CONFIGURATION SPACE THEORY OF 'TRULY THREE-BODY' SCATTERING RATES†

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The configuration space theory of (non-relativistic) three-body scattering is reviewed, with two main objectives in mind: (i) to derive from a very different approach, wherein comparatively little use is made of questionable mathematical manipulations (e.g. operator techniques or the representation of functions by infinite integrals) the general expressions for reaction rates customarily deduced via momentum space procedures; (ii) to determine the 'physical' three-particle transition operator $\boldsymbol{T}^t$, to be distinguished from the conventional $\boldsymbol{T} = V - VGV$, where G is the Green function. The matrix elements $\langle \mathrm{f}|\boldsymbol{T}^t|\mathrm{i}\rangle$ yield the reaction coefficient $\overline{w}(\mathrm{i} \to \mathrm{f})$ expressing the probability of 'true' three-body reactions; contained in the matrix elements $\langle \mathrm{f}|\boldsymbol{T}|\mathrm{i}\rangle$ are terms representing, for example, purely two-body scattering events. Although the possibility of inelastic processes is fully taken into account, for simplicity the detailed analysis is limited to those transition amplitudes representing elastic scattering under the influence of short-range forces; however, it is reasonable to suppose the results obtained are relevant to broader classes of reactions and forces. In essence, the analysis concentrates on the δ-functions occurring in transition amplitudes, as well as in expressions for the solution $\Psi_{\mathrm{i}}^{(+)}(E)$ to Schrödinger's equation presumably satisfying the boundary conditions at real energy E for specified incident wave

$$\psi_{\mathrm{i}} = \exp\{\mathrm{i}(\boldsymbol{k}_1 . \boldsymbol{r}_1 + \boldsymbol{k}_2 \cdot \boldsymbol{r}_2 + \boldsymbol{k}_3 \cdot \boldsymbol{r}_3)\}.$$

It is found that these δ-functions—in a configuration space formulation—always are associated with (and in effect signal) previous illegitimate mathematical operations, e.g. unjustified interchange of order of integration and limit $r \to \infty$, or improper computation of the limit $\epsilon \to 0$ in expressions for $\Psi_{\mathrm{i}}(E + \mathrm{i}\epsilon)$. This last assertion does not negate the fact that the δ-functions so produced often are physically interpretable and indeed desirable, as, for example, the customary total momentum conserving $\delta(\boldsymbol{K}_{\mathrm{f}} - \boldsymbol{K}_{\mathrm{i}})$ factor in laboratory system transition amplitudes. On the other hand, such δ-functions, when on-shell (as can be, for example, either the aforementioned $\delta(\boldsymbol{K}_{\mathrm{f}} - \boldsymbol{K}_{\mathrm{i}})$ or the δ-functions associated with single—i.e. not multiple two-body scattering events), yield meaninglessly infinite reaction rates unless reinterpreted in terms of the (large) volume τ within which the three particles 1, 2, 3 are reacting. Moreover, the 'physical' three-body amplitudes $\langle \mathrm{f}|\boldsymbol{T}^t|\mathrm{i}\rangle$ will contain no δ-functions other than the ever-present $\delta(\boldsymbol{K}_{\mathrm{f}} - \boldsymbol{K}_{\mathrm{i}})$. Thus, the presence of non-three-body contributions to $\langle \mathrm{f}|\boldsymbol{T}|\mathrm{i}\rangle$ is also signalled by anomalous τ-dependence of reaction rates inferred therefrom. In particular, the δ-function contributions to $\langle \mathrm{f}|\boldsymbol{T}|\mathrm{i}\rangle$ from two successive purely two-body scatterings, if retained, would result in predicted three-body scattering rates proportional to $\tau^{\frac{4}{3}}$, whereas the true three-body rate should be proportional to τ. A mathematically correct derivation of $\langle \mathrm{f}|\boldsymbol{T}^t|\mathrm{i}\rangle$, in which these double scattering δ-functions would be wholly avoided, seems very difficult; however, it is possible to subtract these δ-functions from the divergent integral which—in the configuration space formalism—represents the contributions to $\langle \mathrm{f}|\boldsymbol{T}|\mathrm{i}\rangle$ associated with double scattering events. In this fashion it is concluded that $\langle \mathrm{f}|\boldsymbol{T}^t|\mathrm{i}\rangle$ is the sum of all contributions from $n \geqslant 3$ successive purely binary collisions, plus the off-shell contributions from double scattering ($n = 2$) processes. The configuration space and momentum space results for $\langle \mathrm{f}|\boldsymbol{T}|\mathrm{i}\rangle$ agree, as do the configuration space and momentum space expressions for $\langle \mathrm{f}|\boldsymbol{T}^t|\mathrm{i}\rangle$, provided it is granted—as is not apparent from momentum space procedures—that $\langle \mathrm{f}|\boldsymbol{T}^t|\mathrm{i}\rangle$ should include the off-shell double scattering contributions. Including these off-shell double scattering contributions keeps finite the predicted three-body elastic scattering rate observed with fixed counters arranged so as to exclude actual physical (on-shell) double scattering events, but makes infinite the total three-body elastic scattering rate obtained from integration over all counter positions which exclude on-shell double scattering as well as single scattering. Our analysis also relates the τ-dependence to the behaviour of $\Psi_{\mathrm{i}}^{(+)}(E)$ at large distances, and examines off-shell δ-function contributions in certain (not all) formulas for $\langle \mathrm{f}|\boldsymbol{T}|\mathrm{i}\rangle$, whose presence apparently is typically associated with the existence of bound states. In large

† The text makes frequent reference to various sections of these appendices, which, because of their length, have not been included in this paper, but have been placed in the Archives of the Society (for consultation). Copies may be purchased from the National Lending Library, Boston Spa, Yorkshire, LS23 7BQ, United Kingdom. (Reference number SUP 10005.) Copies of the appendices may also be obtained from the author.

part, the text is an amplification (often essentially a correction) of assertions concerning configuration space three-body scattering theory which previously were inferred somewhat offhandedly from conclusions carefully derived for two-body reactions only. The Faddeev equations are mentioned, but the problem with which these equations are mainly concerned—namely the reformulation of Schrödinger's equation as an integral equation permitting solution by Fredholm's method—is not seriously considered in the present work. Setting aside its purely formal implications for scattering theory, the considerations of this publication will be most relevant and least dispensable in the theory of three-body reactions which actually produce three outgoing products; such 'three–three' reactions of actual interest are not uncommon in the field of chemistry. In a sense, therefore, this publication is a first step in the direction of deducing correct formal expressions for important often measurable three–three chemical reaction rates.

1. Introduction and summary

Consider the scattering of three particles† $\alpha = 1, 2, 3$ which for the purposes of this work may be considered elementary, spinless and distinguishable. A major objective of the theory is to determine the physical three-body reaction coefficient

$$\overline{w}(\mathrm{i}\to\mathrm{f}) \equiv \overline{w}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) \equiv \overline{w}(\boldsymbol{k}_{1\mathrm{i}}, \boldsymbol{k}_{2\mathrm{i}}, \boldsymbol{k}_{3\mathrm{i}}\to\boldsymbol{k}_{1\mathrm{f}}, \boldsymbol{k}_{2\mathrm{f}}, \boldsymbol{k}_{3\mathrm{f}}), \tag{1}$$

expressing the probability of three-body elastic scattering in the laboratory system, from initial momenta $\hbar\boldsymbol{k}_{\alpha\mathrm{i}} = m_\alpha \boldsymbol{v}_{\alpha\mathrm{i}}$ to final momenta $\hbar\boldsymbol{k}_{\alpha\mathrm{f}}$. The reaction coefficient $\overline{w}$ is related to observation by

$$\hat{w}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) = N_1 N_2 N_3 \tau \overline{w}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}), \tag{2}$$

where $\hat{w}$ is the observed number of scatterings per unit time into wavenumber ranges $\mathrm{d}\boldsymbol{k}_{1\mathrm{f}}$, $\mathrm{d}\boldsymbol{k}_{2\mathrm{f}}$, $\mathrm{d}\boldsymbol{k}_{3\mathrm{f}}$ in a (large) volume τ containing N_α particles α per unit volume moving with the precise velocities $\boldsymbol{v}_\alpha$, $\alpha = 1, 2, 3$. Presumably $\hat{w}/\tau$ should be independent of τ, i.e. presumably in a correctly formulated theory the computed reaction coefficient $\overline{w}$ will be independent of τ.

If only by analogy with known results (Gerjuoy 1958*a*; Messiah 1962) for collisions between two incident bodies, one expects that

$$\begin{aligned}\overline{w}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) &\equiv \overline{w}(\mathrm{i}\to\mathrm{f})\\ &= \frac{2\pi}{\hbar}\frac{1}{(2\pi)^6}\,|\,\overline{T}^t(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f})|^2\,\delta(E_\mathrm{f}-E_\mathrm{i})\,\delta(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K}_\mathrm{i})\,\mathrm{d}\boldsymbol{k}_{1\mathrm{f}}\,\mathrm{d}\boldsymbol{k}_{2\mathrm{f}}\,\mathrm{d}\boldsymbol{k}_{3\mathrm{f}},\end{aligned} \tag{3}$$

where E and $\hbar\boldsymbol{K}$ are respectively the total energy and momentum in the laboratory system, and where

$$\overline{T}^t(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) \equiv \langle\mathrm{f}|\,\bar{\boldsymbol{T}}^t\,|\mathrm{i}\rangle = \overline{\psi}_\mathrm{f}^*\,\bar{\boldsymbol{T}}^t\overline{\psi}_\mathrm{i} \tag{4}$$

is the centre-of-mass system matrix element of the 'physical' three-particle transition operator $\bar{\boldsymbol{T}}^t$ between initial and final plane wave states $\overline{\psi}$. Evidently determination of the form of $\bar{\boldsymbol{T}}^t$ would fulfil the theoretical objective stated in the preceding paragraph. A determinative definition of $\bar{\boldsymbol{T}}^t$ is not immediately apparent, however. What is apparent is that (granting the validity of (3)) the physical transition operator $\bar{\boldsymbol{T}}^t$ must differ from the customarily employed 'total' transition operator (Watson & Nuttall 1967)

$$\boldsymbol{T}(E) = \boldsymbol{V} - \boldsymbol{V}\boldsymbol{G}^{(+)}(E)\,\boldsymbol{V}, \tag{5}$$

where V is the total interaction and $G^{(+)}$ is the total Green function, defined respectively via (21*b*) and (27) below, and where it is useful to distinguish between the coordinate-dependent

† In this paragraph, and in subsequent paragraphs, the Greek letters α, β are used as running subscripts over the electron indices 1, 2, 3, while the letters i, f are employed to denote respectively initial and final states. Furthermore, barred and unbarred symbols regularly will denote corresponding quantities in the centre of mass and laboratory systems respectively.

function V and its associated operator $\boldsymbol{V} \equiv V\mathbf{1}$ (see (27 *e*) below). Equation (5) is an unsuitable expression for $\boldsymbol{T}^t$ because the centre of mass system matrix elements

$$\langle \mathrm{f}|\, \bar{\boldsymbol{T}}\, |\mathrm{i}\rangle = \overline{\psi}_\mathrm{f}^*\, \boldsymbol{T}\overline{\psi}_\mathrm{i} \tag{6}$$

contain δ-functions (in addition to those already appearing in (3)); as detailed in § 4, these δ-functions—if inserted into (3) and reinterpreted so as to keep finite the integral of (3) over all final momenta—would lead to a $\overline{w}$ depending on τ, i.e. to a result inconsistent with the presumption that the number of three-body scattering events in τ should be strictly proportional to τ at large volumes (in the limit $\tau \to \infty$).

Although the singularities of (6) in the complex energy plane recently have been very thoroughly examined and classified for Yukawa interactions (Rubin, Sugar & Tiktopoulos 1966, 1967 *a*, *b*) and although the Faddeev (1961) reformulation of the Lippmann–Schwinger equation (Lippmann & Schwinger 1950; Gell-Mann & Goldberger 1953) has focused attention on the problem of subtracting out or otherwise eliminating (Weinberg 1964) the troublesome δ-functions contained in (6), the question I am raising—namely, what is the physical three-body transition operator $\bar{\boldsymbol{T}}^t$?—does not appear to have been studied as such. Moreover, because the matrix elements (4) or (6) are computed for plane wave states $\overline{\psi}$, the aforementioned (Rubin *et al.* 1966; Weinberg 1964; Watson & Nuttall 1967) studies of the singularities of (6) and their possible subtractions typically have been performed in the momentum representation, which also happens to be the most natural representation for utilization of diagrammatic methods; for similar reasons, applications of the Faddeev equations (Faddeev 1961) for $\boldsymbol{T}$ generally (Lovelace 1964) have resorted to the momentum representation, even though those equations have a quite representation-independent form. In addition, derivations of (3) in the literature (Lippmann & Schwinger 1950; Gell-Mann & Goldberger 1953; Brenig & Haag 1963; Moller 1945) customarily compute $\overline{w}$ in terms of transition probabilities found by projecting the wavefunction solving Schrödinger's equation onto final plane wave states, i.e. derivations of (3) customarily are couched in the momentum representation essentially *ab initio*. Furthermore, although there is no real basis for doubting the correctness of (3) as it stands, it is fair to state that the aforementioned derivations do not distinguish between $\bar{\boldsymbol{T}}$ and $\bar{\boldsymbol{T}}^t$, and that these derivations characteristically arrive at the result (3) only after considerable use of operator or other so-called symbolic manipulations, whose mathematical validity is very difficult to assess.

On the other hand, previous investigations (Gerjuoy 1958 *a*) have shown that formulating scattering theory in configuration space can be both useful and instructive. This assertion, taken together with those stated in the previous paragraph, provides the motivation for the present work, which in substance presents configuration space derivations of (3) and of a closed form expression for $\bar{\boldsymbol{T}}^t$, after first reviewing the relevant features of configuration space scattering theory. In their totality, the configuration space results obtained furnish a welcome confirmation of the general correctness of the customary momentum space procedures, which usually attain their goals (e.g. a derivation of (3)) much more rapidly than do the configuration space procedures to be described. One very significant reason for the length of this work, however, is its attempt to avoid symbolic manipulations as well as obviously mathematically unsatisfactory operations, e.g. the representations of functions by divergent integrals; this attempt has been largely successful, but unfortunately not entirely so. Moreover, I must point out that while I largely have avoided obviously invalid operations and believe the claimed results of this work are correct, the 'proofs' offered often are barely more than mathematically plausible arguments;

certainly I do not intend to claim that such proofs are rigorous by mathematicians' standards,† not even by the less stringent but still mathematically quite sophisticated standards of Rubin *et al.* (1966, 1967*a*, *b*). There are a few instances (see especially § 5) where the mathematics employed seems sufficiently loose to possibly yield erroneous results; all such instances have been remarked upon in the text, in so far as I have been able to recognize them. I add that of course there would be no reason to doubt momentum space and configuration space predictions of physically observable quantities will be the same, were it not for the fact that the configuration space and momentum space formulations each involve some questionable mathematical manipulations after starting from equally questionable by no means obviously identical physical assumptions. The questionable features of configuration space scattering theory—at least for the elastic collisions of three initially free particles—are a main subject of the present work; discussions, more or less satisfactory, of the assumptions underlying the momentum space procedures for computing reaction rates can be found in the literature (Gell-Mann & Goldberger 1953; Goldberger & Watson 1964; Brenig & Haag 1963).

In the (time-independent) configuration space formulation of scattering theory, reaction coefficients are computed from the probability current at infinity (Gerjuoy 1958*a*). Thus, to determine $\overline{w}(\mathrm{i}\to\mathrm{f})$ defined in (1) and (2), it is necessary to determine the asymptotic behaviour at large $\boldsymbol{r} \equiv \boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3$ of $\Psi_\mathrm{i}^{(+)}(\boldsymbol{r}; E)$, defined as that particular solution of Schrödinger's equation

$$(H-E)\,\Psi = 0, \tag{7}$$

which at real (i.e. physical) energies E satisfies the boundary conditions presumably describing the actual physical situation, namely the collision of three initially free particles moving with momenta $\hbar\boldsymbol{k}_{\alpha\mathrm{i}}$. To be useful, however, this definition must be supplemented by an unambiguous mathematical specification of $\Psi_\mathrm{i}^{(+)}$. It is generally agreed—and has been argued from a variety of physical standpoints (Lippmann & Schwinger 1950; Gell-Mann & Goldberger 1953)—that the desired $\Psi_\mathrm{i}^{(+)}(E)$ solving (7) is obtainable from the Lippmann–Schwinger integral equation. Specifically,‡

$$\Psi_\mathrm{i}^{(+)}(E) = \lim_{\epsilon\to 0} \Psi_\mathrm{i}(E+\mathrm{i}\epsilon) \equiv \lim_{\epsilon\to 0} [\psi_\mathrm{i}(E) + \Phi_\mathrm{i}(E+\mathrm{i}\epsilon)], \tag{8a}$$

where, for $\epsilon > 0$, $\Psi_\mathrm{i}(E+\mathrm{i}\epsilon)$ is the unique bounded (but not necessarily quadratically integrable) solution to

$$\Psi_\mathrm{i}(E+\mathrm{i}\epsilon) = \psi_\mathrm{i}(E) - \frac{1}{H_\mathrm{i}-E-\mathrm{i}\epsilon}\, V_\mathrm{i}\, \Psi_\mathrm{i}(E+\mathrm{i}\epsilon). \tag{8b}$$

Here the incident wave ψ_i satisfies

$$(H_\mathrm{i}-E)\,\psi_\mathrm{i} \equiv (H-V_\mathrm{i}-E)\,\psi_\mathrm{i} = 0 \tag{9}$$

and, for complex λ, the incident Green function

$$G_\mathrm{i}(\lambda) = 1/(H_\mathrm{i}-\lambda) \tag{10a}$$

is the unique quadratically integrable solution of

$$(H_\mathrm{i}-\lambda)\,G_\mathrm{i}(\lambda) = \mathbf{1}. \tag{10b}$$

† To be rigorous by mathematicians' standards (see, for example, Faddeev 1965) requires very much more elaborate analysis than I am able to or desire to give.

‡ At energies E corresponding to bound states of the total Hamiltonian, or to thresholds of inelastic processes, one should not expect the limit (8*a*) to exist. Similarly, $G^{(+)}(E)$ defined by (27*a*) need not exist at such exceptional energies.

Write $$\Psi_i^{(+)}(E) = \psi_1 + \Phi_i^{(+)}, \tag{11a}$$

where $\Phi_i^{(+)}(E)$ is the 'scattered part' of $\Psi_i^{(+)}$. The corresponding centre of mass system defining equation for the scattered part is† $$\bar{\Psi}_i^{(+)}(\bar{E}) = \bar{\psi}_1 + \bar{\Phi}_i^{(+)}, \tag{11b}$$

where barred and unbarred quantities are related as in (33) and (55) below. Contained in $\Phi_i^{(+)}$, $\bar{\Phi}_i^{(+)}$ may be contributions from scattering processes which are not 'truly three-body' and which therefore should not be included in estimates of the three-body coefficient $\bar{w}$; for instance, contributions from the purely two-body scattering of particle 1 by particle 2, wherein particle 3 plays no role (i.e. can be thought to be very far away from the relatively close pair 1, 2), obviously should not be included in $\bar{w}(i \to f)$ of (2). For want of a better term I shall call such presently unwanted contributions to $\Phi_i^{(+)}$, $\bar{\Phi}_i^{(+)}$ 'non-three-body', even though (as amplified below) they can arise from scattering processes which involve all three particles 1, 2, 3, e.g. the double scattering process consisting of the purely two-body scattering of 1 by 2 followed by the similar purely two-body scattering of 2 by 3. Apparently (see § 4) the existence of unwanted δ-function contributions to $\langle f|\, \bar{T}\, |i\rangle$ always can be associated with the presence of non-three-body contributions to $\Phi_i^{(+)}$, $\bar{\Phi}_i^{(+)}$. The physical 'truly three-body' parts of $\Phi_i^{(+)}$, $\bar{\Phi}_i^{(+)}$ which remain after subtracting away the non-three-body contributions will be denoted by $\Phi_i^{t(+)}$, $\bar{\Phi}_i^{t(+)}$ respectively. The desired three-body elastic scattering $\bar{w}(i \to f)$ then is found from the limit of $\bar{\Phi}_i^{t(+)}$ as $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, $\boldsymbol{r}_3$ simultaneously approach infinity along such directions that every

$$\boldsymbol{r}_{\alpha\beta} \equiv \boldsymbol{r}_\alpha - \boldsymbol{r}_\beta = -\boldsymbol{r}_{\beta\alpha} \tag{12}$$

simultaneously becomes infinite.

The organization and contents of this work now can be intelligibly summarized‡ in rather more detail than was possible in earlier paragraphs. In the first place, the present investigation finds that as a quite general rule—in the configuration space formulation of scattering theory, at any rate—the δ-functions encountered (even when capable of perfectly sensible physical interpretation) are associated with improper mathematical manipulations; correspondingly, avoiding such manipulations results in a reformulation in which the associated δ-functions do not explicitly appear, although of course (if the aforementioned physical interpretation really was correct) such reformulation does not eliminate the physical consequences of the δ-functions. For example, it has been shown previously (Gerjuoy 1958*a*), and is redemonstrated in § 4, that in a configuration space formulation the well-known total momentum conserving $\delta(\boldsymbol{K}_f - \boldsymbol{K}_1)$ appearing in the matrix elements $\langle f|\, \boldsymbol{T}\, |i\rangle$ of the laboratory system transition operator $\boldsymbol{T}$, equation (5), is associated with computation of the outgoing probability current in the laboratory system using $\Phi_i^{(+)}$ defined by (11*a*), ignoring the fact that $\Phi_i^{(+)}$ has an incoming plane wave factor (cf. (55*b*) below). This $\delta(\boldsymbol{K}_f - \boldsymbol{K}_1)$ factor in $\langle f|\, \boldsymbol{T}\, |i\rangle$, though obviously physically understandable and desirable, causes the probability current flow involved in the laboratory system derivation of the reaction coefficient to become infinite, necessitating (an also physically understandable) reinterpretation of $\delta(\boldsymbol{K}_f - \boldsymbol{K}_1)$ in terms of the volume τ, as discussed in § 4.2; on the other hand, because $\bar{\Phi}_i^{(+)}$ of (11*b*) does not possess the incoming plane wave factor present in $\Phi_i^{(+)}$, the $\delta(\boldsymbol{K}_f - \boldsymbol{K}_1)$ factor correspondingly is absent from the matrix elements $\langle f|\, \bar{T}\, |i\rangle$, although of course total momentum continues to be conserved and the true laboratory system three-body scattering rate $\hat{w}$ remains proportional to τ, as in (2). Similarly, § 4 shows that the remaining annoying δ-functions in

† See footnote, p. 199.

‡ A brief summary of this work, without any derivations, has appeared in the literature (Gerjuoy 1970).

$\langle \mathrm{f}|\, \bar{\boldsymbol{T}}\, |\mathrm{i}\rangle$, (6), are associated with the fact that $\bar{\Phi}_{\mathrm{i}}^{(+)}$ still does not have the asymptotic behaviour required for a mathematically correct computation of the outgoing three-body probability current.

Further illustrations of the aforementioned thesis—that the δ-functions which are encountered are associated with improper mathematical manipulations—are deduced and discussed in §§ 2 to 4 below. In particular, § 2 is concerned with the consequences of an unjustified interchange—in expressions such as (8 *b*)—of the order of integration and limit $\epsilon \to 0$. Among other results, § 2 shows that whenever stable (negative energy) two-particle bound states $u_j(\boldsymbol{r}_{\alpha\beta})$ exist, then even in the centre of mass system the formal solution†

$$\bar{\Psi}_{\mathrm{i}}^{(+)}(\bar{E}) = \bar{\psi}_{\mathrm{i}}(\bar{E}) - \bar{G}^{(+)}(\bar{E})\, V \bar{\psi}_{\mathrm{i}} \tag{13}$$

to the Lippmann–Schwinger integral equation at real energies involves non-convergent oscillatory integrals—taking the form of δ-functions vanishing (i.e. whose arguments are non-vanishing) on the energy shell. Correspondingly, it can be seen that when such states $u_j(\boldsymbol{r}_{\alpha\beta})$ occur, the interchange of order of integration and limit $\epsilon \to 0$ required to derive (13) is unjustified; moreover, in this instance reformulation so as to avoid unjustified interchange of order of integration and limit $\epsilon \to 0$ results in a formula for $\bar{\Psi}_{\mathrm{i}}^{(+)}$ in which no oscillatory integrals appear, i.e. in this instance the δ-functions are non-physical consequences of the mathematically invalid operations, even though (see § 2.2) the conditions for vanishing of these δ-functions' arguments seem physically quite reasonable.

Section 3 examines the consequences—in integrals arising, for example, from the Lippmann–Schwinger integral equation for the total Green function $G^{(+)}(\boldsymbol{r}; \boldsymbol{r}'; E)$ (Watson & Nuttall 1967) —flowing from unjustified interchange of order of integration and limit as $\boldsymbol{r}$ or $\boldsymbol{r}' \to \infty$. Taking the limit of $G^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$ as $\boldsymbol{r}' \to \infty$ provides an alternative (to (8)) means of specifying $\Psi_{\mathrm{i}}^{(+)}$, because in this limit $G^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$ must become proportional to a solution of (7). In fact, this interchange—of order of integration and limit $\boldsymbol{r}' \to \infty$ in the Lippmann–Schwinger equation for $G^{(+)}$—yields precisely the laboratory system analogue of (13). According to § 2, when bound states exist this analogue of (13) must be considered unsatisfactory (because it involves non-convergent integrals). Correspondingly, among other results, § 3 shows that it is in just these circumstances, namely when bound states can occur, that the interchange of order of integration and limit $\boldsymbol{r}' \to \infty$ in the Lippmann–Schwinger equation for $G^{(+)}$ is unjustified.

As has been indicated, § 4 is concerned with the consequences—in computing the outgoing probability current—of unjustified assumptions about the asymptotic behaviour of, for example, $\Phi_{\mathrm{i}}^{(+)}(\boldsymbol{r})$ at large $\boldsymbol{r}$. Among other results, in addition to those already mentioned, § 4 shows that even after subtraction of purely two-body single scattering contributions the residual part of $\bar{\Phi}_{\mathrm{i}}^{(+)}$ does not have the asymptotic behaviour required to represent truly three-body scattering. Ignoring this fact leads to transition matrix elements $\langle \mathrm{f}|\, \bar{\boldsymbol{T}}\, |\mathrm{i}\rangle$, equation (6), containing δ-functions expressing the consequences of energy and momentum conservation in two successive purely two-body elastic scattering events, i.e. in non-three-body double scattering processes of the type mentioned illustratively following (11 *b*). Moreover, the necessary reinterpretation of these double scattering δ-functions, along the lines of the previously mentioned reinterpretation of $\delta(\boldsymbol{K}_{\mathrm{f}} - \boldsymbol{K}_{\mathrm{i}})$, leads to three-body scattering rates $\hat{w}$ from (2) proportional to $\tau^{\frac{4}{3}}$. This unpleasant result implies (for reasons which have been explained) that the aforementioned double scattering

† Here $\bar{G}^{(+)}(E)$ is the centre of mass analogue of the everywhere outgoing Green function $G^{(+)}(E)$ appearing in (5); for a more precise definition of this Green function, see (36) and (39 *a*).

processes consisting of two successive purely two-body elastic scattering events really are 'non-three-body', whose associated contributions must be subtracted from $\bar{\Phi}_i^{(+)}$ in order to obtain the truly three-body scattered part $\bar{\Phi}_i^{t(+)}$. The correctness of the foregoing reinterpretation of the double scattering δ-functions, and of the implications therefrom, is affirmed by additional essentially geometrical considerations in § 4.2, which indicate that a three-body elastic scattering rate $\hat{w}$ apparently proportional to $\tau^{\frac{4}{3}}$ actually would be observed unless the experimental arrangements (e.g. the locations of particle detectors) exclude counting double scattering events of the aforementioned type. On the other hand, similar geometrical considerations indicate that the contribution to the observed three-body $\hat{w}$ from any number $n \geqslant 3$ of successive purely binary collisions (Doolen 1968) between the three particles 1, 2, 3—unless negligibly infrequent—must be proportional to τ, confirming the finding (still in § 4) that such $n \geqslant 3$ rescattering processes do not yield δ-function contributions to $\langle f|\, \bar{\boldsymbol{T}}\, |i\rangle$.

The results of § 4 described above suggest that the physical $\langle f|\, \bar{\boldsymbol{T}}^t\, |i\rangle$, yielding the truly three-body $\bar{w}$ and $\hat{w}$ via (2) to (4), are obtainable by subtraction—from $\langle f|\, \bar{\boldsymbol{T}}\, |i\rangle$—of the δ-functions which have been discussed. Of course, any derivation of $\langle f|\, \bar{\boldsymbol{T}}^t\, |i\rangle$ involving the subtraction of δ-functions is immediately open to criticism because it perforce is employing improper mathematical manipulations. Nevertheless, the final § 5 details a derivation of $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ via such δ-function subtraction, and examines the expression for $\langle f|\, \bar{\boldsymbol{T}}^t\, |i\rangle$ thereby obtained, including behaviour under time reversal. It is concluded that $\bar{\boldsymbol{T}}^t$ is the sum of all contributions from $n \geqslant 3$ successive purely binary collisions, plus the so-called off-shell contributions from $n = 2$ successive binary collisions, i.e. plus the contributions from double scattering diagrams wherein energy is not conserved in the individual two-body scattering events (although of course the initial and final energies are equal after all scatterings have been completed). As discussed in the closing § 5.3 of the main text, the configuration space results for $\langle f|\, \bar{\boldsymbol{T}}\, |i\rangle$ are wholly consistent with the results for $\langle f|\, \bar{\boldsymbol{T}}\, |i\rangle$ from momentum space procedures. However, momentum space procedures do not seem to provide much basis for deciding what contributions (if any) from double scattering diagrams belong in $\bar{\boldsymbol{T}}^t$; once it has been decided that $\bar{\boldsymbol{T}}^t$ should include the off-shell double scattering contributions, the aforementioned agreement between momentum space and configuration space results for $\langle f|\, \bar{\boldsymbol{T}}\, |i\rangle$ immediately implies that the momentum space and configuration space predictions of $\langle f|\, \bar{\boldsymbol{T}}^t\, |i\rangle$—and therefore of three-body elastic scattering reaction coefficients $\bar{w}(i \to f)$—also will agree. Including these off-shell double scattering contributions in $\bar{\boldsymbol{T}}^t$ keeps finite the three-body elastic scattering rate observed with fixed counters arranged so as to exclude actual physical (i.e. on-shell) double scattering processes. On the other hand, including the off-shell double scattering contributions in $\bar{\boldsymbol{T}}^t$ has the understandable (i.e. physically believable, see § 5.3) consequence that the total three-body elastic scattering rate, obtained from integration of (2) over all $\boldsymbol{k}_{1f}$, $\boldsymbol{k}_{2f}$, $\boldsymbol{k}_{3f}$ which exclude single scattering and on-shell double scattering processes, becomes infinite.

Although it is arguable that the results of this work are relevant to a variety of three-body reactions, including inelastic scattering and rearrangement, for simplicity the actual analysis here presented is restricted specifically to the three-body elastic scattering of a set of three particles obeying (7), where the total Hamiltonian

$$H \equiv T + V = T_1 + T_2 + T_3 + V_{12} + V_{23} + V_{31}. \tag{14}$$

contains only purely two-particle interactions $V_{\alpha\beta}$. Because the particles are supposed spinless, each $V_{\alpha\beta}$ is a function solely of the relative position $\boldsymbol{r}_{\alpha\beta}$. The potentials $V_{\alpha\beta}(\boldsymbol{r}_{\alpha\beta})$ will be

presumed sufficiently short-range and well behaved to guarantee convergence of integrals such as

$$\int \mathrm{d}\boldsymbol{r}_{\alpha\beta} V_{\alpha\beta}(\boldsymbol{r}_{\alpha\beta})\, F(\boldsymbol{r}_{\alpha\beta}) \tag{15}$$

over all $\boldsymbol{r}_{\alpha\beta}$, provided $F(\boldsymbol{r}_{\alpha\beta})$ is bounded and integrable in any infinite volume; in particular the convergence of (15) at infinite $\boldsymbol{r}_{\alpha\beta}$ will be supposed rapid and absolute. The total kinetic energy operator

$$T = \sum_{\alpha} T_{\alpha} = -\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 - \frac{\hbar^2}{2m_3}\nabla_3^2 \tag{16}$$

is not to be confused with the transition operator $\boldsymbol{T}$, of course.

Reactions for which the above claim of relevance is defensible—despite the severe restrictions imposed in the preceding paragraph—include, for example, radiationless electron–ion recombination in a hydrogen plasma

$$\mathrm{e^- + e^- + H^+ \rightarrow e^- + H.} \tag{17a}$$

The results of this publication also should be relevant to the theory of two-body reactions producing three outgoing products, e.g. electron ionization of atomic hydrogen

$$\mathrm{e^- + H \rightarrow e^- + e^- + H^+,} \tag{17b}$$

because transition matrix elements for (17 *b*) frequently (though not necessarily) are expressed in terms of time-reversed wavefunctions, i.e. in terms of wavefunctions describing the collision (17 *a*) inverse to (17 *b*). Similarly, this investigation's results should be relevant to deuteron breakup in collisions with a heavy nucleus A

$$\mathrm{d + A \rightarrow p + n + A.} \tag{17c}$$

Of course, the considerations of this publication will be most relevant and least dispensable in the theory of three-body reactions which actually produce three outgoing products. When estimating the rates of such 'three-three' reactions—unlike the situation with, for example, the 'three-two' reaction (17 *a*) whose rate is related by detailed balancing to the rate of the 'two–three' reaction (17 *b*)—the complicating presence of non-three-body scattered parts cannot be avoided merely by estimating the rate of the time-reversed reaction. As a matter of fact, three–three reactions of actual interest are not uncommon, especially in the field of chemistry. For example, the reaction

$$\mathrm{O_3 + CO + M \rightarrow O_2 + CO_2 + M} \tag{18a}$$

(where M designates any one of many possible third bodies) is a proposed member of the chain of reactions involved in the combustion of $\mathrm{CO + O_2}$. Also, many atomic collisions bearing on chemical reaction rates are of this three-body in, three-body out type, e.g. the recently studied reaction between molecular nitrogen metastables in the presence of a noble gas, namely

$$\mathrm{N_2(^3\Delta_u) + N_2(^3\Delta_u) + Xe \rightarrow N_2(X^1\Sigma_g^+) + N_2(X^1\Sigma_g^+) + Xe^*,} \tag{18b}$$

where the asterisk indicates an excited state of Xe. Furthermore, the generic forms of atomic collision processes frequently cited as important in gaseous discharges or in aeronomy include: three-body associative ionization

$$\mathrm{X + Y + Z \rightarrow X^+ + YZ + e^-} \tag{18c}$$

three-body ion pair formation $\quad X+Y+Z\rightarrow X^{+}+Y^{-}+Z \qquad (18\,d)$

and three-body dissociative recombination

$$e^{-}+XY^{+}+Z\rightarrow X+Y+Z \qquad (18\,e)$$

In a sense, therefore, this publication is a first step in the direction of deducing correct formal expressions for the reaction rates of three–three processes such as (18), especially if—as must happen on occasion—the three–three reaction of interest can proceed via two successive purely two-body reactions. For example, suppose one desires the truly three-body rate of the three–three reaction

$$\{1,2\}+3+4\rightarrow 1+2+\{3,4\}, \qquad (19\,a)$$

involving the four particles 1, 2, 3, 4, where the braces denote a bound state; i.e. in the reaction (19 *a*) particles 1 and 2 are initially bound to each other. Suppose further that (19 *a*) can proceed via the successive two-body reactions

$$\{1,2\}+3\rightarrow 1+\{2,3\}, \qquad (19\,b)$$

$$\{2,3\}+4\rightarrow 2+\{3,4\}, \qquad (19\,c)$$

Then (in complete analogy with the necessary subtraction of on-shell but only on-shell contributions from the double scattering process consisting of 1, 2 scattering followed by 2, 3 scattering when computing the truly three-body elastic scattering of particles 1, 2, 3) computation of the truly three-body rate of the inelastic reaction (19 *a*)—i.e. computation of that rate, proportional to the reaction volume τ, which would be observed under experimental arrangements preventing or eliminating the successive reactions (19 *b*) and (19 *c*)—presumably should subtract δ-function contributions arising from the successive on-shell inelastic two-body reactions (19 *b*) and (19 *c*), but probably should retain contributions from successive off-shell reactions (19 *b*) and (19 *c*). Hopefully, retention of these off-shell contributions will not cause the total truly three-body rate of (19 *a*) to become infinite; although infinite total truly three-body rates are believable for elastic scattering, they are not believable for inelastic processes such as (19 *a*).

I conclude this introductory section with the observation that, to facilitate holding on to the main thread of the discussion in §§ 2 to 4, many mathematical details have been relegated to a (perhaps excessively large) number of appendices.† I add that to a considerable extent the results to be described amount in effect to an amplification (often essentially a correction) of assertions concerning three-body reactions which previously (Gerjuoy 1958 *a*, *b*) were inferred somewhat off-handedly from conclusions which had been carefully derived for two body reactions only. I further remark that a (admittedly not exhaustive) survey of the literature discloses comparatively few authors who have examined three-body scattering from the standpoint of configuration space; illustrative and worthwhile contributions in this category include those of Zickendraht (1967) and Nuttall (1967), as well as (more recently) Noyes (1969) and Lieber, Rosenberg & Spruch (1969).

2. The limit $\epsilon\rightarrow 0$

From the standpoint of configuration space scattering theory, the specification of $\Psi_{\mathrm{i}}^{(+)}(E)$ provided by (8), though undoubtedly valid, is less useful than might have been hoped. For the purpose of predicting $\overline{w}(\mathrm{i}\rightarrow\mathrm{f})$ one requires knowledge of the asymptotic behaviour of $\Psi_{\mathrm{i}}^{(+)}(\boldsymbol{r};E)$

† See footnote, p. 198.

at large r; this asymptotic behaviour is difficult to ascertain from (8), however, because in practice it generally is not possible to evaluate explicitly the limit of $\Psi_\mathrm{i}(E+\mathrm{i}\epsilon)$ as $\epsilon\to 0$. To be more specific, note that (8 *a*) and (11 *a*) imply

$$\Phi_\mathrm{i}^{(+)}(\boldsymbol{r};E) = \lim_{\epsilon\to 0}\Phi_\mathrm{i}(\boldsymbol{r};E+\mathrm{i}\epsilon). \tag{20}$$

Then from (8 *b*) and (20) it is difficult to ascertain what parts of $\Phi_\mathrm{i}^{(+)}$ correspond to two-particle collisions, what parts correspond to true three-particle scattering, etc. In fact, for three-body elastic scattering, when plane waves are incident and the Green function G_i in (8 *b*) becomes identical with the free-space Green function (defined below), it even is difficult to see from (8 *b*) and (20) that $\Phi_\mathrm{i}^{(+)}$ can have parts corresponding to propagation in two-body bound states, representing, for example, recombination reactions like (17 *a*).

For these and similar reasons—in configuration space scattering theory—one seeks alternative (to (8)) specifications of $\Psi_\mathrm{i}^{(+)}$, which avoid the necessity for taking the limit $\epsilon\to 0$. Possible specifications of this sort, and their ensuing difficulties, are examined in §§ 2.2 and 2.3, as well as in § 3; the immediately following § 2.1 explains the notation employed and defines various quantities, e.g. the Green functions, more carefully and thoroughly than was convenient in the preceding introductory section.

2.1. *Definitions and notation*

For the three-particle collisions of present interest, in (8) to (10)

$$\psi_\mathrm{i} = \exp\{\mathrm{i}(\boldsymbol{k}_{1\mathrm{i}}\cdot\boldsymbol{r}_1+\boldsymbol{k}_{2\mathrm{i}}\cdot\boldsymbol{r}_2+\boldsymbol{k}_{3\mathrm{i}}\cdot\boldsymbol{r}_3)\} \equiv \exp\{\mathrm{i}\boldsymbol{k}_\mathrm{i}\cdot\boldsymbol{r}\}, \tag{21 a}$$

$$V_\mathrm{i} = V = V_{12}+V_{23}+V_{31}, \tag{21 b}$$

$$H_\mathrm{i} = T = T_1+T_2+T_3 = \sum_\alpha\left(-\frac{\hbar^2}{2m_\alpha}\nabla_\alpha^2\right), \tag{21 c}$$

$$E = \frac{\hbar^2}{2m_1}k_{1\mathrm{i}}^2+\frac{\hbar^2}{2m_2}k_{2\mathrm{i}}^2+\frac{\hbar^2}{2m_3}k_{3\mathrm{i}}^2, \tag{22}$$

$$\mathbf{1} \equiv \delta(\boldsymbol{r}_1-\boldsymbol{r}_1')\,\delta(\boldsymbol{r}_2-\boldsymbol{r}_2')\,\delta(\boldsymbol{r}_3-\boldsymbol{r}_3'), \tag{23}$$

and $G_\mathrm{i}(\lambda)$ is the known (Gerjuoy 1958*a*) free-space Green function $G_F(\lambda)$ for three particles having masses m_1, m_2, m_3. It will prove useful to have $G_F(\lambda)$ for a system of n particles having masses $m_1, m_2, \ldots, m_n$. Namely, for such a system,

$$G_F(\boldsymbol{r};\boldsymbol{r}';\lambda) = \left(\frac{2m_1}{\hbar^2}\right)^{\frac{3}{2}}\cdots\left(\frac{2m_n}{\hbar^2}\right)^{\frac{3}{2}}\frac{\mathrm{i}}{4}\left(\frac{\sqrt{\lambda}}{2\pi}\right)^D\frac{H_D^{(1)}(\sqrt{\lambda}\,|\boldsymbol{\rho}-\boldsymbol{\rho}'|)}{|\boldsymbol{\rho}-\boldsymbol{\rho}'|^D} \tag{24}$$

where

$$D(n) = \tfrac{1}{2}(3n-2), \tag{25 a}$$

$$\left.\begin{aligned} 0 &< \arg\lambda < 2\pi,\\ 0 &< \arg\sqrt{\lambda} < \pi,\end{aligned}\right\} \tag{25 b}$$

$$H_D^{(1)} = J_D+\mathrm{i}N_D \tag{25 c}$$

is the Bessel function of the third kind; the $3n$-dimensional vector $\boldsymbol{r}$ denotes the collection of 3-dimensional vectors $\boldsymbol{r}_1, \ldots, \boldsymbol{r}_n$; and the $3n$-dimensional vector $\boldsymbol{\rho} = (\boldsymbol{\rho}_1, \ldots, \boldsymbol{\rho}_n)$ is defined by

$$\boldsymbol{\rho}_\alpha = \left(\frac{2m_\alpha}{\hbar^2}\right)^{\frac{1}{2}}\boldsymbol{r}_\alpha. \tag{25 d}$$

For arbitrary incident ψ_1 (not necessarily purely plane wave) the 'outgoing' Green function $G_1^{(+)}(E)$, which presumably† satisfies (10 *b*) for real $\lambda = E$, is defined by

$$G_1^{(+)}(\boldsymbol{r};\boldsymbol{r}';E) = \lim_{\epsilon\to 0} G_1(\boldsymbol{r};\boldsymbol{r}';E+\mathrm{i}\epsilon). \tag{26 a}$$

For ψ_1 of (21 *a*), $G_1^{(+)}$ of course is identical with the outgoing free space Green function for a three-particle system

$$G_F^{(+)}(\boldsymbol{r};\boldsymbol{r}';E) = \lim_{\epsilon\to 0} G_F(\boldsymbol{r};\boldsymbol{r}';E+\mathrm{i}\epsilon), \tag{26 b}$$

where G_F is given by (24). Similarly, the outgoing total Green function $G^{(+)}(E)$ in (5) is defined by‡

$$G^{(+)}(E) = \lim_{\epsilon\to 0} G(E+\mathrm{i}\epsilon) \equiv \lim_{\epsilon\to 0} \frac{1}{H-E-\mathrm{i}\epsilon}, \tag{27 a}$$

where $\epsilon > 0$ and, as in (10), for complex λ

$$G(\lambda) = (H-\lambda)^{-1} \tag{27 b}$$

is the unique quadratically integrable solution to

$$(H-\lambda)\, G = \mathbf{1}. \tag{27 c}$$

It is presumed† that $G^{(+)}(E)$ satisfies

$$(H-E)\, G^{(+)}(E) = \mathbf{1}. \tag{27 d}$$

Equations (26) make explicit the fact that the Green functions $G_1^{(+)}(E)$, $G_1^{(+)}(E+\mathrm{i}\epsilon)$, $G^{(+)}(E)$, etc., are operators, i.e. have configuration space representations depending on both primed and unprimed coordinates. On the other hand, the interactions $V_{\alpha\beta}$ and V appearing in, for example, (8 *b*), (9), (14), (21 *b*), etc., are point functions, in that $V_{\alpha\beta}(\boldsymbol{r}) \equiv V_{\alpha\beta}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)$ depends only on unprimed variables. However, because $\boldsymbol{T}(E)$ on the left side of (5) also is an operator, the first term on the right side of (5) cannot be merely a point function. In fact, in (5) and henceforth,

$$V(\boldsymbol{r};\boldsymbol{r}') = V(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}'). \tag{27 e}$$

Except for occasional instances, such as (5), it is an unnecessary complication to work with the operator $\boldsymbol{V}$ rather than the function V. For example, in (5) itself, the $\boldsymbol{r}$, $\boldsymbol{r}'$ element of the second term on the right side is $V(\boldsymbol{r})\, G^{(+)}(\boldsymbol{r};\boldsymbol{r}')\, V(\boldsymbol{r}')$, where no integration over $\boldsymbol{r}$ or $\boldsymbol{r}'$ is implied; it is

† It is not obvious that $G^{(+)}(E)$ defined by (27 *a*) satisfies (27 *d*), because demonstrating (27 *d*) from (27 *a*) and (27 *c*) involves the demonstration that interchange of the order of differentiation and limit $\epsilon \to 0$ is justified. Clearly such interchange need not be valid, e.g.

$$\frac{\mathrm{d}}{\mathrm{d}r}\left\{\lim_{\epsilon\to 0} \epsilon \sin\left(\frac{r}{\epsilon}\right)\right\} \neq \lim_{\epsilon\to 0}\left\{\frac{\mathrm{d}}{\mathrm{d}r}\,\epsilon \sin\left(\frac{r}{\epsilon}\right)\right\}.$$

Similarly, it is not obvious that $\Psi_1^{(+)}(E)$ defined by (8 *a*) satisfies (7). Nevertheless, on physical grounds, it appears unlikely that either $G(E+\mathrm{i}\epsilon)$ or $\Psi_1(E+\mathrm{i}\epsilon)$ becomes so wildly a fluctuating function of $\boldsymbol{r}$ as $\epsilon \to 0$ that interchange of order of differentiation and $\lim \epsilon \to 0$ becomes unjustified. In any event, excluding exceptional energies E (see footnote ‡, p. 201), the theorem that $\Psi_1^{(+)}(E)$ exists and satisfies (7) apparently is proved in §§ 8 and 9 of Faddeev (1965), subject to some probably inessential restrictions concerning the number of discrete eigenvalues of the associated two-particle Hamiltonians $T_1 + T_2 + V_{12}$, etc. (in their individual two-particle centre of mass systems). Under the same restrictions, moreover, $G^{(+)}(E)$ apparently exists and satisfies (27 *d*). However, I shall not pretend that I have completely mastered all the intricacies and implications of Faddeev's mathematics.

‡ See footnote ‡, p. 201.

equally correct, but obviously pointless, to express this same term on the right side of (5) as $VG^{(+)}V$, whose $\boldsymbol{r}$, $\boldsymbol{r}'$ element consistent with operator notation is

$$\langle \boldsymbol{r}|\, VG^{(+)}V\,|\boldsymbol{r}'\rangle = \int \mathrm{d}\boldsymbol{r}''\,\mathrm{d}\boldsymbol{r}'''\, V(\boldsymbol{r};\boldsymbol{r}'')\, G^{(+)}(\boldsymbol{r}'';\boldsymbol{r}''')\, V(\boldsymbol{r}''';\boldsymbol{r}'), \tag{27f}$$

where integration over the intermediate variables $\boldsymbol{r}''$, $\boldsymbol{r}'''$ now is implied.

Expressions in the centre of mass system tend to be rather more complicated and awkward than in the laboratory system; correspondingly, it is difficult to devise a wholly satisfactory centre of mass system notation. I shall use

$$\boldsymbol{R} = M^{-1}(m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2 + m_3\boldsymbol{r}_3), \tag{28a}$$

$$M = m_1 + m_2 + m_3, \tag{28b}$$

$$\boldsymbol{K} = \boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3, \tag{28c}$$

$$\bar{E} = E - \hbar^2K^2/2M. \tag{28d}$$

Equation (28d) for the centre of mass energy $\bar{E}$ illustrates the previously explained† procedure for symbolizing corresponding quantities in the centre of mass and laboratory systems. I also shall employ

$$\boldsymbol{R}_{12} = \frac{m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2}{m_1 + m_2} = \boldsymbol{R}_{21}, \tag{29a}$$

$$\boldsymbol{q}_{23} = \boldsymbol{r}_1 - \boldsymbol{R}_{23} = \boldsymbol{r}_{12} + \frac{m_3}{m_2 + m_3}\boldsymbol{r}_{23} = \boldsymbol{q}_{32}, \tag{29b}$$

$$\begin{aligned}\boldsymbol{K}_{31} &= M^{-1}[(m_3 + m_1)\,\boldsymbol{k}_2 - m_2(\boldsymbol{k}_3 + \boldsymbol{k}_1)] \\ &= \boldsymbol{k}_2 - \frac{m_2}{M}\boldsymbol{K} = \boldsymbol{K}_{13},\end{aligned} \tag{29c}$$

$$\begin{aligned}\boldsymbol{k}_{23} &= \frac{m_3}{m_2 + m_3}\boldsymbol{k}_2 - \frac{m_2}{m_2 + m_3}\boldsymbol{k}_3 = \boldsymbol{K}_{31} + \frac{m_2}{m_2 + m_3}\boldsymbol{K}_{23} \\ &= -\left(\boldsymbol{K}_{12} + \frac{m_3}{m_2 + m_3}\boldsymbol{K}_{23}\right) = -\boldsymbol{k}_{32},\end{aligned} \tag{29d}$$

$$\mu_{12} = \frac{m_1 m_2}{m_1 + m_2} = \mu_{21}, \tag{29e}$$

$$\mu_{2R} = \frac{m_2(m_3 + m_1)}{M}, \tag{29f}$$

and permutations thereof, which—to avoid error—are best performed cyclically. Quantities like $\boldsymbol{K}$ of (28c) and $\boldsymbol{K}_{31}$ of (29c) should have† subscripts i, f distinguishing between initial and final values; however, to keep the notation as uncomplicated as possible, in what follows the subscripts i, f will be dropped whenever doing so can cause no confusion. It is readily confirmed that $\hbar\boldsymbol{k}_{12}/\mu_{12}$ equals the (classical) relative velocity $\boldsymbol{v}_1 - \boldsymbol{v}_2$ between particles 1 and 2, and that $\hbar\boldsymbol{K}_{12}/\mu_{3R}$ equals the velocity of particle 3 relative to the velocity of the centre of mass of particles 1 and 2; alternatively, $\hbar\boldsymbol{K}_{12}/m_3$ equals the velocity of 3 relative to (the velocity of) the centre of mass of the entire three-particle system.

† See footnote, p. 199.

