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Perturbation Theory for Three-Particle Coulomb Scattering

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The Born series and multiple scattenng expansion for the off-shell wave functions corresponding to a system of three charged particles are studied. Explicit expressions are derived for the anomalous terms and divergences which occur in these perturbation expansions in the energy-shell limit. A prescription is given for canceling these anomalous terms. The resulting "renormalized" perturbation expansions are used to formulate various approximations to the T matrices for excitation and ionization of a neutral fragment by a charged particle.

1. INTRODUCTION

It should be possible to use a perturbational approach to calculate the wave function and T matrix for a quantum mechanical system involving nonsingular forces which go to zero for large particle separation. In the case of short-range forces such an approach can be based on the iterations of the various integral equations satisfied by the wave function and T matrix. However, for scattering involving long-range potentials there are well-known difficulties in basing a perturbation formalism on either the usual off-shell integral equations or equations involving cutoff long-range potentials. These difficulties manifest themselves as anomalous terms and divergences when one attempts to take the limit to physical energies in the off-shell perturbation formalism or remove the cutoff in the perturbation formalism involving cutoff long-range potentials.

In this paper we will show the occurrence of anomalous terms and divergences in the energy-shell limit of the Born and multiple scattering expansions for the off-shell wave functions corresponding to a system of three charged particles. A prescription for canceling these anomalous terms together with a justification of this "renormalization" procedure is given.

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We will concentrate on the wave functions corresponding to the free channel and the channel α consisting of a neutral fragment and a charged particle.

The off-shell wave function corresponding to the free channel, denoted $\phi_{+\varepsilon}(x, p)$, satisfies both the Lippmann–Schwinger equation (see Appendix A for notation)

$$\phi_{+\varepsilon}(x, p)=\phi_0(x, p)-\int dy\, G_0(x, y; E+i\varepsilon)V(y)\phi_{+\varepsilon}(y, p) \qquad (1)$$

and the Weinberg–Van Winter equation (Van Winter, 1964; Weinberg, 1964; Van Winter and Brascamp, 1968; the problem of spurious solutions is discussed in Vanzani, 1978).

$$\begin{aligned}\phi_{+\varepsilon}(x, p)=&\phi_0(x, p)+\sum_{i<j}\left[\phi^{ij}_{+\varepsilon}(x, p)-\phi_0(x, p)\right]\\ &-\sum_{i<j}\int dy\left[G_{ij}(x, y; E+i\varepsilon)-G_0(x, y; E+i\varepsilon)\right]\\ &\times\sum_{\substack{k<l\\(k,l)\neq(i,j)}} V_{kl}(y)\phi_{+\varepsilon}(y, p)\end{aligned} \qquad (2)$$

An argument is given in this paper to show the development of anomalous terms and divergences as $\varepsilon\to+0$ in each term of the Born series corresponding to (1) and the multiple scattering expansion obtained by iterating (2). It has been shown (Zorbas, 1977) that $\phi_{+\varepsilon}(x, p)$ develops an anomalous multiplicative factor as $\varepsilon\to+0$ due to the short-range asymptotic condition which is implicitly assumed in the definition of the off-shell wave function. We will argue that this factor is the source of the anomalous terms and divergences in the Born series and is partially responsible for the divergences in the multiple scattering expansion for $\phi_{+\varepsilon}(x, p)$.

The perturbation formalism for the off-shell wave function corresponding to the channel α illustrates another source of anomalous terms in perturbation theory involving long-range potentials. The α channel wave function, denoted $\phi^{\alpha}_{+\varepsilon}(x, p)$, satisfies the integral equation (see Appendix A and Geltman, 1969)

$$\phi^{\alpha}_{+\varepsilon}(x, p)=\phi^{1;\alpha}_{+\varepsilon}(x, p)-\int dy\, G_1(x, y; E^{\alpha}+i\varepsilon)V_{23}(y)\phi^{\alpha}_{+\varepsilon}(y, p) \qquad (3)$$

An argument is given in this paper to show that the terms of the perturbation expansion, obtained by iterating (3), develop anomalous terms and divergences as $\varepsilon \to +0$. It is not hard to show, using an argument similar to that given in Zorbas (1977), that $\phi^{\alpha}_{+\varepsilon}(x, p)$ does not develop an anomalous multiplicative factor as $\varepsilon \to +0$. This result is directly attributable to the effective short-range interaction between a charged particle and a neutral fragment. We will argue that the anomalous terms appearing in the iterations of (3) are due to an inadequate choice of the "unperturbed" term $\phi^{1;\alpha}_{+\varepsilon}(x, p)$.

In a recent paper (Zorbas, 1978) the occurrence of anomalous terms in the off-shell Born series for two-particle Coulomb-like scattering was examined. For a general class of Coulomb-like potentials it was shown that the anomalous multiplicative factor in the off-shell wave function is the source of the anomalous terms and divergences in the energy-shell limit of the Born series. A prescription was given for canceling the anomalous terms in the off-shell Born series. The resulting perturbation expansion was shown to be term-by-term convergent to the perturbation expansion for the physical Coulomb wave function.

This paper provides a three-particle generalization of these two-particle results. In the case of the Born series corresponding to (1) an argument is given to show that the two-particle prescription (Zorbas, 1978) has a natural extension to three-particle Coulomb scattering.[1] In the case of the multiple scattering expansion corresponding to (2) and the iterations of (3) a prescription is given for canceling anomalous terms so as to obtain term-by-term convergent (in the limit $\varepsilon \to +0$) perturbation expansions for the three-particle wave functions.

The approach taken in this paper is based on the time-dependent theory and the relationship between the time-dependent and stationary scattering formalisms (Amrein et al., 1977; Prugovečki, 1971). The basic idea is to use the $|t| \to \infty$ behavior of various time-dependent expressions to obtain information concerning the $\varepsilon \to +0$ behavior of the corresponding stationary expressions. Many of the arguments given in this paper are formal in that domain problems are not considered. Furthermore, we will conclude convergence of various integrals by formal power counting arguments.

We now give an outline of the contents of this paper. The basic idea of our approach is illustrated in Section 2 by the pedagogical example of a constant perturbation. In Section 3 the occurrence of anomalous terms in the Born series for $\phi_{+\varepsilon}(x, p)$ is shown, and in Section 4 a prescription is given to cancel these terms. In Section 5 we unravel the anomalous terms in the multiple scattering expansion for $\phi_{+\varepsilon}(x, p)$. A "renormalized" multiple

[1] It is straightforward to generalize the results of Sections 3 and 4 of this paper to general N-particle Coulomb systems.

scattering expansion is proposed in Section 6. The perturbation expansions corresponding to the scattering of a charged particle by a fixed neutral "fragment" are discussed in Section 7. The occurrence and cancellation of anomalous terms in the iterations of (3) is shown in Section 8. Applications of these results to excitation and ionization are briefly considered in Section 9, and the paper concludes with a discussion in Section 10.

2. A SIMPLE EXAMPLE

In this section an exactly solvable example is given which illustrates the basic ideas behind our approach.

Consider the Hamiltonian

$$H=H_0+\sum_{i<j}\lambda_{ij}, \qquad \lambda_{ij}\in R^1$$

The correct time-dependent scattering theory for this Hamiltonian is based on the operator $\Omega(t)$ given by

$$\Omega(t)=W(t)\exp[-iG(t)]$$

$$W(t)=\exp(iHt)\exp(-iH_0t), \qquad G(t)=\sum_{i<j}\lambda_{ij}t$$

Note that the usual off-shell formalism is based on the operators $W(t)$, not on the correct operator $\Omega(t)=\mathbb{1}$. In order to see this define the operators $W_{+\varepsilon}$ by

$$W_{+\varepsilon}=\int_0^\infty du\exp(-u)W(-u/\varepsilon)$$

It is not difficult to verify the following equality for appropriate functions ψ (see Appendix B):

$$(W_{+\varepsilon}\psi)(x)=\int dp\,\phi_{+\varepsilon}(x,p)\hat{\psi}(p)$$

where $\phi_{+\varepsilon}(x,p)$ satisfies the off-shell Lippmann–Schwinger equations

$$\phi_{+\varepsilon}(x,p)=\phi_0(x,p)-\sum_{i<j}\int dy\,G_0(x,y;E+i\varepsilon)\lambda_{ij}\phi_{+\varepsilon}(y,p)$$

The above argument shows that $\phi_{+\varepsilon}(x,p)$ and the integral equation satisfied by $\phi_{+\varepsilon}(x,p)$ are directly related to the operators $W(t)$ which do not correctly incorporate the asymptotic condition for a constant potential. That is, the off-shell Lippmann–Schwinger equation corresponds to treating H as a perturbation of H_0; however, for long-range forces H_0 does not generate the correct "free dynamics."

It is straightforward to calculate $\phi_{+\varepsilon}(x, p)$ for each $\varepsilon > 0$:

$$\phi_{+\varepsilon}(x, p) = \frac{i\varepsilon}{i\varepsilon - \sum_{i<j} \lambda_{ij}} \phi_0(x, p)$$

The incorrect choice of asymptotic condition is mirrored in the convergence of $\phi_{+\varepsilon}(x, p)$ to zero as $\varepsilon \to +0$. Furthermore, there are divergences in each term of the Born series for $\phi_{+\varepsilon}(x, p)$ in the energy-shell limit.

In order to avoid the above difficulties one must base the off-shell formalism on the correct asymptotic condition. According to the prescription given by Zorbas (1976), an off-shell stationary formalism should be based on the following "renormalized" off-shell wave function:

$$\phi_{+\varepsilon}(x, p)\Lambda_{+\varepsilon}$$

where

$$\Lambda_{+\varepsilon} = \left\{ \int_0^\infty du \exp[-u + iG(-u/\varepsilon)] \right\}^{-1} = \frac{i\varepsilon - \sum_{i<j} \lambda_{ij}}{i\varepsilon}$$

Clearly the renormalized off-shell wave function is the correct wave function for a constant perturbation.

The simple pedagogical example of this section suggests that one source of anomalous terms in the usual off-shell perturbation formalism involving long-range potentials is the short-range asymptotic condition which forms the basis of this formalism. Furthermore, if the off-shell formalism is based on the correct asymptotic condition it should be possible to formulate a perturbation expansion which is free of anomalous terms and divergences.

