_\alpha)^2}$$

(3.9.26)

it follows that

$$I_3' = -i\,E_{\alpha\alpha} + \int_{\theta_\alpha} dE_\alpha\, d\hat{p}_\alpha \int_{\theta_\alpha'} dE_\alpha'\, d\hat{p}_\alpha\, d\vec{q}_\alpha\, d\vec{q}_\alpha'\, j_\alpha(E_\alpha)\, j_\alpha(E_\alpha') \times$$

$$\times \frac{2\mu}{(E_0-E_\alpha)^2+\mu^2} \frac{-2i\mu}{(E_0'-E_\alpha')^2+\mu^2} \left\{ \text{''} \right\} \left(\frac{\partial}{\partial E_\alpha} \delta(E_\alpha-E_\alpha') \right) \frac{\delta(\hat{p}_\alpha-\hat{p}_\alpha')}{\lambda+i\mu-E_\alpha}$$

(3.9.27)

The substitution of $E_{\alpha\alpha}$ comes from (3.5.10) and the contents of the curve bracket is the same as those in (3.9.25).

In developing the alternative form of I_3' from the other unitarity equation, we have to take special care to obtain the correct result.

$$\tilde{I}_3' = \int_{\theta_\alpha} dE_\alpha\, d\hat{p}_\alpha \int_{\theta_\alpha'} dE_\alpha'\, d\hat{p}_\alpha'\, d\vec{q}_\alpha\, d\vec{q}_\alpha'\, j_\alpha(E_\alpha)\, j_\alpha(E_\alpha')\, \frac{2\mu}{(E_0-E_\alpha)^2+\mu^2}\ \times$$

$$\times\ \frac{-2i\mu}{(E_0'-E_\alpha')^2+\mu^2}\ \frac{\partial}{\partial E_\alpha}\left[\frac{\delta(E_\alpha-E_\alpha')\,\delta(\hat{p}_\alpha-\hat{p}_\alpha')}{\lambda+i\mu-E_\alpha'}\right]\ \times$$

$$\Bigg\{ \frac{\varphi_\alpha(\vec{q}_\alpha')}{\lambda-i\mu-E_\alpha'}\left(\sum_\beta \tilde{G}_{\alpha\beta}(\vec{p}_\alpha';\vec{p}\vec{q};\lambda-i\mu) + \sum_{\beta\neq\alpha} H_{\alpha\beta}(\vec{p}_\alpha',\vec{p}_\beta,\lambda-i\mu)\,\frac{\varphi_\beta^*(\vec{q}_\beta)}{\lambda-i\mu-E_\beta}\right)$$

$$+\left(\sum_\beta G_{\beta\alpha}(\vec{p}'\vec{q}';\vec{p}_\alpha;\lambda-i\mu) + \frac{\varphi_\beta(\vec{q}_\beta')}{\lambda-i\mu-E_\beta'}\sum_{\beta\neq\alpha} H_{\beta\alpha}(\vec{p}_\beta',\vec{p}_\alpha,\lambda-i\mu)\right)\frac{\varphi_\alpha^*(\vec{q}_\alpha)}{\lambda-i\mu-E_\alpha}$$

$$+\ \frac{\varphi_\alpha(\vec{q}_\alpha')}{\lambda-i\mu-E_\alpha'}\, H_{\alpha\alpha}(\vec{p}_\alpha',\vec{p}_\alpha,\lambda-i\mu)\,\frac{\varphi_\alpha^*(\vec{q}_\alpha)}{\lambda-i\mu-E_\alpha}\Bigg\} \tag{3.9.28}$$

Since $\frac{\delta(E_\alpha-E_\alpha')}{\lambda+i\mu-E_\alpha} = \frac{\delta(E_\alpha-E_\alpha')}{\lambda+i\mu-E_\alpha'}$, we are free to choose the most convinient form. We use the first form for I_3' and the later for $\tilde{I}_3'$.

Interchanging the primed and unprimed system in (3.9.28) we have $\tilde{I}_3'$ in a form that is almost the same as $(I_3'+iE_{\alpha\alpha})$ except for $\left(\frac{\partial}{\partial E_\alpha'}\delta(E_\alpha-E_\alpha')\right)$ in $\tilde{I}_3'$ versus $\left(\frac{\partial}{\partial E_\alpha}\delta(E_\alpha-E_\alpha')\right)$ in I_3' .