The kinetic energy operator $\overline{T}$ in the centre of mass system is given in terms of T, (16), by

$$T = -(\hbar^2/2M)\nabla_R^2 + \overline{T}, \tag{30}$$

where, when $\boldsymbol{R}$, $\boldsymbol{r}_{31}$, $\boldsymbol{r}_{23}$ are the new variables replacing $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, $\boldsymbol{r}_3$

$$\overline{T} = -\frac{\hbar^2}{2\mu_{31}}\nabla_{31}^2 - \frac{\hbar}{2\mu_{23}}\nabla_{23}^2 + \frac{\hbar^2}{m_3}\boldsymbol{\nabla}_{31}\cdot\boldsymbol{\nabla}_{23} \tag{31a}$$

on the understanding that $\boldsymbol{\nabla}_{31}$ denotes the gradient with respect to $\boldsymbol{r}_{31}$, while $\boldsymbol{\nabla}_{23}$ denotes the gradient with respect to $\boldsymbol{r}_{23}$. If $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, $\boldsymbol{r}_3$ are replaced by $\boldsymbol{R}$, $\boldsymbol{r}_{31}$, $\boldsymbol{q}_{31}$, the same operator $\overline{T}$ takes the diagonal form

$$\overline{T} = -\frac{\hbar^2}{2\mu_{31}}\nabla_{31}^2 - \frac{\hbar^2}{2\mu_{2R}}\nabla_{q31}^2, \tag{31b}$$

where $\boldsymbol{\nabla}_{q31}$ denotes the gradient with respect to $\boldsymbol{q}_{31}$. The centre of mass system Hamiltonian of course is

$$\overline{H} = \overline{T} + V = \overline{T} + V_{12} + V_{23} + V_{31} \tag{32a}$$

and the centre of mass system Schrödinger equation is

$$(\overline{H} - \bar{E})\,\overline{\Psi} = 0. \tag{32b}$$

The desired solution to (32b) describing the actual physical situation in the centre of mass system can be written in the form (11b), where the incident wave $\overline{\psi}_i$ in the centre of mass system is defined by

$$\psi_i = \exp\{i\boldsymbol{K}\cdot\boldsymbol{R}\}\,\overline{\psi}_i \tag{33a}$$

which makes $$\overline{\psi}_i(\bar{E}) = \exp\{i(\boldsymbol{K}_{31}\cdot\boldsymbol{r}_{23} - \boldsymbol{K}_{23}\cdot\boldsymbol{r}_{31})\} = \exp\{i(\boldsymbol{K}_{31}\cdot\boldsymbol{q}_{31} + \boldsymbol{k}_{31}\cdot\boldsymbol{r}_{31})\} \tag{33b}$$

and cyclical permutations thereof. Evidently, corresponding to (9)

$$(\overline{H}_i - \bar{E})\,\overline{\psi}_i \equiv (\overline{T} + V - V_i - \bar{E})\,\overline{\psi}_i = 0. \tag{33c}$$

Moreover, $\overline{\Psi}_i^{(+)}$ is specified by the analogues of (8). Specifically,†

$$\overline{\Psi}_i^{(+)}(\bar{E}) = \lim_{\epsilon\to 0}\overline{\Psi}_i(\bar{E} + i\epsilon) = \lim_{\epsilon\to 0}[\overline{\psi}_i(\bar{E}) + \overline{\Phi}_i(\bar{E} + i\epsilon)], \tag{34a}$$

where, for $\epsilon > 0$, $\overline{\Psi}_i(\bar{E} + i\epsilon)$ is the unique bounded solution to

$$\overline{\Psi}_i(\bar{E} + i\epsilon) = \overline{\psi}_i(\bar{E}) - \frac{1}{\overline{H}_i - \bar{E} - i\epsilon}V_i\,\overline{\Psi}_i(\bar{E} + i\epsilon). \tag{34b}$$

In (33b) and other preceding equations

$$\bar{E} = \frac{\hbar^2}{2\mu_{31}}K_{23}^2 + \frac{\hbar^2}{2\mu_{23}}K_{31}^2 + \frac{\hbar^2}{m_3}\boldsymbol{K}_{23}\cdot\boldsymbol{K}_{31} = \frac{\hbar^2}{2\mu_{31}}k_{31}^2 + \frac{\hbar^2}{2\mu_{2R}}K_{31}^2. \tag{35}$$

The above definitions, taken together with (54) to (55) below, make believable—and go a long way toward establishing—the simple rule (illustrated by (33) and (34)) that the centre of mass analogue of any formal relation between Ψ_i, ψ_i, G, E, etc., is obtainable simply by barring these laboratory system quantities. However, because they are so important, I shall write down explicitly the definitions of some of the centre of mass system Green functions. In particular, for complex λ, the centre of mass system total Green function

$$\overline{G}(\lambda) = (\overline{H} - \lambda)^{-1} \tag{36a}$$

† See footnote ‡, p. 201 and footnote †, p. 208.

is the unique quadratically integrable solution to

$$(\bar{H}-\lambda)\,\bar{G}(\lambda) = \bar{\mathbf{1}}, \tag{36b}$$

where the unit operator $\bar{\mathbf{1}}$ in the centre of mass system is defined by

$$\mathbf{1} = \delta(\boldsymbol{R}-\boldsymbol{R}')\,\bar{\mathbf{1}}, \tag{37}$$

i.e. $\bar{\mathbf{1}}$ denotes the unit operator in that six-dimensional subspace—of the nine-dimensional space spanned by $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, $\boldsymbol{r}_3$—which is orthogonal to $\boldsymbol{R}$ (for a more precise delineation of this subspace see appendix F). Similarly, in (34*b*)

$$\bar{G}_1(\lambda) = (\bar{H}_1-\lambda)^{-1} \tag{38a}$$

satisfies

$$(\bar{H}_1-\lambda)\,\bar{G}_1 = \bar{\mathbf{1}}. \tag{38b}$$

The centre of mass system outgoing Green function associated with the total Hamiltonian is†

$$\bar{G}^{(+)}(\bar{E}) = \lim_{\epsilon\to 0}\bar{G}(\bar{E}+\mathrm{i}\epsilon). \tag{39a}$$

Correspondingly, the centre of mass system outgoing initial Green function is

$$\bar{G}_1^{(+)}(\bar{E}) = \lim_{\epsilon\to 0}\bar{G}_1(\bar{E}+\mathrm{i}\epsilon). \tag{39b}$$

It is also useful to note that the Jacobians of relevant transformations—e.g. from laboratory frame to centre of mass frame, or between various sets of centre of mass frame coordinates—typically have magnitude unity. Thus

$$\mathrm{d}\boldsymbol{r} \equiv \mathrm{d}\boldsymbol{r}_1\,\mathrm{d}\boldsymbol{r}_2\,\mathrm{d}\boldsymbol{r}_3 = \mathrm{d}\boldsymbol{R}\,\mathrm{d}\tilde{\boldsymbol{r}}, \tag{40a}$$

$$\mathrm{d}\tilde{\boldsymbol{r}} \equiv \mathrm{d}\boldsymbol{r}_{31}\,\mathrm{d}\boldsymbol{r}_{23} = \mathrm{d}\boldsymbol{r}_{12}\,\mathrm{d}\boldsymbol{r}_{31} = \mathrm{d}\boldsymbol{r}_{12}\,\mathrm{d}\boldsymbol{q}_{12}, \quad \text{etc.} \tag{40b}$$

Correspondingly, in (37)

$$\begin{aligned}\bar{\mathbf{1}} &= \delta(\boldsymbol{r}_{31}-\boldsymbol{r}'_{31})\,\delta(\boldsymbol{r}_{23}-\boldsymbol{r}'_{23}) = \delta(\boldsymbol{r}_{12}-\boldsymbol{r}'_{12})\,\delta(\boldsymbol{r}_{31}-\boldsymbol{r}'_{31})\\ &= \delta(\boldsymbol{r}_{12}-\boldsymbol{r}'_{12})\,\delta(\boldsymbol{q}_{12}-\boldsymbol{q}'_{12}), \quad \text{etc.}\end{aligned} \tag{41}$$

Equations (31*b*) and (41) now show that—for the incident $\bar{\psi}_1$ of (33*b*)—the explicit form of $\bar{G}_1^{(+)} \equiv \bar{G}_F^{(+)}$ in the $\boldsymbol{r}_{31}$, $\boldsymbol{q}_{31}$ representation is found from the free space Green function (24) for a system of two particles having masses μ_{31}, μ_{2R} (associated with the coordinates $\boldsymbol{r}_{31}$, $\boldsymbol{q}_{31}$ respectively).

2.2. *The outgoing boundary condition*

I now return to the problem of finding useful—from the standpoint of configuration space scattering theory—specifications of $\Psi_1^{(+)}$, namely specifications which avoid the limit $\epsilon\to 0$. This section will be concerned only with possible specifications of this sort which start from the Lippmann–Schwinger equation for $\Psi_1^{(+)}$, but which then attempt to modify it appropriately (e.g. after iteration). Possible specifications of $\Psi_1^{(+)}$ based on the behaviour of $G^{(+)}(\boldsymbol{r};\boldsymbol{r}')$ as the source $\boldsymbol{r}'$ moves to infinity are examined in § 3. For the reason explained in the previous section following (35), it seems clear that corresponding laboratory and centre of mass frames formulations cannot be essentially inconsistent, although there are the complications (mentioned in § 1 and discussed in § 4.1) associated with the $\delta(\boldsymbol{K}_f-\boldsymbol{K}_1)$ factor appearing in the laboratory system matrix element $\langle \mathrm{f}|\,\boldsymbol{T}\,|\mathrm{i}\rangle$. In the remainder of this work, therefore, especially in § 3 and the rest of the present section, the analysis and discussion often will refer predominantly to the laboratory

† See footnote ‡, p. 201 and footnote †, p. 208.

(or centre of mass) system because application to the centre of mass (or laboratory) system is immediate. When there is no special reason for favouring one frame over the other, the discussion usually will refer to the laboratory frame, mainly with a view toward minimizing notational complexity.

The most obvious means of avoiding the limit $\epsilon \to 0$ in the specification of $\Psi_i^{(+)}(E)$ is to replace $(H_i - E - i\epsilon)^{-1}$ in (8 *b*) by the outgoing initial Green function $G_i^{(+)}$ defined in (26 *a*). In other words (writing in detail the operations implied by the condensed operator notation employed in (8 *b*)), (8 *b*) is replaced by

$$\Psi_i^{(+)}(\boldsymbol{r}; E) = \psi_i(\boldsymbol{r}) - \int d\boldsymbol{r}' G_i^{(+)}(\boldsymbol{r}; \boldsymbol{r}'; E) V_i(\boldsymbol{r}') \Psi_i^{(+)}(\boldsymbol{r}'; E). \tag{42}$$

Although (42) does indeed avoid the limit $\epsilon \to 0$, it is by no means evident that (42) is a valid alternative to (8), i.e. it is by no means evident that a solution $\Psi_i^{(+)}(E)$ to (42) need be identical with the solution $\Psi_i^{(+)}(E)$ specified by (8). The reason there is some question concerning the equivalence of (8) and (42) is that in effect (42) has been obtained by interchanging the order of integration and limit as $\epsilon \to 0$ in (8 *b*). To be specific, the integral on the right side of (42) is

$$\int d\boldsymbol{r}' \{\lim_{\epsilon \to 0} G_i(\boldsymbol{r}; \boldsymbol{r}'; E + i\epsilon)\} V_i(\boldsymbol{r}') \{\lim_{\epsilon \to 0} \Psi(\boldsymbol{r}'; E + i\epsilon)\}. \tag{43 a}$$

Therefore $\Psi_i^{(+)}$ from (42) is identical with $\Psi_i^{(+)}$ from (8) only if

$$\lim_{\epsilon \to 0} \int d\boldsymbol{r}' G_i(\boldsymbol{r}; \boldsymbol{r}'; E + i\epsilon) V_i(\boldsymbol{r}') \Psi_i(\boldsymbol{r}'; E + i\epsilon)$$
$$= \int d\boldsymbol{r}' \lim_{\epsilon \to 0} \{G_i(\boldsymbol{r}; \boldsymbol{r}'; E + i\epsilon) V_i(\boldsymbol{r}') \Psi_i(\boldsymbol{r}'; E + i\epsilon)\}. \tag{43 b}$$

I shall discuss the question of the validity of (43 *b*) later in this section. In the meantime I note that—whether or not the equality (43 *b*) holds for the functions $\Psi_i(E + i\epsilon)$ appearing in (8)—equation (42) cannot be a satisfactory specification of the desired solution $\Psi_i^{(+)}$ to (7) describing the actual collision of three initially free particles, because it is known (Gerjuoy 1958*b*; Foldy & Tobocman 1957)—and is demonstrated in § A.9.2 of appendix A—that the function $\Psi_i^{(+)}$ defined by (8) generally will not be the only solution to (42) when particle rearrangements (e.g. reaction (18 *a*)) can occur. In other words, as Faddeev (1961) stresses, without imposition of additional requirements, for instance the boundary condition that the scattered part $\Phi_i^{(+)}$ of $\Psi_i^{(+)}$ be 'outgoing', (42) does not suffice to determine $\Psi_i^{(+)}(E)$ in collisions of present interest, even though (8 *b*) does have a unique solution $\Psi_i(E + i\epsilon)$ for every $\epsilon > 0$. There is no need here to discuss the by now well-known formal mathematical reasons (Watson & Nuttall 1967; Weinberg 1964; Lovelace 1964)—associated with the fact that the kernel of the Lippmann–Schwinger equation is not of the Hilbert–Schmidt type—underlying the failure of (42) to have unique solutions.

In potential scattering, where (42) is satisfactory because rearrangements cannot occur, use of the 'everywhere outgoing' boundary condition enables replacement of (42) by an explicit formula for $\Psi_i^{(+)}$ (not an integral equation), of course still avoiding the awkward limit $\epsilon \to 0$. The generalization, to many-particle collisions, of this potential scattering procedure for specifying $\Psi_i^{(+)}$ is not wholly obvious, but has been expounded in the literature (Gerjuoy 1958*b*). In particular, it can be proved (see § A. 9.1) that $\Phi_i^{(+)}$ defined by (11 *a*) is given by

$$\Phi_i^{(+)}(\boldsymbol{r}) = -\int d\boldsymbol{r}' G^{(+)}(\boldsymbol{r}; \boldsymbol{r}'; E) V_i(\boldsymbol{r}') \psi_i(\boldsymbol{r}') \equiv -G^{(+)} V_i \psi_i. \tag{44 a}$$

provided the surface integral over the sphere at infinity in the nine-dimensional $\boldsymbol{r}$-space

$$\mathscr{I}(G^{(+)}, \Phi_i^{(+)}) = \int \mathrm{d}\boldsymbol{S} \,.\, \boldsymbol{W}[G^{(+)}(\boldsymbol{r}; \boldsymbol{r}'), \Phi_i^{(+)}(\boldsymbol{r})] = 0 \qquad (44\,b)$$

for all $\boldsymbol{r}'$. In (44), $G^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$ is the configuration space representation of the laboratory system outgoing total Green function defined by (27), while $\boldsymbol{W}$ is a nine-dimensional vector, whose components (along the same unit vectors as the components of $\boldsymbol{r}_\alpha$) are defined by

$$W_\alpha[X, Y] = (\hbar^2/2m_\alpha)\,(X\nabla_\alpha Y - Y\nabla_\alpha X). \qquad (45\,a)$$

In terms of $\boldsymbol{W}$, the Green theorem in $\boldsymbol{r}$-space (the nine-dimensional configuration space) is

$$\int \mathrm{d}\boldsymbol{r} \sum_\alpha \frac{\hbar^2}{2m_\alpha}(X\nabla_\alpha^2 Y - Y\nabla_\alpha^2 X) \equiv -\int \mathrm{d}\boldsymbol{r}(XTY - YTX) = \int_\infty \mathrm{d}\boldsymbol{S} \,.\, \boldsymbol{W}[X, Y]. \qquad (45\,b)$$

Of course, (44 *a*), taken together with (11 *a*), is the laboratory system version of the previously quoted (13).

It can be shown that if (44 *b*) holds then (44 *a*) must hold, and conversely. Moreover, (44 *b*) will be satisfied if $\Phi_i^{(+)}(\boldsymbol{r})$ actually has the same asymptotic behaviour at infinity in $\boldsymbol{r}$-space as does $G^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$. Consequently the condition (44 *b*) appears to be the desired generalization, to many-particle collisions, of the 'everywhere outgoing' condition which prescribes $\Phi_i^{(+)}$ in the case of potential scattering. Correspondingly, because (44 *a*) is a formula, not an integral equation, for $\Phi_i^{(+)}$ in terms of ψ_i, imposition of the condition (44 *b*) indeed uniquely specifies the desired $\Psi_i^{(+)}$ of (11 *a*). Of course, in a sense terming (44 *a*) a 'formula' for $\Phi_i^{(+)}$ is a misnomer, since the total Green function $G^{(+)}$ in (44 *a*) generally is not known in a closed form; in fact, to actually obtain $G^{(+)}$, the Lippmann–Schwinger equation for $G^{(+)}$ in terms of $G_i^{(+)}$ normally would be employed (Watson & Nuttall 1967). Nevertheless, mainly because the asymptotic behaviour of the outgoing $G^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$ as $\boldsymbol{r} \to \infty$ is less complicated and more easily visualized than the corresponding behaviour of $\Phi_i^{(+)}(\boldsymbol{r})$, one can hope that—by being a formula for $\Phi_i^{(+)}(\boldsymbol{r})$ in terms of $G^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$—(44 *a*) has simplified the task of ascertaining the limit of $\Phi_i^{(+)}(\boldsymbol{r})$ as $\boldsymbol{r} \to \infty$. This hope is not unjustified, as subsequent sections discussing modifications of (44 *a*) will show. As they stand, however, (44) do not furnish a satisfactory procedure for specifying $\Psi_i^{(+)}$, by virtue of two not unrelated difficulties. In the first place, (44 *b*) can hold even though $\Phi_i^{(+)}$ has incoming parts. That is to say, the 'outgoing condition' (44 *b*), though it does uniquely specify a solution $\Psi_i^{(+)}$ of (7), does not necessarily guarantee that the scattered part of $\Psi_i^{(+)}$ is 'everywhere outgoing', i.e. has no incoming parts; more particularly, (44 *b*) does not necessarily guarantee that $\Phi_i^{(+)}$ has the same asymptotic behaviour at infinity as does $G^{(+)}$. In the second place, and more seriously, the integral (44 *a*) can be divergent, in which event the proof that (44) yield a formula for $\Phi_i^{(+)}(\boldsymbol{r})$ breaks down. Moreover, even if one assumes that the proof somehow can be fixed up, specification of $\Psi_i^{(+)}$ via a divergent integral (44 *a*) must be considered unsatisfactory unless the divergence is so readily removable that it causes no real difficulties, as, for example, when it can be regarded as a consequence of total momentum conservation, removable merely by formulating the collision in the centre of mass frame.

As a matter of fact, the divergence of the integral (44 *a*) is not readily removable when ψ_i is given by (21 *a*), and when bound two-particle states $u_j(\boldsymbol{r}_{\alpha\beta})$ can exist (see § A. 4). The divergence is manifested by terms—in the laboratory or centre of mass versions of (44 *a*)—which behave like δ-functions. Actually, these δ-functions vanish on the energy shell, i.e. the centre of mass

version of (44 *a*) is not an unbounded integral. More particularly, whenever, for example, a bound state $u_j(\boldsymbol{r}_{12})$ can propagate† at energy E, the integral (to be compared with (44 *a*))

$$-\int \mathrm{d}\boldsymbol{r}' G^{(+)}(\boldsymbol{r};\boldsymbol{r}';E)\,V_1(\boldsymbol{r}')\,\psi_1(\boldsymbol{r}';E') \equiv -G^{(+)}(E)\,V_1\psi_1(E') \tag{46}$$

contains an $\boldsymbol{r}$-dependent term proportional to

$$\delta[\sqrt{(E-\epsilon_j)}-\sqrt{\{E'-(\hbar^2k_{12}'^2/2\mu_{12})\}}]. \tag{47}$$

In the above equations, which have made use of (28 *d*) and (35), $\psi_1(\boldsymbol{r}';E')$ is given by (21 *a*), but E'—defined by (22) in terms of the components of $\boldsymbol{k}_1' \equiv \boldsymbol{k}'$—is not necessarily equal to the energy E characterizing the Green function $G^{(+)}(E)$. Also, the bound state eigenfunction $u_j(\boldsymbol{r}_{12})$ satisfies

$$\left(\frac{-\hbar^2}{2\mu_{12}}\nabla_{12}^2+V_{12}-\epsilon_j\right)u_j(\boldsymbol{r}_{12}) = 0. \tag{48}$$

Because ϵ_j is intrinsically negative, the δ-function (47) assuredly vanishes on the energy shell $E' = E > 0$, where (46) reduces to the integral (44 *a*) for $\Phi_1^{(+)}(\boldsymbol{r};E)$. Similar (vanishing on the energy shell) δ-functions occur in (46)—though not in its centre of mass version—whenever three-body bound states $u_j(\boldsymbol{r}_{12};\boldsymbol{r}_{23})$ exist‡ (see § A 5). It is easily seen (§ A 6) that the argument of the centre of mass analogue of (47)—or equivalently, the argument of the δ-function (47) when conservation of total momentum $\boldsymbol{K}' = \boldsymbol{K}$ is postulated—vanishes when the unprimed and primed speeds of particle 3 relative to the centre of mass of particles 1 and 2 are equal, a result which seems quite reasonable physically.

Although the δ-function (47) vanishes on the energy shell, nevertheless the demonstration that terms such as (47) occur in (46) is very relevant to the validity and utility of the admittedly on-shell formula (44 *a*) for $\Psi_1^{(+)}$. In particular, the result (47) means that the formula (44 *a*)—or its centre of mass version implied by (11 *b*) and (13)—necessarily involves a non-convergent oscillatory integral whenever two-particle bound states exist for any particle pair α, β. Moreover, because many such bound states can exist, the integral (44 *a*)—and its centre of mass version—generally cannot be made convergent in a simple fashion, e.g. by factoring out or subtracting away a δ-function. In addition, these δ-functions (47), though possessing physically quite reasonable arguments as has just been pointed out, appear to be wholly non-physical consequences of the invalid (see also the immediately following paragraphs) mathematical manipulations employed to deduce (44 *a*); it will be shown in § 2.3 below that (44 *a*) for $\Phi_1^{(+)}$ can be replaced by a formula which—while still avoiding the awkward limit $\epsilon \to 0$—expresses $\Phi_1^{(+)}$ in terms of integrals assuredly convergent on the energy shell, and at worst logarithmically divergent off the energy shell, even when two-body bound states exist; in the centre of mass version of the formula developed in § 2.3, integrals remain convergent on the energy shell even if three-body as well as two-body bound states exist. Correspondingly, using (44 *a*) (or its centre of mass version) to determine the asymptotic behaviour of $\Phi_1^{(+)}(\boldsymbol{r})$ at large distances, or to evaluate scattering amplitude integrals involving $\Psi_1^{(+)}(\boldsymbol{r})$, well might result in predicted scattering coefficients which are non-physically divergent or otherwise erroneous. It also is noteworthy that

† With E regarded as a parameter not necessarily > 0, the condition for $u_j(\boldsymbol{r}_{12})$ to propagate, i.e. to reach infinity relative to particle 3, is of course $E-\epsilon_j > 0$.

‡ It is supposed that the energy ϵ_j of the three-body state is < 0. If there ever should be any need to consider (perhaps very long-lived) three-body or two-body states u_j having energy $\epsilon_j > 0$, the assertion referenced—and similar assertions throughout the text—will remain valid provided 'exist' is replaced by 'can propagate', see preceding footnote, this page.

these δ-functions (47) can make non-vanishing (finite or infinite) contributions to (44 *a*) when $\Phi_i^{(+)}(\boldsymbol{r})$ is estimated from an approximate estimate of $G^{(+)}(\boldsymbol{r};\boldsymbol{r}';E)$, even though such non-physical contributions assuredly vanish on the energy shell when the exact $G^{(+)}(E)$ is employed. To put it differently and more generally, use of formally non-convergent expressions like (44 *a*) is dangerous because approximate numerical computations starting from such expressions can produce large contributions from terms which in exact calculation are small or otherwise non-contributing.

I conclude that, for incident waves ψ_i of (21 *a*), specifying $\Psi_i^{(+)}$ via (44) is just as unsatisfactory as specification via (42). I add that from the proof yielding (44) one readily sees that whenever the volume integral (44 *a*) contains δ-functions of the type discussed in the preceding paragraph, the surface integral (44 *b*) contains non-vanishing terms dependent on the radius of the spherical surface at infinity in $\boldsymbol{r}$-space. Therefore, for incident waves ψ_i of (21 *a*) when bound-states can exist, the relation (44 *b*) is neither a meaningful nor a useful statement of the sought-for boundary conditions presumably specifying the desired solution $\Psi_i^{(+)}$ to (7). It follows, still for incident waves ψ_i of (21 *a*), that it generally is impossible (not merely impractical) to employ (44 *b*) to eliminate unwanted solutions of (42).

I now observe that the divergence—and consequent lack of utility—of the integral (44 *a*) can be associated with an unjustified interchange of order of integration and limit $\epsilon \to 0$. To be specific, (8 *b*) implies $\psi_i(E+i\epsilon)$ is the unique solution to the differential equation

$$(H_i - E - i\epsilon)\,\Psi_i = (H_i - E - i\epsilon)\,\psi_i - V_i\,\Psi_i \tag{49 a}$$

which, using (9), can be rewritten in the alternative forms

$$(H - E - i\epsilon)\,\Psi_i = -i\epsilon\psi_i, \tag{49 b}$$

$$(H_i - E - i\epsilon)\,\Phi_i = -V_i\,\Psi_i, \tag{49 c}$$

$$(H - E - i\epsilon)\,\Phi_i = -V_i\,\psi_i, \tag{49 d}$$

where $\Phi_i \equiv \Phi_i(E+i\epsilon)$ defined by (8 *a*). Equation (49 *c*) obviously yields our original starting-point (8 *b*). Equation (49 *d*), however, implies one also can write

$$\Phi_i(E+i\epsilon) = -\frac{1}{H-E-i\epsilon}V_i\psi_i(E), \tag{50 a}$$

where $\psi_i(E)$, the incident wave of (8) and (21 *a*), does not depend on ϵ. Writing in detail the operations implied by the condensed operator notation, (50 *a*) becomes

$$\Phi_i(\boldsymbol{r};E+i\epsilon) = -\int d\boldsymbol{r}'\,G(\boldsymbol{r};\boldsymbol{r}';E+i\epsilon)\,V_i(\boldsymbol{r}')\,\psi_i(\boldsymbol{r}',E). \tag{50 b}$$

Therefore, recalling (20) and (27), $\Psi_i^{(+)}$ obtained from the formula (44 *a*) will be identical with the 'true' $\Psi_i^{(+)}$ defined by (8 *a*) only if

$$\lim_{\epsilon\to 0}\int d\boldsymbol{r}'\,G(\boldsymbol{r};\boldsymbol{r}';E+i\epsilon)\,V_i(\boldsymbol{r}')\,\psi_i(\boldsymbol{r}') = \int d\boldsymbol{r}'\lim_{\epsilon\to 0}\{G(\boldsymbol{r};\boldsymbol{r}';E+i\epsilon)\,V_i(\boldsymbol{r}')\,\psi_i(\boldsymbol{r}')\}, \tag{51 a}$$

i.e. only if (in condensed notation)

$$\lim_{\epsilon\to 0}\{G(E+i\epsilon)\,V_i\psi_i\} = \{\lim_{\epsilon\to 0}G(E+i\epsilon)\}V_i\psi_i. \tag{51 b}$$

In other words, the assertion that (44 *a*) specifies the desired $\Phi_i^{(+)}$ is equivalent to asserting that it is legitimate to interchange the order of integration and limit $\epsilon \to 0$ in the left sides of (51 *a*) or (51 *b*), which furnish our original and correct (though not useful) specification of $\Phi_i^{(+)}(E)$. But it already has been explained that the integrals on the right sides of (51) are divergent when ψ_i is given by (21 *a*) and when there exist bound two-particle or three-particle states. On the other hand, the limits $\epsilon \to 0$ on the left sides of (51) presumably exist, since otherwise—recalling (20) and (50 *b*)—our original specification of $\Psi_i^{(+)}(E)$ via (8) would not have been meaningful. It follows that (51 *a*) cannot hold when bound two-particle or three-particle states can occur, because in these circumstances the limit $\epsilon \to 0$ on the right side of (51 *a*) yields a non-convergent integral (i.e. does not exist), whereas the limit $\epsilon \to 0$ on the left side of (51 *a*) presumably always exists. The incorrect conclusion that $\Phi_i^{(+)}(\boldsymbol{r})$ contains δ-function contributions vanishing on the energy shell results from insistence on the validity of (51 *a*), i.e. insistence that (44 *a*) is a valid formula for $\Phi_i^{(+)}$, in circumstances (existence of bound states) when (51 *a*) in fact is invalid.

It is worth noting that the previous paragraph implies the customarily employed relation

$$V\Psi_i^{(+)}(E) = V[\psi_i - G^{(+)}(E)\, V\psi_i] = [V - VG^{(+)}(E)\, V]\,\psi_i = \boldsymbol{T}(E)\,\psi_i, \tag{51 c}$$

following from (5) and (44 *a*), fails (in configuration space, at any rate) for $\psi_i \equiv \psi_i(E)$ of (21 *a*) whenever bound two-particle or three-particle states exist. Alternatively, because the right side of (51 *c*) involves the integral (44 *a*), the relation

$$\lim_{\epsilon \to 0} \{\boldsymbol{T}(E + i\epsilon)\, \psi_i(E)\} = \{\lim_{\epsilon \to 0} \boldsymbol{T}(E + i\epsilon)\}\, \psi_i(E) \tag{51 d}$$

can be expected to hold in configuration space only when neither bound two-particle states nor bound three-particle states can occur; in (51 *d*) the definition of $\boldsymbol{T}(E + i\epsilon)$ is given by (5), except that $G(E + i\epsilon)$ replaces $G^{(+)}(E)$. Similar assertions pertain to the centre of mass frame wherein, however, the occurrence of three-particle bound states is irrelevant. Note further that when bound states occur, the above considerations do not necessarily rule out the possible validity of (51 *c*) and/or (51 *d*) in the momentum representation, where different integrals are involved.

That (51 *a*) is invalid when bound states occur has been made clear; whether it is valid when bound states do not occur is less clear. In the absence of bound states the integrals

$$\Phi_i^{(+)}(\boldsymbol{r}) = -\int d\boldsymbol{r}' \{G^{(+)}(\boldsymbol{r}; \boldsymbol{r}'; E)\, [V_{12}(\boldsymbol{r}'_{12}) + V_{23}(\boldsymbol{r}'_{23}) + V_{31}(\boldsymbol{r}'_{31})] \exp [i(\boldsymbol{k}_1 . \boldsymbol{r}'_1 + \boldsymbol{k}_2 . \boldsymbol{r}'_2 + \boldsymbol{k}_3 . \boldsymbol{r}'_3)]\} \tag{52 a}$$

$$\bar{\Phi}_i^{(+)}(\bar{\boldsymbol{r}}) = -\int d\bar{\boldsymbol{r}}' \{\bar{G}^{(+)}(\bar{\boldsymbol{r}}; \bar{\boldsymbol{r}}'; \bar{E})\, [V_{12}(\boldsymbol{r}'_{12}) + V_{23}(\boldsymbol{r}'_{23}) + V_{31}(\boldsymbol{r}'_{31})] \exp [i(\boldsymbol{K}_{31} . \boldsymbol{r}'_{23} - \boldsymbol{K}_{23} . \boldsymbol{r}'_{31})]\}, \tag{52 b}$$

expressing respectively (44 *a*) and its centre of mass version for ψ_i of (21 *a*), do converge (see §§ A. 5 and A. 6). On the other hand, the convergence of the integral on the right side of (51 *a*) is by no means mathematically sufficient to imply that (51 *a*) holds. In general (see § A. 8), guaranteeing (51 *a*) requires proving that the sequence of infinite integrals on the left side of (51 *a*) converges uniformly (Whittaker & Watson 1946) as $\epsilon \to 0$, a property not easily demonstrated. It can be argued, however (see § A. 8) that—for Green functions and wavefunctions actually occurring in collisions involving short-range forces—the left side of (51 *a*) indeed will converge uniformly as $\epsilon \to 0$ whenever the right side of (51 *a*) converges. In other words, I argue—and hereafter in this work shall assume—that for relations such as (51 *a*) occurring in scattering theory, the mere existence of the integral on the right side guarantees the interchange of order

of integration and limit $\epsilon \to 0$ actually is valid; it appears (see § A. 9) that this assumption is consistent with—though more generally useful than—a previously employed (Gerjuoy 1958*a*, *b*) criterion for the validity of interchange of order of integration and limit $\epsilon \to 0$. I believe, therefore, that (44*a*) and its centre of mass version are valid specifications, of $\Phi_i^{(+)}$ and $\bar{\Phi}_i^{(+)}$ respectively, when bound states do not occur.

I add that the matrix elements $\langle f| \boldsymbol{T}(E) |i\rangle$ or $\langle f| \bar{\boldsymbol{T}}(\bar{E}) |i\rangle$ defined by (5) and (6) involve precisely the integral (46) we have been discussing. Thus the results of this section bear on the physical significance of bound state contributions to these matrix elements, as well on the validity of the assumption that the limit of $\langle f| \boldsymbol{T}(E+i\epsilon) |i\rangle$ as $\epsilon \to 0$ is identical with $\langle f| \boldsymbol{T}(E) |i\rangle$. On the other hand, I surely do not want to give the impression that the comparatively qualitative considerations of this section can replace detailed quantitative examination of $\langle f| \boldsymbol{T}(\lambda) |i\rangle$ as a function of $\lambda = E+i\epsilon$, for interactions $V_{\alpha\beta}(\boldsymbol{r}_{\alpha\beta})$ wherein the analysis can be carried through (as in the papers of Rubin *et al.* (1966, 1967*a*, *b*)).

I now return to (43*b*). As it happens, the integral on the right side of (43*b*) does converge (see § A. 7) when ψ_i is given by (21*a*), so that the equality (43*b*) apparently does hold for the collisions of three initially free particles. Correspondingly, the integral equation (42) does have a solution which is identical with the desired $\Psi_i^{(+)}$ from (8). Unfortunately, (42) has other solutions than $\Psi_i^{(+)}$ defined by (8), as has been explained. Similar assertions (to those of this paragraph) hold for the centre of mass versions of (42) and (43*b*).

To close this section, I remark that the defining equations (27) and (36) can be shown to imply the expansion (valid whenever $\epsilon > 0$),

$$G(\boldsymbol{r};\boldsymbol{r}';E+i\epsilon) = \frac{1}{(2\pi)^3}\int d\hat{\boldsymbol{K}}\, e^{i\hat{\boldsymbol{K}}\cdot(\boldsymbol{R}-\boldsymbol{R}')}\, \bar{G}\left(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}';E-\frac{\hbar^2\hat{K}^2}{2M}+i\epsilon\right). \tag{53a}$$

Using (53*a*), it then is readily shown that for every ϵ

$$G(E+i\epsilon)\, V_i \psi_i(E) = e^{i\boldsymbol{K}\cdot\boldsymbol{R}}\, \bar{G}(\bar{E}+i\epsilon)\, V_i \bar{\psi}_i(\bar{E}). \tag{53b}$$

Consequently, recalling (33*a*),

$$\Psi_i(\boldsymbol{r};E+i\epsilon) = e^{i\boldsymbol{K}\cdot\boldsymbol{R}}\, \bar{\Psi}_i(\bar{\boldsymbol{r}};\bar{E}+i\epsilon), \tag{54a}$$

$$\Phi_i(\boldsymbol{r};E+i\epsilon) = e^{i\boldsymbol{K}\cdot\boldsymbol{R}}\, \bar{\Phi}_i(\bar{\boldsymbol{r}};\bar{E}+i\epsilon), \tag{54b}$$

where Ψ_i and $\bar{\Psi}_i$ are the unique solutions to (8*b*) and (34*b*) respectively. Correspondingly, letting $\epsilon \to 0$ in (54)

$$\Psi_i^{(+)}(\boldsymbol{r};E) = e^{i\boldsymbol{K}\cdot\boldsymbol{R}}\, \bar{\Psi}_i^{(+)}(\bar{\boldsymbol{r}};\bar{E}), \tag{55a}$$

$$\Phi_i^{(+)}(\boldsymbol{r};E) = e^{i\boldsymbol{K}\cdot\boldsymbol{R}}\, \bar{\Phi}_i^{(+)}(\bar{\boldsymbol{r}};\bar{E}), \tag{55b}$$

which explicitly manifest conservation of total laboratory momentum $\hbar\boldsymbol{K}$ in the laboratory frame wavefunction $\Psi_i^{(+)}$ and its scattered part $\Phi_i^{(+)}$. Of course equations (54) to (55) are well known and as expected; I merely am remarking that these equations are readily derivable in configuration space from the fundamental definitions of the quantities involved, without recourse to operator or diagrammatic techniques. The factor $e^{i\boldsymbol{K}\cdot\boldsymbol{R}}$ relating $\Phi_i^{(+)}$ and $\bar{\Phi}_i^{(+)}$ in (55*b*) makes it manifest that the laboratory frame scattered part $\Phi_i^{(+)}$ need not behave asymptotically like the everywhere outgoing $G^{(+)}$, and even can have incoming parts, as asserted beneath (45*b*). Naturally these $e^{i\boldsymbol{K}\cdot\boldsymbol{R}}$ factors are removed by formulating the collision in the centre of mass frame from the very outset. As will be discussed in the next section, however, neither does the centre of mass frame scattered part $\bar{\Phi}_i^{(+)}(\bar{\boldsymbol{r}})$—as correctly defined by (11*b*) and (34)—behave asymptotically at large $\bar{\boldsymbol{r}}$ as does $\bar{G}^{(+)}(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}')$; indeed there are incoming contributions to $\bar{\Phi}_i^{(+)}(\bar{\boldsymbol{r}})$ as well.

2.3. *Subtraction of two-body scattering terms*

The previous section has explained the deficiencies of (42) and (44 *a*) (and their centre of mass analogues). In this section I shall seek an alternative specification of $\Psi_i^{(+)}$, of a kind which is mathematically unexceptional (i.e. involves neither divergences nor integral equations whose solutions are not unique), but which permits a relatively straightforward determination of how $\Phi_i^{(+)}(\boldsymbol{r})$ behaves at large $\boldsymbol{r}$. In particular, I shall attempt to accomplish this purpose by rewriting the left side of (the centre of mass analogue of) (51 *a*) so as to obtain a form which—for ψ_1 of (21 *a*)—always permits interchange of the order of integration and limit $\epsilon \to 0$. From § A. 8 and the discussion following (52), it appears that what is required is a means of rewriting the left side of (the centre of mass analogue of) (51 *a*) so as to obtain an integral which remains convergent after the interchange in question is performed.

It is reasonable to try to achieve this convergence by iteration of the formula (50 *a*) for $\Phi_1(E+i\epsilon)$. A myriad of different iterations are available, of course. However, a clue as to how to proceed is the fact that elimination of terms representing purely two-body scattering of 1 by 2 (with 3 unaffected), as well as of corresponding terms representing two-body scattering of 2 by 3 and of 3 by 1, apparently replaces the Lippmann–Schwinger equation for the total Green function G by a new integral equation (see the end of this section) whose kernel is better behaved (Weinberg 1964). Moreover, it certainly makes sense physically that two-body scattering terms must be subtracted from $\Psi_i^{(+)}$, i.e. from $\Phi_i^{(+)}$, before specification of three-body scattering becomes possible.

Introduce the Green functions $G_{12}(\lambda)$, $G_{23}(\lambda)$, $G_{31}(\lambda)$ satisfying respectively

$$(H_{12}-\lambda)\,G_{12} \equiv (T+V_{12}-\lambda)\,G_{12} = \mathbf{1}, \tag{56 a}$$

$$(H_{23}-\lambda)\,G_{23} \equiv (T+V_{23}-\lambda)\,G_{23} = \mathbf{1}, \tag{56 b}$$

$$(H_{31}-\lambda)\,G_{31} \equiv (T+V_{31}-\lambda)\,G_{31} = \mathbf{1}. \tag{56 c}$$

Define also

$$G_{12}^{(+)}(E) = \lim_{\epsilon\to 0} G_{12}(E+i\epsilon), \quad \text{etc.} \tag{57}$$

Then (as in (8) and (11)) with the incident wave ψ_1 of (21 *a*) the wavefunction representing purely two-body scattering of 1 by 2, with 3 unaffected, should be

$$\begin{aligned}\Psi_{12}^{(+)}(E) &= \psi_1(E) + \Phi_{12}^{(+)}(E) = \lim_{\epsilon\to 0} \Psi_{12}(E+i\epsilon) \\ &\equiv \lim_{\epsilon\to 0} [\psi_1(E) + \Phi_{12}(E+i\epsilon)]\end{aligned} \tag{58 a}$$

where, recalling (49) to (50), $\Psi_{12}(E+i\epsilon)$ is given by the formula

$$\Psi_{12}(E+i\epsilon) = \psi_1(E) - \frac{1}{H_{12}-E-i\epsilon} V_{12}\psi_1(E). \tag{58 b}$$

Presumably† (58) guarantee

$$(H_{12}-E)\,\Psi_{12}^{(+)} = 0, \tag{59 a}$$

or, equivalently,

$$(H_{12}-E)\,\Phi_{12}^{(+)} = -V_{12}\psi_1, \tag{59 b}$$

where

$$\Phi_{12}^{(+)}(E) = -\lim_{\epsilon\to 0}\left\{\frac{1}{H_{12}-E-i\epsilon} V_{12}\psi_1(E)\right\} \equiv -\lim_{\epsilon\to 0} G_{12}(E+i\epsilon)\,V_{12}\psi_1. \tag{60}$$

† See footnote †, p. 208.

Therefore a suggested alternative way of writing $\Psi_i^{(+)}(E)$—resembling but superior to (11 *a*) in that purely two-body scattering terms explicitly have been subtracted from the 'scattered part'—is

$$\Psi_i^{(+)} = \psi_i + \Phi_{12}^{(+)} + \Phi_{23}^{(+)} + \Phi_{31}^{(+)} + \Phi_i^{s(+)}, \tag{61}$$

where $\Phi_{23}^{(+)}$, $\Phi_{31}^{(+)}$ are defined as in (58) to (60), and where the quantity

$$\Phi_i^{s(+)} = \Phi_i^{(+)} - \Phi_{12}^{(+)} - \Phi_{23}^{(+)} - \Phi_{31}^{(+)}, \tag{62}$$

remaining after subtraction of purely two-body terms now hopefully represents the 'truly three-body' scattered part of $\Psi_i^{(+)}$ (termed $\Phi_i^{t(+)}$ in § 1).

With (61) as a guide, the desired iteration of (50 *a*) is achieved as follows. For complex $\lambda = E + i\epsilon$, the Green functions $G(\lambda)$ and $G_{12}(\lambda)$, etc., are related by (Watson & Nuttall 1967)†

$$G = G_{12} - G_{12}(V_{23}+V_{31})\, G = G_{12} - G(V_{23}+V_{31})\, G_{12}, \tag{63 a}$$

$$G = G_{23} - G_{23}(V_{31}+V_{12})\, G = G_{23} - G(V_{31}+V_{12})\, G_{23}, \tag{63 b}$$

$$G = G_{31} - G_{31}(V_{12}+V_{23})\, G = G_{31} - G(V_{12}+V_{23})\, G_{31}. \tag{63 c}$$

Similarly

$$G = G_F - G_F\, VG = G_F - GVG_F, \tag{63 d}$$

where $G_F(\lambda) \equiv (T-\lambda)^{-1}$ is the free space Green function, in the nine-dimensional space of $\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3 \equiv \boldsymbol{r}$, defined in (24) to (25). Using (63) after substituting (50 *a*) for the last term in (8 *b*), one can write (for ψ_1 of (21 *a*))

$$\begin{aligned}
\Psi_1(E+i\epsilon) &= \psi_1 - G(E+i\epsilon)\,[V_{12}+V_{23}+V_{31}]\,\psi_1 \\
&= \psi_1 + \{-[G_{12} - G(V_{23}+V_{31})\, G_{12}]\, V_{12}\psi_1 \\
&\quad -[G_{23} - G(V_{31}+V_{12})\, G_{23}]\, V_{23}\psi_1 \\
&\quad -[G_{31} - G(V_{12}+V_{23})\, G_{31}]\, V_{31}\psi_1\} \qquad (64\,a) \\
&= \psi_1 - G_{12}V_{12}\psi_1 - G_{23}V_{23}\psi_1 - G_{31}V_{31}\psi_1 \\
&\quad + \{G(V_{23}+V_{31})\, G_{12}V_{12}\psi_1 + G(V_{31}+V_{12})\, G_{23}V_{23}\psi_1 \\
&\quad + G(V_{12}+V_{23})\, G_{31}V_{31}\psi_1\}. \qquad (64\,b)
\end{aligned}$$

In (64), as in (63), $\epsilon \neq 0$, so that all the Green functions are quadratically integrable. Thus the integrals in (63) and (64) are convergent, and (because all integrals involve a Green function) the interchanges of orders of integration implied by the manipulations yielding (64 *b*) should be justifiable.

Taking the limit as $\epsilon \to 0$ in (63 *a*) yields

$$\begin{aligned}
G^{(+)}(E) &= G_{12}^{(+)}(E) - \lim_{\epsilon\to 0} \{G_{12}(E+i\epsilon)\,[V_{23}+V_{31}]\, G(E+i\epsilon)\} \\
&= G_{12}^{(+)}(E) - \lim_{\epsilon\to 0} \{G(E+i\epsilon)\,[V_{23}+V_{31}]\, G_{12}(E+i\epsilon)\}. \qquad (65\,a)
\end{aligned}$$

As discussed in § 2.2, interchanging the order of the limiting and integration processes in (65 *a*) is not obviously legitimate. However, when λ is pure real, i.e. when $\epsilon = 0$, the integrals in (65 *a*), unlike the integral in (44 *a*), converge whether or not bound states exist (see § A. 2). Therefore, again as discussed in §§ 2.2 and A. 8, this paper assumes that

$$\begin{aligned}
G^{(+)}(E) &= G_{12}^{(+)}(E) - G_{12}^{(+)}(E)\,[V_{23}+V_{31}]\, G^{(+)}(E) \\
&= G_{12}^{(+)}(E) - G^{(+)}(E)\,[V_{23}+V_{31}]\, G_{12}^{(+)}(E). \qquad (65\,b)
\end{aligned}$$

† For a configuration space derivation, without appeal to operator algebra, see Gerjuoy (1958 *b*).

For the same reason the relations (63 b, c, d) are assumed to hold at real E, with all the Green functions outgoing. As discussed in § 2.2 in connexion with (44), the validity of (65 b) can be related (see also § A. 9) to the validity of the assertion that

$$\int_{\infty} \mathrm{d}\boldsymbol{S} \cdot \boldsymbol{W}[G^{(+)}(\boldsymbol{r}; \boldsymbol{r}'), G_{12}^{(+)}(\boldsymbol{r}; \boldsymbol{r}'')] = 0 \tag{66}$$

for all $\boldsymbol{r}'$, $\boldsymbol{r}''$, with $\boldsymbol{W}$ defined by (45 a).

Similarly, taking the limit as $\epsilon \to 0$ in (64 b), and recalling (61) and (62)

$$\begin{aligned} \Phi_{\mathrm{i}}^{s(+)}(E) = \lim_{\epsilon \to 0} \{ & G(E+\mathrm{i}\epsilon)\,[V_{23}+V_{31}]\,G_{12}(E+\mathrm{i}\epsilon)\,V_{12}\,\psi_{\mathrm{i}} \\ & + G(E+\mathrm{i}\epsilon)\,[V_{31}+V_{12}]\,G_{23}(E+\mathrm{i}\epsilon)\,V_{23}\,\psi_{\mathrm{i}} \\ & + G(E+\mathrm{i}\epsilon)\,[V_{12}+V_{23}]\,G_{31}(E+\mathrm{i}\epsilon)\,V_{31}\,\psi_{\mathrm{i}} \} \end{aligned} \tag{67 a}$$

which, using (60), can be supposed to yield

$$\begin{aligned} \Phi_{\mathrm{i}}^{s(+)} = {} & G^{+}[V_{23}+V_{31}]\,\{\lim_{\epsilon \to 0} G_{12}\,V_{12}\,\psi_{\mathrm{i}}\} + G^{+}[V_{31}+V_{12}]\,\{\lim_{\epsilon \to 0} G_{23}\,V_{23}\,\psi_{\mathrm{i}}\} \\ & + G^{(+)}[V_{12}+V_{23}]\,\{\lim_{\epsilon \to 0} G_{31}\,V_{31}\,\psi_{\mathrm{i}}\} \end{aligned} \tag{67 b}$$

$$= -G^{+}[(V_{23}+V_{31})\,\Phi_{12}^{(+)} + (V_{31}+V_{12})\,\Phi_{23}^{(+)} + (V_{12}+V_{23})\,\Phi_{31}^{(+)}], \tag{67 c}$$

because the integrals in (67 c) converge in the centre of mass system (see § B. 1). Specifically if

$$\left.\begin{aligned} \Phi_{\mathrm{i}}^{s(+)} &= \mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{R}}\,\bar{\Phi}_{\mathrm{i}}^{s(+)}, \\ \Phi_{12}^{(+)} &= \mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{R}}\,\bar{\Phi}_{12}^{(+)}, \quad \text{etc.} \end{aligned}\right\} \tag{68}$$

then the right side of

$$\bar{\Phi}_{\mathrm{i}}^{s(+)} = -\bar{G}^{(+)}[(V_{23}+V_{31})\,\bar{\Phi}_{12}^{(+)} + (V_{31}+V_{12})\,\bar{\Phi}_{23}^{(+)} + (V_{12}+V_{23})\,\bar{\Phi}_{31}^{(+)}] \tag{69}$$

always is composed of convergent integrals, whether or not bound states exist. I add that the laboratory system integrals (67 c) fail to be assuredly convergent only when three-particle bound states $u_j(\boldsymbol{r}_{12}, \boldsymbol{r}_{23})$ can occur (see § B. 1).

The limit $\epsilon \to 0$ in (60) readily can be evaluated in configuration space, by essentially the same procedure as is used to derive (53) to (55); the result is a mathematically meaningful closed form expression for $\Phi_{12}^{(+)}(E)$. Thus (67 c) (as interpreted by (68) and (69)) yields $\Phi_{\mathrm{i}}^{s(+)}$ in terms of meaningful integrals not involving any limits as $\epsilon \to 0$. Correspondingly, in view of the possibility of evaluating (60) in closed form, (61) becomes a formula—not an integral equation—for $\Psi_{\mathrm{i}}^{(+)}$ in terms of convergent integrals involving Green functions at real energies only (recall, however, the remarks in the paragraph beneath (45 b)). It appears therefore that the set of equations (60), (61) and (67 c) provide the alternative specification of $\Psi_{\mathrm{i}}^{(+)}$ this section has been seeking. Moreover, granting the integrals in (69) really are convergent, it now also is possible to specify $\Psi_{\mathrm{i}}^{(+)}$ in terms of a meaningful new (replacing (44 b)) outgoing condition, namely

$$\int \mathrm{d}\boldsymbol{S} \cdot \boldsymbol{W}[G^{(+)}(\boldsymbol{r}; \boldsymbol{r}'), \Phi_{\mathrm{i}}^{s(+)}(\boldsymbol{r})] = 0, \tag{70}$$

provided it is understood that—because the integrals (67 c) need not converge whereas those in (69) always do (for ψ_{i} of (21 a))—the strictly correct condition is the centre of mass analogue of (70). To verify the immediately preceding assertion, substitute (61) into (7), and use (9) and (59 b). Then, still for ψ_{i} of (21 a),

$$(H-E)\,\Phi_{\mathrm{i}}^{s(+)} = -[(V_{23}+V_{31})\,\Phi_{12}^{(+)} + (V_{31}+V_{12})\,\Phi_{23}^{(+)} + (V_{12}+V_{23})\,\Phi_{31}^{(+)}]. \tag{71}$$

As in the derivation (Gerjuoy 1958*b*) of (44*a*) the equality (71) immediately implies that if (70) holds, then (67*c*) must hold, and conversely; in particular, solutions $\Phi_i^{s(+)}$ to (71) are identical with the 'true' $\Phi_i^{s(+)}$ given by (67*c*) if and only if the $\Phi_i^{s(+)}$ from (71) obeys (70). However, as discussed in § 2.2 in connexion with (44), the condition (70) is not mathematically meaningful when propagation in three-particle bound states is energetically possible (see § B. 1). On the other hand, starting in the centre of mass system leads directly to the strictly correct result that if the assuredly convergent (69) holds, then the assuredly meaningful centre of mass analogue of (70) must hold, and conversely.

The aforementioned closed form expression for the limit in (60) is precisely identical with the result usually quoted, whether obtained by operator techniques, diagrammatic methods, or other procedures. As one expects, $\Phi_i^{(+)}(E)$ from (60)—representing as it does the isolated scattering of the particle pair 1, 2—leaves unaltered the plane wave factors $e^{iK.R}$ and $e^{iK_{12}.q_{12}}$ of (respectively) (33*a*) and the 1, 2 analogue of (33*b*). Specifically,

$$\Phi_i^{(+)}(E) = e^{iK.R}\, e^{iK_{12}.q_{12}}\, \phi_{12}^{(+)}(\boldsymbol{r}_{12}; \boldsymbol{k}_{12}), \tag{72}$$

where the position and momentum vectors appearing in (72) have been defined in (28) and (29), and where

$$\phi_{12}^{(+)}(\boldsymbol{r}_{12}; \boldsymbol{k}_{12}) = -g_{12}^{(+)}(E_{12})\, V_{12}\, e^{i\boldsymbol{k}_{12}.\boldsymbol{r}_{12}} \tag{73a}$$

$$\equiv -\int d\boldsymbol{r}'_{12} g_{12}^{(+)}(\boldsymbol{r}_{12}; \boldsymbol{r}'_{12}; E_{12})\, V_{12}(\boldsymbol{r}'_{12}) \exp\{i\boldsymbol{k}_{12}.\boldsymbol{r}'_{12}\}. \tag{73b}$$

Hence $\phi_{12}^{(+)}$ represents the outgoing wave (as a function of the relative coordinate $\boldsymbol{r}_{12}$) in the centre of mass system of particles 1 and 2, when these particles undergo an isolated collision (no particles 3 involved) with incident wave

$$\psi_{121} = e^{i\boldsymbol{k}_{12}.\boldsymbol{r}_{12}}, \tag{74a}$$

corresponding to a centre of mass system (of particles 1 and 2) energy

$$E_{12} = \frac{\hbar^2 k_{12}^2}{2\mu_{12}}. \tag{74b}$$

It hardly needs to be added that the Green function $g_{12}^{(+)}$ satisfies

$$\left[\frac{-\hbar^2}{2\mu_{12}}\nabla_{12}^2 + V_{12}(\boldsymbol{r}_{12}) - E_{12}\right] g_{12}^{(+)}(\boldsymbol{r}_{12}; \boldsymbol{r}'_{12}; E_{12}) = \delta(\boldsymbol{r}_{12} - \boldsymbol{r}'_{12}). \tag{75}$$

I stress that the (vanishing on the energy shell) δ-functions associated with the divergence of the integral (52*b*) are absent from the right sides of both (69) and (72), i.e. recalling (61) these δ-functions do not appear in a valid specification of $\Psi_i^{(+)}$. To be precise, if (see § B. 1) as in (46) one replaces $\psi_1(E)$ by $\psi_1(E')$, but leaves E unchanged in $G^{(+)}$, $G_{12}^{(+)}$, etc., then $\Phi_{12}^{(+)}$ from (72) and (73) remains a convergent formula; with these modified $\Phi_{\alpha\beta}^{(+)}$, moreover, the right side of (69) remains a convergent formula at all real $\boldsymbol{k}'_1$, $\boldsymbol{k}'_2$, $\boldsymbol{k}'_3$ off the energy shell (provided one makes $\boldsymbol{K}' = \boldsymbol{K}$, consistent with the fact that (69) is a centre of mass system expression). The formula (69) is at worst logarithmically divergent off the energy shell when $\bar{\Phi}_{\alpha\beta}^{(+)}(\bar{E})$ is replaced by $\bar{\Phi}_{\alpha\beta}^{(+)}(\bar{E}')$, which replacement is not identical with altering $\bar{E}$ to $\bar{E}'$ in $\bar{\psi}_1$ while leaving all the Green functions unaltered. In other words, the δ-functions found in (52*b*) really are non-physical artefacts of the particular mathematically faulty derivation leading to the formula (52*b*) for $\bar{\Phi}_i^{(+)}$.