3. DIVERGENCES IN THE BORN SERIES

In this section we examine the development of anomalous terms and divergences in the Born series for $\phi_{+\varepsilon}(x, p)$ as $\varepsilon \to +0$. Our approach is based on the $t \to -\infty$ behavior of the iterations of the time-dependent equations[2]

$$W(t)=\mathbb{1}+i\int_0^t du\, W(u)V(u)$$

$$W(t)=\exp(iHt)\exp(-iH_0t), \qquad V(t)=\exp(iH_0t)V\exp(-iH_0t)$$

The perturbation expansion for $W(t)$ is given by

$$W(t)=\sum_{n=0}^{\infty} W_n(t) \tag{4}$$

where $W_0(t)=\mathbb{1}$ and for $n\geqslant 1$

$$W_n(t)=i^n\int_0^t du_1\int_0^{u_1} du_2\cdots\int_0^{u_{n-1}} du_n V(u_n)V(u_{n-1})\cdots V(u_1)$$

In order to extract the large-$|t|$ behavior of $V(t)=\Sigma_{i<j}V_{ij}(t)$ we rewrite V as follows:

$$V(x)=V^l(x)+V^s(x) \tag{5}$$

where

$$V^l(x)=V_{12}(\mathbf{x}_1)\chi(\mathbf{x}_1)+V_{13}\left(\mathbf{x}_2+\frac{\mu_2}{\mu_1+\mu_2}\mathbf{x}_1\right)$$
$$\times\chi\left(\mathbf{x}_2+\frac{\mu_2}{\mu_1+\mu_2}\mathbf{x}_1\right)+V_{23}\left(\mathbf{x}_2-\frac{\mu_1}{\mu_1+\mu_2}\mathbf{x}_1\right)\chi\left(\mathbf{x}_2-\frac{\mu_1}{\mu_1+\mu_2}\mathbf{x}_1\right)$$

with

$$\chi(\mathbf{x})=\begin{cases}1 & \text{if } |\mathbf{x}|\geqslant 1\\ 0 & \text{if } |\mathbf{x}|<1\end{cases}$$

and $V^s(x)$ defined by (5). The following equality is valid (Alsholm, 1977):

$$\exp(iH_0t)V^l(\mathbf{x}_1,\mathbf{x}_2)\exp(-iH_0t)=\exp\left(-\frac{iL_0}{t}\right)V^l\left(\frac{\mathbf{p}_1t}{m_1},\frac{\mathbf{p}_2t}{m_2}\right)\exp\left(\frac{iL_0}{t}\right) \tag{6}$$

[2]The perturbation expansions for $\phi_{-\varepsilon}(x,p)$ can be studied by a similar argument involving $t\to+\infty$.

where

$$L_0 = \frac{m_1 x_1^2}{2} + \frac{m_2 x_2^2}{2}$$

Using (6) we can rewrite $V(t)$ as follows:

$$V(t) = V^l(t) + V^s(t) = \sum_{i<j} \left[V_{ij}^l(t) + V_{ij}^s(t) \right]$$

$$V^l(t) = V^l\left(\frac{\mathbf{p}_1 t}{m_1}, \frac{\mathbf{p}_2 t}{m_2} \right) = \sum_{i<j} V_{ij}^l \left(\frac{\mathbf{p}_1 t}{m_1}, \frac{\mathbf{p}_2 t}{m_2} \right) \tag{7}$$

where formally $\int_{-\infty}^{+\infty} V_{ij}^s(t)\, dt < \infty$ for $1 \leqslant i < j \leqslant 3$.[3]

We now use (7) to examine the $t \to -\infty$ behavior of $W_n(t)$, $n \geqslant 1$. The first term $W_1(t)$ can be written as

$$\begin{aligned} W_1(t) &= \int_0^t du_1\, iV^l(u_1) + \int_0^t du_1\, iV^s(u_1) \\ &= \int_0^t du_1\, iV^l(u_1) + \eta_1(t) \end{aligned}$$

where $\eta_1(t)$ converges as $t \to -\infty$.

Consider $W_2(t)$, which can be rewritten as follows:

$$\begin{aligned} W_2(t) &= \int_0^t du_1 \left\{ \int_0^{u_1} du_2 \left[iV^l(u_2) \right] + \eta_1(u_1) \right\} \left[iV^l(u_1) + iV^s(u_1) \right] \\ &= \int_0^t du_1 \int_0^{u_1} du_2 \left[iV^l(u_2) \right] \left[iV^l(u_1) \right] + \eta_1(t) \int_0^t du_1 \left[iV^l(u_1) \right] + \eta_2(t) \end{aligned}$$

where $\eta_2(t)$ converges as $t \to -\infty$.

The pattern should be clear and we will state the form of $W_n(t)$. Define $\Lambda_0(t) = \mathbb{1}$ and for $n \geqslant 1$

$$\begin{aligned} \Lambda_n(t) &= \int_0^t du_1 \int_0^{u_1} du_2 \cdots \int_0^{u_{n-1}} du_n \left[iV^l(u_n) \right] \cdots \left[iV^l(u_1) \right] \\ &= \frac{\left[i \int_0^t du\, V^l(u) \right]^n}{n!} \end{aligned}$$

[3]A more precise statement of $\int_{-\infty}^{+\infty} V_{ij}^s(t)\, dt < \infty$ is, for appropriate functions ψ, $\int_{-\infty}^{+\infty} \| V_{ij}^s(t) \psi \|\, dt < \infty$.

We have, using the obvious inductive definition of $\eta_k(t)$, the following equality:

$$W_n(t)=\sum_{k=0}^{n}\eta_k(t)\Lambda_{n-k}(t) \tag{8}$$

where at least formally $\eta_k(t)$ converges as $t\to-\infty$ for each k.

We now relate the divergences as $t\to-\infty$ appearing in (8) to divergences in the nth term of the Born expansion as $\varepsilon\to+0$. The Born expansion for $\phi_{+\varepsilon}(x,p)$ is given by

$$\phi_{+\varepsilon}(x,p)=\sum_{n=0}^{\infty}H^n_{+\varepsilon}(x,p)$$

with $H^0_{+\varepsilon}(x,p)=\phi_0(x,p)$ and for $n\geqslant 1$

$$H^n_{+\varepsilon}(x,p)=-\int dy\,G_0(x,y;E+i\varepsilon)V(y)H^{n-1}_{+\varepsilon}(y,p)$$

It is not difficult to formally show (Prosser, 1964) for appropriate functions ϕ and ψ the following equality:

$$\left\langle\phi,\int_0^\infty du\exp(-u)W_n(-u/\varepsilon)\psi\right\rangle=\int dx\,\overline{\phi(x)}\int dp\,\hat{\psi}(p)H^n_{+\varepsilon}(x,p) \tag{9}$$

where $\hat{\psi}(p)$ is the Fourier transform of $\psi(x)$. The equality (9) provides the link between the $t\to-\infty$ behavior of $W_n(t)$ and the $\varepsilon\to+0$ behavior of $H^n_{+\varepsilon}(x,p)$.

Define $\Lambda^n{}_{+\varepsilon}$ by

$$\Lambda^n{}_{+\varepsilon}=\int_0^\infty du\exp(-u)\Lambda_n(-u/\varepsilon)$$

According to (8) and (9) we have

$$H^n_{+\varepsilon}(x,p)\underset{\varepsilon\to+0}{\to}\sum_{k=0}^{n}\eta_k\Lambda^{n-k}_{+\varepsilon} \tag{10}$$

where η_k is the function of x and p corresponding to the $t\to-\infty$ limit of $\eta_k(t)$. Thus the slow decrease of the Coulomb potential leads to the systematic occurrence of anomalous terms and divergences in each term of the Born series as $\varepsilon \to +0$.

4. A MODIFIED BORN SERIES

In a recent paper (Zorbas, 1977) an off-shell formalism was proposed for Coulomb scattering. In particular it was shown that the three-particle Coulomb wave function $\phi_+(x, p)$ is given by

$$\phi_+(x,p) = \lim_{\varepsilon \to +0} \tilde{\phi}_{+\varepsilon}(x,p)$$

where

$$\tilde{\phi}_{+\varepsilon}(x,p) = \phi_{+\varepsilon}(x,p)\Lambda_{+\varepsilon}(x,p)$$

$$\Lambda_{+\varepsilon} = \Gamma(1-ik)^{-1}\exp(-ik\log\varepsilon)\Lambda_1(p)$$

with $\Lambda_1(p)$ a momentum-dependent phase factor and $k = V(\mathbf{p}_1/m_1, \mathbf{p}_2/m_2)$. The "renormalized" off-shell wave function $\tilde{\phi}_{+\varepsilon}(x,p)$ is based on the correct asymptotic condition for Coulomb scattering and thus the off-shell perturbation formalism should be based on $\tilde{\phi}_{+\varepsilon}(x,p)$ rather than $\phi_{+\varepsilon}(x,p)$. This has previously been done for two-particle Coulomb scattering (Zorbas, 1978), and in this section we use the results of Section 3 to justify a similar perturbation expansion for the three-particle case.

Summing the Born series for $\phi_{+\varepsilon}(x,p)$ and using the small ε behavior of each term given by (10) we obtain

$$\phi_{+\varepsilon}(x,p) = \sum_{n=0}^{\infty} H^n_{+\varepsilon}(x,p) \underset{\varepsilon\to+0}{\to} \sum_{n=0}^{\infty}\sum_{k=0}^{n} \eta_k \Lambda_+^{n-k} = \left(\sum_{n=0}^{\infty}\eta_n\right)\left(\sum_{n=0}^{\infty}\Lambda^n_{+\varepsilon}\right) \tag{11}$$

If $|k|<1$ we have

$$\sum_{n=0}^{\infty}\Lambda^n_{+\varepsilon} = \int_0^{\infty} du \exp\left[-u + i\int_0^{-u/\varepsilon} dt\, V^I(t)\right]$$

$$= \Gamma(1-ik)\exp(+ik\log\varepsilon)\Lambda_2(p)$$

where $\Lambda_2(p)$ is a momentum-dependent phase factor. Thus the anomalous terms appearing in the Born series sum up to an anomalous multiplicative factor which, except for a momentum-dependent factor, cancels $\Lambda_{+\varepsilon}$ appearing in the definition of $\tilde{\phi}_{+\varepsilon}(x, p)$. This result provides a justification for neglecting the anomalous terms appearing in the off-shell Born series for $\phi_{+\varepsilon}(x, p)$.

The prescription for replacing the Born series by a perturbation expansion whose terms are free of anomalous terms is immediate. Each term in $H^n_{+\varepsilon}(x, p)$ which is multiplied by an anomalous factor $\Lambda^k_{+\varepsilon}$ cannot, in the limit $\varepsilon \to +0$, contribute to the physical wave function. Thus we subtract these terms from $H^n_{+\varepsilon}(x, p)$, that is, we replace $H^n_{+\varepsilon}(x, p)$ by the expression $\tilde{H}^n_{+\varepsilon}(x, p)$ which is defined as follows:

$$\tilde{H}^n_{+\varepsilon}(x, p) = H^n_{+\varepsilon}(x, p) - \sum_{k=0}^{n-1} \eta_k \Lambda^{n-k}_{+\varepsilon}$$

The $\varepsilon \to +0$ behavior of $H^n_{+\varepsilon}(x, p)$, given by (10), shows that $\tilde{H}^n_{+\varepsilon}(x, p)$ is free of anomalous terms and divergences. Furthermore the resulting perturbation expansion satisfies

$$\sum_{n=0}^{\infty} \tilde{H}^n_{+\varepsilon}(x, p) \underset{\varepsilon \to +0}{\to} \sum_{n=0}^{\infty} \eta_n$$

where $\sum_{n=0}^{\infty} \eta_n$ yields the Coulomb wave function apart from the momentum-dependent phase factor $\Lambda_1(p)\Lambda_2(p)$.