However, we know that

$$\left(\frac{\partial}{\partial E_\alpha'}\delta(E_\alpha-E_\alpha')\right) = -\frac{\partial}{\partial E_\alpha}\delta(E_\alpha-E_\alpha') \tag{3.9.30}$$

therefore
$$I_3' + \tilde{I}_3' = -i\,E_{\alpha\alpha} \tag{3.9.31}$$

The derivatives on the energy delta function cancel each other.

In conclusion from (3.9.9), (3.9.23) and (3.9.31) we

V.3.10 Conclusion

In this final section we gather all the previous results of Cayley transform and unitarity identity and relate them to time delay. In retrospect, we have developed (3.1.8) in different neighbourhoods. The left hand side is

$$2i \,\mathrm{Im}\, \mathrm{Tr}\left[R(z) - R_0(z) - \sum_{\alpha>0}\left(R_\alpha(z) - R_0(z)\right)\right]$$

We shall gather the right hand side together with unitarity identity to show that it is related to time delay. We divide the right hand side into two parts: the free channel and the three bound state channels.

Without the rescattering terms, the three bound state channels result is particularly simple. Gather together (3.5.4), (3.5.9), (3.5.10) and (3.9.32) for $\sum_{\beta=1}^{3} \theta_\alpha \cup \theta'_\beta$ with $\alpha>0$ and we have the collective result.

$$\begin{aligned} J_\alpha = & \sum_{\beta>0} 4\pi^2 \,\hat{\mathrm{tr}}_\alpha\, \mathcal{H}_{\alpha\beta}(\lambda,\lambda,\lambda-io)\, \mathcal{H}_{\beta\alpha}(\dot\lambda,\dot\lambda,\dot\lambda+io) \\ & - 2\pi i\, \hat{\mathrm{tr}}_\alpha\, \mathcal{H}_{\alpha\alpha}(\dot\lambda,\dot\lambda,\dot\lambda+io) \end{aligned} \qquad (3.10.1)$$

The double pole term $C'_{\alpha\beta}$, $D'_{\alpha\alpha}$ and $E_{\alpha\alpha}$ has been cancelled. Now add to J_α results in $\theta_\alpha \cup \theta'_0$ from (3.6.3), (3.8.10) and (3.8.16),

$$J'_\alpha = \mathrm{Im}\, \hat{\mathrm{tr}}_\alpha\, 4\pi^2 \mathcal{B}_{\alpha 0}(\lambda,\lambda,\lambda-io)\, \mathcal{B}_{0\alpha}(\dot\lambda,\dot\lambda,\dot\lambda+io) \qquad (3.10.2)$$

The double pole term $C'_{\beta 0}$ is cancelled. We note here that the unitarity identity (3.8.10) requires the explicit notation of " Im " to signify that we only consider the pure imaginary part of the right hand side of (3.8.1). The left hand side have established in $\sum_{\alpha,\beta} \theta_\alpha \cup \theta'_\beta$ for $\alpha, \beta > 0$ the collective result:-

$$0 = \sum_{\alpha,\beta>0} \Big[\lim_{\mu \to 0^+} (C'_{\alpha\beta} + D'_{\alpha\beta} + E_{\alpha\alpha}) + $$

$$+ 4\pi^2 \hat{h}_\alpha \mathcal{H}_{\alpha\beta}(\lambda, \lambda, \lambda - i0) \mathcal{H}_{\alpha\beta}(\dot{\lambda}, \dot{\lambda}, \lambda + i0)$$

$$- 2\pi i \hat{h}_\alpha \mathcal{H}_{\alpha\alpha}(\dot{\lambda}, \dot{\lambda}, \lambda + i0) \Big] \qquad (3.9.32)$$

is already explicitly pure imaginary. Together (3.10.1) and (3.10.2) give us the entire α-channel contribution.