Equation (72) makes understandable the assertion (at the end of § 2.2) concerning the asymptotic behaviour of $\bar{\Phi}_i^{(+)}(\bar{\boldsymbol{r}})$ at large $\bar{r}$. Evidently there are incoming contributions to $\bar{\Phi}_i^{(+)}$,

stemming, for example, from the $e^{iK_{12}\cdot q_{12}}$ factor in the $\bar{\Phi}_{12}^{(+)}$ contribution to $\bar{\Phi}_i^{(+)}$. To put it differently, the centre of mass analogue of (44 *b*), even when meaningful (i.e. even when two-particle bound states do not occur), does not specify a $\bar{\Phi}_i^{(+)}$ which is everywhere outgoing in the centre of mass system. These annoying plane wave factors $e^{iK_{\alpha\beta}\cdot q_{\alpha\beta}}$ are not present in $\bar{\Phi}_i^{s(+)}$, however, by virtue of its definition via the centre of mass analogue of (62). Nevertheless, the quantity $\bar{\Phi}_i^{s(+)}$ computed from (69) still does not have the asymptotic behaviour expected of outgoing 'truly three-body scattered' waves. The justification of this assertion is to be found in § 4 below. In other words, despite our hopes, $\bar{\Phi}_i^{s(+)}$ defined by the analogue of (62) is not identical with $\bar{\Phi}_i^{t(+)}$. Correspondingly, it turns out that the limit at large $\tilde{r}$ of $\bar{\Phi}_i^{s(+)}(\tilde{r})$ from the integrals in (69) is not at all readily determinable. Thus, though for the purpose of computing $\bar{w}(i\to f)$ they are an improvement on the specifications discussed in § 2.2, the (centre of mass analogues of) equations (60), (61) and (67 *c*)—despite appearances—do not provide a specification of $\Psi_i^{(+)}$ having all properties demanded at the very outset of this section.

I shall return to the problem of finding a wholly satisfactory specification of $\Psi_i^{(+)}$ in § 3. In the meantime I note that a satisfactory specification cannot be obtained from any integral equation derived by direct iteration of (42) (or of its centre of mass analogue) along the lines of this section, because such iterations merely make use of identities to replace the right side of (42) by more complicated expressions. Thus if $\Psi_i^{(+)}$ solves (42) it will solve any such iteration of (42). In other words—granting the convergence of the integrals therein—all such new integral equations involving real energy Green functions will suffer from the same difficulty as (42), namely they will have non-unique solutions for incident ψ_i of (20).

For three-particle collisions corresponding to incident ψ_i of (20), Faddeev (1961) has shown that a mathematically unexceptional (in the sense of the first paragraph of this section) specification of $\Psi_i^{(+)}$ is furnished by a set of three coupled integral equations for components of $\Phi_i^{(+)}$, the so-called Faddeev equations. The Faddeev equations (which clearly are not merely a direct iteration of (42)) are meaningful at real energies,† i.e. use of the Faddeev equations does avoid legitimately the awkward limit $\epsilon\to 0$. On the other hand, the 'scattered wave' terms in the Faddeev equations represent the same scattered part of $\Psi_i^{(+)}$ as has been identified with $\Phi_i^{s(+)}$. Therefore, the scattered wave terms in the Faddeev equations suffer from the same deficiencies as were ascribed to $\Phi_i^{s(+)}$ in the penultimate paragraph above. Specifically, even in the centre of mass system, the Faddeev equations scattered wave terms do not have the asymptotic behaviour expected of outgoing 'truly three-body scattered waves'; correspondingly, the asymptotic behaviour of these terms at large distances is not readily found.

To demonstrate the assertion in the preceding paragraph, it merely is necessary to observe that the Faddeev equations for the wave function take the form (Faddeev 1961)

$$\left.\begin{aligned} \Phi^{(1)} &= -G_{23}V_{23}\psi_i - G_F\,\boldsymbol{T}_{23}[\Phi^{(2)}+\Phi^{(3)}],\\ \Phi^{(2)} &= -G_{31}V_{31}\psi_i - G_F\,\boldsymbol{T}_{31}[\Phi^{(3)}+\Phi^{(1)}],\\ \Phi^{(3)} &= -G_{12}V_{12}\psi_i - G_F\,\boldsymbol{T}_{12}[\Phi^{(1)}+\Phi^{(2)}], \end{aligned}\right\} \tag{76}$$

where, for $\lambda = E+i\epsilon$,

$$\boldsymbol{T}_{12}(\lambda) = V_{12} - V_{12}G_{12}(\lambda)V_{12}, \quad \text{etc.} \tag{77 a}$$

and

$$\Phi^{(1)}(\lambda) = -G_F(\lambda)V_{23}\Psi_i(\lambda), \quad \text{etc.} \tag{77 b}$$

With respect to (77 *a*), recall (27 *e*) and (27 *f*) and associated remarks. In (77 *b*), Ψ_i is the solution to the Lippmann–Schwinger equation (8 *b*), so that, for ψ_i of (21 *a*),

$$\Phi_i(\lambda) = \Phi^{(1)}(\lambda)+\Phi^{(2)}(\lambda)+\Phi^{(3)}(\lambda), \tag{78}$$

† The key theorems seem to be contained in §§ 7 and 9 of Faddeev (1965), especially theorem 7.1.

where Φ_i is the quantity defined by (8 *a*). All the Green functions, $\Phi^{(\alpha)}$, etc. in (76) to (78) are evaluated at complex energy, but Faddeev has proved† that it is legitimate (other than at exceptional‡ energies) to take the limit of (76) as $\epsilon \to 0$, and that the resulting real energy equations have unique solutions. Taking the limit of (76) as $\epsilon \to 0$, therefore, one sees—making use of (60), (62) and (78)—that

$$\Phi_i^{s(+)} = -\lim_{\epsilon \to 0} \{G_F \boldsymbol{T}_{23}[\Phi^{(2)} + \Phi^{(3)}] + G_F \boldsymbol{T}_{31}[\Phi^{(3)} + \Phi^{(1)}] + G_F \boldsymbol{T}_{12}[\Phi^{(1)} + \Phi^{(2)}]\}. \tag{79}$$

Equation (79) shows§ that the collection of integrals on the right side of (76) indeed represents precisely the same scattered part of $\Psi_i^{(+)}$ as has been identified with $\Phi_i^{s(+)}$.

The set of integral equations (63) for G can be iterated in various ways, thereby yielding new integral equations. In particular, for complex $\lambda = E + i\epsilon$,

$$\begin{aligned} G &= G_F - G_F(V_{12} + V_{23} + V_{31})\, G \\ &= G_F - G_F V_{12}[G_{12} - G_{12}(V_{23} + V_{31})\, G] - G_F V_{23}[G_{23} - G_{23}(V_{31} + V_{12})\, G] \\ &\qquad - G_F V_{31}[G_{31} - G_{31}(V_{12} + V_{23})\, G], \end{aligned} \tag{80 a}$$

or

$$\begin{aligned} G = G_F &- G_F V_{12} G_{12} - G_F V_{23} G_{23} - G_F V_{31} G_{31} + G_F V_{12} G_{12}(V_{23} + V_{31})\, G \\ &+ G_F V_{23} G_{23}(V_{31} + V_{12})\, G + G_F V_{31} G_{31}(V_{12} + V_{23})\, G. \end{aligned} \tag{80 b}$$

At real energies (80 *b*) implies (in essentially the same fashion as (65 *a*) implies (65 *b*))

$$\begin{aligned} G^{(+)} = G_F^{(+)} &- G_F^{(+)} V_{12} G_{12}^{(+)} - G_F^{(+)} V_{23} G_{23}^{(+)} - G_F^{(+)} V_{31} G_{31}^{(+)} \\ &+ \{G_F^{(+)} V_{12} G_{12}^{(+)}\}\, (V_{23} + V_{31})\, G^{(+)} + \{G_F^{(+)} V_{23} G_{23}^{(+)}\}\, (V_{31} + V_{12})\, G^{(+)} \\ &+ \{G_F^{(+)} V_{31} G_{31}^{(+)}\}\, (V_{12} + V_{23})\, G^{(+)}. \end{aligned} \tag{80 c}$$

where it is understood that the integrals in the braces are to be performed first, and where it is obvious, from §§ A. 1 and A. 2 together with

$$G_{12} = G_F - G_F V_{12} G_{12} = G_F - G_{12} V_{12} G_F, \quad \text{etc.} \tag{81 a}$$

and

$$G_{12}^{(+)} = G_F^{(+)} - G_F^{(+)} V_{12} G_{12}^{(+)} = G_F^{(+)} - G_{12}^{(+)} V_{12} G_F^{(+)}, \quad \text{etc.}, \tag{81 b}$$

that all integrals in (80 *c*) are convergent.

Equation (80 *c*) will prove to be useful in § 3. Equation (80 *b*) is Weinberg's integral equation for G mentioned earlier in this section, except that Weinberg (1964) prefers to replace G by the 'completely connected' quantity‖

$$C = -[G - G_F + G_F V_{12} G_{12} + G_F V_{23} G_{23} + G_F V_{31} G_{31}]. \tag{82}$$

Performing on the Lippmann–Schwinger equations (8 *b*) and

$$\Psi_i(E + i\epsilon) = \Psi_{12}(E + i\epsilon) - G_{12}(E + i\epsilon)\, (V_{23} + V_{31})\, \Psi_i(E + i\epsilon), \quad \text{etc.}, \tag{83}$$

† See footnote, p. 222. ‡ See footnote ‡, p. 201.

§ Presumably Faddeev's proofs (Faddeev 1965) mean the order of integration and limit $\epsilon \to 0$ can be interchanged in (79), but performance of this interchange is unnecessary for the purpose of the present discussion of Faddeev's equations.

‖ Note my $G = (H - E)^{-1}$ is the negative of Weinberg's $G = (E - H)^{-1}$.

essentially the same operations as were performed in (80) yields a new (alternative to (42)) real energy integral equation for $\Psi_i^{(+)}(E)$, whose kernel is identical with the kernel in (80*c*). Specifically, recalling (58*b*),

$$\begin{aligned}\Psi_1 &= \psi_1 - G_F(V_{12}+V_{23}+V_{31})\,\Psi_1 \\ &= \psi_1 - G_F V_{12}[\psi_1 - G_{12}V_{12}\psi_1 - G_{12}(V_{23}+V_{31})\,\Psi_1] \\ &\quad - G_F V_{23}[\psi_1 - G_{23}V_{23}\psi_1 - G_{23}(V_{31}+V_{12})\,\Psi_1] \\ &\quad - G_F V_{31}[\psi_1 - G_{31}V_{31}\psi_1 - G_{31}(V_{12}+V_{23})\,\Psi_1], \qquad (84a)\end{aligned}$$

or, using also (81*a*),

$$\begin{aligned}\Psi_1 = \psi_1 &- G_{12}V_{12}\psi_1 - G_{23}V_{23}\psi_1 - G_{31}V_{31}\psi_1 \\ &+ [G_F V_{12}G_{12}(V_{23}+V_{31}) + G_F V_{23}G_{23}(V_{31}+V_{12}) + G_F V_{31}G_{31}(V_{12}+V_{23})]\,\Psi_1, \qquad (84b)\end{aligned}$$

which at real energies E becomes, recalling (60),

$$\begin{aligned}\Psi_i^{(+)} = \psi_i &+ \Phi_{12}^{(+)} + \Phi_{23}^{(+)} + \Phi_{31}^{(+)} \\ &+ [\{G_F^{(+)}V_{12}G_{12}^{(+)}\}(V_{23}+V_{31}) + \{G_F^{(+)}V_{23}G_{23}^{(+)}\}(V_{31}+V_{12}) \\ &+ \{G_F^{(+)}V_{31}G_{31}^{(+)}\}(V_{12}+V_{23})]\,\Psi_i^{(+)}, \qquad (84c)\end{aligned}$$

where, as in (80*c*), the integrals in braces are to be performed first, and where all integrals can be seen to converge (by arguments such as in appendices A and B). Comparing with (61), one sees that $\Phi_i^{s(+)}$ is given by the terms involving $\Psi_i^{(+)}$ in (84*c*).

In a sense, the integral equation (84*c*) bears the same relation to the formula for $\Psi_i^{(+)}$ implied by (61) and (67*c*) as does (42) to the formula for $\Psi_i^{(+)}$ implied by (11*a*) and (44*a*); the essential correctness of this remark will be made more apparent in § 3 below. Neither (80) nor (84) have been the subject of as rigorous a mathematical investigation as have (Faddeev 1965) the Faddeev equations, but one may hope† the better-behaved (than in (42)) kernel ensures the uniqueness of solutions to (84*c*). If unique, the solution to (84*c*) seemingly must be identical with the desired $\Psi_i^{(+)}$ specified by (8), because one can show that

$$\Psi_i(E+i\epsilon) = -i\epsilon G(E+i\epsilon)\,\psi_i(E) \qquad (85)$$

of (8*a*) (recall (49*b*)) satisfies (84*b*). On the other hand, it does not seem possible to show directly from (84*c*) that solutions to (84*c*) necessarily satisfy the original Schrodinger equation (7); to show (7) is satisfied, use of additional real energy integral equations seems required, e.g. corresponding to (83),

$$\Psi_i^{(+)} = \Psi_{12}^{(+)} - G_{12}^{(+)}(V_{23}+V_{31})\,\Psi_i^{(+)}, \quad \text{etc.}, \qquad (86)$$

where $\Psi_{12}^{(+)}$ is specified by the formula (58*a*) plus (72). Equation (86), like (42), can have non-unique solutions, however, i.e. there is no reason to identify solutions $\Psi_i^{(+)}$ to (86) with solutions $\Psi_i^{(+)}$ to (85); in fact, solutions to (86) need not be solutions to the corresponding integral equation for $\Psi_i^{(+)}$ in terms of $\Psi_{23}^{(+)}$. Conversely, unless one knows (84*c*) has a unique solution, there is no reason to identify solutions $\Psi_i^{(+)}$ to (84*c*) with solutions to (86). Actually (84*c*) is not a direct iteration of (42)—and therefore conceivably can have unique solutions—only because the additional integral equations (86) must be used when (84*c*) is derived starting from (42) (and proceeding at real energies as in (84*a*) and (84*b*)).

† The kernel in (84*c*) does have some undesirable properties however (Newton 1967).

3. Green functions at large distances

In this section I shall be concerned primarily with the asymptotic behaviour of the various (real energy) outgoing Green functions which have been introduced, e.g. $G^{(+)}(\boldsymbol{r};\boldsymbol{r}')$, $G_F^{(+)}(\boldsymbol{r};\boldsymbol{r}')$, etc., as $\boldsymbol{r}$ or $\boldsymbol{r}'$ become infinite, usually† along directions $\boldsymbol{\nu}$ or $\boldsymbol{\nu}'$ in the nine-dimensional configuration space corresponding, in physical space, to all particle distances and all interparticle distances simultaneously becoming infinite. For a more precise definition of $\boldsymbol{\nu}$, I observe that all points in $\boldsymbol{r} \equiv \boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3$ space can be specified by the following nine coordinates: the six spherical coordinate angles in ordinary three-dimensional space specifying the directions $\boldsymbol{n}_1, \boldsymbol{n}_2, \boldsymbol{n}_3$ of the vectors $\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3$; the two ratios ζ_{21}, ζ_{31}, where

$$\zeta_{\alpha\beta} = r_\alpha / r_\beta \tag{87}$$

and the distance (in nine dimensions) from the origin

$$r = (r_1^2 + r_2^2 + r_3^2)^{\frac{1}{2}} = r_1(1 + \zeta_{21}^2 + \zeta_{31}^2)^{\frac{1}{2}}. \tag{88}$$

Then the first eight of these coordinates may be said to specify the direction $\boldsymbol{\nu}$ of the nine-dimensional vector $\boldsymbol{r} = (\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)$. In terms of these coordinates the magnitude of the surface element on the sphere at infinity in the nine-dimensional space, at points along $\boldsymbol{\nu}$, is

$$\mathrm{d}S = \frac{\zeta_{21}^2 \zeta_{31}^2 r^8}{(1+\zeta_{21}^2+\zeta_{31}^2)^{\frac{9}{2}}} \mathrm{d}\zeta_{21}\, \mathrm{d}\zeta_{31}\, \mathrm{d}\boldsymbol{n}_1\, \mathrm{d}\boldsymbol{n}_2\, \mathrm{d}\boldsymbol{n}_3 \equiv r^8\, \mathrm{d}\boldsymbol{\nu}, \tag{89a}$$

where of course

$$\mathrm{d}\boldsymbol{n}_\alpha = \sin\theta_\alpha\, \mathrm{d}\theta_\alpha\, \mathrm{d}\phi_\alpha \tag{89b}$$

in terms of the usual three-dimensional spherical coordinates θ_α, ϕ_α of particle α. Along those special directions $\boldsymbol{\nu}$ where r_1 remains finite but, for example, r_2 becomes infinite, one can replace (88) by the corresponding expression involving ζ_{12}, ζ_{32}. The direction in the centre of mass frame corresponding to $\boldsymbol{\nu}$ will be denoted by $\bar{\boldsymbol{\nu}}$; of course in the centre of mass frame only two independent three-dimensional vectors, e.g. $\boldsymbol{q}_{12}$, $\boldsymbol{r}_{12}$, simultaneously become infinite. I also shall employ $\boldsymbol{\nu}_{\alpha\beta}$, $\bar{\boldsymbol{\nu}}_{\alpha\beta}$ to denote directions along which $\boldsymbol{r}_{\alpha\beta}$ remains finite as the sphere at infinity is approached.

The asymptotic behaviour of the laboratory system free space Green function $G_F^{(+)}$ (as well as of its centre of mass frame analogue $\bar{G}_F^{(+)}$) now can be stated. Specifically, for $E > 0$, as $\boldsymbol{r} \to \infty$ along fixed $\boldsymbol{\nu}$, holding $\boldsymbol{r}'$ constant, one sees from (24) that

$$\lim_{r\to\infty||\boldsymbol{\nu}} G_F^{(+)}(\boldsymbol{r};\boldsymbol{r}';E) = \left(\frac{2m_1}{\hbar^2}\right)^{\frac{3}{2}} \cdots \left(\frac{2m_n}{\hbar^2}\right)^{\frac{3}{2}} \frac{\mathrm{e}^{-\mathrm{i}\pi 3(n-1)/4}}{2\sqrt{E}}$$
$$\times \left(\frac{\sqrt{E}}{2\pi\rho}\right)^{(3n-1)/2} \exp\{\mathrm{i}\rho\sqrt{E}\} \exp\{-\mathrm{i}[k_1\boldsymbol{n}_1.\boldsymbol{r}_1' + \ldots + k_n\boldsymbol{n}_n.\boldsymbol{r}_n']\} \tag{90a}$$

$$\equiv C_n(E) \frac{\exp\{\mathrm{i}\rho\sqrt{E}\}}{\rho^{(3n-1)/2}} \exp\{-\mathrm{i}[k_1\boldsymbol{n}_1.\boldsymbol{r}_1' + \ldots + k_n\boldsymbol{n}_n.\boldsymbol{r}_n']\} \tag{90b}$$

† In a correctly formulated theory, those very special directions $\boldsymbol{\nu}_t = \boldsymbol{\nu}_{\alpha\beta}$ (in nine-dimensional configuration space) corresponding to unbound particles α, β moving to infinity (in physical space) with identical velocities (magnitudes and directions) surely must make a negligible contribution to the total three-body elastic scattering rate. Thus, for our present purpose of computing three-body elastic scattering coefficients $\overline{w}$, equation (1), it is not necessary to examine $\lim G^{(+)}(\boldsymbol{r};\boldsymbol{r}')$ as $r \to \infty$ along any $\boldsymbol{\nu}_{\alpha\beta}$, although knowledge of this limit (along $\boldsymbol{\nu}_{\alpha\beta}$) is essential for predicting the rate of two-body bound state $u_j(\boldsymbol{r}_{\alpha\beta})$ production in the three-body collision.

where the directions $\boldsymbol{n}_\alpha$ of $\boldsymbol{r}_\alpha$ are fixed when ν is fixed, and where

$$k_\alpha = \frac{2m_\alpha}{\hbar^2}\sqrt{E}\frac{r_\alpha}{\rho} \quad (\alpha = 1, \ldots, n). \tag{90c}$$

Equation (103 a) shows that the leading term in $\nabla_\alpha G_F^{(+)}$ makes

$$\nabla_\alpha G_F^{(+)}(E) \sim \mathrm{i}\sqrt{E}\frac{2m_\alpha}{\hbar^2}\frac{\boldsymbol{r}_\alpha}{\rho}G_F^{(+)}(E) = \mathrm{i}k_\alpha \boldsymbol{n}_\alpha G_F^{(+)}(E), \tag{91}$$

Also, equations (25 d), (87), (88) and (90 c) imply

$$k_\alpha = \frac{2m_\alpha\sqrt{E}}{\hbar^2}\frac{\zeta_{\alpha 1}}{\sqrt{\left(\frac{2m_1}{\hbar^2}+\frac{2m_2}{\hbar^2}\zeta_{21}^2+\ldots+\frac{2m_n}{\hbar^2}\zeta_{n1}^2\right)}}, \tag{92a}$$

$$\frac{r}{\rho} = \frac{\sqrt{(1+\zeta_{\alpha 1}^2+\ldots+\zeta_{n1}^2)}}{\sqrt{\left(\frac{2m_1}{\hbar^2}+\frac{2m_2}{\hbar^2}\zeta_{21}^2+\ldots+\frac{2m_n}{\hbar^2}\zeta_{n1}^2\right)}}. \tag{92b}$$

The right sides of (92 a) and (92 b) depend on ν but are independent of the magnitude of $\boldsymbol{r}$. Equations (25 d) and (90 c) additionally imply

$$\frac{\hbar_1^2 k_1^2}{2m_1}+\frac{\hbar^2 k_2^2}{2m_2}+\ldots+\frac{\hbar^2 k_n^2}{2m_n} = E. \tag{93}$$

Thus the $3n-1$ variables $\boldsymbol{n}_1, \boldsymbol{n}_2, \ldots, \boldsymbol{n}_n, \zeta_{21}, \ldots, \zeta_{n1}$ specifying the direction ν of the $3n$-dimensional vector $\boldsymbol{r} = (\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_n)$ can be replaced by the components of the n vectors $k_1\boldsymbol{n}_1, \ldots, k_n\boldsymbol{n}_n$ subject to the constraint (93). Moreover, (92 a) makes $k_1, k_2, \ldots, k_n$ exactly equal to the values they would have if k_α had been defined in terms of the classical speed v_α of particle α by

$$\hbar k_\alpha = m_\alpha v_\alpha \quad (\alpha = 1, \ldots, n) \tag{94a}$$

and if

$$\zeta_{\alpha 1} = \frac{v_\alpha}{v_1} \tag{94b}$$

(where, of course, v_1 is supposed $\neq 0$). This interpretation (94 b) of $\zeta_{\alpha 1}$ is consistent with its definition (87) because for short-range forces the classical particle distance r_α should asymptotically approach $v_\alpha t$ at times long after the collision.

The other (than free space) Green functions of interest generally are not known in closed form, so that their asymptotic behaviour at large distances must be computed indirectly, e.g. from relations such as (65 b). Some qualitative understanding of the behaviour to be expected can be obtained from examination of the physical operations corresponding to the mathematical operations $\lim \boldsymbol{r}\to\infty$ or $\lim \boldsymbol{r}'\to\infty$. In particular, consider the laboratory system three-particle Green function $G^{(+)}(\boldsymbol{r};\boldsymbol{r}';E)$ defined by (27). Suppose r_1', r_2' and r_3' each were to be made very large in the δ-functions on the right side of (27 d) (recall (23)); more precisely, suppose for each $\alpha = 1, 2, 3$, $r_\alpha' > L$, L some large distance. Then for values of $r_\alpha < L$ the corresponding $G^{(+)}(\boldsymbol{r};\boldsymbol{r}';E)$ would be a non-singular function of $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, $\boldsymbol{r}_3$ satisfying the homogeneous equation (7). Consequently one expects that in the limits $r_\alpha'\to\infty$, $\alpha = 1, 2, 3$, $G^{(+)}(\boldsymbol{r};\boldsymbol{r}';E)$ becomes proportional to some $\Psi(\boldsymbol{r};E)$ solving (7). In fact, when $r_\alpha'\to\infty$ along $\boldsymbol{n}_\alpha'$ keeping the ratios $r_\alpha'/r_1' = \zeta_{\alpha 1}'$ constant—i.e. when the nine-dimensional vector $\boldsymbol{r}'$ locating the source in (27 d) becomes infinite along the direction ν' specified by the vector $\boldsymbol{k}' = (k_1\boldsymbol{n}_1', k_2\boldsymbol{n}_2', k_3\boldsymbol{n}_3')$ subject to (93)—one expects that the associated $\Psi(\boldsymbol{r};E)$ (obtained from the limit of $G(\boldsymbol{r};\boldsymbol{r}';E)$ as $\boldsymbol{r}'$ becomes infinite along ν') will

represent a solution of (7), wherein particles 1, 2, 3 are incident from a remote source located along the direction $\boldsymbol{k}'$; in other words, $\Psi(\boldsymbol{r};E)$ should represent a solution of (7) wherein particles 1, 2, 3 are initially incident along the direction $-\boldsymbol{k}' = (-\boldsymbol{k}'_1, -\boldsymbol{k}'_2, -\boldsymbol{k}'_3)$ subject to (93). Furthermore, because

$$G^{(+)}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3; \boldsymbol{r}'_1, \boldsymbol{r}'_2, \boldsymbol{r}'_3; E) = G^{(+)}(\boldsymbol{r}'_1, \boldsymbol{r}'_2, \boldsymbol{r}'_3; \boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3; E), \tag{95}$$

it also must be true that

$$\lim_{\substack{r_\alpha\to\infty\,||\,n_\alpha \\ r_\alpha/r_1=\zeta_{\alpha 1}}} G^{(+)}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3; \boldsymbol{r}'_1, \boldsymbol{r}'_2, \boldsymbol{r}'_3; E) \sim \Psi(\boldsymbol{r}'_1, \boldsymbol{r}'_2, \boldsymbol{r}'_3; E), \tag{96}$$

where, in (96), Ψ is a solution to (7) (now written in primed variables) in which particles 1, 2, 3 are incident along $-\boldsymbol{k}$, with $\boldsymbol{k}$ given by (92 *a*), i.e. in which Ψ is interpretable as a solution to (7) whose incident incoming part is the plane wave (21 *a*), with $\boldsymbol{k}_1 = -\boldsymbol{k}$ specified by (92 *a*).

3.1. *Specification of wavefunction*

In essence, (96) asserts that the asymptotic behaviour of the real energy $G^{(+)}(\boldsymbol{r};\boldsymbol{r}'E)$ at large distances can provide an alternative (not considered in previous chapters) specification of the solution to Schrödinger's equation corresponding to any given incoming plane wave (21 *a*). This assertion does seem to be generally true, and it has been made the basis for previous work on the configuration-space formulation of scattering theory. However, the specific results obtained when (96) is applied to the case of three-body scattering have not been very carefully examined heretofore; such examination is the subject of the present § 3.1.

I begin by remarking that the expectations of the last paragraph in the preceding section obviously are explicitly borne out by (90 *b*) for the asymptotic behaviour of $G_F^{(+)}$, i.e. for the asymptotic behaviour of $G^{(+)}$ in the event that there is no scattering because all $V_{\alpha\beta} = 0$. To determine the relation for $G^{(+)}$ analogous to (90 *b*) in the actual case that $V_{\alpha\beta} \neq 0$ and scattering occurs, the most obvious starting-point is the equation for $G^{(+)}$ in terms of $G_F^{(+)}$ implied by (63 *d*), namely (as for (63 *a*) and (65))

$$G^{(+)}(E) = G_F^{(+)}(E) - G_F^{(+)}(E)\,[V_{12}+V_{23}+V_{31}]\,G^{(+)}(E), \tag{97 a}$$

$$= G_F^{(+)}(E) - G^{(+)}(E)\,[V_{12}+V_{23}+V_{31}]\,G_F^{(+)}(E). \tag{97 b}$$

The integrals on the right side of (97) are convergent (see § A. 1). Thus (97 *a*) legitimately yields

$$\begin{aligned}\lim_{r\to\infty\,||\,\nu} G^{(+)}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3; \boldsymbol{r}'_1, \boldsymbol{r}'_2, \boldsymbol{r}'_3; E) &= \lim_{r\to\infty\,||\,\nu} G_F^{(+)}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3; \boldsymbol{r}'_1, \boldsymbol{r}'_2, \boldsymbol{r}'_3; E) \\ &\quad - \lim_{r\to\infty\,||\,\nu} \int \mathrm{d}\boldsymbol{r}''_1\,\mathrm{d}\boldsymbol{r}''_2\,\mathrm{d}\boldsymbol{r}''_3\, G_F^{(+)}(\boldsymbol{r};\boldsymbol{r}'';E) \\ &\quad \times [V_{12}(\boldsymbol{r}''_{12}) + V_{23}(\boldsymbol{r}''_{23}) + V_{31}(\boldsymbol{r}''_{31})]\, G^{(+)}(\boldsymbol{r}'';\boldsymbol{r}';E).\end{aligned} \tag{98}$$

Suppose for the moment that interchanging the order of the limiting and integration processes in (98) is legitimate, i.e. suppose

$$\begin{aligned}&\lim_{r\to\infty\,||\,\nu} \int \mathrm{d}\boldsymbol{r}'' G_F^{(+)}(\boldsymbol{r};\boldsymbol{r}'')\,[V_{12}(\boldsymbol{r}''_{12}) + V_{23}(\boldsymbol{r}''_{23}) + V_{31}(\boldsymbol{r}''_{31})]\, G^{(+)}(\boldsymbol{r}'';\boldsymbol{r}') \\ &\qquad = \int \mathrm{d}\boldsymbol{r}'' \lim_{r\to\infty\,||\,\nu} G_F^{(+)}(\boldsymbol{r};\boldsymbol{r}'')\,[V_{12}(\boldsymbol{r}''_{12}) + V_{23}(\boldsymbol{r}''_{23}) + V_{31}(\boldsymbol{r}''_{31})]\, G^{(+)}(\boldsymbol{r}'';\boldsymbol{r}').\end{aligned} \tag{99}$$

Then, using (90 b), the relation (98) yields

$$\lim_{r\to\infty||\nu_f} G^{(+)}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3; \boldsymbol{r}'_1, \boldsymbol{r}'_2, \boldsymbol{r}'_3; E) = \frac{C_3(E)\, e^{i\rho\sqrt{E}}}{\rho^4} \Psi_f^{(-)*}(\boldsymbol{r}'_1, \boldsymbol{r}'_2, \boldsymbol{r}'_3; E) \qquad (100\,a)$$

where $$\Psi_f^{(-)*}(\boldsymbol{r}'; E) = \psi_f^*(\boldsymbol{r}') - \int d\boldsymbol{r}'' \psi_f^*(\boldsymbol{r}'') [V_{12}(\boldsymbol{r}''_{12}) + V_{23}(\boldsymbol{r}''_{23}) + V_{31}(\boldsymbol{r}''_{31})] G^{(+)}(\boldsymbol{r}''; \boldsymbol{r}'; E) \qquad (100\,b)$$

and $$\psi_f(\boldsymbol{r}') = \exp\{i(\boldsymbol{k}_f . \boldsymbol{r}')\} = \exp\{i(\boldsymbol{k}_{1f} . \boldsymbol{r}'_1 + \boldsymbol{k}_{2f} . \boldsymbol{r}'_2 + \boldsymbol{k}_{3f} . \boldsymbol{r}'_3)\} \qquad (100\,c)$$

Using (95), the formula (100 b) in condensed notation is

$$\Psi_f^{(-)*} = \psi_f^* - G^{(+)}(V_{12} + V_{23} + V_{31})\, \psi_f^* \equiv \psi_f^* - G^{(+)} V_f \psi_f^* \qquad (100\,d)$$

recognizing that for the final plane wave (100 c) the final interaction $V_f = V_1 =$ the total V. Actually, because the definition of $G^{(+)}$ involves no initially incident wave, the subscript† f could have been omitted in (100) without inducing any confusion, just as no subscripts were needed on $\boldsymbol{\nu}$, $\boldsymbol{k}_\alpha$, etc. in (90) to (94). For later purposes, however, it is convenient to distinguish the wave vectors $\boldsymbol{k}_{\alpha i}$ in (21 a) from the 'final' wave vectors $\boldsymbol{k}_{\alpha f}$ (associated with the direction $\boldsymbol{\nu}_f$ along which $r \to \infty$ in (100 a)) appearing in the 'final 'plane wave state (100 c).

Since ψ_f^* of (100 c) is a plane wave propagating along $-\boldsymbol{k}_f$, (100 a) is in good accord with the expectations at the end of the preceding section. In particular, as (100 d) makes clear, the quantity $\Psi_f^{(-)*}$—to which $\lim G^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$ as $r \to \infty$ is proportional—is a formal solution of (7), of the form prescribed by (44 a) together with (11 a). Unfortunately, as has been thoroughly discussed in § 2.2, the right side of (100 b) involves (recall (52 a)) a non-convergent integral whenever two-body or three-body bound states can occur. Consequently, the derivation of (100) from (98) and (99) must be considered unsatisfactory. However, because (100 a) agrees with the physically sensible expectations at the end of the preceding section, it is reasonable to presume that a mathematically correct evaluation of $\lim G^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$ as $r \to \infty$ again will lead to (100 a), but will replace (100 b) by a mathematically meaningful prescription of $\Psi_f^{(-)*}$. It further may be presumed that (100 b) fails because (99) need not be true, i.e. because interchanging the order of integration and limit $r \to \infty$ in (98) need not be legitimate.

The foregoing presumptions are correct, as the remainder of this section shows. Consider, first, the question of the validity of (99). The condition for (97 a) to converge, i.e. the condition for the integral on the left side of (99) to converge, is that—for any fixed $\boldsymbol{r}$ and $\boldsymbol{r}'$—the contribution to the integral from the region $r'' > L''$ approaches zero as the nine-dimensional distance L'' becomes infinite. This condition, which surely is satisfied (see § A. 1), is much too weak to guarantee the validity of (99). In effect, (99) is stating that, for any fixed $\boldsymbol{r}'$, the limiting behaviour at large $\boldsymbol{r}$ of the integral on the left side of (99) is the same as the limiting behaviour of $G_f^{(+)}(\boldsymbol{r}; \boldsymbol{r}'')$ when $r \to \infty$ holding $\boldsymbol{r}''$ fixed. Thus a necessary (though very likely not mathematically rigorously sufficient) condition for (99) to hold is that at sufficiently large $\boldsymbol{r}$, for any fixed $\boldsymbol{r}'$, the contribution to the left side of (99) from the region $r'' > r$ be negligible compared to the contribution from the region $r'' < r$. Recalling (90 b), this latter condition requires that the contribution from $r'' > r$ approach zero more rapidly than r^{-4} as $r \to \infty$, whereas the aforementioned condition for the integral on the left side of (99) to converge at large r requires merely that the contribution from $r'' > r$ approach zero as $r \to \infty$.

It is shown in § C. 1 that in fact the condition for (99) to hold is not obeyed when two-body or three-body bound states can occur; to be specific, in this circumstance the contribution to the left side of (99) from $r'' > r$ is of the same order (namely r^{-4}) as the contribution from $r'' < r$. On

† See footnote, p. 199.

the other hand (see § C. 1), equation (99) is valid in the absence of bound states. Similarly, it is shown in § C. 2 that the centre of mass version of (99), namely

$$\lim_{\bar{r}\to\infty||\bar{v}}\int d\bar{r}''\,\bar{G}_F^{(+)}(\bar{r};\bar{r}'')\,[V_{12}(r_{12}'')+V_{23}(r_{23}'')+V_{31}(r_{31}'')]\,\bar{G}^{(+)}(\bar{r}'';\bar{r}')$$
$$=\int d\bar{r}''\lim_{\bar{r}\to\infty||\bar{v}}\bar{G}_F^{(+)}(\bar{r},\bar{r}'')\,[V_{12}(r_{12}'')+V_{23}(r_{23}'')+V_{31}(r_{31}'')]\,\bar{G}^{(+)}(\bar{r}'';\bar{r}') \quad (101)$$

is invalid when and only when two-body bound states exist. Equation (101) is required to derive the centre of mass analogues of (100) from the centre of mass analogue of (97 *a*); failure of (101) is to be associated with the fact that the centre of mass analogue of (100 *b*) involves a divergent integral (namely (52 *b*)). If, nevertheless, one employs (101), there results, as in (100),

$$\lim_{\bar{r}\to\infty||\bar{v}_f}\bar{G}^{(+)}(\bar{r};\bar{r}';\bar{E})=\frac{C_2(\bar{E})\,e^{i\bar{\rho}\sqrt{\bar{E}}}}{\bar{\rho}^{\frac{5}{2}}}\,\bar{\Psi}_f^{(-)*}(\bar{r}';\bar{E}) \quad (102\,a)$$

where, as in (55), $\bar{\Psi}_f^{(-)*}$ of (102 *a*) is related to $\Psi_f^{(-)*}$ of (100 *b*) (or more accurately, to $\Psi_f^{(-)*}$ of (106), see below) by

$$\Psi_f^{(-)*}(\boldsymbol{r}';E)=\exp\{-i\boldsymbol{K}_f.\boldsymbol{R}'\}\,\bar{\Psi}_f^{(-)*}(\bar{r}';\bar{E}). \quad (102\,b)$$

In (102 *a*), the six-dimensional vector $\bar{\rho}$ has three-dimensional projections

$$\left.\begin{aligned}\bar{\rho}.\boldsymbol{r}_{12}&=\left(\frac{2\mu_{12}}{\hbar^2}\right)^{\frac{1}{2}},\\ \bar{\rho}.\boldsymbol{q}_{12}&=\left(\frac{2\mu_{3R}}{\hbar^2}\right)^{\frac{1}{2}},\end{aligned}\right\} \quad (102\,c)$$

with $\boldsymbol{r}_{12}$, $\boldsymbol{q}_{12}$ understood to be orthogonal vectors in that subspace—of the nine-dimensional space spanned by $\boldsymbol{R}$, $\boldsymbol{r}_{12}$, $\boldsymbol{q}_{12}$—which is independent of, and orthogonal to, $\boldsymbol{R}$. In other words (see Appendix F)

$$\bar{\rho}=\left(\frac{2\mu_{12}}{\hbar^2}\right)^{\frac{1}{2}}\boldsymbol{r}_{12}\oplus\left(\frac{2\mu_{3R}}{\hbar^2}\right)^{\frac{1}{2}}\boldsymbol{q}_{12}=\left(\frac{2\mu_{23}}{\hbar^2}\right)^{\frac{1}{2}}\boldsymbol{r}_{23}\oplus\left(\frac{2\mu_{1R}}{\hbar^2}\right)^{\frac{1}{2}}\boldsymbol{q}_{23}, \quad (102\,d)$$

where the symbol $\oplus$ denotes vector summation in the six-dimensional space. Moreover (recall (90 *a*), (90 *b*)) the two masses appearing in $C_2(\bar{E})$ are the two effective masses in (102 *c*), namely μ_{12} and μ_{3R}.

The significance of the foregoing results is clear, and already has been (briefly) stated in § 1: The integral in (52 *a*) fails to converge, i.e. (52 *a*)—though together with (11 *a*) furnishing a formal solution of (7)—is mathematically meaningless when bound states exist. Therefore, the divergence of (52 *a*) when bound states exist must be a signal that any derivation leading to (52 *a*) is mathematically invalid under these circumstances. In § 2.2 the mathematical errors in two such derivations were pinpointed. The first derivation of (52 *a*) discussed in § 2.2—namely via use of the outgoing condition (44 *b*)—fails because when (44 *a*) diverges (44 *b*) is itself meaningless; indeed the surface integral (44 *b*) does not have a limit zero as the radius of the spherical surface of integration in $\boldsymbol{r}$-space approaches infinity. The second 'derivation' of (52 *a*) examined in § 2.2, namely via interchange of order of integration and limit $\epsilon\to 0$, is seen to be invalid because one can argue (as was done in the paragraph following (51 *b*)) that the left and right sides of (51 *a*) cannot be equal when the right side of (51 *a*) fails to converge; in fact, the same argument implies that when (52 *a*) is non-convergent it surely is not identical with the quantity $\Phi_1^{(+)}(E)$ defined as the $\epsilon\to 0$ limit of $\Phi_1(E+i\epsilon)$. The present section has shown that still a third derivation

of (52 *a*)—namely via the interchange (99) of order of integration and limit $r \to \infty$—fails because (99) indeed is invalid when bound states exist. Similar assertions pertain to derivations of (52 *b*).

There remains the question of deriving (100 *a*) from the limit $G^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$ as $r \to \infty$, but without concomitant introduction of divergent expressions for $\Psi_{\mathfrak{i}}^{(-)*}$, i.e. without making use of mathematically incorrect manipulations, such as (99). A mathematically acceptable procedure is suggested by the form of (67 *c*), which is known to converge in the centre of mass system (see § B. 1) and which, together with (61) and (62), therefore provides an acceptable specification of $\Psi_{\mathfrak{i}}^{(+)}$, as has been discussed in § 2.3. Since (67 *c*) results from iterations of G in the formula (50 *a*), it is reasonable to investigate the effect of similar iterations in the integral equation (97 *a*), which has been used above to derive (100 *a*). Thus the suggested new starting-point for derivation of (100 *a*) is the integral equation (80 *c*) for $G^{(+)}$.

In actuality, (80 *c*) does permit a mathematically unobjectionable extraction of $\lim G^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$ as $r \to \infty$ along directions $\boldsymbol{\nu} = \boldsymbol{\nu}_{\mathfrak{f}}$ corresponding to three-body elastic scattering (wherein (99) fails and (100 *b*) diverges), i.e. along directions $\boldsymbol{\nu}_{\mathfrak{f}}$ such that r_1, r_2, r_3, r_{12}, r_{23}, r_{31} become infinite together.† The key to the procedure is the fact that the asymptotic behaviour of (80 *c*) is determined by the asymptotic behaviour of the integrals $G_F^{(+)} V_{\alpha\beta} G_{\alpha\beta}^{(+)}$, which are more tractable than the integrals $G_F^{(+)} V_{\alpha\beta} G^{(+)}$ appearing in (97 *a*). In particular, one can show (see § D. 1)

$$\int \mathrm{d}\boldsymbol{r}'' G_F^{(+)}(\boldsymbol{r}; \boldsymbol{r}''; E)\, V_{12}(\boldsymbol{r}_{12}'')\, G_{12}^{(+)}(\boldsymbol{r}''; \boldsymbol{r}'; E)$$
$$= \frac{1}{(2\pi)^3}\left(\frac{2M}{\hbar^2}\right)^{\frac{3}{2}}\left(\frac{2\mu_{3R}}{\hbar^2}\right)^{\frac{3}{2}} \int \mathrm{d}\boldsymbol{r}_{12}'' \int_0^\infty \frac{\mathrm{d}\mathscr{E}\mathscr{E}^3 J_2(\mathscr{s}\mathscr{E})}{\mathscr{s}^2} g_F^{+}(\boldsymbol{r}_{12}; \boldsymbol{r}_{12}''; \hat{E}_{12})\, V_{12}(\boldsymbol{r}_{12}'')\, g_{12}^{(+)}(\boldsymbol{r}_{12}''; \boldsymbol{r}_{12}'; \hat{E}_{12}), \tag{103}$$

where $g_{12}^{(+)}$ is defined by (75); $g_F^{(+)}$ is the corresponding one-particle free-space Green function, satisfying (75) with $V_{12} \equiv 0$; J_2 is a Bessel function; and

$$\mathscr{s} = \left[\frac{2M}{\hbar^2}(\boldsymbol{R} - \boldsymbol{R}')^2 + \frac{2\mu_{3R}}{\hbar^2}(\boldsymbol{q}_{12} - \boldsymbol{q}_{12}')^2\right]^{\frac{1}{2}}. \tag{104 a}$$

Also, in the Green functions of (103), the quantity $\hat{E}_{12}$ is not a constant, as in (74 *b*), but instead is defined by

$$\hat{E}_{12} = E - \mathscr{E}^2 \tag{104 b}$$

with the understanding that

$$0 \leqslant \arg \sqrt{\hat{E}_{12}} \leqslant \pi. \tag{104 c}$$

In (103) the presence of the short-range potential $V_{12}(\boldsymbol{r}_{12}'')$ guarantees that at sufficiently large $\boldsymbol{r}_{12}$, for any fixed $\boldsymbol{r}'$, the contribution to the right side of (103) from the region $r_{12}'' > r_{12}$ surely is negligible compared to the contribution from $r_{12}'' < r_{12}$. Thus the limiting behaviour of the right side of (103) at large $\boldsymbol{r}_{12}$ can be found from the limiting behaviour of $g_F^{(+)}(\boldsymbol{r}_{12}; \boldsymbol{r}_{12}'')$ as $r_{12} \to \infty$ holding $\boldsymbol{r}_{12}''$ fixed; i.e. interchanging the order of the integration and limiting (as $r_{12} \to \infty$) processes is legitimate in the integral over $\boldsymbol{r}_{12}''$ on the right side of (103). As a matter of fact, and for the same reason, the order of integration over $\boldsymbol{r}_{12}''$ and limit $r_{12} \to \infty$ also can be interchanged on the left side of (103). However, just as in the case of the term $G_F^{(+)} V_{12} G^{(+)}$ in (98), when bound states exist the integration and limiting (as R and $q_{12} \to \infty$) processes cannot be interchanged for the remaining integration variables $\boldsymbol{R}''$ and $\boldsymbol{q}_{12}''$ on the left side of (103) (see § C. 1).

Fortunately, as (103) makes manifest, the integrations over $\boldsymbol{R}''$ and $\boldsymbol{q}_{12}''$ on the left side of (103) can be performed explicitly, a performance not possible for the corresponding $G_F^{(+)} V_{12} G^{(+)}$ term in (98). Therefore the asymptotic behaviour of the left side of (103) at large

$$\boldsymbol{r} = (\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) \equiv (\boldsymbol{R}, \boldsymbol{q}_{12}, \boldsymbol{r}_{12})$$

† See footnote, p. 225.

and fixed $\boldsymbol{r}'$ is legitimately obtained by replacing J_2 and $g_F^{(+)}$ on the right side of (103) by their asymptotic forms at large $\boldsymbol{r}$, holding $\boldsymbol{r}'$ and $\boldsymbol{r}''$ constant. Now application of the method of stationary phase to the resultant integral over $\mathscr{E}$ yields the sought-for asymptotic behaviour of $G_F^{(+)} V_{12} G_{12}^{(+)}$. One finds (see § D. 1)

$$\lim_{r\to\infty||\nu_f} -\int \mathrm{d}\boldsymbol{r}'' G_F^{(+)}(\boldsymbol{r};\boldsymbol{r}'') V_{12}(\boldsymbol{r}''_{12}) G_{12}^{(+)}(\boldsymbol{r}'';\boldsymbol{r}') = \frac{C_3(E)\,\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}}{\rho^4} \Phi_{12f}^{(-)*}(\boldsymbol{r}';E), \tag{105a}$$

where

$$\Phi_{12f}^{(-)*}(\boldsymbol{r}';E) = \exp(-\mathrm{i}\boldsymbol{K}_f.\boldsymbol{R}') \exp(-\mathrm{i}\boldsymbol{K}_{12f}.\boldsymbol{q}'_{12})\, \phi_{12f}^{(-)*}(\boldsymbol{r}'_{12};\boldsymbol{k}_{12f}), \tag{105b}$$

$$\phi_{12f}^{(-)*}(\boldsymbol{r}'_{12};\boldsymbol{k}_{12f}) = -\int \mathrm{d}\boldsymbol{r}''_{12}\, g_{12}^{(+)}(\boldsymbol{r}'_{12};\boldsymbol{r}''_{12};E_{12f}) V_{12}(\boldsymbol{r}''_{12}) \exp(-\mathrm{i}\boldsymbol{k}_{12f}.\boldsymbol{r}''_{12}), \tag{105c}$$

and E_{12f} now is constant and related to k_{12f} by (74 b). I add that if on the left side of (103) I had wholly (for integration over $\boldsymbol{R}''$ and $\boldsymbol{q}''_{12}$ as well as $\boldsymbol{r}''_{12}$) interchanged the order of integration and limit $\boldsymbol{r}\to\infty$, I again would have obtained (105 a), but with the definition

$$\Phi_{12f}^{(-)*}(\boldsymbol{r}';E) = -\int \mathrm{d}\boldsymbol{r}''\psi_f^*(\boldsymbol{r}'') V_{12}(\boldsymbol{r}''_{12}) G_{12}^{(+)}(\boldsymbol{r}'';\boldsymbol{r}';E), \tag{105d}$$

instead of the more correct (105 b). When bound states $u_j(\boldsymbol{r}_{12})$ exist, the integral (105 d) is divergent, in both the centre of mass and laboratory frames, consistent with the results of § C. 1. Again (recall the remarks following (75)) non-physical (vanishing on the energy shell) δ-functions, absent from the correctly derived (105 b), can appear in the formula (105 d) deduced via incorrect mathematical manipulations. Of course, if one decided to reinterpret the right side of (105 d) as equal to the limit of $G_F(E+\mathrm{i}\epsilon) V_{12}\psi_f^*$ when $\epsilon\to 0$, (105 d) becomes identical with (105 b) (compare (60), (72) and (73)).

Having derived (105 a) to (105 c), they legitimately (see § E. 1) can be directly inserted into (80 c), thereby making manifest the asymptotic behaviour at large $\boldsymbol{r}$ of the term

$$\{G_F^{(+)} V_{12} G^{(+)}\}(V_{23}+V_{31}) G^{(+)}$$

in (80 c). In this way, one proves that (100 a) indeed is correct, but that (100 b) must be replaced by

$$\Psi_f^{(-)*} = \psi_f^* + \Phi_{12f}^{(-)*} + \Phi_{23f}^{(-)*} + \Phi_{31f}^{(-)*} + \Phi_f^{s(-)*}, \tag{106a}$$

$$\Phi_f^{s(-)*} = -G^{(+)}[(V_{23}+V_{31})\Phi_{12f}^{(-)*} + (V_{31}+V_{12})\Phi_{23f}^{(-)*} + (V_{12}+V_{23})\Phi_{31f}^{(-)*}], \tag{106b}$$

where $\Phi_{\alpha\beta f}^{(-)*}$ are defined as in (105 b), and where the integrals in (106 b) are made meaningful by the fact that they surely converge in the centre of mass frame (recall (67 c) and (69)). In view of § 2.3, it is clear that (106) do furnish a meaningful prescription of a solution $\Psi_f^{(-)*}$ to Schrödinger's equation (7); indeed, $\Psi_f^{(-)*}$ must coincide with the limit, as $\epsilon\to 0$, of the solution $\Psi_f(E+\mathrm{i}\epsilon)$ to the Lippmann–Schwinger integral equation

$$\Psi_f(E+\mathrm{i}\epsilon) = \psi_f^*(E) - \frac{1}{H_f - E - \mathrm{i}\epsilon} V_f \Psi_f(E+\mathrm{i}\epsilon), \tag{107a}$$

where, of course, $H_f = H_i = T$ of (21 c).

Starting from (97 b), and (now knowingly naïvely) interchanging the order of integration and limit $\boldsymbol{r}\to\infty$, as in (99), yields, after using the (now mathematically correctly demonstrated) (100 a),

$$\Psi_f^{(-)*} = \psi_f^* - G_F^{(+)}(V_{12}+V_{23}+V_{31})\Psi_f^{(-)*} \tag{107b}$$

as an alternative to (100 *b*) (or (100 *d*)). According to § 2.2, (107 *b*) (compare (42)), the real energy version of (107 *a*), does not involve divergent integrals, even when bound states occur. Correspondingly, one can demonstrate that the interchange of order of integration and limit $r \to \infty$ is justifiable in (97 *b*) (see § C. 3), despite the fact that the similar interchange in (97 *a*) has been shown to be invalid (§ C. 1). This seemingly paradoxical (because the right sides of (97 *a*) and (97 *b*) are equal) conclusion stems from the fact that, according to (98), the $\boldsymbol{r}$, $\boldsymbol{r}'$ element of (97 *a*) involves $G_F^{(+)}(\boldsymbol{r}; \boldsymbol{r}'')\, G^{(+)}(\boldsymbol{r}''; \boldsymbol{r}')$, whereas the $\boldsymbol{r}$, $\boldsymbol{r}'$ element of (97 *b*) involves $G^{(+)}(\boldsymbol{r}; \boldsymbol{r}'')\, G_F^{(+)}(\boldsymbol{r}''; \boldsymbol{r}')$, with integration over $\boldsymbol{r}''$ implied. Therefore the interchange (99)—whose legitimacy depends on the behaviour of the integrand in (98) in the domain $r'' > r$ as $r \to \infty$ holding $\boldsymbol{r}'$ constant and finite—need not be just as valid as the corresponding interchange in (97 *b*).