A somewhat more natural way of stating this prescription is to work directly with $\tilde{\phi}_{+\varepsilon}(x, p)$. Consider $\Lambda_{+\varepsilon}$ and $\phi_{+\varepsilon}(x, p)$ as power series in three variables (k_{12}, k_{13}, k_{23}), where $k_{ij} = V_{ij}(\mathbf{p}_1/m_1, \mathbf{p}_2/m_2)$. Multiply these series to obtain a power series in three variables for $\tilde{\phi}_{+\varepsilon}(x, p)$. The terms of this power series do not involve anomalous terms and divergences as $\varepsilon \to +0$. This is the natural three-particle generalization of the prescription which was recently given for the two-particle case (Zorbas, 1978).

5. DIVERGENCES IN THE MULTIPLE SCATTERING EXPANSION

In this section we examine the multiple scattering expansion for $\phi_{+\varepsilon}(x, p)$ given by

$$\phi_{+\varepsilon}(x, p) = \sum_{n=0}^{\infty} K^n_{+\varepsilon}(x, p) \tag{12}$$

where

$$K^{0}_{+\varepsilon}(x,p)=\phi_0(x,p)+\sum_{i<j}\left[\phi^{ij}_{+\varepsilon}(x,p)-\phi_0(x,p)\right]$$

and for $n\geqslant 1$

$$K^{n}_{+\varepsilon}(x,p)=(-1)^n\sum_{i_n<j_n}\int dy_n\Big[G_{i_nj_n}(x,y_n;E+i\varepsilon)-G_0(x,y_n;E+i\varepsilon)\Big]$$

$$\times\sum_{k_n<l_n}V_{k_nl_n}(y_n)\sum_{i_{n-1}<j_{n-1}}\int dy_{n-1}\Big[G_{i_{n-1}j_{n-1}}(y_n,y_{n-1};E+i\varepsilon)$$

$$-G_0(y_n,y_{n-1};E+i\varepsilon)\Big]$$

$$\times\sum_{k_{n-1}<l_{n-1}}V_{k_{n-1}l_{n-1}}(y_{n-1})\times\cdots$$

$$\times\sum_{i_1<j_1}\int dy_1\Big[G_{i_1j_1}(y_2,y_1;E+i\varepsilon)-G_0(y_2,y_1;E+i\varepsilon)\Big]$$

$$\times\sum_{k_1<l_1}V_{k_1l_1}(y_1)K^{0}_{+\varepsilon}(y_1,p)\qquad(13)$$

with $(k_s,l_s)\neq(i_s,j_s)$ for $s=1,\ldots,n$. Each term of (12) is related to integrals of time-dependent expressions in Appendix B. This relationship is used to extract the anomalous expressions and divergences which occur in each term of (12) in the energy-shell limit. A knowledge of these anomalous terms will allow us to replace (12) by a "renormalized" multiple scattering expansion whose terms are formally free of anomalous terms and divergences as $\varepsilon\to+0$. This is discussed further in Section 6. In this section we give detailed results for $K^{n}_{+\varepsilon}(x,p)$, $n=0$, 1, and 2 together with a brief discussion of the general nth term.

In order to extract the anomalous terms in (12) we require various technical time-dependent results. Define the following operators:

$$\Omega^{ij}(t)=W^{ij}(t)\exp\left[-iG_{ij}(t)\right]$$

$$W^{ij}(t)=\exp(iH_{ij}t)\exp(-iH_0t),\qquad G_{ij}(t)=\int_0^t du\,V^{l}_{ij}\left(\frac{\mathbf{p}_1u}{m_1},\frac{\mathbf{p}_2u}{m_2}\right)$$

According to the time-dependent theory for Coulomb scattering (Dollard, 1963, 1964) we have

$$\Omega^{ij}(t)=\Omega^{ij}_{-}+\zeta(t) \tag{14}$$

where Ω^{ij}_{-} denotes the modified wave operator corresponding to H_{ij}[4] and $\zeta(t)\to 0$ as $t\to-\infty$. There are four types of time-dependent operators appearing in the integrands of (B.12) and (B.13). Applying (7) and (14) we can decompose these operators as follows:

$$\begin{aligned}
V_{kl}(-u)&=V^{l}_{kl}(u)+V^{s}_{kl}(u)\\
W^{rs}(-u)V_{kl}(-u)&=\Omega^{rs}_{-}\exp[iG_{rs}(-u)]V^{l}_{kl}(u)+\xi_1(u)\\
V_{kl}(-u)W^{mn}(-u)^{*}&=V^{l}_{kl}(u)\exp[-iG_{mn}(-u)](\Omega^{mn}_{-})^{*}+\xi_2(u)\\
W^{rs}(-u)V_{kl}(-u)W^{mn}(-u)^{*}&=\Omega^{rs}_{-}\exp[iG_{rs}(-u)]V^{l}_{kl}(u)\\
&\quad\times\exp[-iG_{mn}(-u)](\Omega^{mn}_{-})^{*}+\xi_3(u)
\end{aligned} \tag{15}$$

where formally $\int_0^\infty du\,\xi_i(u)<\infty$ for $i=1$, 2, and 3.

5.1. $K^{0}_{+\varepsilon}(x,p)$. According to (B.3) the term $\phi^{ij}_{+\varepsilon}(x,p)$ corresponds to the following integral:

$$\int_0^\infty du\exp(-u-iH_{ij}u/\varepsilon)\exp(iH_0u/\varepsilon)$$

From (14) we see that as $\varepsilon\to+0$ this integral behaves as follows:

$$\int_0^\infty du\exp(-u)\Omega^{ij}(-u/\varepsilon)\exp(iG_{ij}(-u/\varepsilon))$$

$$\underset{\varepsilon\to+0}{\to}\Omega^{ij}_{-}\int_0^\infty du\exp[-u+iG_{ij}(-u/\varepsilon)]\equiv\Omega^{ij}_{-}\left(\Lambda^{ij}_{+\varepsilon}\right)^{-1}$$

Thus $K^{0}_{+\varepsilon}(x,p)$ has the following small ε behavior:

$$K^{0}_{+\varepsilon}(x,p)\underset{\varepsilon\to+0}{\to}\phi_0(x,p)+\sum_{i<j}\left[\phi^{ij}_{+}(x,p)\left(\Lambda^{ij}_{+\varepsilon}\right)^{-1}-\phi_0(x,p)\right]$$

where $\phi^{ij}_{+}(x,p)$ is the wave function corresponding to Ω^{ij}_{-}.

[4] Ω^{ij}_{-} differs from the modified wave operators of Dollard (1964) by a phase factor.

Clearly the prescription for canceling the anomalous terms in $K^0_{+\varepsilon}(x, p)$ is to replace this expression by $\tilde{K}^0_{+\varepsilon}(x, p)$ defined by

$$\tilde{K}^0_{+\varepsilon}(x, p)=\phi_0(x, p)+\sum_{i<j}\left[\phi^{ij}_{+\varepsilon}(x, p)\Lambda^{ij}_{+\varepsilon}-\phi_0(x, p)\right]$$

5.2. $K^1_{+\varepsilon}(x, p)$. It is shown in Appendix B that there are two types of terms contributing to $K^1_{+\varepsilon}(x, p)$ which correspond to the following two integral expressions:

$$-i\int_0^\infty du \exp(-\varepsilon u)W^{i_1j_1}(-u)V_{k_1l_1}(-u)+i\int_0^\infty du \exp(-\varepsilon u)V_{k_1l_1}(-u) \tag{16}$$

and

$$\begin{aligned}&-i\int_0^\infty du\, W^{i_1j_1}(-u)V_{k_1l_1}(-u)W^{ij}(-u)^*(\varepsilon)\\&\quad\times\int_u^\infty dv \exp(-\varepsilon v)\Omega^{ij}(-v)\exp\left[iG_{ij}(-v)\right]\\&+i\int_0^\infty du\, V_{k_1l_1}(-u)W^{ij}(-u)^*(\varepsilon)\\&\quad\times\int_u^\infty dv \exp(-\varepsilon v)\Omega^{ij}(-v)\exp\left[iG_{ij}(-v)\right]\end{aligned} \tag{17}$$

We first consider (16). Using (15) we obtain the following behavior as $\varepsilon\to+0$:

$$\begin{aligned}&-\Omega^{i_1j_1}_{-}\int_0^\infty du \exp\left[-\varepsilon u+iG_{i_1j_1}(-u)\right]iV^l_{k_1l_1}(u)+\int_0^\infty du \exp(-\varepsilon u)iV^l_{k_1l_1}(u)\\&+i\int_0^\infty du \exp(-\varepsilon u)V^s_{k_1l_1}(u)-i\int_0^\infty du \exp(-\varepsilon u)\xi_1(u)\\&\underset{\varepsilon\to+0}{\to}-\Omega^{i_1j_1}_{-}\int_0^\infty du \exp\left[-\varepsilon u+iG_{i_1j_1}(-u)\right]iV^l_{k_1l_1}(u)\\&+\int_0^\infty du \exp(-\varepsilon u)iV^l_{k_1l_1}(u)+i\int_0^\infty du\left[V^s_{k_1l_1}(u)-\xi_1(u)\right]\end{aligned} \tag{18}$$

The anomalous terms have been isolated in the first two terms of (18).

Translating (18) into the stationary formalism suggests that the terms contributing to $K^1_{+\varepsilon}(x, p)$ which have the form

$$-\int dy\Big[G_{i_1j_1}(x, y; E+i\varepsilon)-G_0(x, y; E+i\varepsilon)\Big]V_{k_1l_1}(y)\phi_0(y, p)$$

should be replaced by

$$-\int dy\Big[G_{i_1j_1}(x, y; E+i\varepsilon)-G_0(x, y; E+i\varepsilon)\Big]V_{k_1l_1}(y)\phi_0(y, p)$$

$$-\Big\{-\phi_+^{i_1j_1}(x, p)\int_0^\infty du \exp\Big[-\varepsilon u+iG_{i_1j_1}(-u)\Big]iV^l_{k_1l_1}(u)$$

$$+\phi_0(x, p)\int_0^\infty du \exp(-\varepsilon u)iV^l_{k_1l_1}(u)\Big\}$$

This expression is free of anomalous terms in the limit $\varepsilon\to+0$.