$$J_\alpha + J_\alpha' = \sum_{\beta=0}^{3} \hat{tr}_\alpha\, s_{\alpha\beta}^{+}(\lambda) \frac{d}{d\lambda} s_{\beta\alpha}(\lambda)$$

$$= -i\, \hat{tr}_\alpha\, q_{\alpha\alpha}(\lambda) \tag{3.10.3}$$

where $\quad s_{\beta\alpha}(\lambda) = \delta_{\alpha\beta}\, e_\alpha - 2\pi i\, \mathcal{M}_{\beta\alpha}(\lambda,\lambda,\lambda+io) \quad$ for $\beta > 0$

and $$s_{0\alpha}(\lambda) = -2\pi i\, \mathcal{B}_{0\alpha}(\lambda,\lambda,\lambda+io) \tag{3.10.4}$$

e_α is the reduced space identity operator. Its kernel is $\delta(\hat{p}_\alpha - \hat{p}_\alpha')$.

The free channel contribution is a little more complicated because of the rescattering term. However, for convenience we propose to write the result in the same form as (3.10.3). From (3.6.4), (3.8.10) and (3.8.16) we gather all the results in $\sum_{\beta=1}^{3} \theta_0\, U\, \theta_\beta'$ as

$$J_0 = \mathcal{I}m\, 4\pi^2\, \hat{tr}_0 \sum_{\beta=1}^{3} \mathcal{B}_{0\beta}(\lambda,\lambda,\lambda-io)\, \mathcal{B}_{\beta 0}(\dot\lambda,\dot\lambda,\dot\lambda+io)$$

$$= \mathcal{I}m\, \hat{tr}_0 \sum_{\beta=1}^{3} s_{0\beta}^{+}(\lambda) \frac{d}{d\lambda} s_{\beta 0}(\lambda) \tag{3.10.5}$$

The double pole term $C_{0\beta}'$ is cancelled.

From $\mathcal{I}m$ (3.4.4) and $4\pi^2$(3.7.19) we have all the three partial derivatives to form the total derivative of all the non-rescattering terms.(3.4.30) and (3.4.38) contains all the regularized rescattering terms. We propose to write all these results as

$$J_0' = \mathcal{I}m\, \hat{tr}_0 \left[s_{00}^{+}(\lambda) \frac{d}{d\lambda} s_{00}(\lambda) \right]_{c,R} \tag{3.10.6}$$

where $$\Delta_{oo}(\lambda) = e_o - 2\pi i \sum_{\alpha,\beta} \mathcal{M}_{\alpha\beta}(\lambda,\lambda,\lambda+io) \tag{3.10.7}$$

The subscript c denotes connectedness and the subscript R denotes regularization. (3.10.6) is only a convenient short natation of the complex results contained in (3.4.4). (3.7.19), (3.4.30) and (3.4.38). We believe that it is sensible to use such simple notation for the same reason that we use $\frac{1}{x \pm io}$ to denote $\frac{P}{x} \mp i\pi\delta(x)$. The generalized function that one gets by substituting (3.10.7) into (3.10.6) would have to be interpreted as (3.4.4), (3.7.19), (3.4.30) and (3.4.38) for the same reason that $\frac{1}{x \pm io}$ is interpreted as $\frac{P}{x} \mp i\pi\delta(x)$.

Now, the free channel contribution from $\sum_{\beta=0}^{3} \theta_o \, U \, \theta'_\beta$ is clearly

$$\begin{aligned} J_o + J_o' &= \operatorname{Im} \hat{tr}_o \sum_{\beta=0}^{3} \left[\Delta_{o\beta}^{+}(\lambda) \frac{d}{d\lambda} \Delta_{\beta o}(\lambda) \right]_{c,R} \\ &= -i \, \hat{tr}_o \, q_{oo}(\lambda) \end{aligned} \tag{3.10.8}$$

Hence, the grand reult from (3.10.8) and (3.10.3) is

$$\begin{aligned} & 2i \operatorname{Im} Tr\left[R(z) - R_o(z) - \sum_{\alpha>0} \left(R_\alpha(z) - R_o(z) \right) \right] \\ &= \sum_{\alpha,\beta=0}^{3} \operatorname{Im} \hat{tr}_\alpha \, \Delta_{\alpha\beta}^{+}(\lambda) \frac{d}{d\lambda} \Delta_{\beta\alpha}(\lambda) \Big|_{c,R} \\ &= -i \sum_{\alpha=0}^{3} \hat{tr}_\alpha \, q_{\alpha\alpha}(\lambda) \Big|_{c} \end{aligned} \tag{3.10.9}$$

We recall that the S-matrix form of $q_{\alpha\alpha}(\lambda)$ in (3.10.3) has been established but that of $q_{oo}(\lambda)$ has not. However, since we have already established (3.10.9) in chapter IV, we can infer from here that (3.10.8) can serve as a proof of the S-matrix form of $q_{oo}(\lambda)$.