Irrespective of validity, the foregoing derivations—of (100 *b*) from (97 *a*), and of (107 *b*) from (97 *b*)—indicate a not altogether apparent relationship between (107 *b*) and (100 *b*), or equivalently between (42) and the formula for $\Psi_i^{(+)}$ implied by (44 *a*) (together with (11 *a*)). Equation (95) means that, in the coordinate representation at any rate, $G^{(+)}$ is a symmetric operator

$$G^{(+)} = \tilde{G}^{(+)}, \tag{108}$$

where the tilde indicates the transpose. One then sees that (97 *b*) is nothing more than the transpose of (97 *a*),

$$\begin{aligned} \tilde{G}^{(+)} = G^{(+)} &= [G_F^{(+)} - G_F^{(+)} V G^{(+)}]_{\text{trans.}} \\ &= \tilde{G}_F^{(+)} - \tilde{G}^{(+)} \tilde{V} \tilde{G}_F^{(+)} = G_F^{(+)} - G^{(+)} V G_F^{(+)}, \end{aligned} \tag{109}$$

wherein, for the purpose of taking the transpose, it now is convenient to write the right side of (97 *a*) in terms of operators only (recall (27 *f*)), i.e. it now is convenient to replace V in (97 *a*) by V of (27 *e*); with this replacement, the operations in (109) are obviously legitimate, recognizing from (27 *e*) that the operator V is diagonal, i.e. symmetric, in the coordinate representation. In other words—now ignoring the distinction between $\Psi_i^{(+)}$ and $\Psi_f^{(-)*}$—(42) and (44 *a*) are the results of (naïvely) taking the limit $\boldsymbol{r} \to \infty$ in a pair of transposed equations for $G^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$.

Similarly, the transpose of (80 *c*) is

$$\begin{aligned} \tilde{G}^{(+)} = G^{(+)} = G_F^{(+)} &- G_{12}^{(+)} V_{12} G_F^{(+)} - G_{23}^{(+)} V_{23} G_F^{(+)} - G_{31}^{(+)} V_{31} G_F^{(+)} + G^{(+)}(V_{23} + V_{31}) \\ &\times \{G_{12}^{(+)} V_{12} G_F^{(+)}\} + G^{(+)}(V_{31} + V_{12}) \{G_{23}^{(+)} V_{23} G_F^{(+)}\} + G^{(+)}(V_{12} + V_{23}) \{G_{31}^{(+)} V_{31} G_F^{(+)}\}, \end{aligned} \tag{110}$$

which of course can be derived directly from the second equality in (63 *d*), via iterations like those in (80 *a*), but substituting always the second equality from each of (63 *a*) to (63 *c*). Now, on the right side of (110), in the second, third and fourth terms *only*, use (81 *b*) to replace $G_{\alpha\beta} V_{\alpha\beta} G_F^{(+)}$ by $G_F^{(+)} V_{\alpha\beta} G_{\alpha\beta}^{(+)}$, and then take the limit $\boldsymbol{r} \to \infty$, recalling (100 *b*) and (105 *a*). There results, in condensed notation

$$\begin{aligned} \Psi_f^{(-)*} = \psi_f^* + \Phi_{12f}^{(-)*} + \Phi_{23f}^{(-)*} + \Phi_{31f}^{(-)*} &+ \{G_F^{(+)} V_{12} G_{12}^{(+)}\} (V_{23} + V_{31})\, \Psi_f^{(-)*} \\ &+ \{G_F^{(+)} V_{23} G_{23}^{(+)}\} (V_{31} + V_{12})\, \Psi_f^{(-)*} + \{G_F^{(+)} V_{31} G_{31}^{(+)}\} (V_{12} + V_{23})\, \Psi_f^{(-)*}. \end{aligned} \tag{111}$$

Equations (111) and (106 *b*) are to be compared with (84 *c*) and (67 *c*) respectively. One concludes, as in the preceding paragraph, that (84 *c*) and (67 *c*) (together with (61)) are the results of taking the limit $\boldsymbol{r} \to \infty$ in another (than (97)) pair of transposed equations for $G^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$, namely (110) and (80 *c*) respectively. This paragraph clarifies and justifies the opening remark in the last paragraph of § 2.3.

3.2. *Finite interparticle distances as* $\boldsymbol{r} \to \infty$

The previous section has examined the limit of $G^{(+)}(\boldsymbol{r};\boldsymbol{r}';E)$ as $r\to\infty$ along directions $\boldsymbol{\nu}=\boldsymbol{\nu}_{\mathrm{f}}$ such that all r_α, $r_{\alpha\beta}$ become infinite together, these being the directions $\boldsymbol{\nu}_{\mathrm{f}}$ which correspond to three-body elastic scattering. For many of the proofs (e.g. in the appendices), however, it is needful also to know the limit of $G^{(+)}(\boldsymbol{r};\boldsymbol{r}';E)$ along directions $\boldsymbol{\nu}$ wherein some $r_{\alpha\beta}$ remains finite as ∞ is approached, i.e. along directions $\boldsymbol{\nu}_{\alpha\beta}$ (as defined at the beginning of this section). The required results in this limit $r\to\infty$ along $\boldsymbol{\nu}_{\alpha\beta}$ are collected in this section.

The need for special treatment when some $\boldsymbol{r}_{\alpha\beta}$ remains finite can be understood from (103). If $\boldsymbol{r}_{12}$ remains finite, one cannot employ assuredly—on the right side of (103)—the asymptotic form of $g_F^{(+)}(\boldsymbol{r}_{12};\boldsymbol{r}''_{12})$ valid at $r_{12}\gg r''_{12}$, even though $V_{12}(\boldsymbol{r}''_{12})$ is a short-range force. Consequently the proof (in § D. 1), leading ultimately to (105 *a*) to (105 *c*), does not necessarily go through when $\boldsymbol{r}_{12}$ remains finite. Correspondingly, use of (100 *a*) with (106) replacing (100 *b*) may not be valid if any pair $\boldsymbol{r}_{\alpha\beta}$ remains finite.

The Green function $\bar{G}_{12}$ has the expansion (analogous to (53 *a*))

$$\bar{G}_{12}(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}';\bar{E}+\mathrm{i}\epsilon)=\sum_{\mathrm{j}}u_{\mathrm{j}}(\boldsymbol{r}_{12})u_j^*(\boldsymbol{r}'_{12})\,g_F(\boldsymbol{q}_{12};\boldsymbol{q}'_{12};\bar{E}-\epsilon_{\mathrm{j}}+\mathrm{i}\epsilon)$$
$$+\int \mathrm{d}\hat{\boldsymbol{k}}_{12}u(\boldsymbol{r}_{12};\hat{\boldsymbol{k}}_{12})\,u^*(\boldsymbol{r}'_{12};\hat{\boldsymbol{k}}_{12})\,g_F(\boldsymbol{q}_{12};\boldsymbol{q}'_{12};\bar{\mathscr{E}}^2+\mathrm{i}\epsilon),\quad(112\,a)$$

where
$$\left[\frac{-\hbar^2}{2\mu_{3R}}\nabla^2_{q12}-\lambda\right]g_F(\boldsymbol{q}_{12};\boldsymbol{q}'_{12};\lambda)=\delta(\boldsymbol{q}_{12}-\boldsymbol{q}'_{12})\quad(112\,b)$$

and
$$\bar{\mathscr{E}}^2=\bar{E}-\frac{\hbar^2\hat{k}_{12}^2}{2\mu_{12}},\quad(112\,c)$$

with the usual understanding, as, for example, in (25 *b*), that

$$0<\arg(\bar{\mathscr{E}}^2+\mathrm{i}\epsilon)<2\pi.\quad(112\,d)$$

The bound state functions u_{j} in (112 *a*) are defined as in (48); the continuum functions $u(\boldsymbol{r}_{12};\hat{\boldsymbol{k}}_{12})$ satisfy

$$\left[-\frac{\hbar^2}{2\mu_{12}}\nabla^2_{12}+V_{12}-\frac{\hbar^2\hat{k}_{12}^2}{2\mu_{12}}\right]u(\boldsymbol{r}_{12};\hat{\boldsymbol{k}}_{12})=0.\quad(113\,a)$$

The sets u_{j} and $u(\hat{\boldsymbol{k}}_{12})$ together presumably form a complete orthonomal set,

$$\sum_{\mathrm{j}}u_{\mathrm{j}}(\boldsymbol{r}_{12})\,u_{\mathrm{j}}^*(\boldsymbol{r}'_{12})+\int \mathrm{d}\hat{\boldsymbol{k}}_{12}u(\boldsymbol{r}_{12};\hat{\boldsymbol{k}}_{12})\,u^*(\boldsymbol{r}'_{12};\hat{\boldsymbol{k}}_{12})=\delta(\boldsymbol{r}_{12}-\boldsymbol{r}'_{12}).\quad(113\,b)$$

A convenient choice of $u(\hat{\boldsymbol{k}}_{12})$ consistent with (113 *b*) is

$$u(\boldsymbol{r}_{12};\hat{\boldsymbol{k}}_{12})=(2\pi)^{-\frac{3}{2}}\left[\exp\{\mathrm{i}\hat{\boldsymbol{k}}_{12}.\boldsymbol{r}_{12}\}-\int \mathrm{d}\boldsymbol{r}'_{12}\,g_{12}^{(+)}\left(\boldsymbol{r}_{12};\boldsymbol{r}'_{12};\frac{\hbar^2\hat{k}_{12}^2}{2\mu_{12}}\right)V_{12}(\boldsymbol{r}'_{12})\exp\{\mathrm{i}\hat{\boldsymbol{k}}_{12}.\boldsymbol{r}'_{12}\}\right],\quad(113\,c)$$

where $g_{12}^{(+)}$ is the same Green function as in (75).

In the discrete sum over j in (112 *a*), the limit as $\epsilon\to 0$ is obvious, i.e. in the discrete terms g_F becomes $g_F^{(+)}$ when $\bar{G}_{12}$ becomes $\bar{G}_{12}^{(+)}$. Therefore, for energies $\bar{E}>0$, (112) and (90) imply that, provided bound states $u_{\mathrm{j}}(\boldsymbol{r}_{12})$ actually exist, $\bar{G}_{12}^{(+)}$ is of order q_{12}^{-1} as $\bar{r}\to\infty$ along directions $\bar{\boldsymbol{\nu}}_{12}$ such that $\boldsymbol{r}_{12}$ remains finite; this result is to be contrasted with the asymptotic behaviour $\sim q_{12}^{-5/2}$ ($\equiv\bar{\rho}^{-5/2}$ for these directions $\boldsymbol{\nu}_{12}$) which would be inferred, incorrectly, to be sure, from, for example, the centre of mass version of (105 *a*), or (equivalently) from (102 *a*) in the case $V_{23}=V_{31}=0$. It has been shown elsewhere (Gerjuoy 1958 *a*) that along these directions $\boldsymbol{\nu}_{12}$ the

outgoing probability current is to be computed from the projections of $\bar{\Phi}_i^{(+)}$ on $u_j(\boldsymbol{r}_{12})$. Correspondingly, when bound states $u_j(\boldsymbol{r}_{12})$ exist, the useful version of the asymptotic behaviour of $\bar{G}_{12}^{(+)}$ along directions $\bar{\boldsymbol{\nu}}_{12}$ is

$$\lim_{q_{12}\to\infty||\bar{\nu}_{12f}}\int d\boldsymbol{r}_{12}u_j^*(\boldsymbol{r}_{12})\,\bar{G}_{12}^{(+)}(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}';\bar{E}) = \frac{\mu_{3R}}{2\pi\hbar^2}\frac{\exp\{i\,K_{12j}q_{12}\}}{q_{12}}u_j^*(\boldsymbol{r}'_{12})\exp\{-i\,K_{12j}\bar{\boldsymbol{\nu}}_{12f}\cdot\boldsymbol{q}'_{12}\}, \quad (114\,a)$$

where

$$\frac{\hbar^2}{2\mu_{3R}}K_{12j}^2+\epsilon_j = \bar{E}. \quad (114\,b)$$

Equations (114 a) and (65 b) then imply

$$\lim_{q_{12}\to\infty||\bar{\nu}_{12f}}\int d\boldsymbol{r}_{12}u_j^*(\boldsymbol{r}_{12})\,\bar{G}^{(+)}(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}';\bar{E}) = \frac{\mu_{3R}}{2\pi\hbar^2}\frac{e^{iK_{12j}q_{12}}}{q_{12}}\bar{\Psi}_{12jf}^{(-)*}(\bar{\boldsymbol{r}}';\bar{E}), \quad (115\,a)$$

$$\bar{\Psi}_{12jf}^{(-)*}(\bar{\boldsymbol{r}}';\bar{E}) = u_j^*(\boldsymbol{r}'_{12})\exp\{-i\,K_{12j}\bar{\boldsymbol{\nu}}_{12f}\cdot\boldsymbol{q}'_{12}\} - \int d\boldsymbol{r}''_{12}\,d\boldsymbol{q}''_{12}\,\bar{G}^{(+)}(\bar{\boldsymbol{r}}';\bar{\boldsymbol{r}}'';\bar{E})\,[V_{23}(\boldsymbol{r}''_{23})+V_{31}(\boldsymbol{r}''_{31})]\,u_j^*(\boldsymbol{r}''_{12})\exp\{-i\,K_{12j}\bar{\boldsymbol{\nu}}_{12f}\cdot\boldsymbol{q}''_{12}\}. \quad (115\,b)$$

Equation (115 b) for $\bar{\Psi}_{12jf}^{(-)*}(\bar{\boldsymbol{r}}')$ has essentially the same form as does (100 b) for $\Psi_i^{(-)*}(\boldsymbol{r}')$, taking into account the differences between the subspaces (defined by $\boldsymbol{\nu}_f$ as opposed to $\bar{\boldsymbol{\nu}}_{12f}$), wherein the limits are being evaluated. However, (115 b), unlike (100 b) or its centre of mass version, is valid, and does not require modification along the lines of (106), because the right side of (115 b) is convergent by virtue of the fact that the V_{12} interaction term has been eliminated from (115 b). The laboratory version of (115 b) fails to converge only when three-body bound states exist (see § A. 5).

Because the continuum terms in (112 a), like the discrete terms, involve merely a one-particle three dimensional Green function g_F, (114) might be thought to imply that—even when no bound states exist—$\bar{G}_{12}^{(+)}$ is of order q_{12}^{-1} as $\bar{r}\to\infty$ along directions $\bar{\boldsymbol{\nu}}_{12}$. This conclusion would be incorrect, however; in the absence of bound states $\bar{G}_{12}^{(+)}$ must behave asymptotically like an outgoing six-dimensional wave along all directions in $\bar{\boldsymbol{r}}$-space, i.e. even along $\bar{\boldsymbol{\nu}}_{12}$ must be proportional to the same $e^{i\bar{\rho}\sqrt{\bar{E}}}/\bar{\rho}^{\frac{5}{2}}$ factor (displayed explicitly in (102 a) for $\bar{G}^{(+)}$) as is found for $\bar{G}_F^{(+)}$ from (90). In fact, an explicit calculation (see § D. 2) starting from (112 a) shows that in the absence of bound states

$$\lim_{q_{12}\to\infty||\bar{\nu}_{12f}}\bar{G}_{12}^{(+)}(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}';\bar{E}) = (2\pi)^3\,C_2(\bar{E})\frac{\exp\{i\bar{\rho}\sqrt{\bar{E}}\}}{\bar{\rho}^{\frac{5}{2}}}u(\boldsymbol{r}_{12};0)\,u^*(\boldsymbol{r}'_{12};0)\exp\{-i\,\boldsymbol{K}_{12f}\cdot\boldsymbol{q}'_{12}\} \quad (116\,a)$$

where $C_2(\bar{E})$ and $\bar{\boldsymbol{\rho}}$ are defined as in (102), with the understanding that in (116 a), because $q_{12}\to\infty$ holding $\boldsymbol{r}_{12}$ finite,

$$\bar{\rho} = \left(\frac{2\mu_{3R}}{\hbar^2}\right)^{\frac{1}{2}}q_{12} \quad (116\,b)$$

and

$$K_{12f} = \left(\frac{2\mu_{3R}\bar{E}}{\hbar^2}\right)^{\frac{1}{2}} \quad (116\,c)$$

plus, of course, $\boldsymbol{K}_{12f} = K_{12f}\bar{\boldsymbol{\nu}}_{12f}$. The functions $u(\boldsymbol{r}_{12};0)$, $u^*(\boldsymbol{r}'_{12};0)$ in (116 a) are given by (113 c), putting $\hat{\boldsymbol{k}}_{12}=0$.

Equations (116) are not quite identical with the result of letting $r_{12}/q_{12}\to 0$ in the centre of mass analogue of (105). To be precise, comparing (105 c) and (113 c), and remembering (81 b), one sees that (105) at $k_{12f}=0$ are identical with (116) except that (116 a) contains an extra factor

$(2\pi)^{\frac{3}{2}}u(\boldsymbol{r}_{12};0)$, which factor approaches unity as $r_{12}\to\infty$ (it is necessary to realize that as $E_{12}\to 0$, but only in this limit,

$$\lim_{E_{12}\to\infty} g_{12}^{(+)}(E_{12}) = \lim_{E_{12}\to\infty} [g_{12}^{(+)}(E_{12})]^* = \lim_{E_{12}\to\infty} g_{12}^{(-)}(E_{12}), \tag{116d}$$

because at $E_{12}=0$, but only at $E_{12}=0$, $g_{12}(E_{12}+\mathrm{i}\epsilon)$ is separated from $g_{12}(E_{12}-\mathrm{i}\epsilon)$ by only an infinitesimal path around the cut running along positive real E_{12} from $E_{12}=0$ to infinity). Equation (116*a*) explicitly demonstrates that—even when there are no bound states—equations (105) are not strictly valid for directions $\boldsymbol{\nu}_{\mathrm{f}}=\boldsymbol{\nu}_{12\mathrm{f}}$ corresponding to having q_{12} and $R\to\infty$ keeping r_{12} finite. Of course, as explained in the second paragraph of this section, there is no reason to expect that (105) remain valid when r_{12} is kept finite.

On the other hand, questions can be raised concerning the correctness of (116*a*) (see § D. 2), so I do not want to insist that (105) are in error along $\boldsymbol{\nu}\equiv\boldsymbol{\nu}_{12\mathrm{f}}$, or that (116*a*) is exact. Evidently, results and remarks similar to the foregoing must pertain to the asymptotic behaviour of $G^{(+)}(\boldsymbol{r};\boldsymbol{r}')$ or $\bar{G}^{(+)}(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}')$ as the unprimed coordinates become infinite along $\boldsymbol{\nu}_{12\mathrm{f}}$ or $\bar{\boldsymbol{\nu}}_{12\mathrm{f}}$ respectively. For all purposes of this work, however, it is sufficient to recognize that when no bound states exist $\lim G^{(+)}(\boldsymbol{r};\boldsymbol{r}')$ must be of order $\mathrm{e}^{\mathrm{i}\rho\sqrt{E}}/\rho^4$, and $\lim \bar{G}^{(+)}(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}')$ must be of order $\mathrm{e}^{\mathrm{i}\bar{\rho}\sqrt{\bar{E}}}/\bar{\rho}^{\frac{5}{2}}$. The above simple and hardly challengeable assertion concerning the asymptotic behaviour of $G^{(+)}$ suffices to make inconsequential (for the purposes of this work) any possible differences, in the absence of bound states, between the actual behaviour of $G^{(+)}(\boldsymbol{r};\boldsymbol{r}')$ along $\boldsymbol{\nu}_{12\mathrm{f}}$ and the behaviour inferred from (100*a*) supplemented by (106); correspondingly, in the absence of bound states any inaccuracies in (102*a*) along directions $\bar{\boldsymbol{\nu}}_{\mathrm{f}}=\bar{\boldsymbol{\nu}}_{12\mathrm{f}}$ are inconsequential for the purposes of the present investigation. In particular, it can be seen that all arguments in the appendices based on the forms of (100*a*) or (102*a*) remain valid (cf., for example, § A. 5), and that the computations of outgoing current flow in § 4 below remain correct (see the remarks in the paragraph immediately preceding § 4.1).

4. Transition amplitudes

The previous chapter has discussed the asymptotic behaviour of the outgoing Green function $G^{(+)}(\boldsymbol{r};\boldsymbol{r}')$ at large $\boldsymbol{r}$. This chapter examines the limit of $\Psi_{\mathrm{i}}^{(+)}(\boldsymbol{r})$ as $\boldsymbol{r}\to\infty$, and interprets the reaction rates inferred therefrom, concentrating primarily on directions $\boldsymbol{\nu}$ corresponding to three-body elastic scattering, i.e. on directions $\boldsymbol{\nu}$ for which no $r_{\alpha\beta}$ remains finite as $r\to\infty$. In this connexion suppose the scattered part $\Phi_{\mathrm{i}}^{(+)}$ of $\Psi_{\mathrm{i}}^{(+)}$ really were everywhere outgoing at infinity in the laboratory system. Then, according to arguments which have been given elsewhere (Gerjuoy 1958*a*), in the laboratory system the outward flow of probability current (associated with $\Phi_{\mathrm{i}}^{(+)}$) across the sphere at infinity should be

$$\mathscr{F} = \frac{1}{\mathrm{i}\hbar}\int \mathrm{d}\boldsymbol{S}\,.\,W[\Phi_{\mathrm{i}}^{(+)*},\Phi_{\mathrm{i}}^{(+)}], \tag{117a}$$

where W is defined as in (45*a*); and where the surface element $\mathrm{d}\boldsymbol{S}$ is perpendicular to $\boldsymbol{\nu}$ and has magnitude $\mathrm{d}S=r^8\,\mathrm{d}\nu$ given by (89). As was mentioned in § 1, in the time-independent configuration space formulation of scattering theory, reaction coefficients are computed from the probability current at infinity. Thus, to be sure that computation of the three-body elastic scattering rate does not involve divergent expressions, it is necessary that along most directions $\boldsymbol{\nu}$

$$|W[\Phi_{\mathrm{i}}^{(+)*},\Phi_{\mathrm{i}}^{(+)}]| \sim \frac{1}{r^8}, \tag{117b}$$

or even smaller. If $|W|$ decreases more slowly than $1/r^8$, the integrand in the surface integral (117 *a*) at infinity is not bounded. Correspondingly, the integral for $\mathscr{F}$ diverges as $r \to \infty$, unless (at fixed large r) the angular integrations over $d\boldsymbol{\nu}$ vanish; of course, the integrations over $d\boldsymbol{\nu}$ in (117 *a*) could not vanish if $\Phi_i^{(+)}$ really were everywhere outgoing at infinity, since then $(i\hbar)^{-1} d\boldsymbol{S} . W$ always would have the same sign.

Equation (117 *b*) would hold if $\Phi_i^{(+)}(\boldsymbol{r}; E)$ behaved asymptotically at large $\boldsymbol{r}$ like $G_F^{(+)}(\boldsymbol{r}; \boldsymbol{r}'; E)$ (recall (90)), i.e. if $\Phi_i^{(+)}(\boldsymbol{r}; E)$ at large $\boldsymbol{r}$ represented three particles moving freely (as if under no forces) outwards from the laboratory system origin and from each other. But (55 *b*) shows the centre of mass motion associated with $\Phi_i^{(+)}$ is that of a plane wave, not an outgoing spherical wave; correspondingly, $|W|$ actually decreases no more rapidly than r^{-5}, and the integrand in (117 *a*) does turn out to be divergent (see § 4.1.1). For three-particle collisions involving two incident bodies only, as, for example, reactions (17 *b*) and (17 *c*), this divergence of (117 *a*) is not a cause for serious concern, however, because: (i) the divergence is interpretable physically, and (more importantly) (ii) manipulations with divergent quantities can be wholly avoided by computing the centre of mass frame probability current flow

$$\bar{\mathscr{F}} = \frac{1}{i\hbar} \int d\bar{\boldsymbol{S}} . \bar{W}[\bar{\Phi}_i^{(+)*}, \bar{\Phi}_i^{(+)}]. \tag{118 a}$$

In particular, in the cited two-body reactions (17 *b*) and (17 *c*), when $\bar{\boldsymbol{r}} \to \infty$ along directions $\bar{\boldsymbol{\nu}}$ corresponding to break-up into three particles, $\bar{\Phi}_i^{(+)}(\bar{\boldsymbol{r}}; \bar{E})$ behaves (Nuttall 1967) like $\bar{G}_F^{(+)}(\bar{\boldsymbol{r}}; \bar{\boldsymbol{r}}'; \bar{E})$, and

$$|\bar{W}[\bar{\Phi}_i^{(+)*}, \bar{\Phi}_i^{(+)}]| \sim 1/\bar{r}^5, \tag{118 b}$$

which suffices to keep finite the total scattered current flow across the sphere at infinite $\bar{r}$, whose surface element $d\bar{S}$ is of order $\bar{r}^5$.

On the other hand, for collisions induced by the incident wave (21 *a*), wherein all three particles are initially free, $\bar{\Phi}_i^{(+)}(\bar{\boldsymbol{r}}; \bar{E})$ does not behave asymptotically like $\bar{G}_F^{(+)}(\bar{\boldsymbol{r}}; \bar{\boldsymbol{r}}'; \bar{E})$; correspondingly, (118 *b*) does not hold and use of (118 *a*) generally does not avoid infinite probability current flows. In fact, (61), (68) and (72) make it obvious that $\bar{\Phi}_i^{(+)}$ generated by (20) contains contributions $\bar{\Phi}_{12}^{(+)}$, $\bar{\Phi}_{23}^{(+)}$, $\bar{\Phi}_{31}^{(+)}$ possessing plane wave factors. For such terms, (118 *b*) fails (see § 4.1.2) because, whereas $\lim \bar{G}_F^{(+)}(\bar{\boldsymbol{r}}; \bar{\boldsymbol{r}}'; \bar{E})$ as $\bar{\boldsymbol{r}} \to \infty$ along $\bar{\boldsymbol{\nu}}$ is of order $\bar{r}^{-5/2}$ (recall (90) and (92)), the corresponding limit of $\bar{\Phi}_{\alpha\beta}^{(+)}(\bar{\boldsymbol{r}}; \bar{E})$ is of order $\bar{r}_{\alpha\beta}^{-1} \cong \bar{r}^{-1}$ along directions $\bar{\boldsymbol{\nu}}$ for which $r_{\alpha\beta}$ becomes infinite with $\bar{r}$. These considerations indicate that at the very least $\bar{\Phi}_{12}^{(+)}$, $\bar{\Phi}_{23}^{(+)}$ and $\bar{\Phi}_{31}^{(+)}$ must be subtracted from $\bar{\Phi}_i^{(+)}$ before there can be any hope of computing—via (118 *a*), but now using $\bar{\Phi}_i^{s(+)}$ from (62) in place of $\bar{\Phi}_i^{(+)}$—non-diverging centre of mass frame scattered current flows.

Unfortunately (as particularly § 4.1.3 will show), use of $\bar{\Phi}_i^{s(+)}$ instead of $\bar{\Phi}_i^{(+)}$ in (118 *a*) still does not eliminate all sources of divergent $\bar{\mathscr{F}}$. To put it differently, it will be shown in § 4.1.3 that—for short-range forces and directions $\bar{\boldsymbol{\nu}}$ corresponding to three-body elastic scattering—$\bar{\Phi}_i^{s(+)}(\bar{\boldsymbol{r}}; \bar{E})$ still is not identical with that part of $\bar{\Phi}_i^{(+)}(\bar{\boldsymbol{r}}; \bar{E})$ which as $\bar{\boldsymbol{r}} \to \infty$ along $\bar{\boldsymbol{\nu}}$ behaves like the corresponding limit of $\bar{G}_F^{(+)}(\bar{\boldsymbol{r}}; \bar{\boldsymbol{r}}'; \bar{E})$ holding $\bar{\boldsymbol{r}}'$ constant; it is this (behaving like $\bar{G}_F^{(+)}$) part of $\bar{\Phi}_i^{(+)}$ which in § 1 was termed its 'truly three-body' part $\bar{\Phi}_i^{t(+)}$. Note that the foregoing definition of $\bar{\Phi}_i^{t(+)}$ is not uniquely prescriptive because it permits adding to (or subtracting from) $\bar{\Phi}_i^{t(+)}$ any part of $\bar{\Phi}_i^{t(+)}$ which at infinity is negligible compared to $\bar{\rho}^{-5/2}$; this indeterminateness in $\bar{\Phi}_i^{t(+)}$ is inconsequential, however, since terms negligible compared to $\bar{\rho}^{-5/2}$ make no contribution to (118 *a*) (when $\bar{\Phi}_i^{t(+)}$ replaces $\bar{\Phi}_i^{(+)}$). The definition does rule out of $\bar{\Phi}_i^{t(+)}$ any terms which at infinity in the centre of mass frame decrease less rapidly than $\bar{\rho}^{-5/2}$, or which are not everywhere outgoing (i.e.

which contain contributions proportional to $e^{-i\bar{\rho}\sqrt{\bar{E}}}$ instead of $e^{i\bar{\rho}\sqrt{\bar{E}}}$). It is understood, of course, that for our present purposes—namely, determining elastic scattering coefficients—nothing need be said nor has been said about the permitted behaviour of $\bar{\Phi}_i^{t(+)}$ along directions $\tilde{\nu} = \tilde{\nu}_{\alpha\beta}$ corresponding to keeping $r_{\alpha\beta}$ finite as $\tilde{r} \to \infty$. As a matter of fact, recombination reactions, e.g. (17 *a*), are 'truly three-body'; moreover, when, for example, particle 1 can be bound to 2,

$$\lim_{q_{12}\to\infty\,||\tilde{\nu}_{12}} \bar{\Phi}_i^{(+)}(\boldsymbol{r}_{12}; \boldsymbol{q}_{12}; \bar{E}) \sim \sum_j a_j(\tilde{\nu}_{12})\, u_j(\boldsymbol{r}_{12}) \frac{e^{iK_{12j}q_{12}}}{q_{12}}, \tag{119}$$

where $a_j(\tilde{\nu}_{12})$ is a number, and where K_{12j} is defined by (114 *b*). At infinite q_{12}, the right side of (119) is proportional to $\bar{\rho}^{-1}$ (recall (116 *b*)). However, because (119) dominates $\bar{\rho}^{-5/2}$ only on that subspace of $d\bar{S}$ corresponding to finite r_{12}, the total contribution of (119) to $\bar{\mathscr{F}}$ of (118 *a*) remains finite (and can be taken to represent the flow of probability current corresponding to reactions such as (17 *a*)).

4.1. *Divergences in transition amplitudes*

This section will show that (in our configuration space formulation) the divergences encountered in transition amplitudes typically are associated with failure to recognize the implications of the above introduction to this chapter. More specifically, this section provides further illustrations of the principle that the δ-functions (even if physically interpretable) encountered in the configuration space formulation of scattering theory are associated with improper mathematical manipulations. The δ-functions considered in this section are those appearing in transition amplitudes; it will be seen that these δ-functions generally are a consequence of an invalid interchange of order of integration and limit $r \to \infty$ in integrals for $\Phi_i^{(+)}$, $\bar{\Phi}_i^{(+)}$, $\Phi_i^{s(+)}$, etc., of the sort discussed in § 3.1 in connexion with integrals for $G^{(+)}$ (e.g. (99)). Failure to recognize that such interchange of order of integration and limit $r \to \infty$ is invalid typically leads to incorrect assumptions about the asymptotic behaviour of the relevant scattered parts (e.g. of $\Phi_i^{(+)}$), and thus to incorrect computations of the scattered current flow (e.g. of $\bar{\mathscr{F}}$ via (117 *a*)). In particular, § 4.1.3 will show that assuming $\bar{\Phi}_i^{s(+)}(\tilde{r}; \bar{E})$ behaves like $\bar{G}^{(+)}(\tilde{r}; \tilde{r}'; \bar{E})$ leads to a divergent transition amplitude, from which follows the (independently verifiable, see § E. 3) conclusion that $\bar{\Phi}_i^{s(+)}$ indeed cannot be identical with $\bar{\Phi}_i^{t(+)}$.

4.1.1. *Divergences associated with momentum conservation*

With the introduction to this chapter in mind, consider the asymptotic behaviour of the integral (52 *a*), which is the simplest expression we have found for the scattered part of $\Psi_i^{(+)}$ when the incident wave is (21 *a*), representing three initially free particles. As has been discussed (in § 2.2), the integral (52 *a*) is divergent when two-body or three-body bound states can occur, so that (52 *a*) is not expected to be a generally useful starting point for determining the asymptotic behaviour of $\Phi_i^{(+)}$. Suppose, nevertheless, (100 *a*) (which is valid providing $\Psi_f^{(-)*}$ is given by (106)) is employed in (52 *a*) to infer

$$\lim_{r\to\infty\,||\nu_f} \Phi_i^{(+)}(\boldsymbol{r}) = -C_3(E) \frac{e^{i\rho\sqrt{E}}}{\rho^4} T(\boldsymbol{k}_i \to \boldsymbol{k}_f), \tag{120 a}$$

where the laboratory system transition amplitude

$$T(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \Psi_f^{(-)*} V_i \psi_i \equiv \int d\boldsymbol{r}' \Psi_f^{(-)*}(\boldsymbol{r}') \left[V_{12}(\boldsymbol{r}'_{12}) + V_{23}(\boldsymbol{r}'_{23}) + V_{31}(\boldsymbol{r}'_{31})\right] \psi_i(\boldsymbol{r}'), \tag{120 b}$$

and where the dependences of ψ_i and $\Psi_f^{(-)*}$ on $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$ are specified by (21 *a*) and (100 *c*), together with (106). Then use of (120 *a*) in (117 *a*), together with (87) to (92), yields

$$\mathscr{F} = \int \mathrm{d}k_{2f}\,\mathrm{d}k_{3f}\,\mathrm{d}\boldsymbol{n}_{1f}\,\mathrm{d}\boldsymbol{n}_{2f}\,\mathrm{d}\boldsymbol{n}_{3f}\,k_{2f}^2\,k_{3f}^2\,k_{1f}\frac{1}{(2\pi)^8}\frac{m_1}{\hbar^3}\,|\,T(\boldsymbol{k}_i\to\boldsymbol{k}_f)\,|^2$$
$$\equiv \int w(\mathrm{i}\to\mathrm{f}), \tag{121 a}$$

wherein the (unphysical, see below) laboratory system three-body scattering coefficient

$$w(\mathrm{i}\to\mathrm{f}) \equiv w(\boldsymbol{k}_i\to\boldsymbol{k}_f) = \frac{2\pi}{\hbar}\frac{1}{(2\pi)^9}\,|\,T(\boldsymbol{k}_i\to\boldsymbol{k}_f)\,|^2\,\delta(E_f-E_i)\,\mathrm{d}\boldsymbol{k}_{1f}\,\mathrm{d}\boldsymbol{k}_{2f}\,\mathrm{d}\boldsymbol{k}_{3f}. \tag{121 b}$$

The energy-conserving $\delta(E_f-E_i)$ factor is employed in (121 *b*) merely as an artifice, to put (121 *b*) into a simple form consistent with the results of time-dependent scattering theory and the 'golden rule'; the directly derived integrand of (121 *a*) contains no $\delta(E_f-E_i)$, and the specification of $\Psi_f^{(-)*}$ in (120 *b*) automatically makes $E_f = E_i$. The laboratory frame quantity w in (121 *a*) and (121 *b*) should be related to the observed scattering rate $\hat{w}$, defined beneath (2), by (see § 4.2)

$$\hat{w}(\boldsymbol{k}_i\to\boldsymbol{k}_f) = N_1 N_2 N_3\, w(\boldsymbol{k}_i\to\boldsymbol{k}_f). \tag{121 c}$$

The form of (120 *a*) seems consistent with the result (117 *b*) required for finite laboratory frame probability current flow $\mathscr{F}$ from (117 *a*). Actually $\mathscr{F}$ is infinite, however (as expected from the introduction to this chapter), because of the customary total momentum-conserving δ-function factor occurring in laboratory system transition amplitudes. Specifically, employing (33 *a*) and (102 *b*), the integral (120 *b*) reduces to

$$T(\boldsymbol{k}_1\to\boldsymbol{k}_f) = (2\pi)^3\,\delta(\boldsymbol{K}_f-\boldsymbol{K}_i)\int \mathrm{d}\bar{\boldsymbol{r}}'\,\overline{\Psi}_f^{(-)*}(\bar{\boldsymbol{r}}';\bar{E}_f)$$
$$\times\,[V_{12}(\boldsymbol{r}'_{12})+V_{23}(\boldsymbol{r}'_{23})+V_{31}(\boldsymbol{r}'_{31})]\,\overline{\psi}_i(\bar{\boldsymbol{r}}';\bar{E}_i), \tag{122}$$

which, when inserted into (121 *a*), causes $\mathscr{F}$ to diverge by virtue of the $[\delta(\boldsymbol{K}_f-\boldsymbol{K}_i)]^2$ factor under the integrand. Note that $\mathscr{F}$ could remain finite if merely $\delta(\boldsymbol{K}_f-\boldsymbol{K}_i)$ (rather than its square) appeared in the integrand of (121 *a*); correspondingly, w from (121 *b*) can be made physically meaningful only by somehow reinterpreting (and thus eliminating) one of the $\delta(\boldsymbol{K}_f-\boldsymbol{K}_i)$ factors in $|\,T(\boldsymbol{k}_i\to\boldsymbol{k}_f)\,|^2$.

Of course, the fact that $T(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ contains a momentum-conserving δ-function factor is gratifying on physical grounds. Nevertheless, from the standpoint of this work's configuration space formulation of scattering theory, this same fact must be regarded as a signal that the computation of the laboratory system transition amplitude has involved unjustified mathematical manipulations. In particular, the assertion in (120 *a*) that $\lim \Phi_i^{(+)}(\boldsymbol{r})$ is $\sim \mathrm{e}^{\mathrm{i}\rho\sqrt{E}}/\rho^4$ is prima facie incorrect by virtue of (55 *b*), as the introduction to this chapter has discussed. Moreover, to derive the pair of equations (120) from (52 *a*) it is necessary to assume (compare (99))

$$\lim_{r\to\infty\,||\,\bar{\nu}_f}\int \mathrm{d}\boldsymbol{r}'\,G^{(+)}(\boldsymbol{r};\boldsymbol{r}')\,V(\boldsymbol{r}')\,\psi_i(\boldsymbol{r}') = \int \mathrm{d}\boldsymbol{r}'\lim_{r\to\infty\,||\,\bar{\nu}_f} G^{(+)}(\boldsymbol{r};\boldsymbol{r}')\,V(\boldsymbol{r}')\,\psi_i(\boldsymbol{r}'). \tag{123}$$

Thus the interchange of order of integration and limit $r\to\infty$ in (123) also must be incorrect, as can be directly verified by comparing (as in the case of (99)) the contributions to the left side of (123) from the regions $r' < r$ and $r' > r$ as $r\to\infty$ (see § C. 4).

Similar remarks (see § C. 4) pertain to the result for $T(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ if, still for ψ_i of (21 *a*), equations (90) together with interchange of order of integration and limit $r\to\infty$ are employed in (42); in this fashion, one again obtains (120 *a*), but now with

$$T(\boldsymbol{k}_i\to\boldsymbol{k}_f) = \psi_f^* V_i \Psi_i^{(+)} \equiv \int \mathrm{d}\boldsymbol{r}'\,\psi_f^*(\boldsymbol{r}')\,[V_{12}(\boldsymbol{r}'_{12})+V_{23}(\boldsymbol{r}'_{23})+V_{31}(\boldsymbol{r}'_{31})]\,\Psi_i^{(+)}(\boldsymbol{r}'). \tag{124 a}$$

As in (122), equation (124 *a*) reduces to

$$T(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) = (2\pi)^3\,\delta(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K}_\mathrm{i})\int \mathrm{d}\bar{\boldsymbol{r}}'\,\overline{\Psi}_\mathrm{f}^{*}(\bar{\boldsymbol{r}}';\bar{E}_\mathrm{f})\,[V_{12}(\boldsymbol{r}'_{12})+V_{23}(\boldsymbol{r}'_{23})+V_{31}(\boldsymbol{r}'_{31})]\,\overline{\Psi}_\mathrm{i}^{(+)}(\bar{\boldsymbol{r}}';\bar{E}_\mathrm{i}). \quad (124\,b)$$

The integral (124 *a*) has a $\delta(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K}_\mathrm{i})$ factor even though the integral in (42) is convergent at real energies (recall § 2.2). Similarly, the integral (120 *b*) contains a $\delta(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K}_\mathrm{i})$ factor whether or not (52 *a*) diverges, i.e. whether or not two-body or three-body bound states exist. On the other hand, it is true (see § 4.1.4 below) that bound states produce additional divergences in (120 *b*), as well as in (124 *a*).

4.1.2. *Divergences associated with two-body scattering*

The preceding subsection implies that if we wish to calculate the reaction coefficient by means which are mathematically valid and do not introduce divergent expressions, we must not make use of the expression (117 *a*) for the laboratory system probability current flow. Let us examine, therefore, the possibility of calculating the probability current flow in the centre of mass system, via (118 *a*). In particular, consider the asymptotic behaviour of the integral (52 *b*), which is the centre of mass analogue of (52 *a*). Then, as in § 4.1.1, ignoring the bound state complications which make (52 *b*) a dubious starting-point, use in (52 *b*) of the valid set of equations (102) and (106), together with

$$\lim_{\bar{r}\to\infty\,||\,\bar{\nabla}\mathrm{f}}\int \mathrm{d}\bar{\boldsymbol{r}}'\,\bar{G}^{(+)}(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}')\,V(\bar{\boldsymbol{r}}')\,\overline{\psi}_\mathrm{i}(\bar{\boldsymbol{r}}') = \int \mathrm{d}\bar{\boldsymbol{r}}'\lim_{\bar{r}\to\infty\,||\,\bar{\nabla}\mathrm{f}}\bar{G}^{(+)}(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}')\,V(\bar{\boldsymbol{r}}')\,\overline{\psi}_\mathrm{i}(\bar{\boldsymbol{r}}') \quad (125)$$

yields

$$\lim_{\bar{r}\to\infty\,||\,\bar{\nabla}\mathrm{f}}\bar{\Phi}_\mathrm{i}^{(+)}(\bar{\boldsymbol{r}}') = -C_2(\bar{E})\,\frac{\mathrm{e}^{\mathrm{i}\bar{\rho}\sqrt{\bar{E}}}}{\bar{\rho}^{\frac{5}{2}}}\,\overline{T}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}), \quad (126\,a)$$

where

$$\overline{T}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) = \overline{\Psi}_\mathrm{f}^{(-)*}V_\mathrm{i}\overline{\psi}_\mathrm{i} \equiv \int \mathrm{d}\bar{\boldsymbol{r}}'\,\overline{\Psi}_\mathrm{f}^{(-)*}(\bar{\boldsymbol{r}}')\,[V_{12}(\boldsymbol{r}'_{12})+V_{23}(\boldsymbol{r}'_{23})+V_{31}(\boldsymbol{r}'_{31})]\,\overline{\psi}_\mathrm{i}(\bar{\boldsymbol{r}}'), \quad (126\,b)$$

and where $C_2(\bar{E})$ and $\bar{\boldsymbol{\rho}}$ are defined as in (102). Correspondingly, using (126 *a*) in (118 *a*), the centre of mass analogues of (121 *a*) and (121 *b*) are found to be

$$\overline{\mathscr{F}} \equiv \int \overline{w}(\mathrm{i}\to\mathrm{f}), \quad (127\,a)$$

$$\overline{w}(\mathrm{i}\to\mathrm{f}) \equiv \overline{w}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) = \frac{2\pi}{\hbar}\frac{1}{(2\pi)^6}\,|\,\overline{T}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f})\,|^2\,\delta(\bar{E}_\mathrm{f}-\bar{E}_\mathrm{i})\,\mathrm{d}\boldsymbol{k}_{12\mathrm{f}}\,\mathrm{d}\boldsymbol{K}_{12\mathrm{f}} \quad (127\,b)$$

$$= \frac{2\pi}{\hbar}\frac{1}{(2\pi)^6}\,|\,\overline{T}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f})\,|^2\,\delta(E_\mathrm{f}-E_\mathrm{i})\,\delta(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K}_\mathrm{i})\,\mathrm{d}\boldsymbol{k}_{1\mathrm{f}}\,\mathrm{d}\boldsymbol{k}_{2\mathrm{f}}\,\mathrm{d}\boldsymbol{k}_{3\mathrm{f}}, \quad (127\,c)$$

where $\overline{w}$ is the reaction coefficient introduced in equations (1) and (2).

In (127 *b*) and (127 *c*), as in (121 *b*), the δ-functions merely are convenient artifices for putting the final result into simple form; moreover, the specification of $\overline{\Psi}_\mathrm{f}^{(-)*}$ does not involve $\boldsymbol{K}_\mathrm{f}$, and automatically makes $\bar{E}_\mathrm{f} = \bar{E}_\mathrm{i}$. Therefore, if $\overline{T}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f})$ contains no divergences, $\overline{\mathscr{F}}$ and $\overline{w}$ given by (127) will be finite and well defined. On the other hand, if $\overline{T}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f})$ contains terms proportional to δ-functions whose arguments can vanish on the energy-momentum shell $E_\mathrm{f} = E_\mathrm{i}$ and $\boldsymbol{K}_\mathrm{f} = \boldsymbol{K}_\mathrm{i}$, then $\overline{\mathscr{F}}$ will diverge because the integrand of (127 *a*) will contain terms proportional to the squares of δ-functions; correspondingly, $\overline{w}$ from (127 *b*) or (127 *c*) will not be physically meaningful unless the singular terms in the integrand somehow can be reinterpreted so as to eliminate all powers of δ-functions higher than the first. Note that a factor $\delta(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K}_\mathrm{i})$ in

$\overline{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ actually would make the integrand of (127 c) proportional to $[\delta(\boldsymbol{K}_f - \boldsymbol{K}_i)]^3$. However, $\overline{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ is independent of $\boldsymbol{K}_f$ or $\boldsymbol{K}_i$; in fact, (120 b) and (126 b) immediately imply

$$T(\boldsymbol{k}_i \to \boldsymbol{k}_f) = (2\pi)^3 \delta(\boldsymbol{K}_f - \boldsymbol{K}_i)\, \overline{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f), \tag{128}$$

consistent with the result (122) previously deduced.

As was mentioned in the introduction to this chapter, this subsection's procedure—namely calculating the probability current flow in the centre of mass system—is mathematically valid for two-body reactions, but not for collisions induced by the incident wave (21 a). To put it differently, $\overline{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ from (126 b) generally is free from (on the energy-momentum shell) divergences for reactions produced by two-body collisions, even when these collisions cause break-up (e.g. ionization) for one of the incident bodies;† for the elastic scattering of three initially free particles, on the other hand, it is well known (Watson & Nuttall 1967; Weinberg 1964) that $\overline{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ contains δ-functions—associated with purely two-body single scattering—whose arguments can vanish on the energy-momentum shell. In particular, consider the contribution to (126 b) from, for example, the first two terms in the centre of mass analogue of (106 a), which validly specifies $\overline{\Psi}_f^{(-)*}$. In other words, recalling (58 a) and (72), replace $\overline{\Psi}_f^{(-)*}(\tilde{\boldsymbol{r}}')$ in (126 b) by

$$\begin{aligned}\overline{\psi}_f^*(\tilde{\boldsymbol{r}}') + \overline{\Phi}_{12f}^{(-)*}(\tilde{\boldsymbol{r}}') &= \overline{\Psi}_{12f}^{(-)*}(\tilde{\boldsymbol{r}}') \\ &= \exp\{-i\boldsymbol{K}_{12f} \cdot \boldsymbol{q}'_{12}\}[\exp\{-i\boldsymbol{k}_{12f} \cdot \boldsymbol{r}'_{12}\} + \phi_{12f}^{(-)*}(\boldsymbol{r}'_{12}; \boldsymbol{k}_{12f})] \\ &\equiv \exp\{-i\boldsymbol{K}_{12f} \cdot \boldsymbol{q}'_{12}\} u_c^{(-)*}(\boldsymbol{r}'_{12}; \boldsymbol{k}_{12f}),\end{aligned} \tag{129 a}$$

where $u_c^{(-)*}(\boldsymbol{r}_{12})$ (which does not contain the $(2\pi)^{-\frac{3}{2}}$ normalization factor attached to $u(\boldsymbol{r}_{12})$ of (113)) obviously solves

$$\left[\frac{-\hbar^2}{2\mu_{12}}\nabla_{12}^2 + V_{12}(\boldsymbol{r}_{12}) - \frac{\hbar^2 k_{12f}^2}{2\mu_{12}}\right] u_c^{(-)*}(\boldsymbol{r}_{12}) = 0, \tag{129 b}$$

and represents scattering of particles 1 and 2 in their own centre of mass system when (in that centre of mass system) the incident plane wave is $e^{-i\boldsymbol{k}_{12f} \cdot \boldsymbol{r}_{12}}$. Then one sees that there is a contribution $\overline{T}_{12}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ to $\overline{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$, from the V_{12} interaction in (126 b), of magnitude

$$\begin{aligned}\overline{\Psi}_{12f}^{(-)*} V_{12} \overline{\psi}_i &= \int d\boldsymbol{r}'_{12}\, d\boldsymbol{q}'_{12} \exp\{-i\boldsymbol{K}_{12f} \cdot \boldsymbol{q}'_{12}\} u_c^{(-)*}(\boldsymbol{r}'_{12}; \boldsymbol{k}_{12f})\, V_{12}(\boldsymbol{r}'_{12}) \\ &\qquad \times \exp\{i(\boldsymbol{K}_{12i} \cdot \boldsymbol{q}'_{12} + \boldsymbol{k}_{12i} \cdot \boldsymbol{r}'_{12})\}, \qquad (130\,a) \\ &= (2\pi)^3 \delta(\boldsymbol{K}_{12f} - \boldsymbol{K}_{12i}) \int d\boldsymbol{r}_{12}\, u_c^{(-)*}(\boldsymbol{r}_{12}; \boldsymbol{k}_{12f})\, V_{12}(\boldsymbol{r}_{12}) \\ &\qquad \times \exp\{i\boldsymbol{k}_{12i} \cdot \boldsymbol{r}_{12}\}, \qquad (130\,b) \\ &= (2\pi)^3 \delta(\boldsymbol{K}_{12f} - \boldsymbol{K}_{12i})\, t_{12}(\boldsymbol{k}_{12i} \to \boldsymbol{k}_{12f}), \qquad (130\,c)\end{aligned}$$

where $t_{12}(\boldsymbol{k}_{12i} \to \boldsymbol{k}_{12f})$ is the transition amplitude representing scattering of the completely isolated pair of particles 1 and 2 in their own centre of mass system. Thus, for incident waves (21 a), the quantities $\overline{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ and $T(\boldsymbol{k}_i \to \boldsymbol{k}_f)$, supposedly representing three-body transition amplitudes in the centre of mass and laboratory frames respectively, actually contain a contribution (130 c) representing purely two-body elastic scattering—of particles 1 and 2 without interaction with 3; according to the remarks following (29), the δ-function in (130 c) guarantees that the laboratory velocity of the non-interacting particle 3 indeed remains unaltered. Similar (to (130 c)) contributions to $\overline{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$, with similar interpretations, result of course from the other interactions in (126 b).

† If, for example, particle 3 is incident on a bound state $u_j(\boldsymbol{r}_{12})$, $\overline{\psi}_i$ is proportional to $u_j(\boldsymbol{r}_{12})$, while $V_i = V - V_{12}$, so that (126 b) surely converges for short-range forces. Of course, to be wholly mathematically correct for reactions causing break-up of the initial $u_j(\boldsymbol{r}_{12})$, $\overline{\Psi}_f^{(-)*}$ in (126 b) must be correctly prescribed, e.g. via the centre of mass analogues of (106).