We now consider (17) which in the limit $\varepsilon\to+0$ can be replaced by

$$-i\int_0^\infty du\, W^{i_1j_1}(-u)V_{k_1l_1}(-u)W^{ij}(-u)^*\Omega^{ij}_-\varepsilon\int_u^\infty dv \exp\big[-\varepsilon v+iG_{ij}(-v)\big]$$

$$+i\int_0^\infty du\, V_{k_1l_1}(-u)W^{ij}(-u)^*\Omega^{ij}_-\varepsilon\int_u^\infty dv \exp\big[-\varepsilon v+iG_{ij}(-v)\big] \tag{19}$$

Using the relations (15) we can rewrite (19) in the limit $\varepsilon\to+0$ as follows:

$$\Omega^{i_1j_1}_-P_1(\varepsilon)+P_2(\varepsilon)+i\int_0^\infty du\big[\xi_2(u)-\xi_3(u)\big]\Omega^{ij}_-\int_0^\infty dv \exp\big[-v+iG_{ij}(-v/\varepsilon)\big] \tag{20}$$

where

$$P_1(\varepsilon)=-\int_0^\infty du\, iV^l_{k_1l_1}(u)\exp\big[iG_{i_1j_1}(-u)-iG_{ij}(-u)\big]\varepsilon$$
$$\times\int_u^\infty dv \exp\big[-\varepsilon v+iG_{ij}(-v)\big] \tag{21}$$

$$P_2(\varepsilon)=\int_0^\infty du\, iV^l_{k_1l_1}(u)\exp\big[-iG_{ij}(-u)\big]\varepsilon\int_u^\infty dv \exp\big[-\varepsilon v+iG_{ij}(-v)\big]$$

From (20) we conclude that the terms contributing to $K^1_{+\varepsilon}(x, p)$ which have the form

$$-\int dy\Big[G_{i_1j_1}(x, y; E+i\varepsilon)-G_0(x, y; E+i\varepsilon)\Big]V_{k_1l_1}(y)\phi^{ij}_{+\varepsilon}(y, p)$$

should be replaced by

$$-\left(\Lambda^{ij}_{+\varepsilon}\right)\int dy\Big[G_{i_1j_1}(x, y; E+i\varepsilon)-G_0(x, y; E+i\varepsilon)\Big]V_{k_1l_1}(y)\phi^{ij}_{+\varepsilon}(y, p)$$

$$-\left(\Lambda^{ij}_{+\varepsilon}\right)\left[\phi^{i_1j_1}_{+}(x, p)P_1(\varepsilon)+\phi_0(x, p)P_2(\varepsilon)\right] \tag{22}$$

The results of this subsection enable us to replace the term $K^1_{+\varepsilon}(x, p)$ by an expression, denoted $\tilde{K}^1_{+\varepsilon}(x, p)$, which is formally free of anomalous terms and divergences in the energy-shell limit.

5.3. $K^2_{+\varepsilon}(x, p)$. The two types of terms contributing to $K^2_{+\varepsilon}(x, p)$ are denoted by $K^0(x, p)$ and $K^{ij}(x, p)$ and are defined by (B.4) and (B.5) with $n=2$. The results of Appendix B show that $K^0(x, p)$ and, in the limit $\varepsilon\to+0$, $K^{ij}(x, p)$ correspond, respectively, to the following integral expressions:

$$\int_0^\infty du_2 W^{i_2j_2}(-u_2)iV_{k_2l_2}(-u_2)W^{i_1j_1}(-u_2)^*$$

$$\times\int_{u_2}^\infty du_1\exp(-\varepsilon u_1)W^{i_1j_1}(-u_1)iV_{k_1l_1}(-u_1)$$

$$-\int_0^\infty du_2 W^{i_2j_2}(-u_2)iV_{k_2l_2}(-u_2)\int_{u_2}^\infty du_1\exp(-\varepsilon u_1)iV_{k_1l_1}(-u_1)$$

$$-\int_0^\infty du_2\, iV_{k_2l_2}(-u_2)W^{i_1j_1}(-u_2)^*$$

$$\times\int_{u_2}^\infty du_1\exp(-\varepsilon u_1)W^{i_1j_1}(-u_1)iV_{k_1l_1}(-u_1)$$

$$+\int_0^\infty du_2\, iV_{k_2l_2}(-u_2)\int_{u_2}^\infty du_1\exp(-\varepsilon u_1)iV_{k_1l_1}(-u_1) \tag{23}$$

and

$$\int_0^\infty du_2 W^{i_2j_2}(-u_2)iV_{k_2l_2}(-u_2)W^{i_1j_1}(-u_2)^*\int_{u_2}^\infty du_1 W^{i_1j_1}(-u_1)iV_{k_1l_1}(-u_1)$$

$$\times W^{ij}(-u_1)^*\Omega_{-}^{ij}\varepsilon\int_{u_1}^\infty dv \exp\left[-\varepsilon v+iG_{ij}(-v)\right]$$

$$-\int_0^\infty du_2 W^{i_2j_2}(-u_2)iV_{k_2l_2}(-u_2)$$

$$\times\int_{u_2}^\infty du_1 iV_{k_1l_1}(-u_1)W^{ij}(-u_1)^*\Omega_{-}^{ij}\varepsilon\int_{u_1}^\infty dv \exp\left[-\varepsilon v+iG_{ij}(-v)\right]$$

$$-\int_0^\infty du_2 iV_{k_2l_2}(-u_2)W^{i_1j_1}(-u_2)^*$$

$$\times\int_{u_2}^\infty du_1 W^{i_1j_1}(-u_1)iV_{k_1l_1}(-u_1)W^{ij}(-u_1)^*$$

$$\times\Omega_{-}^{ij}\varepsilon\int_{u_1}^\infty dv \exp\left[-\varepsilon v+iG_{ij}(-v)\right]+\int_0^\infty du_2 iV_{k_2l_2}(-u_2)$$

$$\times\int_{u_2}^\infty du_1 iV_{k_1l_1}(-u_1)W^{ij}(-u_1)^*\Omega_{-}^{ij}\varepsilon\int_{u_1}^\infty dv \exp\left[-\varepsilon v+iG_{ij}(-v)\right] \quad (24)$$

We first consider (23). By repeated applications of (15) we obtain the following anomalous terms corresponding to (23)[5]:

$$H_1(\varepsilon)+i^2\int_0^\infty du_2[\xi_3(u_2)-\xi_2(u_2)]\Omega_{-}^{i_1j_1}$$

$$\times\int_{u_2}^\infty du_1 \exp[-\varepsilon u_1+iG_{i_1j_1}(-u_1)]V_{k_1l_1}^l(u_1)+i^2\int_0^\infty du_2[V_{k_2l_2}^s(u_2)$$

$$-\xi_1(u_2)]\int_{u_2}^\infty du_1 \exp(-\varepsilon u_1)V_{k_1l_1}^l(u_1) \quad (25)$$

[5]We have neglected all terms having a well-defined limit $\varepsilon\to 0$.

where

$$H_1(\varepsilon)=\Omega^{i_2 j_2}_{-}\int_0^{\infty} du_2 \exp\left[iG_{i_2 j_2}(-u_2)-iG_{i_1 j_1}(-u_2)\right]$$
$$\times iV^l_{k_2 l_2}(u_2)\int_{u_2}^{\infty} du_1 \exp\left(-\varepsilon u_1+iG_{i_1 j_1}(-u_1)\right)iV^l_{k_1 l_1}(u_1)$$
$$-\Omega^{i_2 j_2}_{-}\int_0^{\infty} du_2 \exp\left[iG_{i_2 j_2}(-u_2)\right]iV^l_{k_2 l_2}(u_2)$$
$$\times\int_{u_2}^{\infty} du_1 \exp(-\varepsilon u_1)iV^l_{k_1 l_1}(u_1)$$
$$-\int_0^{\infty} du_2\, iV^l_{k_2 l_2}(u_2)\exp\left[-iG_{i_1 j_1}(-u_2)\right]$$
$$\times\int_{u_2}^{\infty} du_1 \exp\left[-\varepsilon u_1+iG_{i_1 j_1}(-u_1)\right]$$
$$\times iV^l_{k_1 l_1}(-u_1)+\int_0^{\infty} du_2 iV^l_{k_2 l_2}(u_2)\int_{u_2}^{\infty} du_1 \exp(-\varepsilon u_1)iV^l_{k_1 l_1}(u_1) \quad (26)$$

Integrating by parts in (25) it is not hard to show formally that as $\varepsilon\to+0$ the anomalous terms behave as follows:

$$H_1(\varepsilon)+\int_0^{\infty} du_2 i[\xi_3(u_2)-\xi_2(u_2)]\Omega^{i_1 j_1}_{-}$$
$$\times\int_0^{\infty} du_1 \exp\left[-\varepsilon u_1+iG_{i_1 j_1}(-u_1)\right]iV^l_{k_1 l_1}(u_1)$$
$$+\int_0^{\infty} du_2\, i\left(V^s_{k_2 l_2}(u_2)-\xi_1(u_2)\right)\int_0^{\infty} du_1 \exp(-\varepsilon u_1)iV^l_{k_1 l_1}(u_1) \quad (27)$$

Note that the coefficients of the anomalous terms appearing in (27) have been calculated previously [see (18) and (20)]. Thus in principle the anomalous terms are known. Subtracting the function corresponding to (27) from $K^0(x,p)$ yields an expression which is free of anomalous terms in the energy-shell limit.

By an argument similar to that given above one can show that (24) has the following behavior as $\varepsilon\to+0$:

$$\int_0^{\infty} du\,\xi(u)\int_0^{\infty} dv \exp\left[-v+iG_{ij}(-v/\varepsilon)\right]+H_2(\varepsilon)+H_3(\varepsilon) \quad (28)$$

where

$$H_2(\varepsilon)=\Omega^{i_2j_2}_{-}\int_0^\infty du_2\exp\left[iG_{i_2j_2}(-u_2)-iG_{i_1j_1}(-u_2)\right]iV^l_{k_2l_2}(u_2)$$
$$\times\int_{u_2}^\infty du_1\exp\left[iG_{i_1j_1}(-u_1)-iG_{ij}(-u_1)\right]iV^l_{k_1l_1}(u_1)\varepsilon$$
$$\times\int_{u_1}^\infty dv\exp[-\varepsilon v+iG_{ij}(-v)]-\Omega^{i_2j_2}_{-}\int_0^\infty du_2\exp\left[iG_{i_2j_2}(-u_2)\right]$$
$$\times iV^l_{k_2l_2}(u_2)\int_{u_2}^\infty du_1 iV^l_{k_1l_1}(u_1)\times\exp[-iG_{ij}(-u_1)]\varepsilon$$
$$\times\int_{u_1}^\infty dv\exp[-\varepsilon v+iG_{ij}(-v)]-\int_0^\infty du_2 iV^l_{k_2l_2}(u_2)$$
$$\times\exp\left[-iG_{i_1j_1}(-u_2)\right]\int_{u_2}^\infty du_1\exp\left[iG_{i_1j_1}(-u_1)-iG_{ij}(-u_1)\right]$$
$$\times iV^l_{k_1l_1}(u_1)\varepsilon\int_{u_1}^\infty dv\exp[-\varepsilon v+iG_{ij}(-v)]+\int_0^\infty du_2 iV^l_{k_2l_2}(u_2)$$
$$\times\int_{u_2}^\infty du_1 iV^l_{k_1l_1}(u_1)\exp[-iG_{ij}(-u_1)]\varepsilon\int_{u_1}^\infty dv\exp[-\varepsilon v+iG_{ij}(-v)] \tag{29}$$

and

$$H_3(\varepsilon)=\int_0^\infty du_2 i[\xi_3(u_2)-\xi_2(u_2)]\Omega^{i_1j_1}_{-}\int_0^\infty du_1 iV^l_{k_1l_1}(u_1)$$
$$\times\exp\left[iG_{i_1j_1}(-u_1)-iG_{ij}(-u_1)\right]\varepsilon\int_{u_1}^\infty dv\exp[-\varepsilon v+iG_{ij}(-v)]$$
$$+\int_0^\infty du_2 i\left[V^s_{k_2l_2}(u_2)-\xi_1(u_2)\right]\int_0^\infty du_1 iV^l_{k_1l_1}(u_1)\exp[-iG_{ij}(-u_1)]$$
$$\times\varepsilon\int_{u_1}^\infty dv\exp[-\varepsilon v+iG_{ij}(-v)] \tag{30}$$

Note that the coefficients of the anomalous terms appearing in (30) are known from the calculation of $\lim_{\varepsilon\to+0}\tilde{K}^1_{+\varepsilon}(x,p)$. In order to obtain a contribution corresponding to $K^{ij}(x,p)$ which is free of anomalous terms we replace this expression by

$$(\Lambda^{ij}_{+\varepsilon})K^{ij}(x,p)-(\Lambda^{ij}_{+\varepsilon})[H_2(\varepsilon)+H_3(\varepsilon)]$$

where $H_2(\varepsilon)$ and $H_3(\varepsilon)$ are functions corresponding to the operators (29) and (30), respectively.