Let us summarize our conclusions. Starting from the simple two-body time delay theory we have extended these results to arrive at a comparable three-body theory of time delay. We have found an important application of time delay in determining a solution of the virial coefficient problem. Hence, we have illustrated the possibility of studying statistical mechanics entirely in terms of time delay.

While the mathematical problem of disconnectedness has been treated accurately the literature, the other technical difficulty of regularization has not. We have found a simple and complete solution for regularization. This serves as an illustration of the complexity involved in the treatment of N-body time delay. It is hoped that this regularization method may provide new insight into the numerical calculations of virial coefficients.

The different methodologies employed in Chapters IV and V brings forth the richness and fertility of the three-body theory pioneered by Faddeev. While the operator method of Chapter IV brings us to the simple expression of virial coefficient terms of time delay, it does not investigate the actual structure of time delay. In Chapter V we have to solve the problem of regularization to find an expression of three-body time delay in terms of two body t-matrix and three body amplitudes.

One original aim was to show that the trace of the time delay operator can play the role of phase shifts in the three body problem. This goal is achieved in the formula obtained for the third virial coefficient. Such a development is in fact necessary since the scattering amplitudes that characterize the three-body problems do not admit any known phase shift parameterization. Our formula for the second and third virial coefficients also demonstrate that the only effect of the scattering process equilibrium statistical mechanics is sensitive to is the time delay of the collision event.

Appendix A

In this appendix we give proofs of a number of trace related facts used in our derivation of the two body spectral property. In order to specify our notation, we recount the salient features of the trace and of Hilbert Schmidt operators. A bounded operator B acting in some Hilbert space is Schmidt class (notationally $B \varepsilon \sigma C$) if the sum

$$\sigma(B) = \left(\sum_i^\infty \|B \varphi_i\|^2 \right)^{\frac{1}{2}} \tag{A.1}$$

is finite. The norm above is that generated by the Hilbert space inner product. This sum is independent of the basis set $\{\varphi_i\}$. The class of operators that satisfy equation (IV.2.14) is called the trace class and will be denoted by τC. Basic facts about the trace we shall need are:

(1) $A \varepsilon \tau C$ if and only if it can be written as the product $A = BC$ where $B \varepsilon \sigma C$ and $C \varepsilon \sigma C$.

(2) If $B \varepsilon \sigma C$ then $B^+ \varepsilon \sigma C$.

(3) If $B \varepsilon \tau C$ and A is bounded then $BA \varepsilon \tau C$ and $AB \varepsilon \tau C$.

(4) If $B \varepsilon \sigma C$ and $C \varepsilon \sigma C$ then $\mathrm{Tr}\, BC = \mathrm{Tr}\, CB$.

The proof of all these statements can be found in Schatten.[34]

First let us establish the uniform convergence property of $\mathrm{Tr}\, P(R) A$. Here $A \varepsilon \tau C$ and $P(R)$ is the projector defined in section IV.2. Using properties (1) and (4) of the trace we have

$$\mathrm{Tr}\, P(R) A = \mathrm{Tr}\, P(R) B C^{\dagger} = \mathrm{Tr}\, C^{\dagger} P(R) B$$

$$= \sum_i \left(C\varphi_i , P(R) B \varphi_i \right) \quad = \sum_i \left(P(R) C \varphi_i , P(R) B \varphi_i \right) \tag{A.2}$$

The second form of the sum has ultilized the projection operator features of $P(R)$. We now will majorize each term in the sum by a form independent of R, viz.