Recalling the discussion in § 4.1.1, the divergent (on the energy-momentum shell) $\delta(\boldsymbol{K}_{12f}-\boldsymbol{K}_{12i})$ factor in (130 *c*) is a signal that (126) were derived using improper mathematical manipulations. Correspondingly, the interchange of order of integration and limit $\bar{r}\to\infty$ in (125) must be wrong, as can be directly verified (see § C. 4). Nevertheless, as has just been seen—and as in the case of the momentum-conserving $\delta(\boldsymbol{K}_f-\boldsymbol{K}_i)$ factor discussed in the preceding subsection—the divergent term (130 *c*) is readily interpretable physically. I point out that the above conclusion—namely that $\overline{T}(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ contains contributions representing a single purely two-body scattering—was based solely on the form of the contribution (130 *c*) to (126 *b*). But 126 *b*) has been derived from the admittedly not always valid formula (52 *b*) for $\overline{\Phi}_i^{(+)}$; it would have been preferable to obtain $\overline{T}(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ from an always legitimate formula for $\overline{\Phi}_i^{(+)}$, i.e. from (69) supplemented by the centre of mass version of (61). However, starting in this latter fashion, it is immediately obvious that $\overline{T}(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ defined as in (126 *a*) must contain a contribution, stemming from the $\overline{\Phi}_{12}^{(+)}$ term in $\Phi_i^{(+)}$, representing the single purely two-body scattering of 1 and 2. Furthermore, (68) and (72) show explicitly that the assertion $\lim\overline{\Phi}_i^{(+)}(\boldsymbol{r})\cong e^{i\bar{\rho}\sqrt{\bar{E}}}/\bar{\rho}^{\frac{5}{2}}$ (in (126 *a*)) is prima facie incorrect, and that a $\delta(\boldsymbol{K}_{12f}-\boldsymbol{K}_{12i})$ factor in the $\overline{\Phi}_{12}^{(+)}$ contribution to $\overline{T}(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ is to be expected. Alternatively, if, ignoring the accurate result (72) for $\overline{\Phi}_{12}^{(+)}$, one starts from the admittedly not always correct (cf. (60) or (105 *d*)) analogue of (52 *b*)

$$\overline{\Phi}_{12}^{(+)}(\bar{\boldsymbol{r}};\bar{E})=-\int d\bar{\boldsymbol{r}}'\,\overline{G}_{12}^{(+)}(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}')\,V_{12}(\boldsymbol{r}'_{12})\,\overline{\Psi}_1(\bar{\boldsymbol{r}}'),\tag{131 a}$$

and then employs the analogue of (102 *a*) (i.e. (105), in effect) after performing the interchange analogous to (125), one finds

$$\lim_{\bar{r}\to\infty\,||\,\bar{v}_f}\overline{\Phi}_{12}^{(+)}(\bar{\boldsymbol{r}})=-C_2(\bar{E})\frac{e^{i\bar{\rho}\sqrt{\bar{E}}}}{\bar{\rho}^{\frac{5}{2}}}\,\overline{\Psi}_{12f}^{(-)*}V_{12}\overline{\psi}_i.\tag{131 b}$$

Comparing with (130 *a*), one sees that the contribution to $\overline{T}(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ stemming from the $\overline{\Phi}_{12}^{(+)}$ term in $\overline{\Phi}_i^{(+)}$ is precisely the contribution (130 *c*) previously obtained and interpreted. Moreover the contribution to the integral (131 *a*) from $\bar{r}'>\bar{r}$ is not negligible compared to $\bar{\rho}^{-5/2}\cong\bar{r}^{-5/2}$ (see § C. 4), so that the interchange of order of integration and limit $\bar{\boldsymbol{r}}\to\infty$ in (131 *a*) really is unjustified.

The foregoing discussion (especially in the last paragraph) is relevant also to the expression for $\overline{T}(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ obtained from (unjustified) employment of (90) in the centre of mass system version of (42); this procedure again yields (126 *a*), but with

$$\overline{T}(\boldsymbol{k}_i\to\boldsymbol{k}_f)=\overline{\psi}_f^*V_i\,\overline{\Psi}_i^{(+)}\equiv\int d\bar{\boldsymbol{r}}'\overline{\psi}_f^*(\bar{\boldsymbol{r}}')\,[V_{12}(\boldsymbol{r}'_{12})+V_{23}(\boldsymbol{r}'_{23})+V_{31}(\boldsymbol{r}'_{31})]\,\overline{\Psi}_i^{(+)}(\bar{\boldsymbol{r}}').\tag{131 c}$$

Equations (124) and (131 *c*) are consistent with (128). Replacing $\overline{\Psi}_i^{(+)}$ in (131 *c*) by $\overline{\Psi}_{12}^{(+)}=\overline{\psi}_i+\overline{\Phi}_{12}^{(+)}$, and using the V_{12} interaction, once more yields the two-body contribution (130 *c*) to $\overline{T}(\boldsymbol{k}_i\to\boldsymbol{k}_f)$.

If the fact that $\overline{T}(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ given by (131 *c*) is divergent is overlooked, and if (52 *b*) or the centre of mass analogue of (51 *c*) is employed in (131 *c*) despite the fact that (52 *b*) and (51 *c*) fail when two-body bound states exist, then

$$\overline{T}(\boldsymbol{k}_i\to\boldsymbol{k}_f)=\overline{\psi}_f^*\overline{\boldsymbol{T}}(\bar{E}_i)\,\overline{\psi}_i\equiv\langle f|\,\overline{\boldsymbol{T}}(\bar{E}_i)\,|i\rangle,\tag{131 d}$$

where $\overline{\boldsymbol{T}}(\bar{E})$ is the operator defined by the centre of mass analogue of (5). Equation (131 *d*) (but with $\bar{E}_f$ replacing $\bar{E}_i$) also follows from substituting—with similar inattention to questions of mathematical validity—the centre of mass analogue of (100 *b*) in (126 *b*). Although (131 *d*) is quite commonly employed, the foregoing remarks and the entire contents of this § 4.1 make it apparent that—for three independently incident particles described by ψ_i of (21 *a*)—(131 *d*)

implies a connexion between the matrix element $\langle \mathrm{f}|\, \bar{\boldsymbol{T}}(\bar{E})\,|\mathrm{i}\rangle$ and the asymptotic behaviour of $\bar{\Phi}_{\mathrm{i}}^{(+)}(\bar{\boldsymbol{r}})$ at large $\bar{\boldsymbol{r}}$ which has no real mathematical justification (recall (126 *a*) and its difficulties). On the other hand, for the transition amplitude $t_{12}(\boldsymbol{k}_{12\mathrm{i}} \to \boldsymbol{k}_{12\mathrm{f}})$ of (130 *c*) it is mathematically justifiable to write

$$t_{12}(\boldsymbol{k}_{12\mathrm{i}} \to \boldsymbol{k}_{12\mathrm{f}}) = \int \mathrm{d}\boldsymbol{r}_{12}\,\mathrm{d}\boldsymbol{r}'_{12} \exp\{-\mathrm{i}\boldsymbol{k}_{12\mathrm{f}} \cdot \boldsymbol{r}_{12}\}\, \boldsymbol{t}_{12}(\boldsymbol{r}_{12}; \boldsymbol{r}'_{12}; E_{12}) \exp\{\mathrm{i}\boldsymbol{k}_{12\mathrm{i}} \cdot \boldsymbol{r}'_{12}\}$$

$$\equiv \langle \mathrm{f}|\, \boldsymbol{t}_{12}(E_{12})\,|\mathrm{i}\rangle, \tag{131 *e*}$$

where $k_{12\mathrm{f}}^2 = k_{12\mathrm{i}}^2 = k_{12}^2$ satisfying (74 *b*); $\langle \mathrm{f}|\boldsymbol{t}_{12}(E_{12})\,|\mathrm{i}\rangle$ is the limit of $\langle \mathrm{f}|\, \boldsymbol{t}_{12}(E_{12}+\mathrm{i}\epsilon)\,|\mathrm{i}\rangle$ as $\epsilon \to 0$;

$$\boldsymbol{t}_{12}(\boldsymbol{r}_{12}; \boldsymbol{r}'_{12}; \lambda) = V_{12}(\boldsymbol{r}_{12})\,\delta(\boldsymbol{r}_{12} - \boldsymbol{r}'_{12}) - V_{12}(\boldsymbol{r}_{12})\, g_{12}(\boldsymbol{r}_{12}; \boldsymbol{r}'_{12}; \lambda)\, V_{12}(\boldsymbol{r}'_{12}), \tag{131 *f*}$$

and g_{12} is the two-particle Green function, defined as in (75). Moreover, it really is true that as $\boldsymbol{r}_{12} \to \infty$ along the direction of $\boldsymbol{k}_{12\mathrm{f}} = k_{12}\boldsymbol{n}_{12\mathrm{f}}$,

$$\lim_{r_{12}\to\infty\,||\,n_{12\mathrm{f}}} \phi_{12}^{(+)}(\boldsymbol{r}_{12}; \boldsymbol{k}_{12\mathrm{i}}) = -\frac{1}{4\pi}\frac{2\mu_{12}}{\hbar^2}\frac{\mathrm{e}^{\mathrm{i}k_{12}r_{12}}}{r_{12}}\langle \mathrm{f}|\, \boldsymbol{t}_{12}(E_{12})\,|\mathrm{i}\rangle, \tag{131 *g*}$$

where $\phi_{12}^{(+)}$ is defined by (73) and (74). Similarly, it is justified to write

$$\phi_{12}^{(+)}(\boldsymbol{k}_{12\mathrm{i}}) = -g_{12}^{(+)} V_{12}\psi_{12\mathrm{i}} = -[g_F^{(+)} - g_F^{(+)} V_{12} g_{12}^{(+)}]\, V_{12}\psi_{12\mathrm{i}}$$

$$= -g_F^{(+)}[V_{12} - V_{12} g_{12}^{(+)} V_{12}]\,\psi_{12\mathrm{i}} = -g_F^{(+)}\boldsymbol{t}_{12}(E_{12})\,\psi_{12\mathrm{i}}, \tag{131 *h*}$$

as well as

$$V_{12}[\psi_{12\mathrm{i}} + \phi_{12}^{(+)}] = V_{12}[1 - g_{12}^{(+)} V_{12}]\,\psi_{12\mathrm{i}} = \boldsymbol{t}_{12}(E_{12})\,\psi_{12\mathrm{i}}. \tag{131 *i*}$$

Equation (131 *i*) is the two-particle analogue of the not necessarily valid (51 *c*). Note that the first term on the right side of (131 *f*), which term has been denoted by V_{12} in (131 *h*), is not identical with $V_{12}(\boldsymbol{r}; \boldsymbol{r}')$ of (77 *a*) (recall (27 *e*)); V_{12} of (77 *a*) operates in the nine-dimensional three-particle configuration space, whereas V_{12} of (131 *h*) operates in only a three-dimensional space.

4.1.3. *Divergences after subtraction of two-body terms*

The results of the preceding subsection imply that—whether or not divergent, i.e. whether or not bound states occur—the integrals (52) are an unsuitable starting-point for mathematically unobjectionable derivations of formal expressions for the three-body amplitudes $T(\boldsymbol{k}_{\mathrm{i}} \to \boldsymbol{k}_{\mathrm{f}})$ or $\bar{T}(\boldsymbol{k}_{\mathrm{i}} \to \boldsymbol{k}_{\mathrm{f}})$. Similarly, (42) and its centre of mass version, though generally convergent whether or not bound states exist, also have been found to be mathematically unsuitable starting-points for deriving matrix elements of $\boldsymbol{T}$ or $\bar{\boldsymbol{T}}$. To have any hope of deriving non-divergent expressions for $\langle \mathrm{f}|\, \bar{\boldsymbol{T}}\,|\mathrm{i}\rangle$, the purely two-body single scattering parts of $\bar{\Phi}_{\mathrm{i}}^{(+)}$ apparently must be subtracted away at the very outset, before taking the limit $\boldsymbol{r} \to \infty$ (as foreshadowed in the introduction to this chapter). Therefore, I now shall examine the contributions to $T(\boldsymbol{k}_{\mathrm{i}} \to \boldsymbol{k}_{\mathrm{f}})$ and $\bar{T}(\boldsymbol{k}_{\mathrm{i}} \to \boldsymbol{k}_{\mathrm{f}})$ obtained from the asymptotic behaviour of $\Phi_{\mathrm{i}}^{s(+)}$ and $\bar{\Phi}_{\mathrm{i}}^{s(+)}$, specified by (67 *c*) and (69) respectively. In any event, the starting-point (69), taken together with (72) and the centre-of-mass version of (61), has the virtue that it provides a specification of $\bar{\Phi}_{\mathrm{i}}^{(+)}(\bar{\boldsymbol{r}})$ free from divergences or ambiguities.

In (69), assume that

$$\lim_{\bar{r}\to\infty\,||\,\bar{v}_{\mathrm{f}}} \int \mathrm{d}\bar{\boldsymbol{r}}'\, \bar{G}^{(+)}(\bar{\boldsymbol{r}}; \bar{\boldsymbol{r}}')\, V_{23}(\boldsymbol{r}'_{23})\, \bar{\Phi}_{12}^{(+)}(\bar{\boldsymbol{r}}') = \int \mathrm{d}\bar{\boldsymbol{r}}' \lim_{\bar{r}\to\infty\,||\,\bar{v}_{\mathrm{f}}} \bar{G}^{(+)}(\bar{\boldsymbol{r}}; \bar{\boldsymbol{r}}')\, V_{23}(\boldsymbol{r}'_{23})\, \bar{\Phi}_{12}^{(+)}(\bar{\boldsymbol{r}}'). \tag{132}$$

Then in the by now familiar fashion, there results

$$\lim_{\bar{r}\to\infty||\bar{v}_f} \bar{\Phi}_i^{s(+)}(\bar{\boldsymbol{r}}) = -C_2(\bar{E})\frac{e^{i\bar{\rho}\sqrt{\bar{E}}}}{\bar{\rho}^{\frac{5}{2}}}\,\bar{T}^s(\boldsymbol{k}_i\to\boldsymbol{k}_f), \tag{133a}$$

$$\bar{T}^s(\boldsymbol{k}_i\to\boldsymbol{k}_f) = \int d\bar{\boldsymbol{r}}'\,\bar{\Psi}_f^{(-)*}(\bar{\boldsymbol{r}}')\,[(V_{23}+V_{31})\,\bar{\Phi}_{12}^{(+)}(\bar{\boldsymbol{r}}') + (V_{31}+V_{12})\,\bar{\Phi}_{23}^{(+)}(\bar{\boldsymbol{r}}') + (V_{12}+V_{23})\,\bar{\Phi}_{31}^{(+)}(\bar{\boldsymbol{r}}')]. \tag{133b}$$

Similarly, interchanging order of integration and limit $\boldsymbol{r}\to\infty$ in (67 c) yields

$$\lim_{r\to\infty||\bar{v}_f} \Phi_i^{s(+)}(\boldsymbol{r}) = -C_3(E)\frac{e^{i\rho\sqrt{E}}}{\rho^4}\,T^s(\boldsymbol{k}_i\to\boldsymbol{k}_f), \tag{134a}$$

where T^s turns out to obey

$$T^s(\boldsymbol{k}_i\to\boldsymbol{k}_f) = (2\pi)^3\,\delta(\boldsymbol{K}_f-\boldsymbol{K}_i)\,\bar{T}^s(\boldsymbol{k}_i\to\boldsymbol{k}_f), \tag{134b}$$

consistent with (128).

In view of the preceding two subsections, the momentum-conserving $\delta(\boldsymbol{K}_f-\boldsymbol{K}_i)$ in $T^s(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ is to be expected from (68), and requires no further discussion. On the other hand, there are no immediately obvious reasons why the asymptotic behaviour of $\bar{\Phi}_i^{s(+)}$ from (69) should be inconsistent with (133 a). Nevertheless, the integral (133 b) also is divergent. In fact (see § B. 2), the right side of (133 b) contains contributions proportional to

$$\delta\left(k_{12i}-\left|\boldsymbol{K}_{23f}+\frac{m_1}{m_1+m_2}\boldsymbol{K}_{12i}\right|\right) \tag{135a}$$

and cyclic permutations thereof. Using (29) and the relation $\boldsymbol{K}_i = \boldsymbol{K}_f$. the expression (135 a) takes the form

$$\delta(k_{12i}-|\boldsymbol{k}_{12i}+\boldsymbol{k}_{1f}-\boldsymbol{k}_{1i}|), \tag{135b}$$

wherein the argument of the δ-function obviously can be zero on the energy-momentum shell. Consequently the contribution to (133 b) made by (135 a), when squared in (127) after replacing $\bar{T}$ by $\bar{T}^s$, again causes $\bar{w}$ and $\bar{\mathscr{F}}$ to diverge, although the divergence is of lower order with the one-dimensional δ-function (135 a) than with the three-dimensional δ-function contribution (130 c) to $\bar{T}(\boldsymbol{k}_i\to\boldsymbol{k}_f)$.

Judging by our earlier experience in this chapter, therefore, the assertion in (133 a) that $\lim \bar{\Phi}_i^{(+)}$ is $\sim e^{i\bar{\rho}\sqrt{\bar{E}}}/\bar{\rho}^{\frac{5}{2}}$ must be incorrect. In fact, it is shown in § E. 3 that there are contributions to $\bar{\Phi}_i^{s(+)}(\bar{\boldsymbol{r}})$ behaving like $\bar{\rho}^{-2}$ as $\bar{\rho}\to\infty$. Correspondingly (see § E. 2) it can be demonstrated that the contribution to the integral on the left side of (132) from the region $\bar{r}' > \bar{r}$ is non-negligible compared to $\bar{\rho}^{-5/2}$. Thus (as the result of § E. 3 confirms), the subtraction, of terms from $\bar{\Phi}_i^{(+)}$, yielding $\bar{\Phi}_i^{s(+)}$ is not yet sufficient to permit interchange of order of integration and limit $\bar{r}\to\infty$ in (132), although the $\bar{r}' > \bar{r}$ contribution to the left side of (132) is smaller than the corresponding contribution to the left side of (125) (compare the results of §§ E. 2, E. 3 and C. 4). It is additionally noteworthy that these results (of §§ E. 2 and E. 3) hold whether or not bound states exist.

Moreover, still consistent with our previous experience, the result (135 a) is physically interpretable. The particular δ-function (135 a) arises in the contribution to (133 b) made by the term $\bar{\Psi}_f^{(-)*}V_{23}\bar{\Phi}_{12}^{(+)}$; more specifically (see § B. 2), (135 a) is obtained from the

$$\bar{\psi}_f^* + \bar{\Phi}_{23f}^{(-)*} = \bar{\Psi}_{23f}^{(-)*} \tag{136}$$

part of $\overline{\Psi}_{\mathrm{f}}^{(-)*}$ in the aforementioned term. But one sees—using (51), (60), (77 *a*) and (81), together with the Lippmann–Schwinger equation for $\overline{\Psi}_{23\mathrm{f}}^{(-)*}$ analogous to (107)—that

$$\overline{\Psi}_{23\mathrm{f}}^{(-)*} V_{23} \overline{\Phi}_{12}^{(+)} = -\overline{\Psi}_{23\mathrm{f}}^{(-)*} V_{23} \{ \lim_{\epsilon \to 0} \overline{G}_{12}(\bar{E}+\mathrm{i}\epsilon) V_{12} \overline{\psi}_{\mathrm{i}} \} \tag{137 a}$$

$$= -\lim_{\epsilon \to 0} \overline{\Psi}_{23\mathrm{f}}^{(-)*} V_{23} \overline{G}_{12}(\bar{E}+\mathrm{i}\epsilon) V_{12} \overline{\psi}_{\mathrm{i}}$$

$$= -\lim_{\epsilon \to 0} \overline{\Psi}_{23\mathrm{f}}(\bar{E}+\mathrm{i}\epsilon) V_{23} \overline{G}_{F}(\bar{E}+\mathrm{i}\epsilon)\, \overline{\boldsymbol{T}}_{12}(\bar{E}+\mathrm{i}\epsilon) \overline{\psi}_{\mathrm{i}}$$

$$= -\lim_{\epsilon \to 0} \overline{\psi}_{\mathrm{f}}^{*} V_{23} \overline{G}_{23}(\bar{E}+\mathrm{i}\epsilon) \overline{\boldsymbol{T}}_{12}(\bar{E}+\mathrm{i}\epsilon) \overline{\psi}_{\mathrm{i}}$$

$$= -\lim_{\epsilon \to 0} \overline{\psi}_{\mathrm{f}}^{*}\, \overline{\boldsymbol{T}}_{23}(\bar{E}+\mathrm{i}\epsilon)\, \overline{G}_{F}(\bar{E}+\mathrm{i}\epsilon)\, \overline{\boldsymbol{T}}_{12}(\bar{E}+\mathrm{i}\epsilon) \overline{\psi}_{\mathrm{i}}, \tag{137 b}$$

where, for our present purely interpretative purposes, interchange of order of integration and limit $\epsilon \to 0$ in (137 *a*) is permissible. The matrix element (137 *b*) is explicitly discussed on p. 59 of Watson & Nuttall (1967), and obviously is representable by a double scattering diagram (see also § 5.3 below). To be precise, (137 *b*) corresponds to a diagram wherein there is first a purely two-body scattering of particles 1 and 2 (the factor $\overline{\boldsymbol{T}}_{12}$), followed by a period of free propagation (the factor $\overline{G}_F$) and then a second final purely two-body scattering of particles 2 and 3.

The preceding two paragraphs justify the conclusion that the δ-functions (135) arise from contributions to $\overline{\Phi}_{\mathrm{i}}^{s(+)}(\bar{\boldsymbol{r}})$ which, because they arise from two successive purely two-body elastic scatterings, cannot (and do not) behave like truly three-body scattered waves at large $\bar{\boldsymbol{r}}$. This conclusion is reinforced by the fact that the vanishing of the argument of the δ-function (135 *b*) really does guarantee the necessary relations between initial and final momenta following the two independent successive two-particle scattering events associated with the diagram representing (137 *b*)—namely first particle 2 is scattered by 1 with 3 playing no role, after which particle 1 plays no further role as 2 is scattered by 3. Without postulating that the total initial momentum $\hbar \boldsymbol{K} = 0$, let the momenta (in units of $\hbar$) of 1, 2 respectively after the first scattering be $\boldsymbol{k}_1'$, $\boldsymbol{k}_2'$ where

$$\boldsymbol{k}_1' + \boldsymbol{k}_2' = \boldsymbol{k}_{1\mathrm{i}} + \boldsymbol{k}_{2\mathrm{i}}. \tag{138}$$

Since the first scattering is an elastic collision between 1 and 2, $k_{12}' = k_{12\mathrm{i}}$, i.e.

$$(m_1+m_2)\, k_{12\mathrm{i}} = |m_2 \boldsymbol{k}_1' - m_1 \boldsymbol{k}_2'| = |(m_1+m_2)\, \boldsymbol{k}_1' - m_1(\boldsymbol{k}_{1\mathrm{i}} + \boldsymbol{k}_{2\mathrm{i}})|, \tag{139 a}$$

using (138). With the definition (29 *d*) of $\boldsymbol{k}_{12}$, (139 *a*) can be put in the form

$$k_{12\mathrm{i}} = |\boldsymbol{k}_{12\mathrm{i}} + \boldsymbol{k}_1' - \boldsymbol{k}_{1\mathrm{i}}|. \tag{139 b}$$

But since particle 1 is unaffected in the second scattering, $\boldsymbol{k}_1' = \boldsymbol{k}_{1\mathrm{f}}$, making (139 *b*) identical with the condition for which the argument of the δ-function (135 *b*) vanishes. Other permutations of such two successive two-particle scatterings are associated of course with corresponding permutations of (135 *b*), which in turn correspond to other (than (137 *a*)) terms in (133 *b*).

Similar results (to those already discussed) pertain also to derivations of $T^s(\boldsymbol{k}_{\mathrm{i}} \to \boldsymbol{k}_{\mathrm{f}})$ or $\overline{T}^s(\boldsymbol{k}_{\mathrm{i}} \to \boldsymbol{k}_{\mathrm{f}})$ from (134 *a*) or (133 *a*) respectively, starting from the expressions for $\Phi_{\mathrm{i}}^{s(+)}$ or $\overline{\Phi}_{\mathrm{i}}^{s(+)}$ given by (84 *c*) or its centre of mass analogue. In particular, one thus finds

$$\overline{T}^s(\boldsymbol{k}_{\mathrm{i}} \to \boldsymbol{k}_{\mathrm{f}}) = [\overline{\Phi}_{12\mathrm{f}}^{(-)*}(V_{23}+V_{31}) + \overline{\Phi}_{23\mathrm{f}}^{(-)*}(V_{31}+V_{12}) + \overline{\Phi}_{31\mathrm{f}}^{(-)*}(V_{12}+V_{23})]\, \overline{\Psi}_{\mathrm{i}}^{(+)}, \tag{140}$$

while $T^s(\boldsymbol{k}_{\mathrm{i}} \to \boldsymbol{k}_{\mathrm{f}})$ is given by the laboratory system analogue of (140) and obeys (134 *b*). Equation (140) obviously is the time-reversed analogue of (133 *b*), and equally obviously suffers from the same deficiencies—i.e. contains the same double-scattering divergences—as does (133 *b*).

I now observe that the on-shell δ-functions discussed in this subsection, and in §§ 4.1.1 and 4.1.2, illustrate what appears to be a general relation between the asymptotic behaviour of any part of $\Phi_i^{(+)}$ (or $\bar{\Phi}_i^{(+)}$), e.g. $\Phi_{12}^{(+)}$ (or $\bar{\Phi}_{12}^{(+)}$), and the dimensionality of the δ-function in the contribution this same part makes to the laboratory or centre of mass scattering amplitude. Specifically, as $\boldsymbol{r} \to \infty$ along directions $\boldsymbol{\nu}_f \neq \boldsymbol{\nu}_{\alpha\beta}$, i.e. along directions $\boldsymbol{\nu}_f$ not corresponding to the possibility of propagation in bound states: (*a*) $\bar{\Phi}_{12}^{(+)}(\bar{\boldsymbol{r}})$, cf. (72), decreases like $\phi_{12}^{(+)}(\boldsymbol{r}_{12})$, i.e. like $\bar{r}^{-1} \cong \bar{\rho}^{-1}$, and the associated contribution to $\bar{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ contains the three-dimensional δ-function $\delta(\boldsymbol{K}_{12f} - \boldsymbol{K}_{12i})$ (recall the discussion preceding and following (131)); (*b*) the laboratory frame $\Phi_{12}^{(+)}(\boldsymbol{r}_{12})$ still decreases like $\phi_{12}^{(+)}(\boldsymbol{r}_{12})$, i.e. like $r^{-1} \cong \rho^{-1}$, and the associated contribution to $T(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ contains a six-dimensional δ-function, namely $\delta(\boldsymbol{K}_{12f} - \boldsymbol{K}_{12i})$ multiplied by $\delta(\boldsymbol{K}_f - \boldsymbol{K}_i)$; (*c*) according to § E. 3, there are parts of $\bar{\Phi}_i^{s(+)}(\bar{\boldsymbol{r}})$ decreasing like $\bar{\rho}^{-2}$, and these parts apparently give rise to the one-dimensional δ-functions (135) contained in $\bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f)$.

Evidently in the laboratory frame the rule is: as $\boldsymbol{r} \to \infty || \boldsymbol{\nu}_f \neq \boldsymbol{\nu}_{\alpha\beta}$, if the part of $\Phi_i^{(+)}(\boldsymbol{r})$ under consideration decreases like $\rho^{\frac{1}{2}x}\rho^{-4}$, where x is an integer $\geqslant 0$, then the associated contribution to $T(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ contains a δ-function of dimensionality x. Similarly, in the centre-of-mass frame, if as $\bar{\boldsymbol{r}} \to \infty || \bar{\boldsymbol{\nu}}_f \neq \bar{\boldsymbol{\nu}}_{\alpha\beta}$ the part of $\bar{\Phi}_i^{(+)}(\bar{\boldsymbol{r}})$ under consideration decreases like $\bar{\rho}^{\frac{1}{2}y}\bar{\rho}^{-5/2}$, where y is an integer $\geqslant 0$, then the associated contribution to $\bar{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ contains a δ-function of dimensionality y. Of course, because (55*b*) holds, the δ-function dimensionalities associated with corresponding values of x and y are related by $x = y + 3$. Moreover, these rules can be understood. Along directions $\boldsymbol{\nu}_f \neq \boldsymbol{\nu}_{\alpha\beta}$, the scattered part of $\Psi_i^{(+)}(\boldsymbol{r})$ normally would be expected to diverge like an outgoing spherical wave in nine dimensions, i.e. like $G_F^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$, which is of order ρ^{-4} at large r. The amplitude with which $\Phi_i^{(+)}(\boldsymbol{r})$ diverges along $\boldsymbol{\nu}_f$ is measured by $T(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ of (120). Because of special symmetries in the interaction V, however, all or parts of $\Phi_i^{(+)}(\boldsymbol{r})$ may not be able to diverge in a fully nine-dimensional fashion along all $\boldsymbol{\nu}_f \neq \boldsymbol{\nu}_{\alpha\beta}$. These inabilities mean $\Phi_i^{(+)}(\boldsymbol{r})$ or parts thereof are being forced to diverge in a restricted space of less than nine dimensions, i.e. that $\Phi_i^{(+)}(\boldsymbol{r})$ or parts thereof actually will decrease asymptotically like $\rho^{\frac{1}{2}x}\rho^{-4}$, where x is an integer $\geqslant 0$, and where $x > 0$ corresponds to restricted propagation in the sense just described. Correspondingly, for $\Phi_i^{(+)}(\boldsymbol{r})$ or parts thereof with $x > 0$, postulating (120*a*) is wrong; the resultant δ-functions in $T(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ reflect the failure of (120*a*), as has been discussed, but also express the x independent aforementioned restrictions on the directions $\boldsymbol{\nu}_f$ into which—for given $\boldsymbol{\nu}_i$—$\Phi_i^{(+)}(\boldsymbol{r})$ or parts thereof can propagate. For example, the fact that V is independent of $\boldsymbol{R}$ means $\Phi_i^{(+)}(\boldsymbol{r})$ has a factor $e^{i\boldsymbol{K}_i \cdot \boldsymbol{R}}$, so that no part of $\Phi_i^{(+)}(\boldsymbol{r})$ can be diverging in a space of more than six dimensions (the space of $\bar{\boldsymbol{r}} \equiv \boldsymbol{r}_{12}, \boldsymbol{q}_{12}$), i.e. even $\Phi_i^{t(+)}(\boldsymbol{r})$—the 'truly' three-body scattered part of $\Phi_i^{(+)}(\boldsymbol{r})$—decreases asymptotically no more rapidly than $\rho^{-5/2}$; correspondingly, even the truly three-body scattering amplitude $T^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ will have the three-dimensional $\delta(\boldsymbol{K}_f - \boldsymbol{K}_i)$ factor required by (128), which factor also expresses the fact that $\Phi_i^{t(+)}(\boldsymbol{r})$ actually is propagating to infinity only along directions $\boldsymbol{\nu}_f$ consistent with the three independent requirements $\boldsymbol{K}_f = \boldsymbol{K}_i$. The centre-of-mass frame rule cited above is similarly understood. The considerations of this paragraph make it quite clear that the complicated analysis in § E. 3 is basically correct, i.e. it now is quite clear that the presence of the one-dimensional δ-functions (135) deduced in § B. 2 must be associated with the existence of contributions to $\bar{\Phi}_i^{s(+)}(\bar{\boldsymbol{r}})$ behaving asymptotically like $\bar{\rho}^{-2}$.

The conclusion that $\bar{\Phi}_i^{s(+)}(\bar{\boldsymbol{r}})$ generally has contributions $\sim \bar{\rho}^{-2}$ is given added plausibility by the following special illustration. Suppose particles 1 and 2 do not interact with each other, i.e. $V_{12} = 0$, and suppose further that particle 3 is infinitely massive (and thus has zero velocity, or

else its momentum would be infinite). Then the laboratory and centre-of-mass frames are essentially identical, and the collision induced by ψ_1 of (21 *a*) is no different from simultaneous scattering of the mutually non-interacting particles 1 and 2 by a centre of force. For such scattering, with the origin at the centre of force, Schrödinger's equation is

$$\left[-\frac{\hbar^2}{2m_1}\nabla_1^2-\frac{\hbar^2}{2m_2}\nabla_2^2+V_1(\boldsymbol{r}_1)+V_2(\boldsymbol{r}_2)-E\right]\Psi_1^{(+)}=0, \tag{140.1}$$

where the former V_{31}, V_{23} now can be denoted by V_1, V_2 respectively. With the incident wave

$$\psi_1 = e^{i(k_1.r_1+k_2.r_2)} \tag{140.2}$$

(dropping the here unnecessary subscript i in the components of $\boldsymbol{k}_i$), the scattering solution to (140.1) obviously is

$$\Psi_1^{(+)}(\boldsymbol{r}_1,\boldsymbol{r}_2) = \Psi_1^{(+)}(\boldsymbol{r}_1)\,\Psi_2^{(+)}(\boldsymbol{r}_2), \tag{140.3}$$

wherein $\Psi_1^{(+)}(\boldsymbol{r}_1)$, $\Psi_2^{(+)}(\boldsymbol{r}_2)$ represent the independent scattering of 1, 2 respectively by the centre of force. In particular,

$$\left.\begin{aligned}\Psi_1^{(+)}(\boldsymbol{r}_1) &= e^{ik_1.r_1}+\Phi_1^{(+)}(\boldsymbol{r}_1),\\ \Psi_2^{(+)}(\boldsymbol{r}_2) &= e^{ik_2.r_2}+\Phi_2^{(+)}(\boldsymbol{r}_2),\end{aligned}\right\} \tag{140.4}$$

with

$$\left.\begin{aligned}\lim_{r_1\to\infty||\nu_1}\Phi_1^{(+)}(\boldsymbol{r}_1) &= a_1(\boldsymbol{\nu}_1)\frac{e^{ik_1r_1}}{r_1},\\ \lim_{r_2\to\infty||\nu_2}\Phi_2^{(+)}(\boldsymbol{r}_2) &= a_2(\boldsymbol{\nu}_2)\frac{e^{ik_2r_2}}{r_2}.\end{aligned}\right\} \tag{140.5}$$

Substituting (140.4) in (140.3),

$$\Psi_i^{(+)} = e^{i(k_1.r_1+k_2.r_2)}+e^{ik_1.r_1}\Phi_2^{(+)}+e^{ik_2.r_2}\Phi_1^{(+)}+\Phi_1^{(+)}\Phi_2^{(+)}. \tag{140.6}$$

Now compare (140.6) with the defining equation (61) for $\Phi_i^{s(+)}$. The first term on the right side of (140.6) is ψ_1; in the present case there is no purely two-body scattering of 1 by 2 because $V_{12}=0$, i.e. $\Phi_{12}^{(+)}=0$ in (61); moreover, the second term on the right side of (140.6) represents the scattering of 2 by the centre of force with no scattering of 1, i.e. (recall (72)), the second term on the right side of (140.6) corresponds to $\Phi_{23}^{(+)}$ in (61); similarly, $e^{ik_2.r_2}\Phi_1^{(+)}$ in (140.6) corresponds to $\Phi_{31}^{(+)}$ in (61). Therefore, in our present illustration, $\Phi_i^{s(+)}$ of (61) is the product $\Phi_1^{(+)}\Phi_2^{(+)}$. But, from (140.5), this means

$$\lim_{r\to\infty||\nu}\Phi_i^{s(+)}(\boldsymbol{r}_1,\boldsymbol{r}_2) = a_1(\boldsymbol{\nu}_1)\,a_2(\boldsymbol{\nu}_2)\frac{e^{ik_1r_1}}{r_1}\frac{e^{ik_2r_2}}{r_2}=\sim\frac{1}{r^2}, \tag{140.7}$$

where (of course) $\boldsymbol{\nu}$ is specified by $\boldsymbol{\nu}_1$, $\boldsymbol{\nu}_2$ and the ratio r_2/r_1, as explained in the first paragraph of § 3. The result (140.7) explicitly shows that $\bar{\Phi}_i^{s(+)}(\bar{\boldsymbol{r}})\sim r^{-2}=\sim\bar{\rho}^{-2}$ in this special case, remembering that there now is no distinction between the centre-of-mass and laboratory frames. As a matter of fact, the higher order terms in (140.7) are $\sim r^{-3}$, not $r^{-5/2}$, consistent with the expectation that there should be no truly three-particle scattering in the collision between two mutually non-interacting particles and a centre of force.

4.1.4. *Divergences associated with bound states*

In addition to the on-shell δ-functions which have been discussed, the amplitudes T and $\bar{T}$ given respectively by (120) and (126) contain off-shell δ-functions when two-body bound states exist. These off-shell δ-functions in T and $\bar{T}$ have essentially the same form as those (e.g. (47)) occurring in (52), and their presence in the integrals (120 *b*) and (126 *b*) is demonstrated via

essentially the same argument as was employed (in §§ A. 4 to A. 6) for (52). For example, because $\Psi_{\mathfrak{f}}^{(-)*}(\boldsymbol{r}')$ in (120 *b*), like $G^{(+)}(\boldsymbol{r};\boldsymbol{r}')$ in (52 *a*), can contain a term proportional to

$$\exp\{\mathrm{i}\rho'\sqrt{(E-\epsilon_{\mathfrak{j}})}\}\,u_{\mathfrak{j}}(\boldsymbol{r}'_{12})/\rho'^{\frac{5}{2}},$$

the V_{12} term in (120 *b*) contains a contribution behaving like (see § A. 4)

$$\delta(\sqrt{\{E_{\mathfrak{f}}-\epsilon_{\mathfrak{j}}\}}-\sqrt{\{E_{\mathfrak{i}}-(\hbar^2k_{12\mathfrak{i}}^2/2\mu_{12})\}}), \tag{141 a}$$

when there is a bound state $u_{\mathfrak{j}}(\boldsymbol{r}_{12})$ of energy $\epsilon_{\mathfrak{j}}$ into which particles 1 and 2 can combine during the collision. The corresponding contribution to (126 *b*) is proportional to (see § A. 6)

$$\delta(K_{12\mathfrak{j}\mathfrak{f}}-K_{12\mathfrak{i}}), \tag{141 b}$$

where (114 *b*) defines $K_{12\mathfrak{j}\mathfrak{f}}$ in terms of $\bar{E}_{\mathfrak{f}}$; the δ-function (141 *b*) is the result to which (141 *a*) reduces (except for constant factors) when $\boldsymbol{K}_{\mathfrak{f}}$ is set equal to $\boldsymbol{K}_{\mathfrak{i}}$. I note that these δ-function contributions to T or $\overline{T}$ arise from the asymptotic behaviour of $\Phi_{\mathfrak{i}}^{(+)}$ or $\bar{\Phi}_{\mathfrak{i}}^{(+)}$ at large distances, and therefore are associated only with those bound states $u_{\mathfrak{j}}(\boldsymbol{r}_{\alpha\beta})$ which actually can be formed during the collision of three initially free particles; in (52 *a*), on the other hand, δ-functions are associated with all possible bound states of the three-particle system, because all such bound states are present in the asymptotic limit of $G^{(+)}(\boldsymbol{r};\boldsymbol{r}')$ at large $\boldsymbol{r}'$. For example, because energy-momentum conservation prevents three initially free particles from combining into a three-body $u_{\mathfrak{j}}(\boldsymbol{r}_{12},\boldsymbol{r}_{23})$, the existence of three-body states does not cause (120 *b*) to diverge, though such states do produce divergences in (52 *a*) (see § C. 5).

The presence of the divergences (141 *a*) or (141 *b*) has the usual significance, namely that (123) or (125) respectively must be invalid. In particular (see § C. 5), the δ-functions (141 *a*) indicate that at large r the integral on the left side of (123) has non-negligible contributions, compared to r^{-4}, from bound state propagation in the region $r'>r$ along $\boldsymbol{\nu}'_{12}$ (where r'_{12} remains finite as $r'\to\infty$), much as in the analogous integral on the left side of (99) (where the non-negligible contributions arise from $r''\to\infty$ along $\boldsymbol{\nu}''_{12}$). Of course, these contributions to the left side of (123) from $r'\to\infty$ along $\boldsymbol{\nu}'_{12}$ are in addition to, and in now way negate, the contributions dominating r^{-4} from $r'\to\infty$ along arbitrary directions $\boldsymbol{\nu}'$, to which we ascribed the failures of (123) discussed in the preceding subsections. Moreover, as (by now) is to be expected, the δ-functions signalling the failures of (123) or (125) due to bound states are readily interpretable. For instance, the δ-function (141 *b*) corresponds to conservation of the energy of particle 3 relative to an observer moving with the centre of mass of the entire system, as is physically reasonable for a contribution to the V_{12} term in (126 *b*) associated with formation of the bound state $u_{\mathfrak{j}}(\boldsymbol{r}_{12})$.

Nevertheless, despite this possibility of interpretation, it is doubtful that the δ-functions (141) occurring in (120) and (126) have any physical significance whatsoever. I now am contrasting the δ-functions (141) with those discussed in §§ 4.1.1 to 4.1.3. Admittedly the δ-functions in §§ 4.1.1 to 4.1.3, like the δ-functions of this subsection, are encountered in the configuration space formulation of scattering theory under present consideration solely because invalid mathematical manipulations have been performed. Naturally, such invalid manipulations always should be avoided if possible, especially if they lead to expressions for presumably physically meaningful quantities, namely transition amplitudes, involving non-convergent integrals. There is no immediately urgent physical reason for introducing valid mathematical procedures so as to avoid the δ-functions of this subsection, however, since these δ-functions make no contributions to the scattering coefficients w or $\overline{w}$ computed from (121 *b*) or (127 *c*), by virtue of the fact that their

arguments do not vanish on the energy-momentum shell (e.g. remembering $\epsilon_j < 0$, (35) and (114 *b*) show the δ-function (141 *b*) cannot be infinite on the centre-of-mass system energy shell $\bar{E}_f = \bar{E}_i$); the δ-functions of §§ 4.1.1 to 4.1.3, being on-shell, make infinite contributions to (121 *b*) or (127 *c*), and so must be avoided via mathematically acceptable procedures—or at the very least via some sort of reinterpretation (recall the remarks following (122), and see § 4.2)—if physically sensible reaction coefficients are to be computed.

Moreover, the steps which must be taken to avoid the δ-functions of §§ 4.1.1 to 4.1.3 are physically as well as mathematically significant. Section 4.1.1 implies that the probability current flow must be computed in the centre-of-mass frame; § 4.1.2 means that two-body scattering terms must be subtracted from $\bar{\Phi}_i^{(+)}$ before the computation of the three-body scattered current flow is initiated; and § 4.1.3 shows that it will be necessary to initially subtract from $\bar{\Phi}_i^{(+)}$ certain double scattering terms as well. The δ-functions of this subsection, on the other hand, are eliminated without any subtraction merely by starting from the iterated formula for $\bar{\Phi}_i^{(+)}$ implied by (61) and (69), instead of, as heretofore in this section, from the formula (52 *b*). More precisely, start from (61) and (69), but use the formula

$$\bar{\Phi}_{12}^{(+)}(\bar{\boldsymbol{r}}) = -\int \mathrm{d}\bar{\boldsymbol{r}}' \bar{G}_{12}^{(+)}(\bar{\boldsymbol{r}}; \bar{\boldsymbol{r}}') V_{12}(\boldsymbol{r}'_{12}) \bar{\psi}_i(\bar{\boldsymbol{r}}'), \tag{142}$$

in place of the known closed form result for $\bar{\Phi}_{12}^{(+)}$ given by (72). Then, performing on all integrals in the formula for $\bar{\Phi}_i^{(+)}$ the usual invalid interchange of order of integration and limit $\bar{r} \to \infty$, one again obtains (126 *a*), but now with

$$\bar{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \bar{\Psi}_{12f}^{(-)*} V_{12} \bar{\psi}_i + \bar{\Psi}_{23f}^{(-)*} V_{23} \bar{\psi}_i + \bar{\Psi}_{31f}^{(-)*} V_{31} \bar{\psi}_i + \bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f), \tag{143}$$

where $\bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ is given by (133 *b*). Section B. 2 shows that (133 *b*), though of course still containing the δ-functions discussed in § 4.1.3, has no δ-functions of the type (141 *b*) associated with bound states. Similarly, the other terms on the right side of (143) contain no δ-functions associated with bound states; in fact, recalling (105) one sees that, for example, the quantity defined by (130 *a*) and evaluated in (130 *c*) (which obviously contains no δ-functions of type (141 *b*)) is identical with the quantity $\bar{\Psi}_{12f}^{(-)*} V_{12} \bar{\psi}_i$ on the right side of (143). Section E. 2 shows that bound-state propagation does not invalidate (132), consistent with the absence of bound-state δ-function divergences in (133 *b*).

I stress that the preceding two paragraphs do not mean that the presence of these δ-functions (141) in (120 *b*) and (126 *b*) is wholly inconsequential. As §§ 4.1.1 and 4.1.2 taken together illustrate, it may be easier to take account of some on-shell δ-functions than of the off-shell δ-functions (141), which (if the on-shell divergences were not present) would cause the integrals (120 *b*) and (126 *b*) to be oscillatory. In particular, approximate estimates of $\bar{\Psi}_f^{(-)*}$ can be constructed which—when inserted into (126 *b*) so as to obtain approximate estimates of $\bar{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$—enable essentially exact subtraction of the single scattering two-body contributions (known exactly from (130 *c*)) on the right side of (143); however, even if there were not the double scattering complications discussed in § 4.1.3, such approximate $\bar{\Psi}_f^{(-)*}$ probably would give very poor estimates of $\bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ because of now non-vanishing contributions from the δ-functions (141 *b*) (compare the discussion of the significance of the δ-functions (47), in § 2.2 following (48)). Of course, this particular difficulty associated with the δ-functions (141) is perforce avoided when $\bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ is estimated starting from (140). I also point out that the preceding two paragraphs must not be taken to imply that the exact $\bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f)$—or better yet the exact truly

three-body amplitude $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ obtained from the asymptotic behaviour of $\bar{\Phi}_i^{t(+)}$—do not have singularities (as functions of $\boldsymbol{k}_f$) where the arguments of the δ-functions (141 *b*) vanish. I merely am insisting that the presence of off-shell singularities cannot be inferred legitimately from oscillatory (i.e. mathematically undefined) on-shell integrals for $\bar{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$. It is necessary to start with a convergent integral (e.g. $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ or $\bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ with the double-scattering contributions (135) subtracted out). The analytic continuation of this originally convergent integral well might have singularities at $K_{12|f} = K_{12i}$; on the other hand, there is no reason to think these now legitimately inferred singularities at $K_{12|f} = K_{12i}$, if actually found to exist, would be of the δ-function (141 *b*) type.

It is worth noting that the off-shell δ-functions we have been discussing show up in the expression (124 *a*) for $T(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ even though such δ-functions do not appear in the real energy Lippmann–Schwinger integral equation (42) from which (124 *a*) is derived. Correspondingly, bound state propagation invalidates the interchange of order of integration and limit $\boldsymbol{r} \to \infty \| \boldsymbol{\nu}_f$ in the integral on the right side of (42), even though (42), unlike (52 *a*), is convergent; specifically, at large r the integral (42) has contributions of order $r^{-4} \cong \rho^{-4}$ from bound state propagation in the integration region $r' > r$, as shown in § C. 5. Similar comments pertain to the expression (131) for $\bar{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$.

I conclude this subsection with some remarks stemming from the relation (131 *d*). Although the argument leading to (131 *d*) is unsatisfactory (as has been explained), nevertheless, the results of this entire § 4.1 probably are relevant to the physical significance of $\langle f| \bar{\boldsymbol{T}}(\bar{\lambda}) |i\rangle$ and the δ-functions contained therein, when i, f each denote centre-of-mass plane wave states, and when $\bar{\lambda}$ equals one or both of $\bar{E}_i$, $\bar{E}_f$. At the moment, however, I am not prepared to state precisely how the considerations of this particular § 4.1.4 relate to the bound state singularities found by Rubin *et al.* (1966, 1967*a*), who (in the special case of Yukawa interactions $V_{\alpha\beta}$) examine $\langle f| \bar{\boldsymbol{T}}(\bar{\lambda}) |i\rangle$ as a function of $\bar{\lambda}$ for fixed assigned physical values of the vectors $\boldsymbol{y}_{\alpha i} = (2m_\alpha \bar{\lambda})^{-1/2} \boldsymbol{k}_{\alpha i}$ and $\boldsymbol{y}_{\alpha f} = (2m_\alpha \bar{\lambda})^{-1/2} \boldsymbol{k}_{\alpha f}$ associated with the i, f plane waves respectively.

4.2. *Volume dependence of reaction rates*

Equations (2) and (121 *c*) imply that w defined by (121 *a*) and $\bar{w}$ defined by (127 *a*) are related by

$$w(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \tau \bar{w}(\boldsymbol{k}_i \to \boldsymbol{k}_f), \tag{144}$$

where τ is the large volume within which the three-body scattering of present interest is taking place. That the ratio $w/\bar{w}$ must be a quantity having the dimensions of volume can be seen simply from comparison of the right sides of (117 *a*) and (118 *a*). The quantity $\bar{\boldsymbol{W}}$ is defined via the Green Theorem in the centre-of-mass space in complete analogy with (45), and therefore has the same dimensions as $\boldsymbol{W}$ (since the centre-of-mass kinetic energy operator $\bar{T}$ has the same dimensions as T); however, the laboratory system surface element at infinity dS is eight-dimensional in the present three-particle problem, whereas $d\bar{S}$ is merely five-dimensional. The particular relation (144) is obtained from an argument given previously (Gerjuoy 1958*a*). From (128),

$$|T(\boldsymbol{k}_i \to \boldsymbol{k}_f)|^2 = (2\pi)^6 [\delta(\boldsymbol{K}_f - \boldsymbol{K}_i)]^2 |\bar{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)|^2. \tag{145}$$

But, as pointed out beneath (122), to make w physically meaningful, one of the δ-functions in (145 *a*) must be eliminated, presumably via some reinterpretation of $\delta(\boldsymbol{K}_f - \boldsymbol{K}_i)$. A natural reinterpretation is

$$\delta(\boldsymbol{K}_f - \boldsymbol{K}_i) = \frac{1}{(2\pi)^3} \int d\boldsymbol{R}\, e^{i(\boldsymbol{K}_f - \boldsymbol{K}_i)\cdot \boldsymbol{R}}, \tag{146 a}$$

$$[\delta(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K}_\mathrm{i})]^2 = \frac{1}{(2\pi)^6}\int \mathrm{d}\boldsymbol{R}\, \mathrm{e}^{\mathrm{i}(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K}_\mathrm{i})\cdot\boldsymbol{R}}\int \mathrm{d}\boldsymbol{R}'\, \mathrm{e}^{\mathrm{i}(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K})\cdot\boldsymbol{R}'}$$

$$= \frac{1}{(2\pi)^3}\delta(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K}_\mathrm{i})\int \mathrm{d}\boldsymbol{R}'\, \mathrm{e}^{\mathrm{i}(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K}_\mathrm{i})\cdot\boldsymbol{R}'}$$

$$= \frac{1}{(2\pi)^3}\delta(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K}_\mathrm{i})\int \mathrm{d}\boldsymbol{R}' \cong \frac{1}{(2\pi)^3}\delta(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K}_\mathrm{i})\,\tau. \tag{146 b}$$

Using (145) as reinterpreted by (146 *b*) in (121 *b*), and comparing with (127 *c*), yields (144).