Thus we have shown that it is possible to replace $K^2_{+\varepsilon}(x,p)$ by an expression, denoted $\tilde{K}^2_{+\varepsilon}(x,p)$, which is free of anomalous terms and divergences as $\varepsilon\to+0$.

5.4 $K^n_{+\varepsilon}(x,p)$. It should be clear that the arguments used in the previous subsections to extract the anomalous terms for $n=0$, 1, and 2 can be applied to $K^n_{+\varepsilon}(x,p)$ for any positive integer n. Thus by an appropriate multiplication and subtraction of anomalous terms it is possible to associate with $K^n_{+\varepsilon}(x,p)$ an expression, denoted $\tilde{K}^n_{+\varepsilon}(x,p)$, which is formally free of anomalous terms and divergences as $\varepsilon\to+0$.

6. A RENORMALIZED MULTIPLE SCATTERING EXPANSION

A prescription was outlined in Section 5 which enables one to associate with $K^n_{+\varepsilon}(x,p)$ an expression $\tilde{K}^n_{+\varepsilon}(x,p)$ which is free of anomalous terms and divergences as $\varepsilon\to+0$. The resulting perturbation expansion

$$\sum_{n=0}^{\infty}\tilde{K}^n_{+\varepsilon}(x,p) \tag{31}$$

will be referred to as a "renormalized" multiple scattering expansion corresponding to (12).

Our justification of (31) is based on the conjecture that the anomalous expressions in each term of (12) either contribute to the anomalous factor which appears in $\phi_{+\varepsilon}(x,p)$ as $\varepsilon\to+0$ [see (11)] or do not contribute to the physical wave function. In Section 4 it was noted that this anomalous factor should be canceled before the $\varepsilon\to+0$ limit is taken. Since the anomalous expressions do not contribute to the physical wave function it is appropriate to cancel these expressions in each term of (12). Thus in the limit $\varepsilon\to+0$ the renormalized multiple scattering expansion yields the physical wave function apart from a momentum-dependent phase factor.

It should be possible to explicitly show how the various anomalous expressions in each term of (12) sum up to the factor $\Lambda_{+\varepsilon}$ appearing in $\phi_{+\varepsilon}(x,p)$ as $\varepsilon\to+0$. This was easy to do for the Born series; however, the multiple scattering expansion is considerably more involved.

It is straightforward to formulate a renormalized multiple scattering expansion for the infinite-mass case corresponding to the integral equation (A.6). Denote the multiple scattering expansion corresponding to (A.6) by

$$\phi_{+\varepsilon}(x, p) = \sum_{n=0}^{\infty} J^n_{+\varepsilon}(x, p) \tag{32}$$

Using the same type of arguments as given in Section 5 it is possible to associate with $J^n_{+\varepsilon}(x, p)$ an expression, denoted $\tilde{J}^n_{+\varepsilon}(x, p)$, which is free of anomalous terms and divergences as $\varepsilon \to +0$. Thus by the same reasoning used to justify (31) the expansion (32) should be replaced by the renormalized multiple scattering expansion

$$\sum_{n=0}^{\infty} \tilde{J}^n_{+\varepsilon}(x, p) \tag{33}$$

For example, the first term $\tilde{J}^0_{+\varepsilon}(x, p)$ is given by

$$\tilde{J}^0_{+\varepsilon}(x, p) = (\Lambda^1{}_{+\varepsilon})\phi^1{}_{+\varepsilon}(x, p) + \left[(\Lambda^{23}_{+\varepsilon})\phi^{23}_{+\varepsilon}(x, p) - \phi_0(x, p)\right]$$

where

$$(\Lambda^1{}_{+\varepsilon})^{-1} = \int_0^{\infty} du \exp\left[-u + iG_{12}(-u/\varepsilon) + iG_{13}(-u/\varepsilon)\right]$$

7. THE MULTIPLE SCATTERING EXPANSION FOR TWO FIXED CHARGED PARTICLES

In the previous sections we extracted the anomalous terms which occur in the Born series and multiple scattering expansion for the off-shell wave function corresponding to the free channel. It was argued that the source of these anomalous terms is the incorrect asymptotic condition used in the definition of the usual off-shell wave function. In this section we consider a simple scattering situation in which anomalous terms arise in the multiple scattering expansion despite the fact that the off-shell wave function is based on the correct asymptotic condition.

We consider the scattering of a charged particle by two fixed charged particles. The Hamiltonian is given by

$$H = -(2m)^{-1}\Delta + \frac{e^2}{|\mathbf{x}+\mathbf{R}|} - \frac{e^2}{|\mathbf{x}-\mathbf{R}|} = H_0 + V_{13} + V_{23}$$

where **R** is a fixed vector in R^3. This is a two-body problem which, in a sense, mimics the three-body problem of the scattering of a charged particle by a neutral fragment.

Since the two fixed particles have equal but opposite charge the third particle effectively interacts with the neutral "fragment" via a short-range potential. Thus the usual wave operators exist

$$W_{\pm} = s\text{-}\lim_{t\to\pm\infty} W(t)$$

$$W(t) = \exp(iHt)\exp(-iH_0 t)$$

A direct consequence of this result (Zorbas, 1977) is the convergence of the off-shell wave function $\phi_{+\varepsilon}(\mathbf{x},\mathbf{p})$ to the physical wave function $\phi_{+}(\mathbf{x},\mathbf{p})$ as $\varepsilon \to +0$.

In order to study the occurrence of anomalous terms in the Born series and multiple scattering expansion we decompose $V(\mathbf{x})$ as follows:

$$V(\mathbf{x}) = V^l(\mathbf{x}) + V^s(\mathbf{x})$$

where

$$V^l(\mathbf{x}) = [V_{13}(\mathbf{x}) + V_{23}(\mathbf{x})]\chi(\mathbf{x}) = V_{13}^l(\mathbf{x}) + V_{23}^l(\mathbf{x})$$

with

$$\chi(\mathbf{x}) = \begin{cases} 1 & \text{if } |\mathbf{x}| \geqslant 2|\mathbf{R}| \\ 0 & \text{if } |\mathbf{x}| < 2|\mathbf{R}| \end{cases}$$

By an argument similar to that used to justify (7) we can write $V(t) = \exp(iH_0 t)V\exp(-iH_0 t)$ as follows:

$$V(t) = V^l(t) + V^s(t) \tag{34}$$

where

$$V^l(t) = V_{13}^l\left(\frac{\mathbf{p}t}{m}\right) + V_{23}^l\left(\frac{\mathbf{p}t}{m}\right)$$

and formally

$$\int_{-\infty}^{+\infty} dt V^s(t) < \infty$$

In order to examine the Born series for anomalous terms and divergences in the energy-shell limit we study the $t \to -\infty$ behavior of (4) with H and H_0 defined in this section. Using (34) and an argument similar to the one used in Section 3 one can show

$$W_n(t) = \sum_{k=0}^{n} \eta_k(t) \Lambda_{n-k}(t)$$

where the $\eta_k(t)$ formally converge as $t \to -\infty$, $\Lambda_0(t) = \mathbb{1}$, and

$$\Lambda_k(t) = \left[i \int_0^t du V^l(u) \right]^k \Big/ k!$$

Owing to the short-range nature of the potential $V^l(x)$ the expressions $\Lambda_k(t)$, $k = 1, 2, \ldots$, converge as $t \to -\infty$ and thus the nth term of the Born series has a well-defined energy-shell limit, i.e., the Born series does not develop anomalous terms and divergences as $\varepsilon \to +0$.

If we sum $W_n(t)$ over n we obtain

$$W(t) = \left[\sum_{n=0}^{\infty} \eta_n(t) \right] \exp\left[i \int_0^t du V^l(u) \right]$$

The off-shell wave function corresponds to the operator $W_{+\varepsilon}$ which in the limit $\varepsilon \to +0$ behaves as follows:

$$\begin{aligned} W_{+\varepsilon} &= \int_0^{\infty} du \exp(-u) W(-u/\varepsilon) \\ &\underset{\varepsilon \to +0}{\to} \left[\sum_{n=0}^{\infty} \eta_n(-\infty) \right] \int_0^{\infty} du \exp\left[-u + i \int_0^{-u/\varepsilon} dv V^l(v) \right] \\ &\underset{\varepsilon \to +0}{\to} \left[\sum_{n=0}^{\infty} \eta_n(-\infty) \right] \Lambda \end{aligned} \tag{35}$$

where Λ is a momentum-dependent phase factor.

We now consider the Weinberg–Van Winter equations for the off-shell wave function

$$\begin{aligned} \phi_{+\varepsilon}(\mathbf{x},\mathbf{p}) &= \phi_0(\mathbf{x},\mathbf{p}) + \left[\phi^{13}_{+\varepsilon}(\mathbf{x},\mathbf{p}) - \phi_0(\mathbf{x},\mathbf{p}) \right] + \left[\phi^{23}_{+\varepsilon}(\mathbf{x},\mathbf{p}) - \phi_0(\mathbf{x},\mathbf{p}) \right] \\ &\quad - \int d\mathbf{y} \left[G_{13}(\mathbf{x},\mathbf{y};\, E+i\varepsilon) - G_0(\mathbf{x},\mathbf{y};\, E+i\varepsilon) \right] V_{23}(\mathbf{y}) \phi_{+\varepsilon}(\mathbf{y},\mathbf{p}) \\ &\quad - \int d\mathbf{y} \left[G_{23}(\mathbf{x},\mathbf{y};\, E+i\varepsilon) - G_0(\mathbf{x},\mathbf{y};\, E+i\varepsilon) \right] V_{13}(\mathbf{y}) \phi_{+\varepsilon}(\mathbf{y},\mathbf{p}) \end{aligned} \tag{36}$$

Clearly there are anomalous terms and divergences as $\varepsilon \to +0$ in the multiple scattering expansion corresponding to (36). For example, the nonhomogeneous term does not converge as $\varepsilon \to +0$ since $\phi^{ij}_{+\varepsilon}(x, p)$ corresponds to a potential with an $|\mathbf{x}|^{-1}$ behavior as $|\mathbf{x}| \to \infty$.