$$\left| \left(P(R) C \varphi_i , P(R) B \varphi_i \right) \right| \leq \frac{1}{2} \left(\| P(R) B \varphi_i \|^2 + \| P(R) C \varphi_i \| \right)$$
$$\leq \frac{1}{2} \left(\| B\varphi_i \|^2 + \| C\varphi_i \|^2 \right) \tag{A.3}$$

Here the first inequality follows from the definition of the inner product. The final step uses $\|P(R) f\| \leq \|f\|$ which is valid for any f in our Hilbert space. The sums over i of $\| B\varphi_i \|^2$ and $\| C\varphi_i \|^2$ are finite since $B \varepsilon \sigma C$ and $C \varepsilon \sigma C$. Thus the sum defining $Tr\, P(R) A$ is uniformly convergent where is trace class.

Our derivation of the spectral property of time delay requires that we use the diagonal form of the trace,

$$Tr\, A = \int A(y,y)\, dy \tag{A.4}$$

where $A(x,y)$ is the L^2 kernel associated with the trace class operator A. The above formula is not generally true for all trace class operators. However, when $A = BC$ and both $B \varepsilon \sigma C$ and $C \varepsilon \sigma C$ then equation 4 is valid with the diagonal element defined as

$$A(y,y) = \int B(y,x)\, C(x,y)\, dx \tag{A.5}$$

Let us briefly indicate the proof of this result. We first recall that the Schmidt norm can be expressed (cf. Theorem II.4, Schatten 34)

$$\sigma(B)^2 = \iint |B(x,y)|^2 \, dx \, dy \tag{A.6}$$

From the general identity,

$$(f,g) = \left\| \frac{f+g}{2} \right\|^2 - \left\| \frac{f-g}{2} \right\|^2 + i \left\| \frac{f+ig}{2} \right\|^2 \quad i \left\| \frac{f-ig}{2} \right\| \tag{A.7}$$

one can state the trace in terms of σ-norms. In fact

$$\begin{aligned} Tr\, A &= Tr\, BC = \sum_i (B^{+}\varphi_i, C\varphi_i) \\ &= \tfrac{1}{4}\left\{ \sigma(B^{+}+C)^2 - \sigma(B^{+}-C)^2 + i\sigma(B^{+}+iC)^2 - i\sigma(B^{+}-iC)^2 \right\} \end{aligned} \tag{A.8}$$

where we have employed equation 7 and the definition (A.1) of the σ-norm. Inserting (A.6) into the right hand side of (A.8) leads to

$$Tr\, A = \iint B(x,y)\, C(x,y) \, dx \, dy \tag{A.9}$$

The final conclusion, equations 5 and 6 is a consequence of changing the order of integration in the double integral of (A.9). This is justified because both $|B(x,y)|^2$ and $|C(x,y)|^2$ are integrable with respect to $dx\,dy$, so we know the integrand of (A.9) is absolutely integrable. We remark that every use of the formula (A.4) in the main text occurs under the circumstance that A is the product of two Schmidt operators.

The next fact we establish is that if v satisfies condition (IV.2.4) then $\rho(\xi+i\eta) - \rho_0(\xi+i\eta)$ is trace class when $\eta > 0$. To begin we define

$$v(\vec{x}) = W_1(\vec{x})\, W_2(\vec{x}) \tag{A.10}$$

where

$$W_1(\vec{x}) = |v(\vec{x})|^{\frac{1}{2}}, \quad W_2(\vec{x}) = W_1(\vec{x}) \,\mathrm{sgn}\, v(\vec{x}) \tag{A.11}$$

Since $v \varepsilon L^1$, then W_1 and $W_2 \varepsilon L^2$. So W_1 and W_2 are bounded multiplication operators. We first observe that $r_0(\xi+i\eta) W_1$ and $W_2 r_0(\xi+i\eta) \varepsilon \sigma C$. This follows from the integral representation of $r_0(\xi+i\eta) W_1$. The square of the Schmidt norm can be expressed as (cf. A.6)

$$\iint \left|\langle \vec{x} | r_0(\xi+i\eta) | \vec{x}' \rangle W_1(\vec{x}')\right|^2 d\vec{x}\, d\vec{x}'$$

$$= \left(\frac{\mu}{2\pi}\right)^2 \iint \left| \frac{e^{i(2\mu)^{\frac{1}{2}}(\xi+i\eta)^{\frac{1}{2}} |\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|} W_1(\vec{x}')\right|^2 d\vec{x}\, d\vec{x}'$$

$$= \left(\frac{\mu}{2\pi}\right)^2 \int |v(\vec{x})|\, d\vec{x} \int e^{-2(2\mu)^{\frac{1}{2}} \operatorname{Im}(\xi+i\eta)^{\frac{1}{2}} |\vec{y}|} d\hat{y}\, d|\vec{y}| \qquad (A.12)$$