Actually, because of the on-shell divergences discussed in §§ 4.1.2 and 4.1.3, use of (146 *b*) is insufficient to make physically meaningful the quantities w and $\bar{w}$ of (121 *b*) and (127 *c*). However, the procedure of (146) can be employed to eliminate all troublesome squares of δ-functions in (121 *b*) and (127 *c*), thus ultimately yielding finite (in any finite volume τ) probability current flows $\mathscr{F}$ and $\bar{\mathscr{F}}$. Thus, in the contribution (130 *c*) to $\bar{T}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f})$, for example,

$$|\bar{\Psi}_{12\mathrm{f}}^{(-)*}V_{12}\bar{\psi}_\mathrm{i}|^2 = (2\pi)^6[\delta(\boldsymbol{K}_{12\mathrm{f}}-\boldsymbol{K}_{12\mathrm{i}})]^2\,|t_{12}(\boldsymbol{k}_{12\mathrm{i}}\to\boldsymbol{k}_{12\mathrm{f}})|^2$$

$$\cong (2\pi)^3\tau\delta(\boldsymbol{K}_{12\mathrm{f}}-\boldsymbol{K}_{12\mathrm{i}})\,|t_{12}(\boldsymbol{k}_{12\mathrm{i}}\to\boldsymbol{k}_{12\mathrm{f}})|^2. \tag{147}$$

Inserting (147) into (127 *c*), one sees that $\bar{w}(\mathrm{i}\to\mathrm{f})$ has a contribution I will call $\bar{w}_{12}^{(3)}(\mathrm{i}\to\mathrm{f})$—corresponding to purely two-body elastic scattering of 1 and 2 in the three-particle system—given by

$$\bar{w}_{12}^{(3)}(\mathrm{i}\to\mathrm{f}) = \frac{2\pi}{\hbar}\frac{1}{(2\pi)^3}\tau\,|t_{12}(\boldsymbol{k}_{12\mathrm{i}}\to\boldsymbol{k}_{12\mathrm{f}})|^2\,\delta(E_\mathrm{f}-E_\mathrm{i})\,\delta(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K}_\mathrm{i})\,\delta(\boldsymbol{K}_{12\mathrm{f}}-\boldsymbol{K}_{12\mathrm{i}})\,\mathrm{d}\boldsymbol{k}_{1\mathrm{f}}\,\mathrm{d}\boldsymbol{k}_{2\mathrm{f}}\,\mathrm{d}\boldsymbol{k}_{3\mathrm{f}} \tag{148 a}$$

$$= \frac{2\pi}{\hbar}\frac{1}{(2\pi)^3}\tau\,|t_{12}(\boldsymbol{k}_{12\mathrm{i}}\to\boldsymbol{k}_{12\mathrm{f}})|^2\,\delta(E_\mathrm{f}-E_\mathrm{i})\,\delta(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K}_\mathrm{i})\,\delta(\boldsymbol{k}_{3\mathrm{f}}-\boldsymbol{k}_{3\mathrm{i}})\,\mathrm{d}\boldsymbol{k}_{1\mathrm{f}}\,\mathrm{d}\boldsymbol{k}_{2\mathrm{f}}\,\mathrm{d}\boldsymbol{k}_{3\mathrm{f}} \tag{148 b}$$

using the second equality in (29 *c*) for $\boldsymbol{K}_{12}$. Therefore, integrating (148 *b*) over $\mathrm{d}\boldsymbol{k}_{3\mathrm{f}}$

$$\bar{w}_{12}^{(3)}(\mathrm{i}\to\mathrm{f}) = \frac{2\pi}{\hbar}\frac{1}{(2\pi)^3}\tau\,|t_{12}(\boldsymbol{k}_{12\mathrm{i}}\to\boldsymbol{k}_{12\mathrm{f}})|^2\,\delta\left\{\frac{\hbar^2}{2}\left[\left(\frac{k_1^2}{m_1}+\frac{k_2^2}{m_2}\right)_\mathrm{f}-\left(\frac{k_1^2}{m_1}+\frac{k_2^2}{m_2}\right)_\mathrm{i}\right]\right\}$$

$$\times\,\delta(\boldsymbol{k}_{1\mathrm{f}}+\boldsymbol{k}_{2\mathrm{f}}-\boldsymbol{k}_{1\mathrm{i}}-\boldsymbol{k}_{2\mathrm{i}})\,\mathrm{d}\boldsymbol{k}_{1\mathrm{f}}\,\mathrm{d}\boldsymbol{k}_{2\mathrm{f}}. \tag{148 c}$$

Or

$$\bar{w}_{12}^{(3)}(\mathrm{i}\to\mathrm{f}) = \tau\bar{w}_{12}^{(2)}(\mathrm{i}\to\mathrm{f}), \tag{149 a}$$

where

$$\bar{w}_{12}^{(2)}(\mathrm{i}\to\mathrm{f}) = \frac{2\pi}{\hbar}\frac{1}{(2\pi)^3}|t_{12}(\boldsymbol{k}_{12\mathrm{i}}\to\boldsymbol{k}_{12\mathrm{f}})|^2\,\delta\left(\frac{\hbar^2k_{12\mathrm{f}}^2}{2\mu_{12}}-\frac{\hbar^2k_{12\mathrm{i}}}{2\mu_{12}}\right)\mathrm{d}\boldsymbol{k}_{12\mathrm{f}} \tag{149 b}$$

$$= \frac{2\pi}{\hbar}\frac{1}{(2\pi)^3}|t_{12}(\boldsymbol{k}_{12\mathrm{i}}\to\boldsymbol{k}_{12\mathrm{f}})|^2\,\delta(E_\mathrm{f}-E_\mathrm{i})\,\delta(\boldsymbol{K}_\mathrm{f}-\boldsymbol{K}_\mathrm{i})\,\mathrm{d}\boldsymbol{k}_{1\mathrm{f}}\,\mathrm{d}\boldsymbol{k}_{2\mathrm{f}}. \tag{149 c}$$

In (149), $\bar{w}_{12}^{(2)}(\mathrm{i}\to\mathrm{f})$ represents the conventional elastic scattering coefficient for particles 1 and 2 in their centre-of-mass frame; the definitions of the two-particle total energies E and total momenta $\boldsymbol{K}$ in (149 *c*) are obvious. It is understood that particle 3 never appears in the computation of $\bar{w}_{12}^{(2)}$ or its laboratory frame analogue $w_{12}^{(2)}$; in particular, these quantities are computed using Schrödinger's equation for particles 1, 2 only, with incident waves—in the laboratory and centre-of-mass frame respectively—

$$\psi_\mathrm{i} = \mathrm{e}^{\mathrm{i}(\boldsymbol{k}_1\cdot\boldsymbol{r}_1+\boldsymbol{k}_2\cdot\boldsymbol{r}_2)}, \tag{150 a}$$

$$\bar{\psi}_\mathrm{i} = \mathrm{e}^{\mathrm{i}\boldsymbol{k}_{12}\cdot\boldsymbol{r}_{12}}. \tag{150 b}$$

Furthermore, (149 *b*) and (149 *c*), which are the two-particle system analogues of (127 *b*) and (127 *c*), can be derived without any improper mathematical manipulations, because with the

incident wave (150 *b*) the problem of computing $\bar{w}_{12}^{(2)}(\mathrm{i}\to\mathrm{f})$ reduces to potential scattering; correspondingly, $\bar{w}_{12}^{(2)}$ is assuredly τ-independent. But, using (144), to the relation (149 *a*) corresponds

$$w_{12}^{(3)}(\mathrm{i}\to\mathrm{f}) = \tau^2 \bar{w}_{12}^{(2)}(\mathrm{i}\to\mathrm{f}). \tag{151}$$

Therefore, as foreshadowed in § 1, (121 *b*)—taken together with (121 *c*) or (2)—implies the quantity $\tau^{-1}\hat{w}(\boldsymbol{k}_{\mathrm{i}}\to\boldsymbol{k}_{\mathrm{f}})$, supposedly representing the actually observed scattering rate per unit volume into wavenumber ranges $\mathrm{d}\boldsymbol{k}_{1\mathrm{f}}$, $\mathrm{d}\boldsymbol{k}_{2\mathrm{f}}$, $\mathrm{d}\boldsymbol{k}_{3\mathrm{f}}$, will not be independent of the volume in the limit $\tau\to\infty$ for all $\boldsymbol{k}_{1\mathrm{f}}$, $\boldsymbol{k}_{2\mathrm{f}}$, $\boldsymbol{k}_{3\mathrm{f}}$. Rather, at $\boldsymbol{k}_{1\mathrm{f}}$, $\boldsymbol{k}_{2\mathrm{f}}$, $\boldsymbol{k}_{3\mathrm{f}}$ consistent with the restrictions imposed by the three δ-functions in (148 *a*) or (148 *b*), $\tau^{-1}\hat{w}$ seemingly will be proportional to the reaction volume τ.

The above result is just another way of seeing that w and $\bar{w}$ of (121 *b*) and (127 *c*) are not the 'true' three-body elastic scattering coefficients; these, as discussed in § 1, still will be computed from (121 *b*) and (127 *c*), except that the true three-body amplitudes $T^t(\boldsymbol{k}_{\mathrm{i}}\to\boldsymbol{k}_{\mathrm{f}})$ and $\bar{T}^t(\boldsymbol{k}_{\mathrm{i}}\to\boldsymbol{k}_{\mathrm{f}})$ —determined by the asymptotic forms of $\Phi_{\mathrm{i}}^{t(+)}$ and $\bar{\Phi}_{\mathrm{i}}^{t(+)}$—will replace T and $\bar{T}$ respectively. This last remark suggests that the result (151)—having been deduced by a somewhat questionable argument (147), starting from formally divergent expressions (for T or $\bar{T}$) derived via invalid mathematical manipulations—does not have any physical significance. This suggestion is incorrect, however, as the immediately following subsection shows. Instead, the volume dependence of (151)—like the δ-functions of (128) and (130 *c*) which are its source—is physically interpretable and, in fact, to be expected.

4.2.1. *Volume dependence and incident wave normalization*

One subject which has been ignored thus far in this work is the genesis of the relations (2) or (121 *c*). To be more explicit, there is the following question which should be answered: because the normalization of the incident wave (21 *a*), namely unit amplitude, is a purely arbitrary choice, how do I know that (2) or (121 *c*) relate the actually observed scattering rate to the probability current flows computed from ψ_{i} of (21 *a*)? Or, to put it differently, granted I somehow have managed to determine the asymptotic forms of the truly three-body $\Phi_{\mathrm{i}}^{t(+)}$ or $\bar{\Phi}_{\mathrm{i}}^{t(+)}$ corresponding to the unit amplitude incident wave (21 *a*), how do I know that the corresponding (presumably divergence-free and therefore τ-independent) centre-of-mass frame 'true' three-body coefficient $\bar{w}(\mathrm{i}\to\mathrm{f})$ yields the expected laboratory frame reaction rate after multiplication by precisely $N_1 N_2 N_3 \tau$?

Before trying to answer these questions for three-body scattering, let me try to answer their analogues for conventional two-body scattering of species 1 and 2, in the complete absence of species 3. In this latter event, the analogue of (2) is

$$\hat{w}_{12}^{(2)}(\boldsymbol{k}_{1\mathrm{i}}, \boldsymbol{k}_{2\mathrm{i}}\to\boldsymbol{k}_{1\mathrm{f}}, \boldsymbol{k}_{2\mathrm{f}}) = N_1 N_2 \tau \bar{w}_{12}^{(2)}(\boldsymbol{k}_{1\mathrm{i}}, \boldsymbol{k}_{2\mathrm{i}}\to\boldsymbol{k}_{1\mathrm{f}}, \boldsymbol{k}_{2\mathrm{f}}), \tag{152 a}$$

where $\bar{w}_{12}^{(2)}$ is given by (149 *b*) or (149 *c*) and where $\hat{w}_{12}^{(2)}$ represents the observed scattering rate of particles 1, 2 into $\mathrm{d}\boldsymbol{k}_{1\mathrm{f}}$, $\mathrm{d}\boldsymbol{k}_{2\mathrm{f}}$, in a large volume τ containing particle species 1 and 2 only. Then the customary (and quite satisfactory) way of understanding the volume dependence of (152 *a*) is as follows. One first observes that (130) and (149 *b*) imply

$$\bar{w}_{12}^{(2)}(\mathrm{i}\to\mathrm{f}) = |\boldsymbol{v}_1 - \boldsymbol{v}_2|\ \bar{\sigma}(\boldsymbol{k}_{12\mathrm{i}}\to\boldsymbol{k}_{12\mathrm{f}})\,\mathrm{d}\boldsymbol{n}_{12\mathrm{f}}, \tag{152 b}$$

where $\bar{\sigma}(\boldsymbol{k}_{12\mathrm{i}}\to\boldsymbol{k}_{12\mathrm{f}})$ is the conventional centre-of-mass frame differential cross-section for elastic scattering into the direction $\boldsymbol{n}_{12\mathrm{f}}$ of $\boldsymbol{k}_{12\mathrm{f}}$, computed as if for potential scattering of a particle having

mass μ_{12} and incident wave vector $\boldsymbol{k}_{12}$; $\boldsymbol{v}_1$, $\boldsymbol{v}_2$ are the classical particle velocities, of course, and it is understood that scattering occurs only into $\boldsymbol{k}_{1f}$, $\boldsymbol{k}_{2f}$ consistent with energy-momentum conservation. By definition of the cross-section, however, if a beam of particles 1, containing N_1 particles/c.c. with velocity $\boldsymbol{v}_1$, is incident on a single particle 2, the number of elastic scattering events per second into $\mathrm{d}\boldsymbol{n}_{12f}$ is

$$N_1 |\boldsymbol{v}_1 - \boldsymbol{v}_2| \, \bar{\sigma}(\boldsymbol{k}_{12i} \to \boldsymbol{k}_{12f}) \, \mathrm{d}\boldsymbol{n}_{12f}. \tag{152c}$$

The scattering rate $\hat{w}$ with $\hat{N}_2 = N_2 \tau$ scatterers will be $\hat{N}_2$ times (152 c), which, using (152 b), is precisely the result (152 a).

The foregoing interpretation of (152 a) is not readily generalized to collisions involving three incident particles because, for three-body collisions, it is not readily possible to find a quantity playing the role of the cross-section; there is no useful analogue of the cross-section because the three-particle centre-of-mass frame incident wave (33 b) propagates in six rather than three dimensions, so that going to the centre-of-mass frame does not reduce the three-particle collision to potential scattering. However, I now shall give an alternative interpretation of (152 a) which, because it rests on considerations of the laboratory frame six-dimensional two-particle incident wave (150 a), is easily generalizable to collisions between three (or more) particles.

Obviously the average scattering rate from a volume τ containing randomly and uniformly distributed particles 1 and 2, in numbers $\hat{N}_1 = N_1 \tau$ and $\hat{N}_2$, will be $\hat{N}_1 \hat{N}_2$ times the average scattering rate from the same volume containing only a single particle 1 and a single particle 2, assuming these single particles each may be found anywhere in τ with uniform probability per unit volume. The incident plane wavefunction corresponding to (150 a), but normalized to one particle 1 in τ and one particle 2 in τ is

$$\psi_i' = \frac{1}{\tau} e^{i(k_1 . r_1 + k_2 . r_2)} \tag{153a}$$

because, for example, the probability of finding particle 1 in any $\mathrm{d}\boldsymbol{r}_1$ within τ is

$$\mathrm{d}\boldsymbol{r}_1 \int_\tau \mathrm{d}\boldsymbol{r}_2 \, |\psi_i'(\boldsymbol{r}_1, \boldsymbol{r}_2)|^2 = \mathrm{d}\boldsymbol{r}_1 \frac{1}{\tau^2} \int \mathrm{d}\boldsymbol{r}_2 = \frac{1}{\tau} \mathrm{d}\boldsymbol{r}_1. \tag{153b}$$

On the other hand, because (50 a) shows $\Phi_i(E + i\epsilon)$, and therefore also its limit $\Phi_i^{(+)}(E)$, rigorously is multiplied by τ^{-1} when ψ_i is multiplied by τ^{-1}, it follows from (45 a) and (117 a) that the outgoing probability current flow computed with ψ_i' of (153 a) is precisely τ^{-2} times the corresponding flow computed with ψ_i of (150 a). In other words, recognizing that the definition (121 a) of w applies to two-particle as well as to three-particle systems, the scattered probability current flow computed with ψ_i' of (153 a) yields precisely

$$\hat{w}_{12}'^{(2)}(i \to f) = \tau^{-2} w_{12}^{(2)}(i \to f) = \tau^{-1} \bar{w}_{12}^{(2)}(i \to f), \tag{154}$$

wherein the second equality holds because the conventional laboratory and centre-of-mass frame two-particle scattering coefficients, $w_{12}^{(2)}$ and $\bar{w}_{12}^{(2)}$ respectively, also satisfy (144). Moreover, $\hat{w}_{12}'^{(2)}$ of (154), with $\bar{w}_{12}^{(2)}$ given by (149 b), represents the scattering rate when a single particle 1 and a single particle 2 are to be found in τ. Multiplying (154) by $\hat{N}_1 \hat{N}_2 = N_1 N_2 \tau^2$ again yields (152 a).

The fact that (154) represents the scattering rate for a single pair of particles also can be understood on the following less exact but very physical basis. In a genuinely two-body collision involving short-range forces, it can be assumed that scattering takes place only if the two particles 1 and 2 manage to get within a (possibly dependent on $|\boldsymbol{v}_1 - \boldsymbol{v}_2|$) distance b of each

other, where the total elastic scattering cross-section $\bar{\sigma} \cong \pi b^2$. In effect this relation defines the (dependent on relative velocity) quantity b; of course, often, but not necessarily, b turns out to equal approximately the range at which the interaction $V_{12}(\boldsymbol{r}_{12})$ becomes negligibly different from zero. Now again consider a large volume τ containing precisely one particle 1 and one particle 2, each of which may be located anywhere in τ with equal probability per unit volume. Then at any given instant, in any given volume $\tau_0 = b^3$, the probability of finding particle 1 in τ_0 is τ_0/τ. Hence the probability that particles 1 and 2 are scattering within τ_0 at any given instant $= (\tau_0/\tau)^2$, the probability of simultaneously finding 1 and 2 within τ_0. The number of such volumes τ_0 in τ is τ/τ_0. At any given instant, therefore, with one particle 1 and one particle 2 in τ, the probable number of scatterings taking place is τ_0/τ. To convert this result to a scattering rate per particle pair, one must divide by a time t_c representing the average 'duration' of a collision, i.e. the average time a pair of particles remains within scattering range; this division by t_c recognizes that even with a large number of particle pairs in τ, scattering continues at a steady average rate only because particles complete one scattering event and move into a new volume τ_0, where they again have a chance τ_0/τ of scattering against any other given particle in τ. Hence the scattering rate per particle pair in τ is $\cong \tau_0/\tau t_c$. Since $t_c \cong |\boldsymbol{v}_1 - \boldsymbol{v}_2|^{-1} b$, this scattering rate per particle pair has exactly the form (154), recalling (152 b) as well as the definitions in this paragraph relating τ_0 and $\bar{\sigma}$ to b.

Now, having managed to give simple laboratory system interpretations of (152 a), I turn to its analogous three-body relation (2). First, let me proceed inexactly, though qualitatively correctly, as in the preceding paragraph. A true three-body collision between particles 1, 2, 3 occurs only if the three particles simultaneously find themselves within some volume τ_0 (possibly, but not necessarily, of the same order b^3 as in individual two-particle collisions between individual pairs α, β). With a single particle of each species α ($\alpha = 1, 2, 3$) in a large volume τ, the probability of simultaneously finding all three particles in a given τ_0 is $(\tau_0/\tau)^3$. Letting t_c again denote the average collision duration (now not as readily related as previously to the relative particle velocities), the true three-body scattering rate per triplet 1, 2, 3 in τ is

$$\hat{w}'(\mathrm{i} \to \mathrm{f}) \cong \left(\frac{\tau_0}{\tau}\right)^3 \frac{\tau}{\tau_0} \frac{1}{t_c} = \frac{\tau_0^2}{\tau^2 t_c}. \tag{155 a}$$

Therefore, the laboratory frame scattering rate with $\hat{N}_\alpha = N_\alpha \tau$ particles in τ is

$$\hat{w}(\mathrm{i} \to \mathrm{f}) = \hat{N}_1 \hat{N}_2 \hat{N}_3 \hat{w}' \cong N_1 N_2 N_3 \tau \frac{\tau_0^2}{t_c}. \tag{155 b}$$

Equation (155 b) has the form (2); in particular, it asserts that the measured laboratory scattering rate should be proportional to τ, as well as to $N_1 N_2 N_3$. If (2) now is regarded merely as a definition of the proportionality factor $\bar{w}$ between the actually observed three-body scattering rate $\hat{w}$ and $N_1 N_2 N_3 \tau$, then (155 b) shows

$$\bar{w} \cong \frac{\tau_0^2}{t_c}. \tag{155 c}$$

Thus, if (2) really provides a prediction of the measured $\hat{w}$ in terms of the true three-body reaction coefficient $\bar{w}$ determined from $\bar{\Phi}_i^{t(+)}$ (as this paper has been asserting), then calculations of this $\bar{w}$ from $\bar{\Phi}_i^{t(+)}$ should be consistent with (155 c). In other words, the computed true three-body scattering coefficient $\bar{w}$ should turn out to be τ-independent, and should be interpretable as the square of a reaction volume divided by the collision duration.

I also can argue as in the next to the last paragraph above, wherein no approximations were made and no ill-defined average quantities (e.g. t_c) were introduced. The incident wavefunction corresponding to (21 *a*), but normalized to one particle of each species 1, 2 and 3 in τ is (compare (153 *a*))

$$\psi_i' = \frac{1}{\tau^{\frac{3}{2}}} e^{i(k_1 \cdot r_1 + k_2 \cdot r_2 + k_3 \cdot r_3)}. \tag{156 a}$$

Thus the true three-particle collision rate with one particle of each species in τ is precisely

$$\hat{w}'(i \to f) = \tau^{-3} w(i \to f) = \tau^{-2} \overline{w}(i \to f), \tag{156 b}$$

where w, $\overline{w}$ here are supposed to be the true reaction coefficients determined from $\Phi_i^{t(+)}$, $\overline{\Phi}_i^{t(+)}$ corresponding to the conventional incident wave (21 *a*), i.e. determined from the truly three-body parts of the conventional $\Phi_i^{(+)}$, $\overline{\Phi}_i^{(+)}$ whose asymptotic forms were examined in § 4.1. Multiplying the precise scattering rate (156 *b*) per triplet by the number of triplets

$$\hat{N}_1 \hat{N}_2 \hat{N}_3 = N_1 N_2 N_3 \tau^3$$

in τ yields precisely (2); in other words, the argument of this paragraph implies that the measured scattering rate $\hat{w}$, and the reaction coefficient $\overline{w}$ determined as described in the preceding sentence, indeed must be related as in (2). Note that this present argument does not imply $\hat{w}$ is proportional to τ; $\overline{w}$ in (156 *b*) might be τ-dependent, for all this present argument knows. However, the fact that the true three-body reaction coefficient $\overline{w}$ is independent of τ will become apparent when $\overline{w}$ is calculated correctly, i.e. starting from $\overline{\Phi}_i^{t(+)}$ and not employing any improper mathematical manipulations. Alternatively, having now shown $\overline{w}$ in (2) indeed must be the true three-body reaction coefficient, I can appeal to the considerations of the preceding paragraph, in particular to (155 *c*), thus inferring (without actual calculation of $\overline{w}$ from $\overline{\Phi}_i^{t(+)}$) that such calculation will yield a $\overline{w}$ independent of τ. In fact, once (155 *a*) and (156 *b*) each have been deduced, the relation (155 *c*) for the true three-body reaction coefficient $\overline{w}$ of (156 *b*) follows immediately, without any necessity for referring to (2).

This result answers the questions raised in the first paragraph of this subsection. I turn therefore to the problem of understanding (151). The quantity $w_{12}^{(3)}$ of (151) represents the laboratory frame coefficient for two-body scattering of 1, 2, when computed from the solution $\Psi_i^{(+)}$ to the three-particle Lippmann–Schwinger equation corresponding to the three-particle incident wave (21 *a*). Now what two-body rate $w_{12}'^{(3)}$ of 1, 2 scattering should be expected with the incident wave ψ_i' of (156 *a*)? The answer to this question, clearly, is the same rate (154) as was computed using the two-particle ψ_i' of (153 *a*), because both these incident waves correspond to one particle 1 and one particle 2 in τ. In other words, it must be true that

$$\hat{w}_{12}'^{(3)}(i \to f) = \hat{w}_{12}'^{(2)}(i \to f) = \tau^{-1} \overline{w}_{12}^{(2)}(i \to f). \tag{157 a}$$

But, as explained previously following (153 *b*), the probability current flow computed with ψ_i' of (156 *a*) is precisely τ^{-3} times the corresponding flow computed with ψ_i of (21 *a*). Therefore I see that with the incident wave (21 *a*) I must expect to find a laboratory frame two-body coefficient

$$w_{12}^{(3)}(i \to f) = \tau^3 \hat{w}_{12}'^{(3)}(i \to f) = \tau^2 \overline{w}_{12}^{(2)}(i \to f), \tag{157 b}$$

which is precisely the result (151) obtained earlier from the expressions for $w_{12}^{(2)}$ and $w_{12}^{(3)}$ in terms of the matrix elements $\hat{T}_{12}(i \to f)$.

The argument in the preceding paragraph makes it apparent that the τ^2 dependence in

$w_{12}^{(3)}(\mathrm{i}\to\mathrm{f})$ is necessary if the predicted observed two-body scattering rate $\hat{w}_{12}^{(3)}$ using the three-body incident wave (21 *a*) is to agree with the conventional prediction $\hat{w}_{12}^{(2)}$ of (152 *a*) obtained using the two-body incident wave (150 *a*). Indeed, one can say flatly that if adding an irrelevant particle 3 to the pair 1, 2 had changed the physical predictions, this publication's whole approach to many-particle collisions would have become very questionable. The preceding paragraph and earlier discussion in this subsection also suggest a simple series of rules for making the connexion between collision theory and experiment, for any collision process and whatever the number of particles involved: (i) compute the reaction coefficient using unit amplitude waves; (ii) if the mathematics has involved invalid manipulations, so that on-shell δ-functions appear in the transition amplitudes, reinterpret them along the lines of (146) and (147), permitting only the first powers of δ-functions to remain in w or $\bar{w}$; (iii) renormalize so as to correspond to an incident wave with one particle of each species in a volume τ; (iv) multiply by the appropriate number of particle pairs, triplets, tetrads, etc. (e.g. by $\hat{N}_1\hat{N}_2 = N_1N_2\tau^2$ for two-particle processes, by $N_1N_2N_3\tau^3$ for three-particle processes, etc.), to obtain the laboratory system reaction rate $\hat{w}$ in τ.

Granted I have not proved the legitimacy of the above rules, this subsection makes it unlikely that they are not quite generally applicable. On the other hand, I must point out that especially rule (ii) above is dubious; certainly I have not shown that the prescribed replacement of powers of on-shell δ-functions by powers of τ always will make good physical sense, although the likelihood that this will be the case now seems much greater than previously might have been supposed. In particular, the next subsection will demonstrate that the τ-dependence implied by the double-scattering δ-functions (135) can be understood physically. Nevertheless, it is apparent that the results of this subsection in no way negate the results of previous sections. The presence of δ-functions in transition amplitudes still signals improper mathematical manipulations, generally reflecting the fact that erroneous assumptions have been made concerning the asymptotic dependence of the scattered wave terms whose limit as $\boldsymbol{r}\to\infty$ is being extracted; the corresponding anomalous τ-dependences of computed reaction coefficients indicate the same fact from a different point of view, i.e. they indicate that physical processes other than those desired have been included, e.g. two-body scattering in the supposed three-body reaction coefficient.

Section 4.3 below illustrates the fact that qualitative arguments like those leading to (155) can lead to a predicted centre-of-mass reaction coefficient proportional to a negative power of τ. I believe that in this event the corresponding collision process either really is unobservedly small in any large volume (in comparison with related competing processes), or at most has a laboratory system rate $\hat{w}(\mathrm{i}\to\mathrm{f})$ proportional to τ; it also is possible that a predicted $\bar{w}$ proportional to τ^{-z}, $z>0$, means simply that the process under examination is essentially meaningless within the theoretical formulation adopted. In either case, the above rules probably are not applicable. It also seems reasonable that reaction coefficients $\bar{w}$ which really are physically proportional to τ^{-z}, $z>0$, correspond to processes which, in the particular theoretical formulation adopted, depend on parts of $\bar{\Phi}_{\mathrm{i}}^{(+)}(\bar{\boldsymbol{r}})$ decreasing more rapidly at large $\bar{\boldsymbol{r}}$ than does the relevant free-space Green function $\bar{G}_F^{J(+)}(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}')$, i.e. more rapidly than $\bar{r}^{-[3(J-1)-1]/2}$; here J is the number of independent aggregates moving outward to infinity in the laboratory system ($J=2$ in a three-particle collision resulting in formation of bound states $u_{\mathrm{j}}(\boldsymbol{r}_{12})$ as, for example, in (17 *a*)), and $\bar{G}_F^{J(+)}$ has the dimensionality of the centre-of-mass frame free space Green function for a system of J elementary particles. Needless to say, I have not proved the immediately preceding assertion concerning $\bar{w}\sim\tau^{-z}$, $z>0$; we have seen, however, that δ-functions in transition amplitudes generally lead to $\bar{w}$ proportional to positive powers of τ, and seem to be associated with terms in

$\bar{\Phi}_i^{(+)}(\bar{\boldsymbol{r}})$ decreasing less rapidly than the relevant free space Green function $\bar{G}_F^{J(+)}(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}')$ (recall the rules cited at the end of § 4.1.3).

4.2.2. *Double scattering contributions*

In this subsection I shall discuss the volume dependence implied by the δ-functions (135). To begin with, the briefest consideration of the contributions made by these δ-functions to w and $\bar{w}$ of (121 *b*) and (127 *b*) makes it evident that there is little hope of being able to compute precisely the anomalous τ-dependences these δ-functions yield. It is easily seen that the δ-functions (135) make contributions to $\bar{w}(\mathrm{i}\to\mathrm{f})$ proportional to $\tau^{\frac{1}{3}}$, but the precise magnitudes of these contributions are essentially incalculable.

To make these last assertions more explicit, suppose I write, as in (146) and (147),

$$\delta(k_{12\mathrm{i}}-|\boldsymbol{k}_{12\mathrm{f}}+\boldsymbol{k}_{1\mathrm{f}}-\boldsymbol{k}_{1\mathrm{i}}|)\equiv\delta(k_{12\mathrm{i}}-Q)=\frac{1}{2\pi}\int \mathrm{d}x\,\mathrm{e}^{\mathrm{i}x(k_{12\mathrm{i}}-Q)}, \tag{158 a}$$

$$[\delta(k_{12\mathrm{i}}-Q)]^2=\frac{1}{(2\pi)^2}\int \mathrm{d}x\,\mathrm{e}^{\mathrm{i}x(k_{12}-Q)}\int \mathrm{d}x'\,\mathrm{e}^{\mathrm{i}x'(k_{12\mathrm{i}}-Q)}$$

$$=\frac{1}{2\pi}\delta(k_{12\mathrm{i}}-|\boldsymbol{k}_{12\mathrm{f}}+\boldsymbol{k}_{1\mathrm{f}}-\boldsymbol{k}_{1\mathrm{i}}|)\int \mathrm{d}x'. \tag{158 b}$$

Then the one-dimensional integral over $\mathrm{d}x'$ in (158 *b*) is not as readily interpretable as the three-dimensional integral over $\mathrm{d}\boldsymbol{R}'$ in (146 *b*). Certainly the integral over $\mathrm{d}x'$ in (158 *b*) can be assumed proportional to some average dimension of τ, i.e. proportional to $\tau^{\frac{1}{3}}$. The proportionality factor is ill-defined, however, and probably will depend on the shape of the large volume τ. In other words, the best I seem able to do is to replace (158 *b*) by

$$[\delta(k_{12\mathrm{i}}-|\boldsymbol{k}_{12\mathrm{f}}+\boldsymbol{k}_{1\mathrm{f}}-\boldsymbol{k}_{1\mathrm{i}}|)]^2\cong\frac{1}{2\pi}C\delta(k_{12\mathrm{i}}-|\boldsymbol{k}_{12\mathrm{f}}+\boldsymbol{k}_{1\mathrm{f}}-\boldsymbol{k}_{1\mathrm{i}}|)\,\tau^{\frac{1}{3}}, \tag{158 c}$$

where C is an unknown factor, dependent on the shape of the scattering region τ, but not on the magnitude of its volume. Recalling that (135 *a*) is a contribution to $\bar{T}^s$ of (133 *b*), and comparing with (147) and (148), one sees that insertion of $\bar{T}^s$ into (127 *b*) will yield a $\bar{w}(\mathrm{i}\to\mathrm{f})$ containing terms surely proportional to $\tau^{\frac{1}{3}}$, but with unknown coefficients dependent on the shape of τ. The corresponding double-scattering contributions to $w(\mathrm{i}\to\mathrm{f})$ will be proportional to $\tau^{\frac{4}{3}}$, using the still applicable (144). I add that the rules cited at the end of § 4.1.3 now make it evident that when a part of $\Phi_i^{(+)}(\boldsymbol{r})$ decreases like $\rho^{\frac{1}{2}x}\rho^{-4}$ along $\boldsymbol{\nu}_\mathrm{f}+\boldsymbol{\nu}_{\alpha\beta}$, $x\geqslant 0$, the associated contribution to $w(\mathrm{i}\to\mathrm{f})$ will be proportional to $\tau^{\frac{1}{3}x}$; equivalently, when a part of $\bar{\Phi}_i^{(+)}(\bar{\boldsymbol{r}})$ decreases like $\bar{\rho}^{\frac{1}{2}y}\bar{\rho}^{-5/2}$ along $\bar{\boldsymbol{\nu}}_\mathrm{f}+\bar{\boldsymbol{\nu}}_{\alpha\beta}$, the associated contribution to $\bar{w}(\mathrm{i}\to\mathrm{f})$ will be proportional to $\tau^{\frac{1}{3}y}$, assuming $y\geqslant 0$.

I now show that this $\tau^{\frac{4}{3}}$ dependence of double-scattering contributions to $w(\mathrm{i}\to\mathrm{f})$—like the τ^2 dependence of two-body scattering contributions to $w(\mathrm{i}\to\mathrm{f})$ discussed in § 4.2.1—is physically understandable and, in fact, to be expected. As in the case of true three-body collisions, in a large volume τ containing $\hat{N}_\alpha$ particles α, $\alpha=1,2,3$, the double-scattering rate corresponding to (135 *b*)—namely (recall the discussion of (136) to (139)) the average number of times per second that a two-body scattering event between 1 and 2 is followed by a two-body scattering between 2 and 3—will be precisely $\hat{N}_1\hat{N}_2\hat{N}_3$ times the corresponding rate when τ contains a single particle of each species. The desired double scattering rate in this latter situation will be the integral—over all possible intermediate momenta $\boldsymbol{k}_2'$ resulting from the first scattering—of the product

between the rate at which 1, 2 scatterings produce $\boldsymbol{k}_2'$ and the probability that particle 2 will scatter from 3 as it moves through the volume τ with momentum $\boldsymbol{k}_2'$. This latter probability is $\cong L\bar{\sigma}_{23}/\tau$, where $\bar{\sigma}_{23}$ is the cross-section for two-body scattering of 2 by 3, and L is some average dimension of τ, depending on the site of the first scattering, the direction of $\boldsymbol{k}_2'$, the shape of τ, etc.; evidently $L\bar{\sigma}_{23}$ is an estimate of the volume wherein scattering of 2 by 3 can occur as 2 moves through τ. The rate of 1, 2 scatterings for a single pair 1, 2 in τ is given by (154). Therefore, after performing all the complicated averages, the desired double-scattering rate $\hat{w}_{\mathrm{d}}'$ (12, 23) with one particle of each species in τ will turn out to be

$$\hat{w}_{\mathrm{d}}'(12,23) \cong \left\langle \left(\frac{\bar{w}_{12}^{(2)}}{\tau}\right)\left(\frac{L\bar{\sigma}_{23}}{\tau}\right)\right\rangle_{\mathrm{av}} \cong C\tau^{-5/3}, \tag{159a}$$

where C again is an effectively unknown factor, dependent on the shape of the scattering region τ, but not on the magnitude of its volume. Here $\hat{w}_{\mathrm{d}}'(12,23)$ represents the double-scattering contribution to the probability current flow when the incident wave is ψ_{i}' of (156 a). Hence the corresponding contribution to $w(\mathrm{i}\to\mathrm{f})$ of (121 b) must be proportional to $\tau^3\tau^{-5/3} = \tau^{\frac{4}{3}}$, with a shape-dependent factor C, as found in the preceding paragraph beneath (158 c). The corresponding observed double-scattering rate $\hat{w}_{\mathrm{d}}(12,23)$ when τ contains $\hat{N}_\alpha$ particles of each species will be

$$\hat{w}_{\mathrm{d}}(12,23) = \hat{N}_1\hat{N}_2\hat{N}_3\,\hat{w}_{\mathrm{d}}'(12,23) \cong N_1N_2N_3C\tau^{\frac{4}{3}}. \tag{159b}$$

I want to contrast this result (159 b) for the δ-functions (135) with the corresponding result in § 4.2.1 for the δ-function (130 c). In the case of the δ-functions (135) the computed $w(\mathrm{i}\to\mathrm{f})$ using ψ_1 of (21 a) has terms proportional to $\tau^{\frac{4}{3}}$; to these terms will correspond observed laboratory frame scattering rates $\hat{w}(\mathrm{i}\to\mathrm{f})$ proportional to $N_1N_2N_3$ and to $\tau^{\frac{4}{3}}$. For the δ-function (130 c), on the other hand, though the computed $w(\mathrm{i}\to\mathrm{f})$ using ψ_1 of (21 a) is proportional to τ^2, the corresponding observable laboratory frame $\hat{w}(\mathrm{i}\to\mathrm{f})$ is proportional merely to τ, as well as merely to N_1N_2 (being independent of N_3). Note also that the experimentalist attempting to measure the true three-body elastic scattering coefficient by crossing three beams (let us ignore the present utter infeasibility of such an experiment) will have to avoid placing his coincidence counters at directions and distances corresponding to vanishing of the arguments of the δ-function (135 b) and its analogues, if he wishes to avoid measuring double scattering rather than true three-body scattering. Of course, he also must avoid counter locations corresponding to a single purely two-body scattering.

4.3. *Truly three-body scattering*

I return now to our original objective of determining the physical three-body $\bar{w}(\mathrm{i}\to\mathrm{f})$, i.e. to the problem of finding expressions for the true three-body matrix elements $\langle\mathrm{f}|\,\bar{T}^t\,|\mathrm{i}\rangle$ of (4). It is argued in § 4.3.1 immediately below that the contributions to $\bar{\Phi}_{\mathrm{i}}^{s(+)}$ of (69) from triple and higher rescattering processes (namely, from processes involving any number $n \geqslant 3$ of successive purely two-body collisions between pairs of the three particles 1, 2, 3) behave asymptotically like $\bar{G}_F^{(+)}(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}';\bar{E})$ as $\bar{\boldsymbol{r}}\to\infty$ along essentially all $\bar{\boldsymbol{\nu}}_{\mathrm{f}}$ which keep no $\boldsymbol{r}_{\alpha\beta}$ finite. In other words, as this chapter (especially in its introduction and in § 4.1.3) has made abundantly clear, such $n \geqslant 3$ rescattering processes legitimately can be termed 'truly three-body', and are expected to contribute neither δ-functions to $\bar{T}^s(\boldsymbol{k}_{\mathrm{i}}\to\boldsymbol{k}_{\mathrm{f}})$ of (133 b) nor anomalous τ-dependences to $\bar{w}(\mathrm{i}\to\mathrm{f})$. A direct way of attaining our desired objective, therefore, is to develop a procedure for subtracting the double-scattering contributions to $\bar{\Phi}_{\mathrm{i}}^{s(+)}$ of (69), thereby hopefully obtaining $\bar{\Phi}_{\mathrm{i}}^{t(+)}$. If this could be done, one should be able to compute $\lim \bar{\Phi}_{\mathrm{i}}^{t(+)}$ as $\bar{\boldsymbol{r}}\to\infty\|\bar{\boldsymbol{\nu}}_{\mathrm{f}}$, therewith determining

$\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ in closed form; correspondingly, using the centre-of-mass analogues of (105) and (106), one would have a closed form expression for the true (or physical) three-body elastic scattering transition operator $\bar{\boldsymbol{T}}^t$ introduced in § 1. I add that because the shape-dependent factor C in (158 c) is essentially incalculable, there seems to be no practical way to obtain the theoretical physical three-body $\bar{w}(i \to f)$ by subtraction of $\tau^{\frac{4}{3}}$ contributions from the $\bar{w}(i \to f)$ computed using $\bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ of (133 b). Thus, to obtain the physical $\bar{w}(i \to f)$, the necessary subtraction of non-three-body contributions must be performed before carrying out the probability current flow computations and δ-function reinterpretations discussed in §§ 4.1 and 4.2. The experimentalist, on the other hand, actually might be able to perform this subtraction by varying the scattering volume while keeping its shape constant, thus in effect determining the shape-dependent factor C empirically.

4.3.1. *Subtraction of double-scattering terms*

Although there is no obvious reason why it should be impossible to do so, I have not been able to perform the desired subtraction of double scattering contributions to $\bar{\Phi}_i^{s(+)}$ described in the introduction to this section. The difficulty lies in the need not to subtract too much; otherwise there would be no problem. The two-body scattering δ-function appearing as a multiplicative factor in (130 c) has its origin in the plane wave factor $e^{iK_{12}\cdot q_{12}}$ in the $\bar{\Phi}_{12}^{(+)}$ (72) part of $\bar{\Phi}_i^{(+)}$. But the presence of this plane wave factor means the entire term $\bar{\Phi}_{12}^{(+)}(\bar{\boldsymbol{r}})$ fails to behave like $\bar{G}_F(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}')$ as $\bar{\boldsymbol{r}} \to \infty$ along $\bar{\boldsymbol{\nu}}_f$ corresponding to elastic scattering, so that in seeking $\bar{\Phi}_i^{t(+)}$ one assuredly can subtract the entire term $\bar{\Phi}_{12}^{(+)}$ from $\bar{\Phi}_i^{(+)}$ (recall the discussion preceding (119)). However, the double scattering δ-functions (135), which appear as additive components of $\bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f)$, correspondingly arise from additive components of $\bar{\Phi}_i^{s(+)}$. To obtain $\bar{\Phi}_i^{t(+)}$ from $\bar{\Phi}_i^{s(+)}$, one must subtract from $\bar{\Phi}_i^{s(+)}(\bar{\boldsymbol{r}})$ all terms behaving asymptotically like $\bar{\rho}^{-2}$ as $\bar{\boldsymbol{r}} \to \infty$ along elastic scattering $\bar{\boldsymbol{\nu}}_f$, but, as is clear from the rules and discussion at the end of subsection 4.1.3, one must retain in $\bar{\Phi}_i^{t(+)}(\bar{\boldsymbol{r}})$ all (outgoing) terms in $\bar{\Phi}_i^{s(+)}(\bar{\boldsymbol{r}})$ behaving asymptotically like $\bar{\rho}^{-5/2}$.

To make more explicit the difficulty of performing this delicate subtraction, let me indicate the results of one reasonable attempt to single out the double-scattering terms in $\bar{\Phi}_i^{s(+)}$. According to § E. 3.2, the $\bar{\rho}^{-2}$ contribution in the $\bar{G}^{(+)}V_{23}\bar{\Phi}_{12}^{(+)}$ part of $\bar{\Phi}_i^{s(+)}$ (equation (69)) is contained entirely in

$$\bar{G}_{23}^{(+)}V_{23}\bar{\Phi}_{23}^{(+)} = -\bar{G}_{23}^{(+)}V_{23}\{\lim_{\epsilon\to 0}\bar{G}_{12}(\bar{E}+i\epsilon)V_{12}\bar{\psi}_1(\bar{E})\}$$
$$= -\bar{G}_{23}^{(+)}V_{23}\left\{e^{iK_{12i}\cdot q_{12}}\left[g_{12}^{(+)}\left(\frac{\hbar^2 k_{12i}^2}{2\mu_{12}}\right)\right]V_{12}\,e^{ik_{12i}\cdot r_{12}}\right\}, \qquad (160)$$

recalling the centre-of-mass versions of (60) and (72). Therefore I will perform an iteration on (69), as follows. In the V_{23} terms of (67 c) use the second equality in (63 b), proceeding as in (64) to (67 c), and similarly for the V_{31} and V_{12} terms in (67 c). Then, after taking the limit $\epsilon \to 0$, one finds

$$\Phi_i^{s(+)} = \Phi_{23}^{s(+)} + \Phi_{31}^{s(+)} + \Phi_{12}^{s(+)} + \Phi_i^{d(+)}, \qquad (161\,a)$$

where

$$\Phi_{23}^{s(+)} = -G_{23}^{(+)}V_{23}[\Phi_{12}^{(+)} + \Phi_{31}^{(+)}], \qquad (161\,b)$$

$$\Phi_{31}^{s(+)} = -G_{31}^{(+)}V_{31}[\Phi_{23}^{(+)} + \Phi_{12}^{(+)}], \qquad (161\,c)$$

$$\Phi_{12}^{s(+)} = -G_{12}^{(+)}V_{12}[\Phi_{31}^{(+)} + \Phi_{23}^{(+)}], \qquad (161\,d)$$

and where the result of double iteration and subtraction (on the original formula (52 a) for $\Psi_i^{(+)}$) is

$$\Phi_i^{d(+)} = -G^{(+)}[(V_{23}+V_{31})\Phi_{12}^{s(+)} + (V_{31}+V_{12})\Phi_{23}^{s(+)} + (V_{12}+V_{23})\Phi_{31}^{s(+)}]. \qquad (162)$$

The centre-of-mass version of (162) involves no divergent integrals, and is the desired iteration of (69); obviously, I could have obtained the same result by iterating directly on (69), using the centre-of-mass versions of (63).

Because $\bar{\Phi}^{s(+)}_{\alpha\beta}(\bar{\boldsymbol{r}})$ decreases no less slowly than $\bar{\rho}^{-2}$ as $\bar{r}\to\infty$ along $\bar{\boldsymbol{\nu}}_{\mathrm{f}} \neq \bar{\boldsymbol{\nu}}_{\alpha\beta}$, it can be seen from the arguments at the end of § E. 2 that interchange of order of integration and limit $\bar{\boldsymbol{r}}\to\infty\|\bar{\boldsymbol{\nu}}_{\mathrm{f}}$ is justified in the integrals (162) for $\bar{\Phi}^{d(+)}_{\mathrm{i}}(\bar{\boldsymbol{r}})$, except possibly along certain special $\bar{\boldsymbol{\nu}}_{\mathrm{f}}$. As § E. 2 explains, it has not been shown that these special $\bar{\boldsymbol{\nu}}_{\mathrm{f}}$ really exist; we merely have not ruled out the possibility that such $\bar{\boldsymbol{\nu}}_{\mathrm{f}}$ occur. However, the discussion in § 4.3.2 below strongly indicates that such special $\bar{\boldsymbol{\nu}}_{\mathrm{f}}$ (even if they actually occur) are inconsequential for the purposes of this work. Therefore we infer that for our present purposes interchange of order of integration and limit $\bar{\boldsymbol{r}}\to\infty\|\bar{\boldsymbol{\nu}}_{\mathrm{f}}$ in (162) is justified; correspondingly, we may conclude that $\bar{\Phi}^{d(+)}_{\mathrm{i}}$ is outgoing and decreases no less rapidly than $\bar{\rho}^{-5/2}$ as $\bar{\boldsymbol{r}}\to\infty\|\bar{\boldsymbol{\nu}}_{\mathrm{f}}$, except possibly for these same special inconsequential $\bar{\boldsymbol{\nu}}_{\mathrm{f}}$. In other words, it appears legitimate to conclude that the anomalously propagating double-scattering contributions to $\bar{\Phi}^{s(+)}_{\mathrm{i}}$ all are contained in $\bar{\Phi}^{s(+)}_{23}$, $\bar{\Phi}^{s(+)}_{31}$ and $\bar{\Phi}^{s(+)}_{12}$; thus subtracting these terms from $\bar{\Phi}^{s(+)}_{\mathrm{i}}$ should leave a $\bar{\Phi}^{d(+)}_{\mathrm{i}}$ which represents true three-body scattering only.

On the other hand, I see no reason to think that $\bar{\Phi}^{s(+)}_{\alpha\beta}$ represent anomalous double scattering only, i.e. contain no parts which should be included in $\bar{\Phi}^{t(+)}_{\mathrm{i}}$. For one thing, § E. 3.2 can be seen to imply

$$-\bar{G}^{(+)}_{F}V_{23}\bar{G}^{(+)}_{23}V_{23}\bar{\Phi}^{(+)}_{12} = [\bar{G}^{(+)}_{23}-\bar{G}^{(+)}_{F}]V_{23}\bar{\Phi}^{(+)}_{12} \tag{163}$$

decreases no less rapidly than $\bar{\rho}^{-5/2}$. But this result immediately means that $\bar{\Phi}^{s(+)}_{23}$ on the right side of (161 *a*) contains a part, namely the left side of (163), belonging in $\bar{\Phi}^{t(+)}_{\mathrm{i}}$ (because it is most unlikely that the $\bar{\rho}^{-5/2}$ contribution to the left side of (163) is everywhere incoming); in other words, $\bar{\Phi}^{d(+)}_{\mathrm{i}}$ of (162) does not contain all parts of $\bar{\Phi}^{(+)}_{\mathrm{i}}$ contributing to $\bar{\Phi}^{t(+)}_{\mathrm{i}}$.

Alternatively, (163) means

$$\bar{G}^{(+)}_{F}V_{23}\bar{\Phi}^{(+)}_{12} = -\bar{G}^{(+)}_{F}V_{23}\left\{\mathrm{e}^{\mathrm{i}\boldsymbol{K}_{12\mathrm{i}}\cdot\boldsymbol{q}_{12}}\left[g^{(+)}_{12}\left(\frac{\hbar^2k^2_{12\mathrm{i}}}{2\mu_{12}}\right)\right]V_{12}\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}_{12\mathrm{i}}\cdot\boldsymbol{r}_{12}}\right\} \tag{164 a}$$

contains the entire $\bar{\rho}^{-2}$ contribution in (160), just as (160) contains the entire $\bar{\rho}^{-2}$ contribution in $\bar{G}^{(+)}V_{23}\bar{\Phi}^{(+)}_{12}$. However, replacing $g^{(+)}_{12}$ in (164 *a*) by $g^{(+)}_{F}$ would not retain the entire $\bar{\rho}^{-2}$ contribution. Sections E. 2 and E. 3 show the $\bar{\rho}^{-2}$ behaviour in (164 *a*) stems from the fact that the integral (73 *b*) behaves like r^{-1}_{12} as $\boldsymbol{r}_{12}\to\infty$; evidently

$$[g^{(+)}_{12}-g^{(+)}_{F}]V_{12}\exp\{\mathrm{i}\boldsymbol{k}_{12\mathrm{i}}\cdot\boldsymbol{r}_{12}\} = -\int \mathrm{d}\boldsymbol{r}'_{12}\,\mathrm{d}\boldsymbol{r}''_{12}g^{(+)}_{F}(\boldsymbol{r}_{12};\boldsymbol{r}'_{12})V_{12}(\boldsymbol{r}'_{12}) \times g^{(+)}_{12}(\boldsymbol{r}'_{12};\boldsymbol{r}''_{12})V_{12}(\boldsymbol{r}''_{12})\exp\{\mathrm{i}\boldsymbol{k}_{12\mathrm{i}}\cdot\boldsymbol{r}''_{12}\} \tag{164 b}$$

also behaves like r^{-1}_{12} as $\boldsymbol{r}_{12}\to\infty$, recognizing that V_{12} is short range. In any event, even if one could find some iteration of (164 *a*) that retained all $\bar{\rho}^{-2}$ terms in an integral of convenient or transparent form, there remains the complication that the $\bar{\rho}^{-2}$ contribution to (160) (i.e. to (164 *a*)) was obtained in § E. 3 by application of the principle of stationary phase. It readily can be seen that this method of obtaining the $\bar{\rho}^{-2}$ contribution amounts to computing the leading term in an expansion in powers of $\bar{\rho}^{-1/2}$. Therefore, along with the $\bar{\rho}^{-2}$ contribution to (160) or (164 *b*), or to any $\bar{\rho}^{-2}$-retaining iteration thereof, there generally will be $\bar{\rho}^{-5/2}$ contributions.

It follows (from the material presented thus far in this subsection) that it is very difficult to find any set of scattering terms—or, equivalently, any set of scattering diagrams—which represent the anomalous double scattering part of $\bar{\Phi}^{(+)}_{\mathrm{i}}$ without any truly three-body scattering contributions, and which therefore could be subtracted from $\bar{\Phi}^{s(+)}_{\mathrm{i}}$ to yield the entire $\bar{\Phi}^{t(+)}_{\mathrm{i}}$. In this connexion it is worth noting that $\bar{\Phi}^{d(+)}_{\mathrm{i}}$ of (162)—which, according to the penultimate paragraph

above lies wholly in $\bar{\Phi}_i^{t(+)}$—can be thought to result from scattering processes involving no less than three successive purely two-body collisions. It has been explained above that interchange of order of integration and limit $\bar{r}\to\infty\|\bar{\nu}_f$ in (162) is justified for essentially all $\bar{\nu}_f \neq \bar{\nu}_{\alpha\beta}$; thus we obtain as, for example, in (133)

$$\lim_{\bar{r}\to\infty\|\bar{\nu}_f} \bar{\Phi}_i^{d(+)}(\bar{r}) = -C_2(\bar{E})\frac{e^{i\bar{\rho}\sqrt{\bar{E}}}}{\bar{\rho}^{\frac{5}{2}}}\bar{T}^d(\boldsymbol{k}_i\to\boldsymbol{k}_f), \tag{165a}$$

$$\bar{T}^d(\boldsymbol{k}_i\to\boldsymbol{k}_f) = \int d\bar{r}'\,\bar{\Psi}_f^{(-)*}(\bar{r}')\,[(V_{23}+V_{31})\,\bar{\Phi}_{12}^{s(+)}(\bar{r}') + (V_{31}+V_{12})\,\bar{\Phi}_{23}^{s(+)}(\bar{r}') + (V_{12}+V_{23})\,\bar{\Phi}_{31}^{s(+)}(\bar{r}')]. \tag{165b}$$

Now consider, for example, the first term on the right side of (165 *b*); in particular, consider the contribution to $\bar{\Psi}_f^{(-)*}V_{23}\bar{\Phi}_{12}^{s(+)}$ made by the $\bar{\Psi}_{23f}^{(-)*}$ part of $\bar{\Psi}_f^{(-)*}$, where $\bar{\Psi}_{23f}^{(-)*}$ is given by (136). From (161 *d*),

$$\bar{\Psi}_{23f}^{(-)*}V_{23}\bar{\Phi}_{12}^{s(+)} = -\bar{\Psi}_{23f}^{(-)*}V_{23}\bar{G}_{12}^{(+)}V_{12}[\bar{\Phi}_{31}^{(+)}+\bar{\Phi}_{23}^{(+)}]. \tag{166a}$$

The first term on the right side of (166 *a*) can be re-expressed, as in (137), in the interpretable form

$$\begin{aligned}
&\bar{\Psi}_{23f}^{(-)*}V_{23}\bar{G}_{12}^{(+)}V_{12}\bar{\Phi}_{31}^{(+)}\\
&\quad = -\lim_{\epsilon\to 0}\bar{\Psi}_{23f}(\bar{E}+i\epsilon)\,V_{23}\,\bar{G}_{12}(\bar{E}+i\epsilon)\,V_{12}\,\bar{G}_{31}(\bar{E}+i\epsilon)\,V_{31}\,\bar{\psi}_i\\
&\quad = -\lim_{\epsilon\to 0}\bar{\Psi}_{23f}(\bar{E}+i\epsilon)\,V_{23}\,\bar{G}_F(\bar{E}+i\epsilon)\;\bar{\boldsymbol{T}}_{12}(\bar{E}+i\epsilon)\,\bar{G}_F(\bar{E}+i\epsilon)\;\bar{\boldsymbol{T}}_{31}(\bar{E}+i\epsilon)\,\bar{\psi}_i\\
&\quad = -\lim_{\epsilon\to 0}\bar{\psi}_f^*\;\bar{\boldsymbol{T}}_{23}\,\bar{G}_F\,\bar{\boldsymbol{T}}_{12}\,\bar{G}_F\,\bar{\boldsymbol{T}}_{31}\,\bar{\psi}_i,
\end{aligned} \tag{166b}$$

where $\bar{\boldsymbol{T}}_{\alpha\beta}$ and $\bar{G}_F$ are evaluated at the complex energy $\bar{E}+i\epsilon$. The integral (166 *b*) obviously corresponds to a diagram wherein there are three successive purely two-body scatterings: first of the pair 3, 1; next of the pair 1, 2; and finally of the pair 2, 3. Similar results hold for the other terms on the right sides of (165 *b*) and (166 *a*). Moreover, further iteration of $\bar{\Psi}_f^{(-)*}$ in (165 *b*), or, for example, replacing $\bar{\Psi}_f^{(-)*}$ by $\bar{\Phi}_{12f}^{s(-)*}$ in $\bar{\Psi}_f^{(-)*}V_{23}\bar{\Phi}_{12}^{s(+)}$, yields integrals corresponding to even higher order scattering diagrams.