The multiple scattering expansion is given by

$$\phi_{+\varepsilon}(\mathbf{x},\mathbf{p}) = \sum_{n=0}^{\infty} K^{n}_{+\varepsilon}(\mathbf{x},\mathbf{p}) \tag{37}$$

where $K^{0}_{+\varepsilon}(\mathbf{x},\mathbf{p})$ denotes the nonhomogeneous terms of (36) and for $n \geqslant 1$

$$K^{n}_{+\varepsilon}(\mathbf{x},\mathbf{p}) = -\int d\mathbf{y}\{[G_{13}(\mathbf{x},\mathbf{y};E+i\varepsilon) - G_0(\mathbf{x},\mathbf{y};E+i\varepsilon)]V_{23}(\mathbf{y})$$
$$+[G_{23}(\mathbf{x},\mathbf{y};E+i\varepsilon) - G_0(\mathbf{x},\mathbf{y};E+i\varepsilon)]V_{13}(\mathbf{y})\}K^{n-1}_{+\varepsilon}(\mathbf{y},\mathbf{p})$$

It should be clear from the similarity of the multiple scattering expansions (37) and (12) that the same argument as used in Section 5 to extract the anomalous terms in each term of (12) can be applied to (37). Using the same renormalization prescription as given in Section 5 we can associate with $K^{n}_{+\varepsilon}(x, p)$ an expression, denoted $\tilde{K}^{n}_{+\varepsilon}(x, p)$, which is free of anomalous terms. Thus it is possible to replace the multiple scattering expansion (37) by a renormalized multiple scattering expansion

$$\sum_{n=0}^{\infty} \tilde{K}^{n}_{+\varepsilon}(\mathbf{x},\mathbf{p}) \tag{38}$$

which is formally free of anomalous terms and divergences in the energy-shell limit. The argument is the same as given in Section 5 and we will not give details.

Our justification of the above renormalization prescription is based on the assumption that the various anomalous expressions appearing in the terms of (37) contribute to the factor

$$\int_0^{\infty} du \exp\left[-u + i\int_0^{-u/\varepsilon} dv\, V^{l}(v)\right]$$

which appears in (35). In the limit $\varepsilon \to +0$ the cancellation of the anomalous terms in the multiple scattering expansion is thus the same as neglecting the momentum-dependent factor Λ in the physical wave function. Thus the renormalized multiple scattering expansion (38) allows one to calculate $\Lambda^{-1}\phi_{+}(\mathbf{x},\mathbf{p})$.

The occurrence of anomalous terms and divergences in the multiple scattering expansion is a consequence of an inadequate choice of unperturbed term in (36). One should consider the wave function corresponding to H as a perturbation of the physical wave functions corresponding to H_0, H_0+V_{13}, and H_0+V_{23}. This is not the case for the integral equation (36) in the energy-shell limit.

8. A MODIFIED PERTURBATION EXPANSION FOR A NEUTRAL FRAGMENT

In this section we consider the perturbation expansion, obtained by iterating (3), for the off-shell wave function $\phi^{\alpha}_{+\varepsilon}(x,p)$ corresponding to the channel α consisting of a charged particle and a neutral fragment. The neutral fragment is assumed to consist of charged particles 1 and 2 with particle 1 having an infinite mass (see Appendix A for notation). This problem is similar to the two-center problem considered in the previous section. We will show the systematic occurrence of anomalous terms in the perturbation expansion corresponding to (3). These anomalous terms cannot contribute to the off-shell wave function, since $\phi^{\alpha}_{+\varepsilon}(x,p)$ has a well-defined limit $\varepsilon\to+0$. The explicit cancellation of anomalous terms is shown.

We first rewrite (3) as follows:

$$\phi^{\alpha}_{+\varepsilon}(x,p)=\phi^{1;\alpha}_{+\varepsilon}(x,p)-\int dy\,G_1(x,y;E^{\alpha}+i\varepsilon)\left[V^s(y)-V^l_{13}(y)\right]\phi^{\alpha}_{+\varepsilon}(y,p) \tag{39}$$

where $V^s(y)=V_{23}(y)+V^l_{13}(y)$ is a short-range potential. The perturbation expansion associated with (39) is denoted by

$$\phi^{\alpha}_{+\varepsilon}(x,p)=\sum_{n=0}^{\infty}H^{\alpha,n}_{+\varepsilon}(x,p) \tag{40}$$

where

$$H^{\alpha,0}_{+\varepsilon}(x,p)=\phi^{1;\alpha}_{+\varepsilon}(x,p)$$

and for $n\geqslant 1$

$$H^{\alpha,n}_{+\varepsilon}(x,p)=-\int dy\,G_1(x,y;E^{\alpha}+i\varepsilon)\left[V^s(y)-V^l_{13}(y)\right]H^{\alpha,n-1}_{+\varepsilon}(y,p)$$

We now use the time-dependent formalism to examine the terms of (40).

The term $H^{\alpha,0}_{+\varepsilon}(x,p)$ corresponds to the expression

$$\int_0^\infty du \exp(-u-iH_1u/\varepsilon)\exp(iH_{12}u/\varepsilon)P^\alpha$$

$$=\int_0^\infty du \exp(-u-iK_{13}u/\varepsilon)\times\exp\left[-i(2m_3)^{-1}\Delta_3 u/\varepsilon-iG_{13}(-u/\varepsilon)\right]$$

$$\times\exp\left[iG_{13}(-u/\varepsilon)\right]P^\alpha \tag{41}$$

where P^α is the projection onto the α-channel subspace, $K_{13}=-(2m_3)^{-1}\Delta_3 + V_{13}$ and $G_{13}(t)=\int_0^t du\, V^l_{13}(u)$. As $\varepsilon\to+0$, (41) behaves as follows:

$$\Omega^{13}_{-}P^\alpha\int_0^\infty du \exp\left[-u+iG_{13}(-u/\varepsilon)\right]=\Omega^{13}_{-}P^\alpha\left(\Lambda^{13}_{+\varepsilon}\right)^{-1}$$

where Ω^{13}_{-} denotes the modified wave operator corresponding to K_{13}. Thus the expression $\tilde{H}^{\alpha,0}_{+\varepsilon}(x,p)$ defined as follows:

$$\tilde{H}^{\alpha,0}_{+\varepsilon}(x,p)=\left(\Lambda^{13}_{+\varepsilon}\right)\phi^{1,\alpha}_{+\varepsilon}(x,p)$$

is free of anomalous terms and divergences in the energy-shell limit.

We now consider $H^{\alpha,1}_{+\varepsilon}(x,p)$ which corresponds to the following expression:

$$-i\int_0^\infty du \exp(-iH_1u)\left(V^s-V^l_{13}\right)\exp(iH_1u)\varepsilon$$

$$\times\int_u^\infty dv \exp(-\varepsilon v-iH_1v)\exp(iH_{12}v)P^\alpha \underset{\varepsilon\to+0}{\to} -i\int_0^\infty du \exp(-iH_1u)\left(V^s-V^l_{13}\right)$$

$$\times\exp(iH_1u)\Omega^{13}_{-}P^\alpha\varepsilon\int_u^\infty dv \exp\left[-\varepsilon v+iG_{13}(-v)\right]$$

$$\tag{42}$$

By a similar argument as used to verify (15) we have

$$\exp(-iH_1u)\left(V^s-V^l_{13}\right)\exp(iH_1u)\Omega^{13}_{-}P^\alpha=-\Omega^{13}_{-}P^\alpha V^l_{13}(u)+\eta(u) \tag{43}$$

where formally $\int_0^\infty du\,\eta(u)<\infty$.

Using (43) we can rewrite (42) in the limit $\varepsilon \to +0$ as follows:

$$-i\int_0^\infty du\,\eta(u)\int_0^\infty dv\exp[-v+iG_{13}(-v/\varepsilon)]$$
$$+\Omega_-^{13}P^\alpha\int_0^\infty du\exp[-u+iG_{13}(-u/\varepsilon)]\int_0^{u/\varepsilon}dv\,iV_{13}^l(v)$$

Thus, in order to avoid divergences and anomalous terms, $H_{+\varepsilon}^{\alpha,1}(x, p)$ should be replaced by $\tilde{H}_{+\varepsilon}^{\alpha,1}(x, p)$, which is defined by

$$\tilde{H}_{+\varepsilon}^{\alpha,1}(x,p)=(\Lambda_{+\varepsilon}^{13})H_{+\varepsilon}^{\alpha,1}(x,p)-\phi_+^{13}(x,p)(\Lambda_{+\varepsilon}^{13})$$
$$\times\int_0^\infty du\exp[-u+iG_{13}(-u/\varepsilon)]\int_0^{u/\varepsilon}dv\,iV_{13}^l(v)$$

where $\phi_+^{13}(x, p)$ is the product of the bound state wave function and the wave function corresponding to Ω_-^{13}.

The similarity of equations (1) and (3) suggests that there is a simple pattern to the development of anomalous terms in (40). It is not difficult to convince oneself, using the same type of argument as given above for $n=0$ and 1, that as $\varepsilon \to +0$ the nth term $H_{+\varepsilon}^{\alpha,n}(x, p)$ corresponds to the following expression:

$$\sum_{k=0}^{n}\eta_k\int_0^\infty dv\exp[-v+iG_{13}(-v/\varepsilon)]\frac{1}{(n-k)!}\left[i\int_0^{v/\varepsilon}du\,V_{13}^l(u)\right]^{n-k} \tag{44}$$

where η_k are appropriate functions of x and p. If we sum over n we obtain (for $|k_{13}|<1$)

$$\sum_{n=0}^{\infty}H_{+\varepsilon}^{\alpha,n}(x,p)\underset{\varepsilon\to+0}{\to}\sum_{n=0}^{\infty}\sum_{k=0}^{n}\eta_k\int_0^\infty dv\exp[-v+iG_{13}(-v/\varepsilon)]$$
$$\times\frac{1}{(n-k)!}\left[i\int_0^{v/\varepsilon}du\,V_{13}^l(u)\right]^{n-k}$$
$$=\left(\sum_{n=0}^{\infty}\eta_n\right)\sum_{n=0}^{\infty}\int_0^\infty dv\exp[-v+iG_{13}(-v/\varepsilon)]$$
$$\times\frac{1}{n!}\left[i\int_0^{v/\varepsilon}du\,V_{13}^l(u)\right]^n=\sum_{n=0}^{\infty}\eta_n$$

This result shows that the anomalous terms appearing in (44) do not contribute to the physical wave function, which justifies our renormalization prescription for canceling the anomalous expressions appearing in each term of (40).

It is straightforward to associate with $H^{\alpha;n}_{+\varepsilon}(x, p)$ an expression, denoted $\tilde{H}^{\alpha;n}_{+\varepsilon}(x, p)$, which is free of anomalous terms in the energy-shell limit. The resulting renormalized perturbation expansion

$$\sum_{n=0}^{\infty} \tilde{H}^{\alpha;n}_{+\varepsilon}(x, p) \tag{45}$$

formally converges as $\varepsilon \to +0$ to $\phi^{\alpha}_{+}(x, p)$.

9. APPLICATIONS

In this section we use the renormalized perturbation expansions developed in this paper to generate various approximate expressions for the T matrices corresponding to the excitation and ionization of a neutral fragment by a charged particle.