In (A.12) we have used the standard coordinate space form of the free resolvent $r_0(\xi+i\eta)$. A change of variables $\vec{y} = \vec{x}-\vec{x}'$ leads to the last form of the integral. For $\eta > 0$ the $\vec{y}$ integral converges. Because $v \varepsilon L^1$ the $\vec{x}$ integration is finite. Thus $r_0(z) W_1 \varepsilon \sigma C$. The same treatment shows $W_2 r_0(z) \varepsilon \sigma C$.

Consider now

$$r_0(z)\, v\, r_0(z) = r_0(z)\, W_1 W_2\, r_0(z) \qquad (A.13)$$

Thus $r_0(z) v r_0(z) \varepsilon \tau C$, since it is the product of two Schmidt class operators. Finally weemploy these facts to show that $r(z) - r_0(z)$ is trace class. The definitions of the resolvents imply

$$r(z) - r_0(z) = -r_0(z)\, v\, r(z) = -r_0(z)\, v\, r_0(z) \left[e - v\, r(z)\right] \qquad (A.14)$$

For $\eta = \operatorname{Im} z \neq 0$ the operator in the square bracket is bounded. First note for z not part of the spectrum of h that $\|r(z)\| < \infty$. Second, $v \varepsilon L^2$ means v is a bounded operator.

Thus $\Lambda(z)-\Lambda_0(z)$ is the product of a bounded operator times a trace class operator. Properties (1) and (3) imply that such an operator is trace class. So our proof is complete.

We conclude this appendix by demonstrating that the operators $P(R)[\Lambda_0(z)-\Lambda_0^{\dagger}(z)]P(R)$ and $P(R)[\Lambda(z)-\Lambda^{\dagger}(z)]P(R)$ are trace class for $\mathcal{I}m\, z \neq 0$ and finite R. To prove this for the first mentioned of the above operators use the Hilbert identity to write

$$P(R)[\Lambda_0(z)-\Lambda_0^{\dagger}(z)]P(R) = -2i\, \mathcal{I}m\, z\; P(R)\Lambda_0(z)\Lambda_0^{\dagger}(z)P^{\dagger}(R) \tag{A.15}$$

The argument given in equation 10 to show $\Lambda_0(z)W_1 \in \sigma\mathcal{C}$ can easily be modified to show $P(R)\Lambda_0(z) \in \sigma\mathcal{C}$, $\mathcal{I}m \neq 0$, $R<\infty$. Thus the operator on the left of equation 15 is trace class by virtue of (1) and (2). Turning to our second operator, we note that equation 13 still applies with $\Lambda_0(z)$ replaced by $\Lambda(z)$. Thus we only need prove $P(R)\Lambda(z) \in \sigma\mathcal{C}$. But this is easy since

$$P(R)\Lambda(z) = P(R)\Lambda_0(z)\left[e - v\Lambda(z)\right] \tag{A.16}$$

As noted before the operator in the square bracket is bounded. Thus property (3) tells us $P(R)\Lambda(z) \in \sigma\mathcal{C}$. Now appealing to property (1) tells us that $P(R)[\Lambda(z)-\Lambda^{\dagger}(z)]P(R)$ is trace class.

Appendix B

This appendix collects together the technical details concerning the trace of the three-body resolvents. The proof given in section IV.3 rests on the fact that the operators $A(z)$ defined by (IV.3.59) are trace class for $z \in \Pi_\delta$. Further $\mathrm{Tr}\, A(z)$ must be an analytic function in Π_δ that is the sum of a uniformly convergent series of analytic functions on Π_δ. We state the circumstances under whcih these results are known. We shall rely on the proof given by Buslaev and Merkuriev. Although their proof is rather long we have not been able to find a more direct one.