4.3.2. *Volume dependence of triple scattering contributions*

The integrals (165 *b*) are convergent, except possibly along special directions $\boldsymbol{k}_f$ (for given $\boldsymbol{k}_i$) where some of the integrals in (165 *b*) may be logarithmically divergent (see § B. 2). However, there is no reason to think that the centre-of-mass frame probability current flow $\bar{\mathscr{F}}$ of (127)—when integrated over an infinitesimal range $d\boldsymbol{k}_f$ in the vicinity of these special (here meaning isolated) $\boldsymbol{k}_f$ where $\bar{T}^d(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ from (165 *b*) is undefined—receives finite contributions from these comparatively weak divergences (see § B. 2). Thus the possible existence of these special $\boldsymbol{k}_f$ seemingly does not require reinterpretations along the lines of § 4.2, i.e. seemingly does not introduce any anomalously τ-dependent contributions into the reaction coefficient $\bar{w}(i\to f)$. Moreover, there is no indication that the integrals (165 *b*) contain any other $\boldsymbol{k}_f$-dependent parts which, after squaring, will be non-integrable over $d\boldsymbol{k}_f$ (recall the form of (127 *c*)). Therefore, it does seem to be true that the doubly-iterated $\bar{\Phi}_i^{d(+)}(\bar{r})$ of (162), comprising contributions from numbers $n \geqslant 3$ of successive two-body collisions, in essence behaves asymptotically like $\bar{G}_F^{(+)}(\bar{r};\bar{r}';\bar{E})$ and entirely represents truly three-body scattering (as concluded in § 4.3.1). I remark that, as in the case of the special $\bar{\nu}_f$ discussed in § 4.3.1, it has not been shown that the

special $\boldsymbol{k}_f$ of the present subsection actually exist; rather, because their effects apparently are inconsequential for the purposes of this work, it is not worth the very considerable effort which would be required to decide whether or not the logarithmic divergences of (165 *b*) ever can occur at physically allowed real $\boldsymbol{k}_f$. Nor is there any evidence that the possible existence of real or imaginary values of $\boldsymbol{k}_f$ where (165 *b*) is logarithmically divergent should be associated with actual singularities of $\overline{T}^d(\boldsymbol{k}_1 \to \boldsymbol{k}_f)$, computed via analytic continuation (as a function of $\boldsymbol{k}_f$ for fixed $\boldsymbol{k}_1$) from values of $\overline{T}^d(\boldsymbol{k}_1 \to \boldsymbol{k}_f)$ for which the integrals (165 *b*) surely are well behaved; it is conceivable, for instance, that the logarithmic divergences of the integrals (165 *b*) at special $\boldsymbol{k}_f$ have no physical significance,† but simply are manifestations of the fact that the interchange of order of integration and limit $\bar{r} \to \infty \| \bar{\nu}_f$ in (162) is not justified at special $\bar{\nu}_f$. It does seem worthwhile to stress, much as in the discussion following (48), that the integrals (165 *b*) are convergent except possibly on an inconsequential subset of the allowed real $\boldsymbol{k}_f$, whereas the integrals (133 *b*) always are divergent, although it is true that the divergences in (133 *b*) arise from δ-functions (135) which can be considered non-contributory except when their arguments vanish.

To further confirm our conclusion that $\bar{\Phi}_i^{d(+)}$ represents truly three-body scattering, I now shall demonstrate, by arguments along the lines of §§ 4.2.1 and 4.2.2, that three or more successive binary collisions cannot make contributions to the three-body reaction coefficient $\overline{w}(\mathrm{i} \to \mathrm{f})$ which increase as any positive power of τ. Consider, for example, the sequence of three two-body scatterings: 1, 2 collide; 2, 3 collide; 3, 1 collide. Then, as in § 4.2.2, I first compute the reaction rate for the above sequence under the circumstances that the volume τ contains precisely one particle of each species α. After the collision between 2 and 3, whenever it may take place, the laboratory frame speed and direction with which 3 moves through τ are strictly correlated. It follows that in order to rescatter from particle 1—whose trajectory has been fixed by the first collision between 1 and 2—particle 3 must be scattered by 2 into a very narrow solid angle, of the order $\overline{\sigma}_{31}/L^2$ where $L \cong \tau^{-1/3}$. Hence, referring to (159 *a*), the postulated sequence of three binary collisions will have the rate

$$\hat{w}_i'(12;23;31) \cong \left\langle \frac{\overline{w}_{12}^{(2)}}{\tau} \frac{L\overline{\sigma}_{23}}{\tau} \frac{\overline{\sigma}_{31}}{L^2} \right\rangle_{\mathrm{av}} \cong \tau^{-7/3}. \tag{167}$$

This result for $\hat{w}_i'$ corresponds to the incident wave ψ_i' of (156 *a*), so that the laboratory frame $w(\mathrm{i} \to \mathrm{f})$ is proportional to $\tau^3 \tau^{-7/3} = \tau^{\frac{2}{3}}$, implying this sequence of three binary collisions makes a contribution to $\overline{w}(\mathrm{i} \to \mathrm{f})$ which is proportional to $\tau^{-1/3}$. Therefore, recalling the discussion at the end of § 4.2.1, it is reasonable to infer that successions of $n \geqslant 3$ purely two-body scatterings, if observable at all in a large volume τ, will be indistinguishable from (and apparently should be included in) what I have termed truly three-body scattering. Note that the diagram corresponding to (166 *b*) represents successive two-body scatterings in which energy is not necessarily conserved in the intermediate states (e.g. between the first 3, 1 scattering and the second 1, 2 scattering); the physical purely two-body scatterings yielding the just estimated $\tau^{-1/3}$ contribution to $\overline{w}(\mathrm{i} \to \mathrm{f})$ are energy-conserving, and therefore are only a subset of the whole class of three successive two-body scatterings represented by the diagram corresponding to (166 *b*) (see § 5.3.3).

† On the other hand, these logarithmic divergences may be related to the so-called pinch singularities (Eden, Landshoff, Olive & Polkinghorne 1966) in the scattering amplitudes; however, I have not attempted to see if the conditions for the logarithmic divergences coincide with the conditions for pinch singularities.

5. The physical three-body transition amplitude

This, our final chapter, is concerned with an attempt to actually determine a useful expression for the physical three-body transition amplitude $\bar{T}^t(\boldsymbol{k}_i - \boldsymbol{k}_f)$. As § 5.1 explains, attempting to find $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ using mathematically defensible procedures is impractical; to avoid extremely difficult and complicated calculations, employment of some not obviously justified mathematical short cuts seems necessary. One such plausible attempt to determine $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ actually is carried out in § 5.1. The formula for $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ obtained in this fashion is shown to be consistent with detailed balancing in § 5.2, while its interpretation is discussed in § 5.3. Section 5.3 also compares the configuration space expression for $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$, as well as for the entire $\bar{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$, with the corresponding expressions inferred via the more customary momentum space procedures.

5.1. *Derivation by subtraction of δ-functions*

Among the concerns of the preceding section has been the possibility of expressing $\bar{\Phi}_i^{s(+)}$ in the form

$$\bar{\Phi}_i^{s(+)}(\bar{\boldsymbol{r}}) = \bar{\Phi}_i^{a(+)}(\bar{\boldsymbol{r}}) + \bar{\Phi}_i^{t(+)}(\bar{\boldsymbol{r}}), \tag{168}$$

where $\bar{\Phi}_i^{a(+)}$ is that part of $\bar{\Phi}_i^{s(+)}$ which represents unwanted contributions such as anomalous double scattering, but which is wholly devoid of any truly three-body scattering contributions. In fact, § 4.3.1 has examined, and found to be impractical though not obviously impossible, one suggested means of constructing $\bar{\Phi}_i^{a(+)}$, namely by seeking a set of scattering diagrams which separate out the anomalous double-scattering terms from the truly three-body contributions to $\bar{\Phi}_i^{s(+)}$. Alternatively, one could try to find a closed form analytic expression for $\bar{\Phi}_i^{a(+)}(\bar{\boldsymbol{r}})$ by carrying through the calculation—of the asymptotic form of $\bar{\Phi}_i^{s(+)}(\bar{\boldsymbol{r}})$—outlined in § E. 3. A glance at § E. 3.1, however—especially (E 40 b) and the discussion immediately thereafter—makes it evident that this suggested procedure for finding $\bar{\Phi}_i^{a(+)}$ also is not very practical, though again not obviously impossible.

For many purposes—e.g. the construction of variational principles for three-body elastic scattering—complete knowledge of the asymptotic behaviour of $\bar{\Phi}_i^{s(+)}$ may be essential. On the other hand, it is conceivable that only partial knowledge of the asymptotic behaviour of $\bar{\Phi}_i^{s(+)}$—in particular, only partial knowledge of the asymptotic behaviour of $\bar{\Phi}_i^{t(+)}$ in (168)—can suffice to determine the physical three-body scattering amplitude $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$. Thus it may be possible to find $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ without having to carry through either of the difficult calculations discussed in the preceding paragraph. It seems clear, however, that any argument which leads to $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ while avoiding exact construction of $\bar{\Phi}_i^{t(+)}(\bar{\boldsymbol{r}})$—or of its leading $\bar{\rho}^{-5/2}$ part at the very least—will have to involve some mathematically questionable steps, i.e. will lead to a possibly erroneous result for $\bar{T}^t$. Nevertheless, because determination of $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ has been a major objective of this work (recall our opening remarks in § 1), I now shall describe an attempt to deduce $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ via a plausible argument which indeed does avoid finding first the leading $\bar{\rho}^{-5/2}$ part of $\bar{\Phi}_i^{t(+)}(\bar{\boldsymbol{r}})$.

We have seen that $\bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ of (133 *b*) contains δ-functions (135), ascribable to the fact that the interchange of order of integration and limit $\bar{\boldsymbol{r}} \to \infty$ in (132) was unjustified; this interchange led to the erroneous assertion (133 *a*) whereas actually $\bar{\Phi}_i^{s(+)}(\bar{\boldsymbol{r}})$ contains contributions behaving like $\bar{\rho}^{-2}$ at large $\bar{\rho}$. Suppose, therefore, I am able to express $\bar{T}^s$ of (133) in the form

$$\bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \bar{T}^a(\boldsymbol{k}_i \to \boldsymbol{k}_f) + \bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f), \tag{169 a}$$

where $\bar{T}^t$ is wholly composed of convergent integrals (except possibly for inconsequential

logarithmic divergences at special $\boldsymbol{k}_f$, recall § 4.3.2), whereas $\bar{T}^a$ is a sum of terms proportional to δ-functions and thus has no finite part. Then from the entire body of this work, especially the rules and discussion at the end of § 4.1.3, it seems reasonable to infer that $\bar{T}^a(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ in (169 *a*) represents the contribution to $\bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ from that part of $\bar{\Phi}_i^{s(+)}(\bar{\boldsymbol{r}})$ which behaves like $\bar{\rho}^{-2}$ at large $\bar{\rho}$, but which has no $\bar{\rho}^{-5/2}$ components at large $\bar{\rho}$. In other words, it seems reasonable to conclude that $\bar{T}^a(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ is the contribution to $\bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ made by $\bar{\Phi}_i^{a(+)}(\bar{\boldsymbol{r}})$ of (168), implying $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ of (169 *a*) will be the desired entire truly three-body scattering amplitude associated with $\bar{\Phi}_i^{t(+)}(\bar{\boldsymbol{r}})$. I stress that this conclusion, though reasonable enough, depends on a number of unproved assumptions. For instance, I am assuming that any mathematically well-behaved $\bar{\rho}^{-5/2}$ component of $\bar{\Phi}_i^{s(+)}(\bar{\boldsymbol{r}})$—that is to say, any component of $\bar{\Phi}_i^{s(+)}(\bar{\boldsymbol{r}})$ which is finite at $\bar{\boldsymbol{r}} = 0$ and propagates to infinity without restriction in the six-dimensional $\bar{\boldsymbol{r}}$-space (recall the discussion at the end of § 4.1.3)—indeed is everywhere outgoing, i.e. behaves everywhere at infinity like the outgoing $\bar{G}_F^{(+)}(\bar{\boldsymbol{r}}; \bar{\boldsymbol{r}}')$, not like the incoming free space Green function $\bar{G}_F^{(-)}(\bar{\boldsymbol{r}}; \bar{\boldsymbol{r}}')$. I also am assuming that the unjustified interchange of order of integration and limit $\bar{\boldsymbol{r}} \to \infty \| \bar{\boldsymbol{\nu}}_f$ in (132) is not so wrong that (169 *a*) becomes a quite misleading indication of the actual form of $\bar{T}^t$. Without making these and similar assumptions, there is little basis for arguing that $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ obtained from (169 *a*) and (133 *b*) can be identified with the 'truly' three-body transition amplitudes of (3) and (4). Of course, explicit verification of these assumptions would involve finding closed form analytic expressions for $\bar{\Phi}_i^{a(+)}(\bar{\boldsymbol{r}})$ and $\bar{\Phi}_i^{t(+)}(\bar{\boldsymbol{r}})$, an impractical task (as explained at the beginning of this subsection) whose performance, if achieved, simultaneously would obviate the need for computing the physical $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ via the present dubious argument.

Granting the legitimacy of using (133 *b*) and (169 *a*), $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ is found as follows. In the terms on the right side of (133 *b*) involving the product $\bar{\Psi}_f^{(-)*} V_{12}$, use

$$\bar{\Psi}_f^{(-)*} = \bar{\Psi}_{12f}^{(-)*} - \bar{\Psi}_f^{(-)*}(V_{23} + V_{31})\, \bar{G}_{12}^{(+)}, \tag{169 b}$$

which is the time-reversed analogue of (86), written in the notational style of (100 *b*) or (105 *d*), i.e. with the Green function on the right, as here will be convenient; (169 *b*) also can be inferred directly from the centre-of-mass analogue of the second equality in (65 *b*), via the methods of § 3. Furthermore, in the $\bar{\Psi}_f^{(-)*} V_{23}$ and $\bar{\Psi}_f^{(-)*} V_{31}$ terms of (133 *b*), use respectively the 2, 3 and 3, 1 analogues of (169 *b*). Then, employing (161) as well, one obtains

$$\begin{aligned}\bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \int \mathrm{d}\bar{\boldsymbol{r}}' \{ &\bar{\Psi}_{23f}^{(-)*}(\bar{\boldsymbol{r}}')\, V_{23}[\bar{\Phi}_{12}^{(+)}(\bar{\boldsymbol{r}}') + \bar{\Phi}_{31}^{(+)}(\bar{\boldsymbol{r}}')] + \bar{\Psi}_{31f}^{(-)*}(\bar{\boldsymbol{r}}')\, V_{31}[\bar{\Phi}_{23}^{(+)}(\bar{\boldsymbol{r}}') + \bar{\Phi}_{12}^{(+)}(\bar{\boldsymbol{r}}')] \\ &+ \bar{\Psi}_{12f}^{(-)*}(\bar{\boldsymbol{r}}')\, V_{12}[\bar{\Phi}_{31}^{(+)}(\bar{\boldsymbol{r}}') + \bar{\Phi}_{23}^{(+)}(\bar{\boldsymbol{r}}')]\} + \bar{T}^d(\boldsymbol{k}_i \to \boldsymbol{k}_f)\end{aligned} \tag{169 c}$$

in place of (133 *b*), where $\bar{T}^d(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ is given by (165 *b*). The same (169 *c*) is obtained from the interchange of order of integration and $\lim \boldsymbol{r} \to \infty \| \boldsymbol{\nu}_f$ in the right sides of (161) and (162); of course, this interchange—though justified in (162) (recall the discussion in § 4.3.1)—is unjustified in the $\Phi_{\alpha\beta}^{s(+)}$ terms of (161) (recall the discussion of (132) to (135)).

Returning now to the discussion of (135) to (137) in § 4.1.3, one sees from comparison of (169 *c*) and (133 *b*) that all the double scattering δ-functions of type (135) contributing to $\bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ are entirely contained in the integral on the right side of (169 *c*); in particular (a term proportional to) the specific δ-function (135 *a*) arises entirely from the $\bar{\Psi}_{23f}^{(-)*} V_{23} \bar{\Phi}_{12}^{(+)}$ term in (169 *c*). Let us consider this term, therefore. Using (72), (105 *b*) and (136), one finds

$$\bar{\Psi}_{23f}^{(-)*} V_{23} \bar{\Phi}_{12}^{(+)} = \int \mathrm{d}\boldsymbol{q}_{23}\, \mathrm{d}\boldsymbol{r}_{23}\, \mathrm{e}^{-\mathrm{i}K_{23f} \cdot q_{23}}\, u_{23cf}^{(-)*}(\boldsymbol{r}_{23}; \boldsymbol{k}_{23f})\, V_{23}(\boldsymbol{r}_{23})\, \mathrm{e}^{\mathrm{i}K_{12i} \cdot q_{12}}\, \phi_{12}^{(+)}(\boldsymbol{r}_{12}; \boldsymbol{k}_{12i}), \tag{170 a}$$

where u_{23cf} is defined as was $u_c^{(-)*}$ in (129a), i.e.

$$u_{23cf}^{(-)*}(\boldsymbol{r}_{23};\boldsymbol{k}_{23f}) = e^{-i\boldsymbol{k}_{23f}\cdot\boldsymbol{r}_{23}} + \phi_{23f}^{(-)*}(\boldsymbol{r}_{23};\boldsymbol{k}_{23f}), \tag{170b}$$

with $\phi_{23f}^{(-)*}$ given by the 2, 3 analogue of (105c). Replacing the integration variable $\boldsymbol{q}_{23}$ by $\boldsymbol{r}_{12}$, the six-dimensional integral (170a) factorizes into a product of two independent three-dimensional integrals, namely

$$\int d\boldsymbol{r}_{12}\, e^{-i\boldsymbol{r}_{12}\cdot\boldsymbol{A}}\phi_{12}^{(+)}(\boldsymbol{r}_{12};\boldsymbol{k}_{12i})\int d\boldsymbol{r}_{23}\, u_{23cf}^{(-)*}(\boldsymbol{r}_{23};\boldsymbol{k}_{23f})\, V_{23}(\boldsymbol{r}_{23})\, e^{-i\boldsymbol{B}\cdot\boldsymbol{r}_{23}} \tag{170c}$$

where in this section I henceforth shall employ the notation

$$\left.\begin{aligned}\boldsymbol{A} &= \boldsymbol{K}_{23f} + \frac{m_1}{m_1+m_2}\boldsymbol{K}_{12i},\\ \boldsymbol{B} &= \frac{m_3}{m_2+m_3}\boldsymbol{K}_{23f} + \boldsymbol{K}_{12i},\end{aligned}\right\} \tag{171a}$$

along with

$$\left.\begin{aligned}\boldsymbol{C} &= \boldsymbol{K}_{23f} + \frac{m_1}{m_3+m_1}\boldsymbol{K}_{31i},\\ \boldsymbol{D} &= \frac{m_2}{m_2+m_3}\boldsymbol{K}_{23f} + \boldsymbol{K}_{31i}.\end{aligned}\right\} \tag{171b}$$

The integral over $d\boldsymbol{r}_{23}$ in (170c) is convergent, and in fact can be identified with a matrix element of $\boldsymbol{t}_{23}$ (see § E. 4). The integral over $d\boldsymbol{r}_{12}$ in (170c) fails to converge, and in fact contains a contribution proportional to the δ-function (135a); the exact magnitude of this δ-function (135a) contribution to (170c), as well as of a second related δ-function contribution, is computed in § E. 4.

Specifically, § E. 4 shows that

$$\begin{aligned}\int d\boldsymbol{r}_{12}\, e^{-i\boldsymbol{r}_{12}\cdot\boldsymbol{A}}\phi_{12}^{(+)}(\boldsymbol{r}_{12};\boldsymbol{k}_{12i}) = \int d\boldsymbol{r}_{12}\Bigg\{ & e^{-i\boldsymbol{r}_{12}\cdot\boldsymbol{A}}\phi_{12}^{(+)}(\boldsymbol{r}_{12};\boldsymbol{k}_{12i}) + \frac{i\mu_{12}}{\hbar^2}\frac{e^{ik_{12i}r_{12}}}{r_{12}}\langle k_{12i}\boldsymbol{\nu}_{12}|\,\boldsymbol{t}_{12i}\,|\boldsymbol{k}_{12i}\rangle \\ & \times\left[\delta(\boldsymbol{\nu}_{12}-\boldsymbol{\nu}_A)\frac{e^{-iAr_{12}}}{Ar_{12}} - \delta(\boldsymbol{\nu}_{12}+\boldsymbol{\nu}_A)\frac{e^{iAr_{12}}}{Ar_{12}}\right]\Bigg\} \\ & - \frac{i\mu_{12}}{\hbar^2 A}\langle k_{12i}\boldsymbol{\nu}_A|\,\boldsymbol{t}_{12i}\,|\boldsymbol{k}_{12i}\rangle\int_0^\infty dr_{12}\, e^{i(k_{12i}-A)r_{12}} \\ & + \frac{i\mu_{12}}{\hbar^2 A}\langle -k_{12i}\boldsymbol{\nu}_A|\,\boldsymbol{t}_{12i}\,|\boldsymbol{k}_{12i}\rangle\int_0^\infty dr_{12}\, e^{i(k_{12i}+A)r_{12}},\end{aligned} \tag{172a}$$

where $\boldsymbol{r}_{12} = r_{12}\boldsymbol{\nu}_{12}$; $\boldsymbol{A} = A\boldsymbol{\nu}_A$; while the truly two-body transition operators (third particle completely irrelevant and absent) $\boldsymbol{t}_{\alpha\beta i}$, and their matrix elements, are defined by (131e) and (131f), together with the shorthand notation

$$\boldsymbol{t}_{12i} \equiv \boldsymbol{t}_{12}(E_{12i}) = \boldsymbol{t}_{12}\left(\frac{\hbar^2 k_{12i}^2}{2\mu_{12}}\right), \quad \text{etc.} \tag{172b}$$

$$\boldsymbol{t}_{23f} \equiv \boldsymbol{t}_{23}(E_{23f}) = \boldsymbol{t}_{23}\left(\frac{\hbar^2 k_{23f}^2}{2\mu_{23}}\right), \quad \text{etc.} \tag{172c}$$

The notation (172c), though not employed in (172a), will be made use of below.

In (172a), integrals of the individual terms, e.g. of the term $e^{-i\boldsymbol{r}_{12}\cdot\boldsymbol{A}}\phi_{12}^{(+)}(\boldsymbol{r}_{12};\boldsymbol{k}_{12i})$ originally appearing in (170c), do not converge. However, the δ-function terms inside the braces in (172a) cancel the leading ($\sim r_{12}^{-2}$) terms in the asymptotic expansion of $e^{-i\boldsymbol{r}_{12}\cdot\boldsymbol{A}}\Phi_{12}^{(+)}(\boldsymbol{r}_{12};\boldsymbol{k}_{12i})$; in other words, provided it is treated as a single $\boldsymbol{r}_{12}$-dependent function, the quantity within the braces in

(172 *a*) is of order $r_{12}^{-1}\,e^{i(k_{12}\pm A)r_{12}}$ at large r_{12}. Consequently the integral involving the braces in (172 *a*) fails to converge only at the special values of $\boldsymbol{k}_f$ satisfying $A^2 = k_{12i}^2$ for given $\boldsymbol{k}_i$, whereas the left side of (172 *a*) (the first integral factor in (170 *c*)) diverges at all $\boldsymbol{A}$, $\boldsymbol{k}_{12i}$. The remaining pair of one-dimensional integrals on the right side of (172 *a*)—multiplying the matrix elements $\langle k_{12i}\boldsymbol{\nu}_A|\boldsymbol{t}_{12i}|\boldsymbol{k}_{12i}\rangle$ and $\langle -k_{12i}\boldsymbol{\nu}_A|\boldsymbol{t}_{12i}|\boldsymbol{k}_{12i}\rangle$ respectively—are obviously divergent, i.e. strictly speaking are mathematically undefined. To accomplish our present objective of finding an expression for $\overline{T}^t(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ of (169 *a*), it is necessary to somehow reinterpret these last two divergent integrals on the right side of (172 *a*). There is no doubt but that the convergent first integral on the right side of (172 *a*) contributes wholly to $\overline{T}^t(\boldsymbol{k}_i\to\boldsymbol{k}_f)$. The problem is to decide whether or not the last two integrals on the right side of (172 *a*) also contribute to $\overline{T}^t(\boldsymbol{k}_i\to\boldsymbol{k}_f)$; referring to the discussion following (169 *a*), this problem amounts to deciding whether or not the integrals in question plausibly can be interpreted as a sum of terms proportional to δ-functions, with no residual finite parts.

5.1.1. *Formula for* $\overline{T}^t(\boldsymbol{k}_i\to\boldsymbol{k}_f)$

It is argued in § E. 4 that the relations

$$\int_0^\infty dx\,e^{ikx} = \frac{i}{k} \quad (k \neq 0), \tag{173 a}$$

$$\int_0^\infty dx\,e^{ikx} = \pi\delta(k) \quad (k = 0), \tag{173 b}$$

provide a plausible interpretation, as a function of k, of the divergent integral on the left sides of (173). Equations (173) are consistent with the more customary formula (Brenig & Haag 1963)†

$$\int_0^\infty dx\,e^{ikx} = \pi\delta(k) + iP\frac{1}{k}, \tag{174 a}$$

where P signifies the principal part when integrated over k, i.e. where it is asserted that for any reasonably well-behaved function $f(k)$

$$\int_{-\infty}^\infty dk f(k)\int_0^\infty dx\,e^{ikx} = \pi f(0) + i\lim_{\epsilon\to 0}\left[\int_{-\infty}^{\epsilon}\frac{dk f(k)}{k} + \int_\epsilon^\infty \frac{dk f(k)}{k}\right]. \tag{174 b}$$

Use of Equations (173) in (172 *a*) specifies the magnitudes of the δ-function contributions to $\overline{\Psi}_{23f}^{(-)*}V_{23}\overline{\Phi}_{12}^{(+)}$ of (170 *a*), thereby making it obvious how to express this $\overline{\Psi}_{23f}^{(-)*}V_{23}\overline{\Phi}_{12}^{(+)}$ part of $\overline{T}^s(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ in the form (169 *a*). Thus (see § E. 4) we conclude from (169 *a*) and (169 *c*) that

$$\begin{aligned}\overline{T}^t(\boldsymbol{k}_i\to\boldsymbol{k}_f) = {}& \overline{T}^d(\boldsymbol{k}_i\to\boldsymbol{k}_f) + \overline{T}^t_{2312}(\boldsymbol{k}_i\to\boldsymbol{k}_f) + \overline{T}^t_{2331}(\boldsymbol{k}_i\to\boldsymbol{k}_f)\\ &+ \overline{T}^t_{3123}(\boldsymbol{k}_i\to\boldsymbol{k}_f) + \overline{T}^t_{3112}(\boldsymbol{k}_i\to\boldsymbol{k}_f)\\ &+ \overline{T}^t_{1231}(\boldsymbol{k}_i\to\boldsymbol{k}_f) + \overline{T}^t_{1223}(\boldsymbol{k}_i\to\boldsymbol{k}_f),\end{aligned} \tag{175 a}$$

† It is possible that use of the methods of functional analysis would give some of the derivations which follow a mathematically more acceptable (though probably not yet wholly rigorous) foundation. As a matter of fact, Gel'fand & Shilov (1964) quote i/k rather than $iP(k^{-1})$ for the imaginary part of the integral on the left side of (174 *a*). I do not believe this difference—which probably is purely formal—would affect any of the results obtained via use of (173) and (174); moreover, as §§ 5.2 and 5.3 point out, use of equations (173) and (174) as they stand leads to formulas for $\overline{T}^t(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ which are consistent with detailed balance, with physical expectation, and with momentum space procedures. Nevertheless, it must be admitted that I have not examined carefully the functional analysis implications for the present work. I wish to thank Professor M. R. C. McDowell for making me aware of Gel'fand & Shilov's alternative to (174 *a*).

where for $A^2 \neq k_{12i}^2$

$$\bar{T}^t_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \langle \boldsymbol{k}_{23f} | \boldsymbol{t}_{23f} | -\boldsymbol{B} \rangle \int d\boldsymbol{r}_{12} \Big\{ e^{-i\boldsymbol{r}_{12}\cdot\boldsymbol{A}} \phi^{(+)}_{12}(\boldsymbol{r}_{12}; \boldsymbol{k}_{12i}) + \frac{i\mu_{12}}{\hbar^2} \frac{e^{ik_{12i}r_{12}}}{r_{12}} \langle k_{12i}\boldsymbol{\nu}_{12} | t_{12i} | k_{12i} \rangle \Big[\delta(\boldsymbol{\nu}_{12} - \boldsymbol{\nu}_A) \frac{e^{-iAr_{12}}}{Ar_{12}} - \delta(\boldsymbol{\nu}_{12} + \boldsymbol{\nu}_A) \frac{e^{iAr_{12}}}{Ar_{12}} \Big] \Big\}$$
$$+ \frac{\mu_{12}}{\hbar^2} \langle \boldsymbol{k}_{23f} | \boldsymbol{t}_{23f} | -\boldsymbol{B} \rangle \Big[\frac{\langle k_{12i}\boldsymbol{\nu}_A | t_{12i} | k_{12i} \rangle}{A(k_{12i} - A)} - \frac{\langle -k_{12i}\boldsymbol{\nu}_A | t_{12i} | k_{12i} \rangle}{A(k_{12i} + A)} \Big], \qquad (175\,b)$$

while for $C^2 \neq k_{31i}^2$

$$\bar{T}^t_{2331}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \langle \boldsymbol{k}_{23f} | \boldsymbol{t}_{23f} | \boldsymbol{D} \rangle \int d\boldsymbol{r}_{31} \Big\{ e^{i\boldsymbol{r}_{31}\cdot\boldsymbol{C}} \phi^{(+)}_{31}(\boldsymbol{r}_{31}; \boldsymbol{k}_{31i}) + \frac{i\mu_{31}}{\hbar^2} \frac{e^{ik_{31}r_{31}}}{r_{31}} \langle k_{31i}\boldsymbol{\nu}_{31} | t_{31i} | k_{31i} \rangle \Big[\delta(\boldsymbol{\nu}_{31} + \boldsymbol{\nu}_C) \frac{e^{-iCr_{31}}}{Cr_{31}} - \delta(\boldsymbol{\nu}_{31} - \boldsymbol{\nu}_C) \frac{e^{iCr_{31}}}{Cr_{31}} \Big] \Big\}$$
$$+ \frac{\mu_{31}}{\hbar^2} \langle \boldsymbol{k}_{23f} | \boldsymbol{t}_{23f} | \boldsymbol{D} \rangle \Big[\frac{\langle -k_{31i}\boldsymbol{\nu}_C | t_{31i} | k_{31i} \rangle}{C(k_{31i} - C)} - \frac{\langle k_{31i}\boldsymbol{\nu}_C | t_{31i} | k_{31i} \rangle}{C(k_{31i} + C)} \Big]. \qquad (175\,c)$$

In (175) we employ the notation (172 c), along with $\boldsymbol{r}_{31} = r_{31}\boldsymbol{\nu}_{31}$, $\boldsymbol{C} = C\boldsymbol{\nu}_C$; the two-particle scattered waves $\phi^{(+)}_{\alpha\beta}$ are given by (73), as always. The quantities $\bar{T}^t_{3123}$, $\bar{T}^t_{1231}$ of (175) are cyclic permutations of $\bar{T}^t_{2312}$; the quantities $\bar{T}^t_{3112}$, $\bar{T}^t_{1223}$ are cyclic permutations of $\bar{T}^t_{2331}$. Evidently $\bar{T}^t_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ is the contribution to $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ made by $\bar{\Psi}^{(-)*}_{23f} V_{23} \bar{\Phi}^{(+)}_{12}$ in (169 c); $\bar{T}^t_{2331}$ is the contribution to $\bar{T}^t$ made by $\bar{\Psi}^{(-)*}_{23f} V_{23} \bar{\Phi}^{(+)}_{31}$. In (175 b), as in its generating expression (172 a), integrals of the individual terms within the braces (e.g. of the term $e^{-i\boldsymbol{r}_{12}\cdot\boldsymbol{A}} \phi^{(+)}_{12}$) do not converge, but the entire integral in (175 b) does converge provided the quantity within the braces is treated as a single $\boldsymbol{r}_{12}$-dependent function. Equation (173 a) means that the divergent integrals in (172 a) have residual finite parts in addition to their δ-function parts from (173 b); these residual parts are the terms not under the integral sign in (175 b). Equation (175 b) does not specify

$$\bar{T}^t_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f) \quad \text{at} \quad A = \pm k_{12i}$$

(although of course only $A = k_{12i}$ can occur for real $\boldsymbol{k}_i$, $\boldsymbol{k}_f$, where $A > 0$ by definition); in fact, as was the case for the corresponding integral in (172 a), at $A = \pm k_{12i}$ the integral in (175 b) is logarithmically divergent, i.e. strictly speaking is mathematically undefined. That these deficiencies of (175 b) at $A = \pm k_{12i}$ are inconsequential for the purpose of this publication has been explained in § 4.3.2; in any event, the experimenter attempting to measure truly three-body scattering would not be placing his counters at locations consistent with $A = k_{12i}$, because these locations also are those at which the argument of the δ-function (135 a) vanishes (recall the remarks at the end of § 4.2.2). The rather awkward form of the right side of (175 b) actually reduces to a quite convenient and readily interpretable expression for $\bar{T}^t_{2312}$ (see § 5.2.3 below). Similar remarks (to those of this paragraph) pertain to (175 c), which converges except when $C = \pm k_{31i}$.

The derivation of (175) (§ E. 4) simultaneously shows that in (169 a)

$$\bar{T}^a(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \bar{T}^a_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f) + \bar{T}^a_{2331}(\boldsymbol{k}_i \to \boldsymbol{k}_f) + \bar{T}^a_{3123}(\boldsymbol{k}_i \to \boldsymbol{k}_f) + \bar{T}^a_{3112}(\boldsymbol{k}_i \to \boldsymbol{k}_f) + \bar{T}^a_{1231}(\boldsymbol{k}_i \to \boldsymbol{k}_f) + \bar{T}^a_{1223}(\boldsymbol{k}_i \to \boldsymbol{k}_f), \qquad (176\,a)$$

where
$$\bar{T}^a_{2312}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) = -\frac{\mu_{12}\pi\mathrm{i}}{\hbar^2 k_{12\mathrm{i}}}\langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|-\boldsymbol{B}\rangle\langle -k_{12\mathrm{i}}\boldsymbol{\nu}_A|\,\boldsymbol{t}_{12\mathrm{i}}\,|\,\boldsymbol{k}_{12\mathrm{i}}\rangle\,\delta(k_{12\mathrm{i}}+A)$$
$$-\frac{\mu_{12}\pi\mathrm{i}}{\hbar^2 k_{12\mathrm{i}}}\langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|-\boldsymbol{B}\rangle\langle k_{12\mathrm{i}}\boldsymbol{\nu}_A|\,\boldsymbol{t}_{12\mathrm{i}}\,|\,\boldsymbol{k}_{12\mathrm{i}}\rangle\,\delta(k_{12\mathrm{i}}-A), \qquad (176\,b)$$

$$\bar{T}^a_{2331}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) = -\frac{\mu_{31}\pi\mathrm{i}}{\hbar^2 k_{31\mathrm{i}}}\langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|\boldsymbol{D}\rangle\langle k_{31\mathrm{i}}\boldsymbol{\nu}_C|\,\boldsymbol{t}_{31\mathrm{i}}\,|\,\boldsymbol{k}_{31\mathrm{i}}\rangle\,\delta(k_{31\mathrm{i}}+C)$$
$$-\frac{\mu_{31}\pi\mathrm{i}}{\hbar^2 k_{31\mathrm{i}}}\langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|\boldsymbol{D}\rangle\langle -k_{31\mathrm{i}}\,\boldsymbol{\nu}_C|\,\boldsymbol{t}_{31\mathrm{i}}\,|\,\boldsymbol{k}_{31\mathrm{i}}\rangle\,\delta(k_{31\mathrm{i}}-C). \qquad (176\,c)$$

The quantities $\bar{T}^a_{3123}$, $\bar{T}^a_{1231}$, in (176 *a*) are cyclic permutations of $\bar{T}^a_{2312}$; the quantities $\bar{T}^a_{3112}$, $\bar{T}^a_{1223}$ are cyclic permutations of $\bar{T}^a_{2331}$. Evidently $\bar{T}^a_{2312}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f})$ is the contribution to $\bar{T}^a(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f})$ made by $\bar{\Psi}^{(-)*}_{23\mathrm{f}}V_{23}\bar{\Phi}^{(+)}_{12}$ in (169 *c*); $\bar{T}^a_{2331}$ is the contribution to $\bar{T}^a$ made by $\bar{\Psi}^{(-)*}_{23\mathrm{f}}V_{23}\bar{\Phi}^{(+)}_{31}$.

In (176 *b*), only the second δ-function on the right can have a vanishing argument at real $\boldsymbol{k}_\mathrm{i}$, $\boldsymbol{k}_\mathrm{f}$. Referring to (171 *a*), one sees explicitly that this second term on the right side of (176 *b*) is proportional to precisely the δ-function (135 *a*) interpreted in § 4.1.3. In particular, (137) to (139), and the discussion thereof, showed the presence of the δ-function (135 *a*) could be interpreted as resulting from two independent successive two-particle scatterings, namely first particles 1, 2 are scattered by each other, after which particle 2 is scattered by 3. The precise form of the $\delta(k_{12\mathrm{i}}-A)$ term in (176 *b*) is consistent with this interpretation, in that this term is proportional to the product of the truly two-body matrix elements $\langle k_{12\mathrm{i}}\boldsymbol{\nu}_A|\,\boldsymbol{t}_{12\mathrm{i}}\,|\,\boldsymbol{k}_{12\mathrm{i}}\rangle$ and $\langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|-\boldsymbol{B}\rangle$. Indeed, at $k_{12\mathrm{i}}=A$, the final relative momentum $k_{12\mathrm{i}}\boldsymbol{\nu}_A$ in the two-body matrix element $\langle k_{12\mathrm{i}}\boldsymbol{\nu}_A|\,\boldsymbol{t}_{12\mathrm{i}}\,|\,\boldsymbol{k}_{12\mathrm{i}}\rangle$ associated with the first 1, 2 scattering is identical with $\boldsymbol{A}$ of (171 *a*), which in turn is identical with the intermediate (after the first scattering) $\boldsymbol{k}'_{12}$ of (138) and (139), because, using (29) and (138) as well as $\boldsymbol{K}_\mathrm{i}=\boldsymbol{K}_\mathrm{f}$ and $\boldsymbol{k}_{1\mathrm{f}}=\boldsymbol{k}'_1$,

$$\boldsymbol{A} = \boldsymbol{K}_{23\mathrm{f}}+\frac{m_1}{m_1+m_2}\boldsymbol{K}_{12\mathrm{i}} = \boldsymbol{k}_{1\mathrm{f}}-\frac{m_1}{M}\boldsymbol{K}_\mathrm{f}+\frac{m_1}{m_1+m_2}\left(\boldsymbol{k}_{3\mathrm{i}}-\frac{m_3}{M}\boldsymbol{K}_\mathrm{i}\right)$$
$$= \boldsymbol{k}_{1\mathrm{f}}-\frac{m_1}{m_1+m_2}(\boldsymbol{k}_{1\mathrm{i}}+\boldsymbol{k}_{2\mathrm{i}}) = \boldsymbol{k}'_1-\frac{m_1}{m_1+m_2}(\boldsymbol{k}'_1+\boldsymbol{k}'_2) = \boldsymbol{k}'_{12}. \qquad (177\,a)$$

Similarly,

$$-\boldsymbol{B} = -\frac{m_3}{m_2+m_3}\boldsymbol{K}_{23\mathrm{f}}-\boldsymbol{K}_{12\mathrm{i}} = -\frac{m_3}{m_2+m_3}\left(\boldsymbol{k}_{1\mathrm{f}}-\frac{m_1}{M}\boldsymbol{K}_\mathrm{f}\right)-\left(\boldsymbol{k}_{3\mathrm{i}}-\frac{m_3}{M}\boldsymbol{K}_\mathrm{i}\right)$$
$$= -\boldsymbol{k}_{3\mathrm{i}}+\frac{m_3}{m_2+m_3}(\boldsymbol{k}_{2\mathrm{f}}+\boldsymbol{k}_{3\mathrm{f}}) = -\boldsymbol{k}'_3+\frac{m_3}{m_2+m_3}(\boldsymbol{k}'_2+\boldsymbol{k}'_3) = \boldsymbol{k}'_{23}. \qquad (177\,b)$$

Equation (177 *b*) shows that, in the $\delta(k_{12}-A)$ term of (176 *b*), the initial momentum $-\boldsymbol{B}$ in the two-body matrix element $\langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|-\boldsymbol{B}\rangle$ associated with the second 2, 3 scattering is identical with the intermediate $\boldsymbol{k}'_{23}$. Moreover, at $k_{12\mathrm{i}}=A$ this second scattering matrix element $\langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|-\boldsymbol{B}\rangle$, like the first scattering matrix element $\langle k_{12\mathrm{i}}\boldsymbol{\nu}_A|\,\boldsymbol{t}_{12\mathrm{i}}\,|\,\boldsymbol{k}_{12\mathrm{i}}\rangle$, is on the two-body energy shell (i.e. $B=k_{23\mathrm{f}}$) because

$$A^2 = K^2_{23\mathrm{f}}+\left(\frac{m_1}{m_1+m_2}\right)^2 K^2_{12\mathrm{i}}+\frac{2m_1}{m_1+m_2}\boldsymbol{K}_{23\mathrm{f}}.\boldsymbol{K}_{12\mathrm{i}} = k^2_{12\mathrm{i}} \qquad (178\,a)$$

implies
$$B^2 = \left(\frac{m_3}{m_2+m_3}\right)^2 K^2_{23\mathrm{f}}+K^2_{12\mathrm{i}}+\frac{2m_3}{m_2+m_3}\boldsymbol{K}_{23\mathrm{f}}.\boldsymbol{K}_{12\mathrm{i}}$$
$$= \frac{m_3}{m_1}\left(\frac{m_1+m_2}{m_2+m_3}\right)k^2_{12\mathrm{i}}+\frac{m_2 M}{(m_2+m_3)(m_1+m_2)}K^2_{12\mathrm{i}}-\frac{m_2 m_3 M}{m_1(m_2+m_3)^2}K^2_{23\mathrm{f}}. \qquad (178\,b)$$

But conservation of the total energy of the three particles, along with $\boldsymbol{K}_i = \boldsymbol{K}_f$, further implies (via (35)) that

$$\frac{k_{23f}^2}{\mu_{23}} + \frac{K_{23f}^2}{\mu_{1R}} = \frac{k_{12i}^2}{\mu_{12}} + \frac{K_{12i}^2}{\mu_{3R}}. \tag{178c}$$

Use of (178 c) to eliminate k_{12i}^2 in (178 b) immediately yields $B^2 = k_{23f}^2$ (recalling (29 e) and (29f)).

Similar considerations to those of the preceding two paragraphs pertain to the cyclic permutations of (176 b), as well as to (176 c) and its cyclic permutations. In particular, the precise form of the $\delta(k_{31i} - C)$ term in (176 c) is consistent with the interpretation that this term results from the purely two-particle scattering of 3 and 1, followed by a second purely two-particle scattering of 3 by 2. More specifically, at $k_{31i} = C$ it can be seen that: (i) the vector $-k_{31i}\boldsymbol{\nu}_c = -\boldsymbol{C}$ of (171 b) is identical with the expected intermediate (after the first 3, 1 scattering) $\boldsymbol{k}'_{31}$; (ii) the vector $\boldsymbol{D}$ now is identical with the expected intermediate $\boldsymbol{k}'_{23}$; (iii) now $D = k_{23f}$, so that each two-body matrix element multiplying $\delta(k_{31i} - C)$ in (176 c) lies on the two-body energy shell.

5.2. *Detailed balancing*

From very general time reversal considerations (Goldberger & Watson 1964) one expects that the matrix elements of the total three-body transition operator $\bar{T}$ (defined by (5)) satisfy

$$\bar{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \bar{T}(-\boldsymbol{k}_f \to -\boldsymbol{k}_i). \tag{179a}$$

Similarly, one expects that the truly three-body part $\bar{T}^t$ of $\bar{T}$ obeys

$$\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \bar{T}^t(-\boldsymbol{k}_f \to -\boldsymbol{k}_i). \tag{179b}$$

For purely two-body collisions—where the integrals $\bar{\Psi}_f^{(-)*} V \bar{\psi}_i$ and $\bar{\psi}_f^* V \bar{\Psi}_i^{(+)}$ of (126 b) and (131c) always converge, and where correspondingly the scattered parts $\bar{\Phi}_i^{(+)}$, $\bar{\Phi}_f^{(-)*}$ of $\bar{\Psi}_i^{(+)}$, $\bar{\Psi}_f^{(-)*}$ are everywhere outgoing—the result (179 a) easily is demonstrated (Gerjuoy 1958a) directly from the formulas (126 b) and (131 c). In the three-body case of present interest this previous demonstration of (179 a) is not applicable, however, because now the integrals (126 b) and (131 c) need not converge, and because correspondingly $\bar{\Phi}_i^{(+)}$ and $\bar{\Phi}_f^{(-)*}$ now are not everywhere outgoing. The truly three-body amplitudes of (179 b) are expressible in terms of convergent integrals (as the last § 5.1 has shown), but these expressions are so complicated that the previous two-body proof of the reciprocity relation (179 a) also is inapplicable to (179 b). Thus it is needful to investigate here whether or not the expressions (175) for $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ really are consistent with the reciprocity relation (179 b). This investigation is particularly necessary because the formulas (175) for $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ were derived on the basis of some mathematically questionable (though plausible) manipulations, as discussed in § 5.1. One also could adopt the viewpoint that (179 b) obviously holds because, as will be discussed in § 5.3, the formulas (165 b) and (175) for the various component parts of $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ reduce to momentum space matrix elements, for which there presumably are general proofs (Goldberger & Watson 1964) of time reversal invariance; this viewpoint does not really simplify the problem of proving (179 b), however, since the proofs of detailed balance in §§ 5.2.1 to 5.2.3 below largely involve carrying out this reduction of our configuration space expressions for $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ to recognizable momentum space matrix elements.

Recalling (175 a), to demonstrate (179 b) it is sufficient to show

$$\bar{T}^d(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \bar{T}^d(-\boldsymbol{k}_f \to \boldsymbol{k}_i), \tag{180a}$$

$$\bar{T}^t_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \bar{T}^t_{1223}(-\boldsymbol{k}_f \to -\boldsymbol{k}_i), \tag{180b}$$

because (180 *b*) obviously implies the cyclic relations

$$\bar{T}^{t}_{3123}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \bar{T}^{t}_{2331}(-\boldsymbol{k}_f \to -\boldsymbol{k}_i), \tag{180 c}$$

$$\bar{T}^{t}_{1231}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \bar{T}^{t}_{3112}(-\boldsymbol{k}_f \to -\boldsymbol{k}_i), \tag{180 d}$$

as well as

$$\bar{T}^{t}_{1223}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \bar{T}^{t}_{2312}(-\boldsymbol{k}_f \to -\boldsymbol{k}_i). \tag{180 e}$$

Equation (180 *e*) is obtained from (180 *b*) by replacing $\boldsymbol{k}_i$, $\boldsymbol{k}_f$ with $-\boldsymbol{k}_f$, $-\boldsymbol{k}_i$ respectively.

5.2.1. *Triple and higher scattering terms*

First I shall prove (180 *a*) holds, i.e. I shall prove detailed balancing for those terms in $\bar{T}^{t}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ associated with $n \geqslant 3$ successive two-body scatterings (recall the discussion at the end of subsection 4.3.1). Using (165 *b*), one sees (180 *a*) is equivalent to the assertion that

$$\begin{aligned}\bar{\Psi}^{(-)*}_{f}(\boldsymbol{k}_f)\,[(V_{23}+V_{31})\,\bar{\Phi}^{s(+)}_{12i}(\boldsymbol{k}_i) + (V_{31}+V_{12})\,\bar{\Phi}^{s(+)}_{23i}(\boldsymbol{k}_i) + (V_{12}+V_{23})\,\bar{\Phi}^{s(+)}_{31i}(\boldsymbol{k}_i)] \\ = \bar{\Psi}^{(-)*}_{f}(-\boldsymbol{k}_i)\,[(V_{23}+V_{31})\,\bar{\Phi}^{s(+)}_{12i}(-\boldsymbol{k}_f) + (V_{31}+V_{12})\,\bar{\Phi}^{s(+)}_{23i}(-\boldsymbol{k}_f) + (V_{12}+V_{23})\,\bar{\Phi}^{s(+)}_{31i}(-\boldsymbol{k}_f)],\end{aligned} \tag{181}$$

where the notation indicates that $\bar{\Psi}^{(-)*}_{f}$ on the left side of (181) is the limit as $\epsilon \to 0$ of the solution to the centre-of-mass version of the Lippmann–Schwinger equation (107 *a*) with ψ_f of (100 *c*), whereas $\bar{\Psi}^{(-)*}_{f}$ on the right side of (181) is the limit as $\epsilon \to 0$ of the solution to the centre of mass version of (107 *a*) using

$$\psi_f \equiv \psi_f(\boldsymbol{r}, -\boldsymbol{k}_i) = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_i\cdot\boldsymbol{r}}. \tag{182 a}$$

Similarly $\bar{\Phi}^{s(+)}_{12i}(\boldsymbol{k}_i)$ in (181) is the quantity defined by (161 *d*) with the understanding that in (161 *d*) the functions $\Phi^{(+)}_{\alpha\beta} \equiv \Phi^{(+)}_{\alpha\beta i}$ are defined by (58 *a*) for ψ_i from (21 *a*), whereas $\bar{\Phi}^{s(+)}_{12i}(-\boldsymbol{k}_f)$ is defined by (161 *d*) and (58 *a*) using

$$\psi_i \equiv \psi_i(\boldsymbol{r}, -\boldsymbol{k}_f) = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_f\cdot\boldsymbol{r}}. \tag{182 b}$$

Equations (182), together with (8) and (107 *a*), immediately imply

$$\bar{\Psi}^{(-)*}_{f}(-\boldsymbol{k}_i) = \bar{\Psi}^{(+)}_{i}(\boldsymbol{k}_i). \tag{183 a}$$

Similarly, (72), (73) and (105), along with (106) and (160), imply

$$\bar{\Phi}^{(+)}_{12i}(-\boldsymbol{k}_f) = \bar{\Phi}^{(-)*}_{12f}(\boldsymbol{k}_f), \tag{183 b}$$

$$\bar{\Phi}^{s(+)}_{12i}(-\boldsymbol{k}_f) = -\bar{G}^{(+)}_{12}V_{12}[\bar{\Phi}^{(-)*}_{31f}(\boldsymbol{k}_f) + \bar{\Phi}^{(-)*}_{23f}(\boldsymbol{k}_f)] \equiv \bar{\Phi}^{s(-)*}_{12f}(\boldsymbol{k}_f). \tag{183 c}$$

Thus the right sides of (180 *a*) and (181) become

$$\bar{T}^{d}(-\boldsymbol{k}_f \to -\boldsymbol{k}_i) = [\bar{\Phi}^{s(-)*}_{12f}(V_{23}+V_{31}) + \bar{\Phi}^{s(-)*}_{23f}(V_{31}+V_{12}) + \bar{\Phi}^{s(-)*}_{31f}(V_{12}+V_{23})]\,\bar{\Psi}^{(+)}_{i}, \tag{184 a}$$

where now, as always in the past, the subscript i on the right side of a matrix element is associated with the incident wave vector $\boldsymbol{k}_i$, while the subscript f on the left side of a matrix element is associated with the final wave vector $\boldsymbol{k}_f$.