The prior version of the on-shell T matrix for excitation is given by[6]

$$(-\pi)^{-1} \int dx\, \overline{\phi^{\beta}_{-}(x, p)}\, V_{23}(x) \phi_{\alpha}(x, k) \tag{46}$$

where $\phi_{\alpha}(x, k)$ denotes the wave function for the incoming α-channel Hamiltonian and $\phi^{\beta}_{-}(x, p)$ is the wave function corresponding to W^{β}_{+}. In the case of ionization the prior version of the on-shell T matrix has the form (Zorbas, 1979)

$$(-\pi)^{-1} \int dx\, \overline{\phi_{-}(x, p)}\, [V_{13}(x) + V_{23}(x)] \phi_{\alpha}(x, k) \tag{47}$$

where $\phi_{-}(x, p)$ corresponds to Ω_{+}. Replacing the wave functions appearing in (46) and (47) by the renormalized perturbation expansions derived in this paper yields perturbation expansions for the excitation and ionization T matrices.

We first consider the excitation T matrix. By a similar argument as given in Section 8 the wave function $\phi^{\beta}_{-}(x, p)$ can be calculated via a

[6]This expression is derived from the S operator $(2\pi i)^{-1}(W^{\beta}_{+})^{*} W^{\alpha}_{-}$ by a standard argument. It is assumed that particle 1 has an infinite mass and $P^{\alpha} P^{\beta} = 0$.

renormalized perturbation expansion

$$\phi_-^{\beta}(x,p)=\lim_{\varepsilon\to+0}\sum_{n=0}^{\infty}\tilde{H}_{-\varepsilon}^{\beta,n}(x,p)$$

If we approximate $\phi_-^{\beta}(x,p)$ by the $n=0$ term of this expansion we obtain the following approximate expression for the excitation T matrix:

$$(-\pi)^{-1}\int dx\,\overline{\phi_-(\mathbf{x}_3,\mathbf{p}_3)\psi(\mathbf{x}_2)}\,V_{23}(x)\phi_\alpha(x,k)$$

where $\psi(\mathbf{x}_2)$ is the β-channel bound state wave function and $\phi_-(\mathbf{x}_3,\mathbf{p}_3)$ is the wave function corresponding to Ω_+^{13}. This approximate expression corresponds, apart from a phase factor, to the well-known Coulomb-projected Born approximation for excitation (Geltman, 1969; Geltman and Hidalgo, 1974).

We now consider the problem of ionization with all three particles having a finite mass. A renormalized scattering expansion for $\phi_-(x,p)$ can be derived in analogy with (31). If we approximate $\phi_-(x,p)$ by the first term of this expansion and substitute this approximate wave function in (47) we obtain, apart from momentum-dependent phase factors, the approximation recently proposed by Zorbas (1979).

In the case of ionization with one particle having an infinite mass it is natural to use the renormalized multiple scattering expansion for $\phi_-(x,p)$ corresponding to (33). If we approximate $\phi_-(x,p)$ by the first term of this expansion we obtain the Coulomb-projected Born approximation for ionization (Geltman and Hidalgo, 1974) (except for a phase factor) together with an additional term corresponding to the interaction of the two finite-mass particles.

The renormalized perturbation expansions proposed in this paper provide a theoretical framework for understanding the known approximations for excitation and ionization. Furthermore, these perturbation expansions yield new approximations for the ionization T matrix and allow one, at least in principle, to calculate higher-order corrections to the T matrices for excitation and ionization of an uncharged fragment by a charged particle.

The use of the prior version of the T matrix enabled us to circumvent the well-known difficulties associated with the post version of the ionization T matrix (Prugovečki and Zorbas, 1978). It has been shown, however, that it is possible to calculate the ionization T matrix via the post version if one performs a "renormalization" before going to physical energies (McCartor and Nuttall, 1971; Prugovečki and Zorbas, 1978). If one considers the ionization of a charged fragment by a charged particle, neither the post or prior versions of the T matrix are well defined. In this case one must consider the renormalized expressions for the T matrix.

10. CONCLUDING REMARKS

In recent years there has been considerable progress in understanding the difficulties associated with multiparticle scattering when Coulomb forces are present. Various stationary formalisms have been proposed for circumventing these problems (Veselova, 1970, 1972; McCartor and Nuttall, 1971; Rosenberg, 1973; Prugovečki and Zorbas, 1973; Gibson and Chandler, 1974; Zorbas, 1974, 1977; Alt et al., 1978; Mekur'ev, 1979). Many of these formalisms are of a theoretical nature and have not yet led to practical computational results. The most promising results have been based on the "renormalization" of screened scattering amplitudes (Alt et al., 1978) and have so far been restricted to multiparticle scattering involving at most two charged particles.

In the present paper we have shown that the "off-shell renormalization" prescription, proposed by Zorbas (1977), can be carried out on the level of perturbation theory. We have restricted our attention to scattering involving three charged particles. It should be possible, however, to use the techniques of this paper to obtain at least a formal understanding of perturbation theory for general scattering systems involving long-range forces. For example, the problem of anomalous terms in perturbation theory for screened Coulomb potentials, general long-range potentials, general N-particle systems, and the problem of infrared divergences in quantum electrodynamics are natural candidates for study via the techniques of this paper.

APPENDIX A: THREE-BODY OFF-SHELL INTEGRAL EQUATIONS

A derivation of various off-shell integral equations is given in this appendix together with a brief discussion of the notation used in this paper.

We first consider three particles labeled 1, 2, and 3 with particle i having mass μ_i and position coordinate $\mathbf{r}_i$. After eliminating the center-of-mass motion the internal full Hamiltonian is given by

$$H = H_0 + V, \qquad V = \sum_{i<j} V_{ij}, \qquad V_{ij}(\mathbf{x}) = \frac{\lambda_{ij}}{|\mathbf{x}|}$$

For example, choosing $\mathbf{x}_1=\mathbf{r}_2-\mathbf{r}_1$ and $\mathbf{x}_2=\mathbf{r}_3-(\mu_1\mathbf{r}_1+\mu_2\mathbf{r}_2)/(\mu_1+\mu_2)$ then

$$H_0=-\sum_{i=1}^{2}(2m_i)^{-1}\Delta_i$$

with $m_i^{-1}=\mu_{i+1}^{-1}+(\Sigma_{j\leqslant i}\mu_j)^{-1}$ and

$$V(x)=V_{12}(\mathbf{x}_1)+V_{13}\left(\mathbf{x}_2+\frac{\mu_2}{\mu_1+\mu_2}\mathbf{x}_1\right)+V_{23}\left(\mathbf{x}_2-\frac{\mu_1}{\mu_1+\mu_2}\mathbf{x}_1\right)$$

where x denotes collectively $(\mathbf{x}_1,\mathbf{x}_2)$ and p will denote collectively $(\mathbf{p}_1,\mathbf{p}_2)$, where $\mathbf{p}_i$ is the momentum conjugate to $\mathbf{x}_i$.

The Green's functions corresponding to the resolvents $(H-z)^{-1}$, $(H_0-z)^{-1}$, and $(H_{ij}-z)^{-1}$, $H_{ij}=H_0+V_{ij}$, are denoted, respectively, by $G(x,y;z)$, $G_0(x,y;z)$, and $G_{ij}(x,y;z)$. The various off-shell wave functions corresponding to the free channel are defined by the following integrals:

$$\phi_{+\varepsilon}(x,p)=(-i\varepsilon)\int dy\,\phi_0(y,p)G(x,y;E+i\varepsilon)$$

$$\phi_{+\varepsilon}^{ij}(x,p)=(-i\varepsilon)\int dy\,\phi_0(y,p)G_{ij}(x,y;E+\varepsilon)$$

$$\phi_0(x,p)=(2\pi)^{-3}\exp(ip\cdot x)$$

where $E=p_1^2/2m_1+p_2^2/2m_2$.

The following identities are satisfied by the various resolvents

$$(H-z)^{-1}=(H_0-z)^{-1}-(H_0-z)^{-1}V(H-z)^{-1} \tag{A.1}$$

$$(H-z)^{-1}=(H_{ij}-z)^{-1}-(H_{ij}-z)^{-1}\sum_{\substack{k<l\\(k,l)\neq(i,j)}}V_{kl}(H-z)^{-1} \tag{A.2}$$

Adding (A.2) with $(i,j)=(1,2)$, $(1,3)$, and $(2,3)$ and subtracting two times (A.1) yields the Weinberg–Van Winter equations for the resolvent

$$\begin{aligned}(H-z)^{-1}=&(H_0-z)^{-1}+\sum_{i<j}\left[(H_{ij}-z)^{-1}-(H_0-z)^{-1}\right]\\&-\sum_{i<j}\left[(H_{ij}-z)^{-1}-(H_0-z)^{-1}\right]\sum_{\substack{k<j\\(k,l)\neq(i,j)}}V_{kl}(H-z)^{-1}\end{aligned} \tag{A.3}$$

Expressing (A.1) and (A.3) in terms of Green's functions and using the various definitions of the off-shell wave functions yields (1) and (2), respectively.

A considerable simplification occurs if we assume one of the particles, say particle 1, has an infinite mass. In this case the Hamiltonian is given by

$$H = H_0 + V$$

$$H_0 = -(2m_2)^{-1}\Delta_2 - (2m_3)^{-1}\Delta_3,$$

$$V(x) = V_{12}(\mathbf{x}_2) + V_{13}(\mathbf{x}_3) + V_{23}(\mathbf{x}_3 - \mathbf{x}_2)$$

where $\mathbf{x}_i$ represents the position coordinate of particle i with respect to particle 1 which is located at the origin. We will use the same notation for H_{ij}, the Green's functions, and the wave functions as in the finite-mass case.

It is convenient to consider the operator $H_1 = H_0 + V_{12} + V_{13}$. The resolvent $(H_1 - z)^{-1}$ satisfies

$$(H-z)^{-1} = (H_1 - z)^{-1} - (H_1 - z)^{-1} V_{23} (H-z)^{-1} \tag{A.4}$$

Since H_1 can be written as a sum of two operators which commute it is possible to obtain (Geltman, 1969) an explicit integral representation for the Green's function $G_1(x, y; z)$ corresponding to $(H_1 - z)^{-1}$. We require the following off-shell wave functions corresponding to the free channel and to the channel α with particles 1 and 2 bound:

$$\phi^1_{+\varepsilon}(x, p) = (-i\varepsilon)\int dy\, \phi_0(y, p) G_1(x, y; E + i\varepsilon)$$

$$\phi^\alpha_{+\varepsilon}(x, p) = (-i\varepsilon)\int dy\, \phi_\alpha(y, p) G(x, y; E^\alpha + i\varepsilon)$$

$$\phi^{1,\alpha}_{+\varepsilon}(x, p) = (-i\varepsilon)\int dy\, \phi_\alpha(y, p) G_1(x, y; E^\alpha + i\varepsilon)$$

$$\phi_\alpha(x, p) = (2\pi)^{-3/2}\phi(\mathbf{x}_2)\exp(i\mathbf{p}_3\cdot\mathbf{x}_3)$$

where $\phi(\mathbf{x}_2)$ denotes the bound-state wave function corresponding to the energy E_b and $E^\alpha = E_b + p_3^2/2m_3$. Lippmann–Schwinger-type integral equations for $\phi_{+\varepsilon}(x, p)$ and $\phi^\alpha_{+\varepsilon}(x, p)$ follow immediately from (A.4).