The fundamental structures equations (IV.3.11 - 19) were established by Faddeev[1] for interactions whose momentum space potentials satisfy the two restrictions,

$$|v(\vec{q})| \leq C\,(1+|\vec{q}|)^{-(1+\theta)}, \quad \theta > \tfrac{1}{2} \tag{B.1}$$

$$|v(\vec{q}) - v(\vec{q}+\Delta\vec{q})| \leq C\,|\Delta\vec{q}|^{\mu}\,(1+|\vec{q}|)^{-(1+\theta)} \tag{B.2}$$

for $|\Delta\vec{q}| < 1$ and $\mu > 0$. Physically, the variable $\vec{q}$ is the momentum transfer. The first property ensures us that integrals over momentum are convergent. The second is necessary to make sure the operator $v R_0(\zeta + i\eta)$ is well defined in a suitable Banach space as $\eta \to 0$. An addition restriction is needed for Buslaev and Merkuriev's analysis. Let $\{q_1, q_2, q_3\}$ be the Cartesian components of the vector $\vec{q}$. Then $v(\vec{q})$ must satisfy

$$\left| \frac{\partial^k}{\partial^n q_1\, \partial^m q_2\, \partial^\ell q_3} v(\vec{q}) \right| \le C(1+|\vec{q}|)^{-(1+\theta)}, \quad k \le 5, \quad \theta > \tfrac{1}{2} \tag{B.3}$$

where $k = n + m + \ell$. In all three of the restrictions above C is a constant dependent only on v . We shall let τ denote the trace norm on the space $\mathcal{H}$. Its definition in terms of the trace is

$$\tau(B) = \mathrm{Tr}\,|B| \tag{B.4}$$

where B is any trace-class operator acting on $\mathcal{H}$. Under assumptions (B.1 -3) Buslaev and Merkuriev establish (second reference in 19) , Theorem 2.1) that

$$\tau\big(A(z)\big) \le C\,\big(1+|z|\big)^{a}, \quad z \in \Pi_\delta \tag{B.5}$$

where a is a positive number. The operator $A(z)$ is given by equation (IV.3.59).

It follows from (B.5) and general features of the resolvent that $\mathrm{Tr}\,A(z)$ is a uniformly convergent series of analytic functions in $\mathcal{H}$. Let us prove this. Suppose $\{\phi_i\}$ is a complete orthonormal set in $\mathcal{H}$ that is used to define the trace. Then

$$(\phi_i, R^2(z)\,\phi_i) = \int (\varsigma - z)^{-2}\, d(\phi_i, E(\varsigma)\,\phi_i) , \tag{B.6}$$

clearly defines an analytic function for every $\phi_i \in \mathcal{H}$, and $z \in \Pi_\delta$. The same holds with $R^2(z)$ replaced by $R_\alpha^2(z)$ or $R_0^2(z)$. Thus each term $(\phi_i, A(z)\,\phi_i)$ is analytic. We need only show the series defining $\mathrm{Tr}\,A(z)$ is uniformly convergent. Choose D to be any finite region in Π_δ . Let M be

$$\sup_{z \varepsilon D} C(1+|z|)^a = M < \infty \tag{B.7}$$

It follows from the general properties of the trace[34] that

$$\sum_i^{\infty} |(\phi_i, A(z)\phi_i)| \leq \tau(A(z)) \leq M, \quad \forall z \varepsilon D \tag{B.8}$$

this, of course, tells us that

$$Tr\ A(z) = \sum_i^{\infty} (\phi_i, A(z)\phi_i) \tag{B.9}$$

is pointwise convergent for each $z \varepsilon D$. Inequality (B.8) also implies

$$\left| \sum_i^{n} (\phi_i, A(z)\phi_i) \right| \leq M, \quad \forall n, \forall z \varepsilon D \tag{B.10}$$

We recall from analytic function theory Vitali's theorem (Titchmarsh[39], Theorem 5.21). Under hypothesis (B.10) and (B.9) then the convergent series (B.9) must be uniformly convergent in any region interior to D . Since D was chosen arbitrarily we have that (B.9) is uniformly convergent in any compact domain of Π_δ .