A set of Weinberg–Van Winter-type integral equations involving the Green's function and wave function corresponding to H_1 can also be derived. Adding (A.2) with $(i, j) = (2,3)$ to (A.4) and subtracting (A.1) yields

$$(H-z)^{-1}=(H_1-z)^{-1}+(H_{23}-z)^{-1}-(H_0-z)^{-1}$$
$$-\left[(H_1-z)^{-1}-(H_0-z)^{-1}\right]V_{23}(H-z)^{-1}$$
$$-\left[(H_{23}-z)^{-1}-(H_0-z)^{-1}\right](V_{12}+V_{13})(H-z)^{-1} \tag{A.5}$$

Thus in the infinite mass case $\phi_{+\varepsilon}(x, p)$ satisfies the integral equation

$$\phi_{+\varepsilon}(x, p)=\phi^1_{+\varepsilon}(x, p)+\left[\phi^{23}_{+\varepsilon}(x, p)-\phi_0(x, p)\right]$$
$$-\int dy\left[G_1(x, y; E+i\varepsilon)-G_0(x, y; E+i\varepsilon)\right]V_{23}(y)\phi_{+\varepsilon}(y, p)$$
$$-\int dy\left[G_{23}(x, y; E+i\varepsilon)-G_0(x, y; E+i\varepsilon)\right]$$
$$\times\left[V_{12}(y)+V_{13}(y)\right]\phi_{+\varepsilon}(y, p) \tag{A.6}$$

APPENDIX B: TIME-DEPENDENT THEORY AND THE MULTIPLE SCATTERING EXPANSION

In this appendix we give a formal argument to relate the terms appearing in the multiple scattering expansion (12) to the time-dependent formalism.

We first consider the expression $\phi^{ij}_{+\varepsilon}(x, p)$ appearing in $K^0_{+\varepsilon}(x, p)$. It is not difficult to verify the following equality for appropriate ψ (see Section 4 of Zorbas, 1977):

$$\left(\int_{-\infty}^{+\infty}\frac{-i\varepsilon}{H_{ij}-\lambda-i\varepsilon}d_\lambda E^{H_0}_\lambda\psi\right)(x)=\int dp\,\phi^{ij}_{+\varepsilon}(x, p)\hat{\psi}(p) \tag{B.1}$$

Furthermore the identity

$$\frac{-i\varepsilon}{H_{ij}-\lambda-i\varepsilon}=\int_0^\infty du\exp\left(-u-iH_{ij}\frac{u}{\varepsilon}+i\lambda\frac{u}{\varepsilon}\right) \tag{B.2}$$

together with an interchange of integrals yields

$$\left(\int_0^{\infty} du \exp\left(-u-iH_{ij}\frac{u}{\varepsilon}\right)\exp\left(iH_0\frac{u}{\varepsilon}\right)\psi\right)(x)=\int dp\, \phi^{ij}_{+\varepsilon}(x,p)\hat{\psi}(p) \tag{B.3}$$

Clearly the $t\to-\infty$ behavior of $W^{ij}(t)=\exp(iH_{ij}t)\exp(-iH_0 t)$ is directly related to the $\varepsilon\to+0$ behavior of $\phi^{ij}_{+\varepsilon}(x,p)$.

We now consider $K^n_{+\varepsilon}(x,p)$ for $n\geqslant 1$. The two types of terms, denoted by $K^0(x,p)$ and $K^{ij}(x,p)$, which contribute to $K^n_{+\varepsilon}(x,p)$ have the following general form:

$$\begin{aligned}K^0(x,p)=(-1)^n\int dy_n\Big[G_{i_nj_n}(x,y_n;E+i\varepsilon)-G_0(x,y_n;E+i\varepsilon)\Big]V_{k_nl_n}(y_n)\\ \times\int dy_{n-1}\Big[G_{i_{n-1}j_{n-1}}(y_n,y_{n-1};E+i\varepsilon)-G_0(y_n,y_{n-1};E+i\varepsilon)\Big]\\ \times\cdots\times\int dy_1\Big[G_{i_1j_1}(y_2,y_1;E+i\varepsilon)-G_0(y_2,y_1;E+i\varepsilon)\Big]\\ \times V_{k_1l_1}(y_1)\phi_0(y_1,p)\end{aligned} \tag{B.4}$$

and

$$\begin{aligned}K^{ij}(x,p)=(-1)^n\int dy_n\Big[G_{i_nj_n}(x,y_n;E+i\varepsilon)-G_0(x,y_n;E+i\varepsilon)\Big]V_{k_nl_n}(y_n)\\ \times\int dy_{n-1}\Big[G_{i_{n-1}j_{n-1}}(y_n,y_{n-1};E+i\varepsilon)-G_0(y_n,y_{n-1};E+i\varepsilon)\Big]\\ \times\cdots\times\int dy_1\Big[G_{i_1j_1}(y_2,y_1;E+i\varepsilon)-G_0(y_2,y_1;E+i\varepsilon)\Big]\\ \times V_{k_1l_1}(y_1)\phi^{ij}_{+\varepsilon}(y_1,p)\end{aligned} \tag{B.5}$$

where $(k_s,l_s)\neq(i_s,j_s)$ for $s=1,2,\ldots,n$.

By an argument similar to the one used to verify (B.1) we have for each $\varepsilon>0$ and for appropriate ψ the following equalities:

$$(K^0\psi)(x)=\int dp\, K^0(x,p)\hat{\psi}(p) \tag{B.6}$$

and

$$(K^{ij}\psi)(x)=\int dp\, K^{ij}(x,p)\hat{\psi}(p) \tag{B.7}$$

where the operators K^0 and K^{ij} are defined by the following spectral integrals (Amrein et al., 1977; Prugovečki, 1971):

$$K^0=(-1)^n\int_{-\infty}^{+\infty}\left(\frac{1}{H_{i_nj_n}-\lambda-i\varepsilon}-\frac{1}{H_0-\lambda-i\varepsilon}\right)$$

$$\times V_{k_nl_n}\left(\frac{1}{H_{i_{n-1}j_{n-1}}-\lambda-i\varepsilon}-\frac{1}{H_0-\lambda-i\varepsilon}\right)$$

$$\times\cdots\times\left(\frac{1}{H_{i_1j_1}-\lambda-i\varepsilon}-\frac{1}{H_0-\lambda-i\varepsilon}\right)V_{k_1l_1}d_\lambda E_\lambda^{H_0} \tag{B.8}$$

and

$$K^{ij}=(-1)^n\int_{-\infty}^{+\infty}\left(\frac{1}{H_{i_nj_n}-\lambda-i\varepsilon}-\frac{1}{H_0-\lambda-i\varepsilon}\right)V_{k_nl_n}\times\cdots$$

$$\times\left(\frac{1}{H_{i_1j_1}-\lambda-i\varepsilon}-\frac{1}{H_0-\lambda-i\varepsilon}\right)V_{k_1l_1}\frac{-i\varepsilon}{H_{ij}-\lambda-i\varepsilon}d_\lambda E_\lambda^{H_0} \tag{B.9}$$

Using (B.2) and interchanging integrals we can rewrite K^0 and K^{ij} as follows:

$$K^0=(-i)^n\int_0^\infty du_n\exp(-\varepsilon u_n)\left[\exp\left(-iH_{i_nj_n}u_n\right)-\exp(-iH_0u_n)\right]V_{k_nl_n}$$

$$\times\cdots\times\int_0^\infty du_1\exp(-\varepsilon u_1)\left[\exp\left(-iH_{i_1j_1}u_1\right)-\exp(-iH_0u_1)\right]$$

$$\times V_{k_1l_1}\exp[+iH_0(u_1+\cdots+u_n)] \tag{B.10}$$

and

$$K^{ij}=(-i)^n\int_0^{\infty}du_n\exp(-\varepsilon u_n)\Big[\exp\big(-iH_{i_nj_n}u_n\big)-\exp(-iH_0u_n)\Big]V_{k_nl_n}$$
$$\times\cdots\times\int_0^{\infty}du_1\exp(-\varepsilon u_1)\Big[\exp\big(-iH_{i_1j_1}u_1\big)-\exp(-iH_0u_1)\Big]$$
$$\times V_{k_1l_1}(\varepsilon)\int_0^{\infty}dv\exp(-\varepsilon v-iH_{ij}v)\exp\big[iH_0(v+u_1+\cdots+u_n)\big] \tag{B.11}$$

Multiplying the various terms making up (B.10) and (B.11) and then performing the substitutions $u_1'=u_n+\cdots+u_1$ in the u_1 integral, $u_2'=u_n+\cdots+u_2$ in the u_2 integral,..., and finally $u_n'=u_n$ in the u_n integral, we obtain

$$K^0=(-i)^n\int_0^{\infty}du_n\exp\big(-iH_{i_nj_n}u_n\big)\exp(iH_0u_n)V_{k_nl_n}(-u_n)$$
$$\times\exp(-iH_0u_n)\exp\big(+iH_{i_{n-1}j_{n-1}}u_n\big)\int_{u_n}^{\infty}du_{n-1}\exp\big(iH_{i_{n-1}j_{n-1}}u_{n-1}\big)$$
$$\times\exp(iH_0u_{n-1})V_{k_{n-1}l_{n-1}}(-u_{n-1})\times\cdots\times V_{k_2l_2}(-u_2)\exp(-iH_0u_2)$$
$$\times\exp\big(iH_{i_1j_1}u_2\big)\int_{u_2}^{\infty}du_1\exp\big(-\varepsilon u_1-iH_{i_1j_1}u_1\big)\exp(iH_0u_1)$$
$$\times V_{k_1l_1}(-u_1)+\cdots+(i)^n\int_0^{\infty}du_nV_{k_nl_n}(-u_n)\int_{u_n}^{\infty}du_{n-1}V_{k_{n-1}l_{n-1}}(-u_{n-1})$$
$$\times\cdots\times\int_{u_2}^{\infty}du_1\exp(-\varepsilon u_1)V_{k_1l_1}(-u_1) \tag{B.12}$$

and

$$K^{ij}=(-i)^n\int_0^{\infty}du_n\exp\big(-iH_{i_nj_n}u_n\big)\exp(+iH_0u_n)V_{k_nl_n}(-u_n)$$
$$\times\exp(-iH_0u_n)\exp\big(iH_{i_{n-1}j_{n-1}}u_n\big)\int_{u_n}^{\infty}du_{n-1}\exp\big(-iH_{i_{n-1}j_{n-1}}u_{n-1}\big)$$
$$\times\cdots\times\exp(iH_{ij}u_1)(\varepsilon)\int_{u_1}^{\infty}dv\exp(-\varepsilon v-iH_{ij}v)\exp(+iH_0v)$$
$$+\cdots+(i)^n\int_0^{\infty}du_nV_{k_nl_n}(-u_n)\int_{u_n}^{\infty}du_{n-1}V_{k_{n-1}l_{n-1}}(-u_{n-1})$$
$$\times\cdots\times V(-u_1)(\varepsilon)\int_{u_1}^{\infty}dv\exp(-\varepsilon v-iH_{ij}v)\exp(iH_0v) \tag{B.13}$$

The equalities (B.6) and (B.7) together with (B.12) and (B.13) provide the link between the time-dependent formalism and the terms in the multiple scattering expansion.

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