The topic that remains for this appendix is to discuss the Schmidt character of operators like $\mathcal{P}(\rho) R_0^2(z)$. We shall investigate a more general class of operators. Special examples of this class will turn out to be those we need in the main text. Let Σ denote an arbitrary compact set of points in the $\vec{x}$, $\vec{y}$ space. Denote by $V(\Sigma)$ the finite volume of this set. In the main text, Σ was always a sphere with possible different radii ρ . Define by $\phi(\cdot)$ any continuous real function with arguments from the positive real line. We shall study the Schmidt character of $\mathcal{P}(\Sigma)\phi(H_0)$. The symbol $\mathcal{P}(\Sigma)$ denotes the projection onto the set Σ .

The Schmidt norm, when defined in momentum space is (cf. A.6)

$$\sigma(\mathcal{P}(\Sigma)\,\phi(H_0))^2 = \iint \left|\langle \vec{p}_0 | \mathcal{P}(\Sigma)\,\phi(H_0) | \vec{p}_0{}' \rangle\right|^2 d\vec{p}_0\, d\vec{p}_0{}' \tag{B.11}$$

and the kernel $\langle \vec{p}_0 | \mathcal{P}(\Sigma) | \vec{p}_0{}' \rangle$ is given by

$$\langle \vec{p}_0 | \mathcal{P}(\Sigma) | \vec{p}_0{}' \rangle = F_\Sigma(\vec{p}_0 - \vec{p}_0{}') = \int_\Sigma e^{i(\vec{p}_0 - \vec{p}_0{}')\cdot \vec{r}_0}\, d\vec{r}_0 \tag{B.12}$$

where $\vec{r}_0 = (\vec{x}_\alpha, \vec{y}_\alpha)$. Note that if we integrate $|F_\Sigma(\vec{p}_0)|^2$ over all $\vec{p}_0$ then its definition (B.12) leads to

$$\int |F_\Sigma(\vec{p}_0)|^2 d\vec{p}_0 = \frac{V(\Sigma)}{(2\pi)^6} \tag{B.13}$$

Thus if we use the fact that $\phi(H_0)$ is diagonal in $\vec{p}_0$ and change the variables of integration in (B.11) from $d\vec{p}_0\, d\vec{p}_0{}'$ to $d(\vec{p}_0 - \vec{p}_0{}')\, d\vec{p}_0{}'$ then,

$$\sigma(\mathcal{P}(\Sigma)\,\phi(H_0))^2 = \frac{V(\Sigma)}{(2\pi)^6} \int \left|\phi(p_0^2/2m_0)\right|^2 d\vec{p}_0 \tag{B.14}$$

The measure $d\vec{p}_0$ can be represented as $p_0^5\, dp_0\, d\hat{p}_0$ – the appropriate six dimensional spherical coordinates.

Consider now, several choices for ϕ. If $\phi(H_0) = R_0(z)$ then the integral in (B.14) is infinite. So $\mathcal{P}(\Sigma)\, R_0(z)$ is not Schmidt class. Try next $\phi(H_0) = R_0^2(z)$. Now the denominator vanishes as p_0^8 and the measure remains $p_0^5\, dp_0$. Thus the integral converges and $\mathcal{P}(\Sigma) R_o^2(z)$ has finite Schmidt norm. The same conclusion also applies to $\phi(H_o) = e^{-\beta H_o}$.

Our derivations in section IV.3 also require that $\mathcal{P}(\Sigma) R_\alpha^2(z)$ and $\mathcal{P}(\Sigma) R^2(z)$ are Schmidt class. Examine the last operator. Take the square of the usual resolvent relation between $R(z)$ and $R_o(z)$ and multiply from the left by $\mathcal{P}(\Sigma)$. This gives one

$$\mathcal{P}(\Sigma) R^2(z) = \mathcal{P}(\Sigma) R_o^2(z) \left[E - \sum_{\alpha=1}^{3} V_\alpha R(z) \right]^2 \tag{B.15}$$

The operator in the square bracket is bounded and multiplied by a Schmidt class operator. Thus $\mathcal{P}(\Sigma) R^2(z)$ is Schmidt class. The same argument applies to $\mathcal{P}(\Sigma) R_\alpha^2(z)$.

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