Using the symmetry relation (95), valid for all the Green functions employed in this work, (183 *c*) permits rewriting (184 *a*) in the form

$$\begin{aligned}\bar{T}^{d}(-\boldsymbol{k}_f \to -\boldsymbol{k}_i) = &-[(\bar{\Phi}^{(-)*}_{31f} + \bar{\Phi}^{(-)*}_{23f})\,V_{12}\,\bar{G}^{(+)}_{12}(V_{23}+V_{31}) \\ &+ (\bar{\Phi}^{(-)*}_{12f} + \bar{\Phi}^{(-)*}_{31f})\,V_{23}\,\bar{G}^{(+)}_{23}(V_{31}+V_{12}) \\ &+ (\bar{\Phi}^{(-)*}_{23f} + \bar{\Phi}^{(-)*}_{12f})\,V_{31}\,\bar{G}^{(+)}_{31}(V_{12}+V_{23})]\,\bar{\Psi}^{(+)}_{i}.\end{aligned} \tag{184 b}$$

In (184 b), $\overline{\Psi}_{\mathrm{i}}^{(+)}$ can be replaced by $\lim \overline{\Psi}_{\mathrm{i}}(\bar{E}+\mathrm{i}\epsilon)$, from (34 a); correspondingly, recalling (60), (72) and (105), $\bar{\Phi}_{12\mathrm{f}}^{(-)*}$ can be replaced by

$$-\lim_{\epsilon\to 0}\{\bar{G}_{12}(\bar{E}+\mathrm{i}\epsilon)\,V_{12}\,\overline{\psi}_{\mathrm{f}}^{*}\}=-\lim_{\epsilon\to 0}\{\overline{\psi}_{\mathrm{f}}^{*}V_{12}\,\bar{G}_{12}(\bar{E}+\mathrm{i}\epsilon)\}. \tag{184 c}$$

Moreover, as written the right side of (184 b) is wholly composed of convergent integrals. According to §§ 2.2 and A. 8, therefore, it is legitimate to replace (184 b) by

$$\begin{aligned}\overline{T}^{d}(-\boldsymbol{k}_{\mathrm{f}}\to-\boldsymbol{k}_{\mathrm{i}})=\lim_{\epsilon\to 0}\overline{\psi}_{\mathrm{f}}^{*}[&(V_{31}\bar{G}_{31}+V_{23}\bar{G}_{23})V_{12}\bar{G}_{12}(V_{23}+V_{31})+(V_{12}\bar{G}_{12}+V_{31}\bar{G}_{31})\\&\times V_{23}\bar{G}_{23}(V_{31}+V_{12})+(V_{23}\bar{G}_{23}+V_{12}\bar{G}_{12})V_{31}\bar{G}_{31}(V_{12}+V_{23})]\,(1-\bar{G}V)\overline{\psi}_{\mathrm{i}},\end{aligned} \tag{185 a}$$

where all the Green functions are evaluated at the same complex energy $\bar{\lambda}=\bar{E}+\mathrm{i}\epsilon$. Similarly, the left sides of (180 a) and (181) are

$$\begin{aligned}\overline{T}^{d}(\boldsymbol{k}_{\mathrm{i}}\to\boldsymbol{k}_{\mathrm{f}})=\lim_{\epsilon\to 0}\overline{\psi}_{\mathrm{f}}^{*}(1-V\bar{G})\,[&(V_{23}+V_{31})\,\bar{G}_{12}V_{12}(\bar{G}_{31}V_{31}+\bar{G}_{23}V_{23})+(V_{31}+V_{12})\\&\times\bar{G}_{23}V_{23}(\bar{G}_{12}V_{12}+\bar{G}_{31}V_{31})+(V_{12}+V_{23})\,\bar{G}_{31}V_{31}(\bar{G}_{23}V_{23}+\bar{G}_{12}V_{12})]\,\overline{\psi}_{\mathrm{i}}.\end{aligned} \tag{185 b}$$

I stress that (185) hold even though the integral (52 b) need not converge, i.e. even though it is not legitimate to replace $\overline{\Psi}_{\mathrm{i}}^{(+)}$ by $[1-\bar{G}^{(+)}V]\,\overline{\psi}_{\mathrm{i}}$.

I now show that the matrix elements on the right sides of (185 a) and (185 b) are identical at every $\bar{\lambda}=\bar{E}+\mathrm{i}\epsilon$ ($\epsilon>0$), which is sufficient to demonstrate (180 a). Because all the Green functions in (185) are exponentially decreasing at infinity for $\epsilon>0$, the orders of integration in (185) (and in subsequent expressions in this subsection) can be and will be rearranged essentially at will. Moreover, to ease the notational complexity, for the moment I shall drop the bars in (185), which here introduces no error even though the right sides of (184 a) and (184 b) are not convergent in the laboratory system.

In (185 b) use (63) to replace, for example, $G(V_{23}+V_{31})\,G_{12}$ by $G_{12}-G$. Then (also dropping temporarily the irrelevant lim as $\epsilon\to 0$) the matrix element on the right side of (185 b) reduces to

$$\begin{aligned}&\psi_{\mathrm{f}}^{*}\{(V_{23}+V_{31})\,G_{12}V_{12}(G_{31}V_{31}+G_{23}V_{23})\\&\quad+(V_{31}+V_{12})\,G_{23}V_{23}(G_{12}V_{12}+G_{31}V_{31})+(V_{12}+V_{23})\,G_{31}V_{31}(G_{23}V_{23}+G_{12}V_{12})\\&\quad+V[(G-G_{12})V_{12}(G_{31}V_{31}+G_{23}V_{23})+(G-G_{23})V_{23}(G_{12}V_{12}+G_{31}V_{31})\\&\quad+(G-G_{31})V_{31}(G_{23}V_{23}+G_{12}V_{12})]\}\psi_{\mathrm{i}}\end{aligned} \tag{186 a}$$

$$\begin{aligned}&=\psi_{\mathrm{f}}^{*}\{VG[(V_{12}+V_{23})\,G_{31}V_{31}+(V_{23}+V_{31})\,G_{12}V_{12}+(V_{31}+V_{12})\,G_{23}V_{23}]\\&\quad-V_{12}G_{12}V_{12}(G_{31}V_{31}+G_{23}V_{23})-V_{23}G_{23}V_{23}(G_{12}V_{12}+G_{31}V_{31})\\&\quad-V_{31}G_{31}V_{31}(G_{23}V_{23}+G_{12}V_{12})\}\psi_{\mathrm{i}},\end{aligned} \tag{186 b}$$

where in going from (186 a) to (186 b) I have rearranged the terms in G, and have noted that $V_{23}+V_{31}=V-V_{12}$, etc. Now in (186 b), use (63) again in the terms involving G, and recall (77 a) as well as the manipulations in (137) and (166 b). Then (186 b) further reduces to

$$\begin{aligned}&\psi_{\mathrm{f}}^{*}\{V[(G_{31}-G)V_{31}+(G_{12}-G)V_{12}+(G_{23}-G)V_{23}]+(\boldsymbol{T}_{12}-V_{12})\,(G_{31}V_{31}+G_{23}V_{23})\\&\quad+(\boldsymbol{T}_{23}-V_{23})\,(G_{12}V_{12}+G_{31}V_{31})+(\boldsymbol{T}_{31}-V_{31})\,(G_{23}V_{23}+G_{12}V_{12})\}\psi_{\mathrm{i}}\end{aligned} \tag{186 c}$$

$$\begin{aligned}&=\psi_{\mathrm{f}}^{*}\{-VGV+V_{31}G_{31}V_{31}+V_{12}G_{12}V_{12}+V_{23}G_{23}V_{23}+\boldsymbol{T}_{12}(G_{31}V_{31}+G_{23}V_{23})\\&\quad+\boldsymbol{T}_{23}(G_{12}V_{12}+G_{31}V_{31})+\boldsymbol{T}_{31}(G_{23}V_{23}+G_{12}V_{12})\}\psi_{\mathrm{i}},\end{aligned} \tag{186 d}$$

which, recalling our starting-point for (184 d) was (185 b), implies finally

$$\bar{T}^d(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \lim_{\epsilon \to 0} \bar{\psi}_f^* \{\bar{\boldsymbol{T}} - \bar{\boldsymbol{T}}_{12} - \bar{\boldsymbol{T}}_{23} - \bar{\boldsymbol{T}}_{31} + \bar{\boldsymbol{T}}_{12} \bar{G}_F \bar{\boldsymbol{T}}_{31} + \bar{\boldsymbol{T}}_{12} \bar{G}_F \bar{\boldsymbol{T}}_{23} + \bar{\boldsymbol{T}}_{23} \bar{G}_F \bar{\boldsymbol{T}}_{12} + \bar{\boldsymbol{T}}_{23} \bar{G}_F \bar{\boldsymbol{T}}_{31} + \bar{\boldsymbol{T}}_{31} \bar{G}_F \bar{\boldsymbol{T}}_{23} + \bar{\boldsymbol{T}}_{31} \bar{G}_F \bar{\boldsymbol{T}}_{12}\} \bar{\psi}_i. \quad (187\,a)$$

A similar (to those employed in (186 a) and (187 a)) sequence of manipulations reduces the right side of (185 a) to the right side of (187 a). Therefore, the equality (180 a) has been demonstrated.

It is worth remarking that the changes of sign on the right side of (187 a) are consistent with the expectation that $\bar{T}^d(\boldsymbol{k}_i \to \boldsymbol{k}_f)$, being the contribution to $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ associated with $n \geqslant 3$ successive two-body scatterings, must be identifiable with the matrix element of $\boldsymbol{T}$ minus all single and double scattering contributions; these double scattering contributions, contained in $\bar{T}^s(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ of (133 b), have been evaluated in (137). Actually, if convergence difficulties are ignored, a much simpler sequence of iterations than was employed in deriving (187 a) from (165 b) yields (see § 5.3 below)

$$\bar{\psi}_f^* \bar{\boldsymbol{T}} \bar{\psi}_i = \bar{\psi}_f^* \{\bar{\boldsymbol{T}}_{12} + \bar{\boldsymbol{T}}_{23} + \bar{\boldsymbol{T}}_{31} - \bar{\boldsymbol{T}}_{23} \bar{G}_F \bar{\boldsymbol{T}}_{12} - \bar{\boldsymbol{T}}_{23} \bar{G}_F \bar{\boldsymbol{T}}_{31} - \bar{\boldsymbol{T}}_{31} \bar{G}_F \bar{\boldsymbol{T}}_{23} - \bar{\boldsymbol{T}}_{31} \bar{G}_F \bar{\boldsymbol{T}}_{12} - \bar{\boldsymbol{T}}_{12} \bar{G}_F \bar{\boldsymbol{T}}_{31} - \bar{\boldsymbol{T}}_{12} \bar{G}_F \bar{\boldsymbol{T}}_{23}\} \bar{\psi}_i + \bar{T}^d(\boldsymbol{k}_i \to \boldsymbol{k}_f) \quad (187\,b)$$

where now $\bar{G}_F$, $\bar{\boldsymbol{T}}_{\alpha\beta}$ are evaluated at real centre of mass energy $\bar{E}_i = \bar{E}_f$. The form of (187 b) evidently is consistent with (187 a), as asserted. However, because both the right and left sides of (187 b) are composed of divergent integrals (containing the trivial and non-trivial δ-function contributions which have been discussed in § 4.1), (187 b) is not a useful formula for actually computing $\bar{T}^d(\boldsymbol{k}_i \to \boldsymbol{k}_f)$. Instead, one must use (187 a), or, if one wants to avoid taking the limit $\epsilon \to 0$, the original formula (165 b).

I further remark that (180 a) also can be demonstrated by showing that the right side of (184 b) is precisely the expression one would deduce for $\bar{T}^d(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ starting from the integral equation (84 c). Specifically, in (84 c)

$$\{G_F^{(+)} V_{12} G_{12}^{(+)}\} V_{23} \Psi_i^{(+)} = \{G_F^{(+)} V_{12} G_{12}^{(+)}\} V_{23} [\Psi_{23}^{(+)} - G_{23}^{(+)} (V_{12} + V_{31}) \Psi_i^{(+)}] \quad (188\,a)$$

using (86). Thus one infers

$$\Phi_i^{s(+)} = \lim_{\epsilon \to 0} \{G_F(\lambda) V_{12} G_{12}(\lambda) [V_{23} \Psi_{23}^{(+)} + V_{31} \Psi_{31}^{(+)}] + \text{etc.}\} - \{G_F^{+} V_{12} G_{12}^{(+)}\} [V_{23} G_{23}^{(+)} (V_{12} + V_{31}) + V_{31} G_{31}^{(+)} (V_{23} + V_{12})] \Psi_i^{(+)} + \text{etc.}, \quad (188\,b)$$

where, as always, $\lambda = E + i\epsilon$. But in (188 b)

$$\lim_{\epsilon \to 0} \{G_F V_{12} G_{12} [V_{23} \Psi_{23}^{(+)} + V_{31} \Psi_{31}^{(+)}]\} = \lim_{\epsilon \to 0} \{G_{12} V_{12} G_F [V_{23} \Psi_{23}^{(+)} + V_{31} \Psi_{31}^{(+)}]\} = -G_{12}^{(+)} V_{12} [\Phi_{23}^{(+)} + \Phi_{31}^{(+)}] = \Phi_{12}^{s(+)}. \quad (189\,a)$$

Therefore, comparing with (161) and (162), $\Phi_i^{d(+)}$ is given by the terms involving $\Psi_i^{(+)}$ in (188 b). Correspondingly, using the defining equation (165 a) for $\bar{T}^d(\boldsymbol{k}_i \to \boldsymbol{k}_f)$,

$$\bar{T}^d(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \bar{\psi}_f^* V_{12} \bar{G}_{12}^{(+)} [V_{23} \bar{G}_{23}^{(+)} (V_{12} + V_{31}) + V_{31} \bar{G}_{31}^{(+)} (V_{23} + V_{12})] \bar{\Psi}_i^{(+)} + \text{etc.} = -\bar{\Phi}_{12f}^{(-)*} [V_{23} \bar{G}_{23}^{(+)} (V_{12} + V_{31}) + V_{31} \bar{G}_{31}^{(+)} (V_{23} + V_{12})] \bar{\Psi}_i^{(+)} + \text{etc.} \quad (189\,b)$$

The right side of (189 b) is seen to be identical with the (slightly rearranged) right side of (184 b).

5.2.2. *Double scattering δ-function terms*

In this subsection I show that the amplitudes $\bar{T}^a(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ of (176 *a*) also obey detailed balancing, i.e. that

$$\bar{T}^a(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \bar{T}^a(-\boldsymbol{k}_f \to -\boldsymbol{k}_i). \tag{190a}$$

In particular, I shall prove $\bar{T}^a_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \bar{T}^a_{1223}(-\boldsymbol{k}_f \to -\boldsymbol{k}_i)$, (190 *b*)

which is sufficient to demonstrate (190 *a*) (recall the analogous case of (180)). It will be presumed (in the remainder of this subsection) that for any given $\boldsymbol{k}_i$ the final $\boldsymbol{k}_f$ are chosen consistent with energy and momentum conservation. These restrictions on $\boldsymbol{k}_f$ are convenient, as will be seen; $\boldsymbol{k}_f$ can be so restricted because—for the purposes of this section 5.2—detailed balancing need not be investigated for values of $\boldsymbol{k}_i$, $\boldsymbol{k}_f$ which cannot occur in actual collisions.

Referring to (176 *b*), the left side of (190 *b*) can be written in the form

$$\begin{aligned}\bar{T}^a_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f) &= \frac{-\mu_{12}\pi i}{\hbar^2 k_{12i}} \langle \boldsymbol{k}_{23f} | \boldsymbol{t}_{23f} | -\boldsymbol{B}\rangle \langle \boldsymbol{A} | \boldsymbol{t}_{12i} | \boldsymbol{k}_{12i}\rangle [\delta(k_{12i}+A)+\delta(k_{12i}-A)] \\ &= \frac{-2\mu_{12}\pi i}{\hbar^2} \langle \boldsymbol{k}_{23f} | \boldsymbol{t}_{23f} | -\boldsymbol{B}\rangle \langle \boldsymbol{A} | \boldsymbol{t}_{12i} | \boldsymbol{k}_{12i}\rangle \delta(k^2_{12i}-A^2),\end{aligned} \tag{191a}$$

where we have used

$$\delta[f(x)] = \sum_r \frac{1}{f'(x_r)} \delta(x-x_r) \tag{191b}$$

summed over all roots x_r satisfying $f(x_r) = 0$. Similarly, from (171 *b*) and (176 *c*),

$$\bar{T}^a_{1223}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \frac{-2\mu_{23}\pi i}{\hbar^2} \langle \boldsymbol{k}_{12f} | \boldsymbol{t}_{12f} | \hat{\boldsymbol{D}}\rangle \langle -\hat{\boldsymbol{C}} | \boldsymbol{t}_{23i} | \boldsymbol{k}_{23i}\rangle \delta(k^2_{23i}-\hat{C}^2), \tag{192a}$$

where

$$\left.\begin{aligned}\hat{\boldsymbol{C}} &= \boldsymbol{K}_{12f} + \frac{m_3}{m_2+m_3}\boldsymbol{K}_{23i}, \\ \hat{\boldsymbol{D}} &= \frac{m_1}{m_1+m_2}\boldsymbol{K}_{12f} + \boldsymbol{K}_{23i}.\end{aligned}\right\} \tag{192b}$$

When $\boldsymbol{k}_i$, $\boldsymbol{k}_f$ are replaced by $-\boldsymbol{k}_f$, $-\boldsymbol{k}_i$ respectively, (192 *b*) implies that $\hat{\boldsymbol{C}}$, $\hat{\boldsymbol{D}}$ are replaced by $-\boldsymbol{B}$, $-\boldsymbol{A}$ respectively, where $\boldsymbol{A}$, $\boldsymbol{B}$ again are the vectors defined in (171 *a*). Therefore

$$\bar{T}^a_{1223}(-\boldsymbol{k}_f \to -\boldsymbol{k}_i) = \frac{-2\mu_{23}\pi i}{\hbar^2} \langle -\boldsymbol{k}_{12i} | \boldsymbol{t}_{12i} | -\boldsymbol{A}\rangle \langle \boldsymbol{B} | \boldsymbol{t}_{23f} | -\boldsymbol{k}_{23f}\rangle \delta(k^2_{23f}-B^2). \tag{193}$$

Now, as explained at the very beginning of this section, we know that the matrix elements of the two-body operators $\boldsymbol{t}_{12i}$, $\boldsymbol{t}_{23f}$ do obey detailed balancing, i.e. for any two vectors $\boldsymbol{X}$, $\boldsymbol{Y}$ (whether on the energy-momentum shell or not)

$$\langle \boldsymbol{X} | \boldsymbol{t}_{12i} | \boldsymbol{Y}\rangle = \langle -\boldsymbol{Y} | \boldsymbol{t}_{12i} | -\boldsymbol{X}\rangle \tag{194a}$$

and similarly for $\boldsymbol{t}_{23f}$. Equation (194 *a*) can be proved, e.g. by noting that (108) and the definition (131*f*) of $\boldsymbol{t}_{12}$ imply $\boldsymbol{t}_{12}$ is a symmetric operator in the coordinate representation,

$$\boldsymbol{t}_{12}(\boldsymbol{r}_{12}; \boldsymbol{r}'_{12}; \lambda_l) = \boldsymbol{t}_{12}(\boldsymbol{r}'_{12}; \boldsymbol{r}_{12}; \lambda), \tag{194b}$$

whereat (194 *a*) follows immediately, recalling the fundamental defining relation (131 *e*) for the matrix elements of $\boldsymbol{t}_{12}$.

Comparing (191 *a*) with (193), and employing (194 *a*), we see that (190 *b*) will hold if

$$\mu_{12}\delta(k^2_{12i}-A^2) = \mu_{23}\delta(k^2_{23f}-B^2), \tag{195a}$$

i.e. if
$$\frac{k_{12i}^2}{\mu_{12}}-\frac{A^2}{\mu_{12}}=\frac{k_{23f}^2}{\mu_{23}}-\frac{B^2}{\mu_{23}}. \tag{195 b}$$

But using (178 *a*) and (178 *b*), we see that (195 *b*) reduces to the relation (178 *c*) required by conservation of energy and momentum. Therefore (195 *b*) does hold, and the detailed balancing relations (190) are satisfied, for $\boldsymbol{k}_i$, $\boldsymbol{k}_f$ on the energy-momentum shell, Q.E.D.

5.2.3. *Residual terms*

I now return to $\overline{T}^t(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ of (175 *a*); in particular I now shall investigate the detailed balancing properties of the residual terms $\overline{T}^t_{2312}(\boldsymbol{k}_i\to\boldsymbol{k}_f)$, etc., not examined in § 5.2.1. If we ignore convergence questions casting doubt on the legitimacy of interchange of order of integration and limit $\epsilon\to 0$, then, according to (137), the integral (170 *a*) is

$$\overline{\Psi}^{(-)*}_{23f}(\boldsymbol{k}_f)\,V_{23}\,\overline{\Phi}^{(+)}_{12}(\boldsymbol{k}_i)=-\lim_{\epsilon\to 0}\overline{\psi}^*_f(\boldsymbol{k}_f)\,\overline{\boldsymbol{T}}_{23}(\bar{E}+i\epsilon)\,\overline{G}_F(\bar{E}+i\epsilon)\,\overline{\boldsymbol{T}}_{12}(\bar{E}+i\epsilon)\,\overline{\psi}_i(\boldsymbol{k}_i), \tag{196 a}$$

where $\psi_i(\boldsymbol{k}_i)$, $\psi_f(\boldsymbol{k}_f)$ are respectively the initial and final plane wave states ψ_i, ψ_f we have been employing throughout, defined by (21 *a*) and (100 *c*). The time-reversed matrix element in $\overline{\boldsymbol{T}}^s(-\boldsymbol{k}_f\to-\boldsymbol{k}_i)$ corresponding to (196 *a*) would be (referring to (169 *c*) and using the notation of (181) and (182))

$$\overline{\Psi}^{(-)*}_{12f}(-\boldsymbol{k}_i)\,V_{12}\,\overline{\Phi}^{(+)}_{23}(-\boldsymbol{k}_f)=-\lim_{\epsilon\to 0}\overline{\psi}^*_f(-\boldsymbol{k}_i)\,\overline{\boldsymbol{T}}_{12}(\bar{E}+i\epsilon)\,\overline{G}_F(\bar{E}+i\epsilon)\,\overline{\boldsymbol{T}}_{23}(\bar{E}+i\epsilon)\,\psi_i(-\boldsymbol{k}_f), \tag{196 b}$$

via manipulations as in (137). But, as in (183),

$$\overline{\psi}^*_f(-\boldsymbol{k}_i)=\overline{\psi}_i(\boldsymbol{k}_i),\quad \overline{\psi}_i(-\boldsymbol{k}_f)=\overline{\psi}^*_f(\boldsymbol{k}_f). \tag{197}$$

Moreover, the fundamental definition (77 *a*) implies the three-body $\boldsymbol{T}_{12}$, like the purely two-body $\boldsymbol{t}_{12}$ in (194 *b*), is a symmetric operator in the coordinate representation. Consequently, granting the validity of (196),

$$\overline{\Psi}^{(-)*}_{23f}(\boldsymbol{k}_f)\,V_{23}\,\overline{\Phi}^{(+)}_{12}(\boldsymbol{k}_i)=\overline{\Psi}^{(-)*}_{12f}(-\boldsymbol{k}_i)\,V_{12}\,\overline{\Phi}^{(+)}_{23}(-\boldsymbol{k}_f). \tag{198}$$

Section E. 4 in essence shows that

$$\overline{\Psi}^{(-)*}_{23f}(\boldsymbol{k}_f)\,V_{23}\,\overline{\Phi}^{(+)}_{12}(\boldsymbol{k}_i)=\overline{T}^t_{2312}(\boldsymbol{k}_i\to\boldsymbol{k}_f)+\overline{T}^a_{2312}(\boldsymbol{k}_i\to\boldsymbol{k}_f), \tag{199 a}$$

where the quantities on the right side of (199 *a*) are given by (175 *b*) and (176 *b*). Similarly,

$$\overline{\Psi}^{(-)*}_{12f}(-\boldsymbol{k}_i)\,V_{12}\,\overline{\Phi}^{(+)}_{23}(-\boldsymbol{k}_f)=\overline{T}^t_{1223}(-\boldsymbol{k}_f\to-\boldsymbol{k}_i)+\overline{T}^a_{1223}(-\boldsymbol{k}_f\to-\boldsymbol{k}_i). \tag{199 b}$$

Comparison of (199 *a*) and (199 *b*), together with (190 *b*) and (198), now implies the desired reciprocity relation (180 *b*) which, along with the already proved (180 *a*), is sufficient to guarantee (179 *b*), as explained at the beginning of § 5.2.

The foregoing demonstration that $\overline{T}^t(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ obeys (179 *b*) is merely suggestive rather than compelling, for the following two reasons. First, the interchange of order of integration and limit $\epsilon\to 0$ leading to the symmetric expression (196 *a*) for $\overline{\Psi}^{(-)*}_{23f}V_{23}\overline{\Phi}^{(+)}_{12}$ really is not justified, for reasons amply discussed in this and earlier sections. Secondly, even if the validity of (196) is granted, it is not clear that the specific formulas (175 *b*) and (175 *c*) are consistent with detailed balancing, because these formulas were derived via some mathematically questionable manipulations, e.g. the use of (173) to reinterpret† the divergent integrals in (172 *a*). What is required, therefore, is a proof that (175 *b*) and (175 *c*), as they stand, satisfy (180 *b*). This proof I now proceed to give.

† Recall the footnote, p. 265.

Recalling (192) to (194), it is seen that (175 c) yields

$$\bar{T}^{t}_{1223}(-\boldsymbol{k}_{\mathrm{f}}\to-\boldsymbol{k}_{\mathrm{i}}) = \langle \boldsymbol{A}|\,\boldsymbol{t}_{12\mathrm{i}}\,|\boldsymbol{k}_{12\mathrm{i}}\rangle \int \mathrm{d}\boldsymbol{r}_{23}\Big\{\mathrm{e}^{-\mathrm{i}\boldsymbol{r}_{23}\cdot\boldsymbol{B}}\,\phi^{(+)}_{23}(\boldsymbol{r}_{23};-\boldsymbol{k}_{23\mathrm{f}}) + \frac{\mathrm{i}\mu_{23}}{4\pi\hbar^2}\frac{\mathrm{e}^{\mathrm{i}k_{23\mathrm{f}}r_{23}}}{r_{23}}\Big[\langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|-k_{23\mathrm{f}}\boldsymbol{\nu}_B\rangle\frac{\mathrm{e}^{-\mathrm{i}Br_{23}}}{Br_{23}} - \langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|k_{23\mathrm{f}}\boldsymbol{\nu}_B\rangle\frac{\mathrm{e}^{\mathrm{i}Br_{23}}}{Br_{23}}\Big]\Big\} + \frac{\mu_{23}}{\hbar^2}\langle \boldsymbol{A}|\,\boldsymbol{t}_{12\mathrm{i}}\,|\boldsymbol{k}_{12\mathrm{i}}\rangle\Big[\frac{\langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|-k_{23\mathrm{f}}\boldsymbol{\nu}_B\rangle}{B(k_{23\mathrm{f}}-B)} - \frac{\langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|k_{23\mathrm{f}}\boldsymbol{\nu}_B\rangle}{B(k_{23\mathrm{f}}+B)}\Big]. \tag{200 a}$$

In (200 a) it has been convenient to rewrite (175 c) and its analogues in a fashion that trivially eliminates the δ-functions under the integral; as in (175 c), the integral in (200 a) is convergent provided the quantity within the braces is treated as a single $\boldsymbol{r}_{23}$-dependent function. It is further convenient to rewrite (200 a) as

$$\bar{T}^{t}_{1223}(-\boldsymbol{k}_{\mathrm{f}}\to-\boldsymbol{k}_{\mathrm{i}}) = \langle \boldsymbol{A}|\,\boldsymbol{t}_{12\mathrm{i}}\,|\boldsymbol{k}_{12\mathrm{i}}\rangle\Big\{F_{23}(\boldsymbol{k}_{23\mathrm{f}};\boldsymbol{B};\boldsymbol{t}_{23\mathrm{f}}) + \frac{\mu_{23}}{\hbar^2}\Big[\frac{\langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|-k_{23\mathrm{f}}\boldsymbol{\nu}_B\rangle}{B(k_{23\mathrm{f}}-B)} - \frac{\langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|k_{23\mathrm{f}}\boldsymbol{\nu}_B\rangle}{B(k_{23\mathrm{f}}+B)}\Big]\Big\} \tag{200 b}$$

where

$$F_{23}(\boldsymbol{k}_{23\mathrm{f}};\boldsymbol{B};\boldsymbol{t}_{23\mathrm{f}}) = \int \mathrm{d}\boldsymbol{r}_{23}\Big\{\mathrm{e}^{-\mathrm{i}\boldsymbol{r}_{23}\cdot\boldsymbol{B}}\,\phi^{(+)}_{23}(\boldsymbol{r}_{23};-\boldsymbol{k}_{23\mathrm{f}}) + \frac{\mathrm{i}\mu_{23}}{4\pi\hbar^2}\frac{\mathrm{e}^{\mathrm{i}k_{23\mathrm{f}}r_{23}}}{Br_{23}^2}\big[\langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|-k_{23\mathrm{f}}\boldsymbol{\nu}_B\rangle\,\mathrm{e}^{-\mathrm{i}Br_{23}} - \langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|k_{23\mathrm{f}}\boldsymbol{\nu}_B\rangle\,\mathrm{e}^{\mathrm{i}Br_{23}}\big]\Big\}. \tag{200 c}$$

Rewriting (175 b) in the same way, we obtain

$$\bar{T}^{t}_{2312}(\boldsymbol{k}_{\mathrm{i}}\to\boldsymbol{k}_{\mathrm{f}}) = \langle \boldsymbol{k}_{23\mathrm{f}}|\,\boldsymbol{t}_{23\mathrm{f}}\,|-\boldsymbol{B}\rangle\Big\{F_{12}(\boldsymbol{k}_{12\mathrm{i}};\boldsymbol{A};\boldsymbol{t}_{12\mathrm{i}}) + \frac{\mu_{12}}{\hbar^2}\Big[\frac{\langle k_{12\mathrm{i}}\boldsymbol{\nu}_A|\,\boldsymbol{t}_{12\mathrm{i}}\,|\boldsymbol{k}_{12\mathrm{i}}\rangle}{A(k_{12\mathrm{i}}-A)} - \frac{\langle -k_{12\mathrm{i}}\boldsymbol{\nu}_A|\,\boldsymbol{t}_{12\mathrm{i}}\,|\boldsymbol{k}_{12\mathrm{i}}\rangle}{A(k_{12\mathrm{i}}+A)}\Big]\Big\} \tag{201 a}$$

where

$$F_{12}(\boldsymbol{k}_{12\mathrm{i}};\boldsymbol{A};\boldsymbol{t}_{12\mathrm{i}}) = \int \mathrm{d}\boldsymbol{r}_{12}\Big\{\mathrm{e}^{-\mathrm{i}\boldsymbol{r}_{12}\cdot\boldsymbol{A}}\,\phi^{(+)}_{12}(\boldsymbol{r}_{12};\boldsymbol{k}_{12\mathrm{i}}) + \frac{\mathrm{i}\mu_{12}}{4\pi\hbar^2}\frac{\mathrm{e}^{\mathrm{i}k_{12\mathrm{i}}r_{12}}}{Ar_{12}^2}\big[\langle k_{12\mathrm{i}}\boldsymbol{\nu}_A|\,\boldsymbol{t}_{12\mathrm{i}}\,|\boldsymbol{k}_{12\mathrm{i}}\rangle\,\mathrm{e}^{-\mathrm{i}Ar_{12}} - \langle -k_{12\mathrm{i}}\boldsymbol{\nu}_A|\,\boldsymbol{t}_{12\mathrm{i}}\,|\boldsymbol{k}_{12\mathrm{i}}\rangle\,\mathrm{e}^{\mathrm{i}Ar_{12}}\big]\Big\}. \tag{201 b}$$

With the aid of (131 f) and the two-particle analogue of (63 a), equation (73 b) takes the form

$$\phi^{(+)}_{12}(\boldsymbol{r}_{12};\boldsymbol{k}_{12\mathrm{i}}) = -\int \mathrm{d}\boldsymbol{r}'_{12}\,g^{(+)}_{12F}(\boldsymbol{r}_{12};\boldsymbol{r}'_{12};E_{12\mathrm{i}})\int \mathrm{d}\boldsymbol{r}''_{12}\,\boldsymbol{t}_{12}(\boldsymbol{r}'_{12};\boldsymbol{r}''_{12};E_{12\mathrm{i}})\exp\{\mathrm{i}\boldsymbol{k}_{12\mathrm{i}}\cdot\boldsymbol{r}''_{12}\} \tag{202 a}$$

$$= -\lim_{\epsilon\to0}\int \mathrm{d}\boldsymbol{r}'_{12}\,\mathrm{d}\boldsymbol{r}''_{12}\,g_{12F}(\boldsymbol{r}_{12};\boldsymbol{r}'_{12};\lambda)\,\boldsymbol{t}_{12}(\boldsymbol{r}'_{12};\boldsymbol{r}''_{12};\lambda)\exp\{\mathrm{i}\boldsymbol{k}_{12\mathrm{i}}\cdot\boldsymbol{r}''_{12}\} \tag{202 b}$$

$$\equiv -\lim_{\epsilon\to0} g_{12F}(\lambda)\,\boldsymbol{t}_{12}(\lambda)\,\psi_{12\mathrm{i}}(\boldsymbol{k}_{12\mathrm{i}}), \tag{202 c}$$

where $\psi_{12\mathrm{i}}$ is defined by (74 a), and

$$\lambda = E_{12\mathrm{i}}+\mathrm{i}\epsilon = \frac{\hbar^2k_{12\mathrm{i}}^2}{2\mu_{12}}+\mathrm{i}\epsilon. \tag{202 d}$$

Then from (201 b) we see

$$F_{12}(\boldsymbol{k}_{12\mathrm{i}};\boldsymbol{A};\boldsymbol{t}_{12\mathrm{i}}) = \int \mathrm{d}\boldsymbol{r}_{12}\lim_{\epsilon\to0}\Big\{-\mathrm{e}^{\mathrm{i}\boldsymbol{r}_{12}\cdot\boldsymbol{A}}\,g_{12F}(\lambda)\,\boldsymbol{t}_{12}(\lambda)\,\psi_{12\mathrm{i}}(\boldsymbol{k}_{12\mathrm{i}}) + \frac{\mathrm{i}\mu_{12}}{4\pi\hbar^2}\frac{\exp\{\mathrm{i}(2\mu_{12}\lambda/\hbar^2)^{\frac{1}{2}}r_{12}\}}{Ar_{12}^2} \times\big[\langle k_{12\mathrm{i}}\boldsymbol{\nu}_A|\,\boldsymbol{t}_{12\mathrm{i}}\,|\boldsymbol{k}_{12\mathrm{i}}\rangle\,\mathrm{e}^{-\mathrm{i}Ar_{12}} - \langle -k_{12\mathrm{i}}\boldsymbol{\nu}_A|\,\boldsymbol{t}_{12\mathrm{i}}\,|\boldsymbol{k}_{12\mathrm{i}}\rangle\,\mathrm{e}^{\mathrm{i}Ar_{12}}\big]\Big\}. \tag{203 a}$$

But, by our usual rule (§ A. 8), interchange of order of integration and limit $\epsilon \to 0$ is permissible in (203 *a*), because the integral (201 *b*) is convergent (except at $A = \pm k_{12i}$). Hence

$$F_{12}(\boldsymbol{k}_{12i}; \boldsymbol{A}; \boldsymbol{t}_{12i}) = \lim_{\epsilon \to 0} \int \mathrm{d}\boldsymbol{r}_{12} \Big\{ -\mathrm{e}^{-\mathrm{i}\boldsymbol{r}_{12}\cdot\boldsymbol{A}}\, g_{12F}(\lambda)\, \boldsymbol{t}_{12}(\lambda)\, \psi_{12i}(\boldsymbol{k}_{12i}) + \frac{\mathrm{i}\mu_{12}}{4\pi\hbar^2} \frac{\exp\{\mathrm{i}(2\mu_{12}\lambda/\hbar^2)^{\frac{1}{2}} r_{12}\}}{A r_{12}^2} \times [\langle k_{12i}\boldsymbol{\nu}_A | \boldsymbol{t}_{12i} | \boldsymbol{k}_{12i}\rangle \mathrm{e}^{-\mathrm{i}Ar_{12}} - \langle -k_{12i}\boldsymbol{\nu}_A | \boldsymbol{t}_{12i} | \boldsymbol{k}_{12i}\rangle \mathrm{e}^{\mathrm{i}Ar_{12}}] \Big\}, \quad (203\,b)$$

where now each of the terms inside the braces in (203 *b*) are individually convergent integrals.

Using the expansion
$$g_{12F}(\boldsymbol{r}_{12}; \boldsymbol{r}'_{12}; \lambda) = \frac{1}{(2\pi)^3} \int \mathrm{d}\hat{\boldsymbol{k}}_{12} \frac{\exp \mathrm{i}\hat{\boldsymbol{k}}_{12}\cdot(\boldsymbol{r}_{12} - \boldsymbol{r}'_{12})}{(\hbar^2 \hat{k}_{12}^2/2\mu_{12}) - \lambda} \quad (204)$$

the integrals (203 *b*) yield

$$F_{12}(\boldsymbol{k}_{12i}; \boldsymbol{A}; \boldsymbol{t}_{12i}) = \lim_{\epsilon \to 0} \frac{2\mu_{12}}{\hbar^2} \Big\{ -\frac{\langle \boldsymbol{A} | \boldsymbol{t}_{12}(\lambda) | \boldsymbol{k}_{12i}\rangle}{A^2 - (2\mu_{12}\lambda/\hbar^2)} + \frac{1}{2} \frac{\langle k_{12i}\boldsymbol{\nu}_A | \boldsymbol{t}_{12i} | \boldsymbol{k}_{12i}\rangle}{A[A - (2\mu_{12}\lambda/\hbar^2)^{\frac{1}{2}}]} + \frac{1}{2} \frac{\langle -k_{12i}\boldsymbol{\nu}_A | \boldsymbol{t}_{12i} | \boldsymbol{k}_{12i}\rangle}{A[A + (2\mu_{12}\lambda/\hbar^2)^{\frac{1}{2}}]} \Big\} \quad (205\,a)$$

Hence, evaluating the limit $\epsilon \to 0$ in (204 *a*), we obtain finally

$$F_{12}(\boldsymbol{k}_{12i}; A\boldsymbol{\nu}_A; \boldsymbol{t}_{12i}) = \frac{2\mu_{12}}{\hbar^2} \Big\{ -\frac{\langle A\boldsymbol{\nu}_A | \boldsymbol{t}_{12i} | \boldsymbol{k}_{12i}\rangle}{A^2 - k_{12i}^2} + \frac{1}{2} \frac{\langle k_{12i}\boldsymbol{\nu}_A | \boldsymbol{t}_{12i} | \boldsymbol{k}_{12i}\rangle}{A(A - k_{12i})} + \frac{1}{2} \frac{\langle -k_{12i}\boldsymbol{\nu}_A | \boldsymbol{t}_{12i} | \boldsymbol{k}_{12i}\rangle}{A(A + k_{12i})} \Big\}. \quad (205\,b)$$

The result (205 *b*) is well-defined and finite at all values of $\boldsymbol{A}$, $\boldsymbol{k}_{12i}$ such that $A \neq \pm k_{12i}$. In fact, (205 *b*) is finite even at $A \pm k_{12i}$—where the integral (201 *b*) (from which we deduced (205 *b*)) diverges—provided it is understood that the values of F_{12} at $A = \pm k_{12i}$ are given by the limits of (205 *b*) as $A \to \pm k_{12i}$, namely

$$F_{12}(\boldsymbol{k}_{12i}; k_{12i}\boldsymbol{\nu}_A; \boldsymbol{t}_{12i}) \equiv \lim_{A \to k_{12i}} F_{12} = \frac{\mu_{12}}{2\hbar^2 k_{12i}^2} \langle -k_{12i}\boldsymbol{\nu}_A | \boldsymbol{t}_{12i} | \boldsymbol{k}_{12i}\rangle \quad (205\,c)$$

$$F_{12}(\boldsymbol{k}_{12i}; -k_{12i}\boldsymbol{\nu}_A; \boldsymbol{t}_{12i}) \equiv \lim_{A \to -k_{12i}} F_{12} = \frac{\mu_{12}}{2\hbar^2 k_{12i}^2} \langle k_{12i}\boldsymbol{\nu}_A | \boldsymbol{t}_{12i} | \boldsymbol{k}_{12i}\rangle. \quad (205\,d)$$

Equations (205 *c*) and (205 *d*) are consistent with each other, in the sense that changing $\boldsymbol{\nu}_A$ to $-\boldsymbol{\nu}_A$ in (205 *c*) gives (205 *d*).

Combining (205 *b*) and (201) leads to

$$\overline{T}^t_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = -\frac{2\mu_{12}}{\hbar^2} \frac{\langle \boldsymbol{k}_{23f} | \boldsymbol{t}_{23f} | -\boldsymbol{B}\rangle \langle \boldsymbol{A} | \boldsymbol{t}_{12i} | \boldsymbol{k}_{12i}\rangle}{A^2 - k_{12i}^2} \quad (206)$$

valid at $A^2 \neq k_{12i}^2$. Equation (206), which has been deduced from (175 *b*), obviously is a generally more convenient and more readily interpretable formula for $\overline{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ than is (175 *b*) itself. Similarly, (200 *c*) leads to

$$F_{23}(\boldsymbol{k}_{23f}; B\boldsymbol{\nu}_B; \boldsymbol{t}_{23f}) = \frac{2\mu_{23}}{\hbar^2} \Big\{ -\frac{\langle B\boldsymbol{\nu}_B | \boldsymbol{t}_{23f} | -\boldsymbol{k}_{23f}\rangle}{B^2 - k_{23f}^2} + \frac{1}{2} \frac{\langle \boldsymbol{k}_{23f} | \boldsymbol{t}_{23f} | -k_{23f}\boldsymbol{\nu}_B\rangle}{B(B - k_{23f})} + \frac{1}{2} \frac{\langle \boldsymbol{k}_{23f} | \boldsymbol{t}_{23f} | k_{23f}\boldsymbol{\nu}_B\rangle}{B(B + k_{23f})} \Big\} \quad (207)$$

which, when combined with (200), yields

$$\overline{T}^t_{1223}(-\boldsymbol{k}_f \to -\boldsymbol{k}_i) = -\frac{2\mu_{23}}{\hbar^2} \frac{\langle \boldsymbol{A} | \boldsymbol{t}_{12i} | \boldsymbol{k}_{12i}\rangle \langle \boldsymbol{B} | \boldsymbol{t}_{23f} | -\boldsymbol{k}_{23f}\rangle}{B^2 - k_{23f}^2} \quad (208)$$

valid at $B^2 \neq k_{23f}^2$.

Using (194 *a*) and (195 *b*), we now see that (206) and (208) indeed are consistent with the detailed balancing relation (180 *b*), Q.E.D. I further note that according to (173 *b*) the term involving $(k_{12i}-A)^{-1}$ in (175 *b*) should be dropped at $A = k_{12i}$; correspondingly, the term in (175 *b*) involving $(k_{12i}+A)^{-1}$ should be dropped when $A = -k_{12i}$. If these strictures are included in (201 *a*), and then combined with (205 *c*) and (205 *d*), we see that (206) should be supplemented by

$$\bar{T}^t_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = 0 \tag{209 a}$$

at $A^2 = k^2_{12i}$. Similarly (208) is supplemented by

$$\bar{T}^t_{1223}(-\boldsymbol{k}_f \to -\boldsymbol{k}_i) = 0 \tag{209 b}$$

at $B^2 = k^2_{23f}$, again consistent with detailed balancing. For completeness, I also note that (175 *c*) reduces to

$$\bar{T}^t_{2331}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = -\frac{2\mu_{31}}{\hbar^2}\frac{\langle \boldsymbol{k}_{23f}|\, \boldsymbol{t}_{23f}\,|\boldsymbol{D}\rangle\langle -\boldsymbol{C}|\, \boldsymbol{t}_{31i}\,|\boldsymbol{k}_{31i}\rangle}{C^2 - k^2_{31i}} \tag{210 a}$$

at $C^2 \neq k^2_{31i}$, supplemented by $\qquad \bar{T}^t_{2331}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = 0 \tag{210 b}$

at $C^2 = k^2_{31i}$.

I close this section with two remarks. First, because our conclusion that the detailed balancing relation (180 *b*) is satisfied rests so heavily on the result (205 *b*), in appendix A. 10 I deduce (205 *b*) from (201 *b*) by a method which avoids the (made to seem reasonable, but not really proved in Appendix A. 8) interchange (203 *a*) and (203 *b*) of order of integration and limit $\epsilon \to 0$; this alternative derivation confirms the conclusions of the present subsection and provides further evidence that our claims and arguments in Appendix A. 8 really are correct. Secondly, it readily can be verified that (175 *b*) and (175 *c*) would not be consistent with (180 *b*) if the contributions (173 *a*) to the singular integrals in (172 *a*) had been omitted.†

5.3. *Momentum space procedures*

The iterations which have been employed in this work on numerous occasions—to obtain, for example, (64) or (162)—clearly are independent of representation, i.e. equally well could have been performed in momentum space. Moreover, relations such as (63), (81) and the three-particle analogue of (131 *h*) ultimately make it possible to express all iterations of the scattered wave $\Phi_i^{(+)}$—or of various contributions to $\Phi_i^{(+)}$ such as $\Phi^{s(+)}_{\alpha\beta}$ of (161)—in terms of expressions beginning with $G_F^{(+)}$ (that is to say, expressions whose left-most factor is $G_F^{(+)}$) and whose right-most factor is ψ_i. In addition, as (96) argues and (90) make explicit, it is the case that the limit of $G_F^{(+)}(\boldsymbol{r};\boldsymbol{r}';E)$ as $\boldsymbol{r} \to \infty$ is proportional to $\psi_f^*(\boldsymbol{r}')$ defined by (100 *c*). Therefore, granting that the variety of possible iterations must lead to self-consistent results provided questions concerning convergence and interchanging orders of integration can be ignored, it really is not surprising that the transition amplitude matrix elements obtained from our configuration space approach agree formally with the corresponding matrix elements in the more customary momentum space procedures.

Thus, for example, it is no surprise that (187) take the form they do. In the discussion of (165) and (166) we have argued that $\bar{T}^d(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ defined by (165 *b*) represents the contribution to $\bar{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ resulting from scattering processes involving three or more successive purely two-body collisions. Hence (187 *b*) merely states that $\langle f|\, \bar{\boldsymbol{T}}\,|i\rangle$ consists of $\bar{T}^d(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ plus the contributions $\langle f|\, \bar{\boldsymbol{T}}_{\alpha\beta}\,|i\rangle$ from individual purely two-body collisions, plus the contributions

† Recall the footnote, p. 265.

$-\langle \mathrm{f}|\, \bar{\boldsymbol{T}}_{\alpha\beta}\bar{G}_F\bar{\boldsymbol{T}}_{\gamma\delta}\,|\mathrm{i}\rangle$ from all possible pairs of successive purely two-body collisions; that the minus signs in (187 *b*) preceding the double scattering matrix elements are consistent with this interpretation follows from (133 *b*) and (137). In the text I have given a long-winded derivation of (187 *a*) (which except for its explicit inclusion of the limit $\epsilon\to 0$ is the same as (187 *b*)) only because I have insisted: (i) on starting from an expression (165 *b*) for $\bar{T}^d(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f})$ composed solely of convergent integrals, and (ii) on employing no mathematically illegitimate manipulations in going from (165 *b*) to (187 *a*). If I am willing to employ mathematically questionable operations, (187 *b*) can be derived more readily than was (187 *a*). Specifically, start from (131 *d*), which with the aid of (63) can be rewritten in the form (once again simplifying the notation by dropping the bars)

$$\begin{aligned}\psi_\mathrm{f}^*\,\boldsymbol{T}\psi_\mathrm{i} &= \psi_\mathrm{f}^*(V-VGV)\,\psi_\mathrm{i}\\ &= \psi_\mathrm{f}^*\{V-V[G_{12}-G(V_{23}+V_{31})\,G_{12}]\,V_{12}-V[G_{23}-G(V_{31}+V_{12})\,G_{23}]\,V_{23}\\ &\quad -V[G_{31}-G(V_{12}+V_{23})\,G_{31}]\,V_{31}\}\psi_\mathrm{i} \qquad (211\,a)\\ &= \psi_\mathrm{f}^*\{V-V_{12}G_{12}V_{12}-(V_{23}+V_{31})\,G_{12}V_{12}+VG(V_{23}+V_{31})\,G_{12}V_{12}\\ &\quad -V_{23}G_{23}V_{23}-(V_{31}+V_{12})\,G_{23}V_{23}+VG(V_{31}+V_{12})\,G_{23}V_{23}\\ &\quad -V_{31}G_{31}V_{31}-(V_{12}+V_{23})\,G_{31}V_{31}+VG(V_{12}+V_{23})\,G_{31}V_{31}\}\psi_\mathrm{i}. \qquad (211\,b)\end{aligned}$$

Next, employ (60) and (77 *a*), which reduce (211 *b*) to

$$\begin{aligned}\psi_\mathrm{f}^*\,\boldsymbol{T}\psi_\mathrm{i} = \psi_\mathrm{f}^*(\boldsymbol{T}_{12}+\boldsymbol{T}_{23}+\boldsymbol{T}_{31})\,\psi_\mathrm{i}-\psi_\mathrm{f}^*(-1+VG)\,(V_{23}+V_{31})\,\Phi_{12}^{(+)}\\ -\psi_\mathrm{f}^*(-1+VG)\,(V_{31}+V_{12})\,\Phi_{23}^{(+)}-\psi_\mathrm{f}^*(-1+VG)\,(V_{12}+V_{23})\,\Phi_{31}^{(+)}, \qquad (211\,c)\end{aligned}$$

and then use (100 *b*), which converts (211 *c*) to

$$\psi_\mathrm{f}^*\,\boldsymbol{T}\psi_\mathrm{i} = \psi_\mathrm{f}^*(\boldsymbol{T}_{12}+\boldsymbol{T}_{23}+\boldsymbol{T}_{31})\,\psi_\mathrm{i}+\Psi_\mathrm{f}^{(-)*}[(V_{23}+V_{31})\,\Phi_{12}^{(+)}+(V_{31}+V_{12})\,\Phi_{23}^{(+)}+(V_{12}+V_{23})\,\Phi_{31}^{(+)}]. \qquad (211\,d)$$

The $\Psi_\mathrm{f}^{(-)*}$ terms in (211 *d*) are precisely $T^s(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f})$ of (133 *b*); equations (137) and (169 *c*) have shown

$$\begin{aligned}T^s(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) = T^d(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f})-\psi_\mathrm{f}^*[\boldsymbol{T}_{23}G_F\,\boldsymbol{T}_{12}+\boldsymbol{T}_{23}G_F\,\boldsymbol{T}_{31}\\ +\boldsymbol{T}_{31}G_F\,\boldsymbol{T}_{23}+\boldsymbol{T}_{31}G_F\,\boldsymbol{T}_{12}+\boldsymbol{T}_{12}G_F\,\boldsymbol{T}_{31}+\boldsymbol{T}_{12}G_F\,\boldsymbol{T}_{23}]\psi_\mathrm{i}. \qquad (211\,e)\end{aligned}$$

Equations (211 *d*) and (211 *e*) yield (187 *b*).

5.3.1. *Diagrammatic techniques*

The above derivation of (187 *b*), as well as the derivation of (187 *a*) in § 5.2.1, can be paralleled step by step in the momentum representation. Alternatively, one can obtain a quite direct and simple demonstration of (187 *b*) via diagrammatic techniques (Watson & Nuttall 1967; Weinberg 1964). Although it really is not necessary to do so, we already have two independent derivations of (187 *b*), for completeness sake I shall give this diagrammatic derivation. It is convenient first to introduce as propagators the negatives of the Green functions we have been using; in this section these negatives will be denoted by the caret, i.e. $\hat{G}=-G$, $\hat{G}_F=-G_F$, $\hat{g}_{12}=-g_{12}$, etc. Then (131 *f*) becomes

$$\boldsymbol{t}_{12} = \boldsymbol{V}_{12}+V_{12}\hat{g}_{12}V_{12}. \qquad (212\,a)$$

Correspondingly, the two-particle analogue of (81) is

$$\hat{g}_{12} = \hat{g}_F+\hat{g}_F V_{12}\hat{g}_{12}. \qquad (212\,b)$$

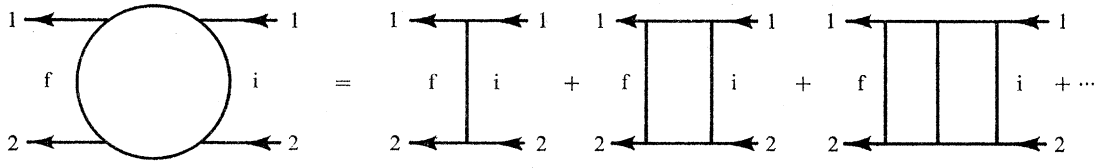
Using (212 *b*) to iterate (212 *a*) yields

$$t_{12} = V_{12} + V_{12}\hat{g}_F V_{12} + V_{12}\hat{g}_F V_{12}\hat{g}_F V_{12} + \ldots, \tag{212 c}$$

wherein all terms are of positive sign (the reason for introducing these careted propagators in place of our former g_F, g_{12}). Taking matrix elements of (212 *c*),

$$\overline{\psi}^*_{12\mathrm{f}} t_{12} \overline{\psi}_{12\mathrm{i}} = \overline{\psi}^*_{12\mathrm{f}} V_{12} \overline{\psi}_{12\mathrm{i}} + \overline{\psi}^*_{12\mathrm{f}} V_{12}\hat{g}_F V_{12} \overline{\psi}_{12\mathrm{i}} + \overline{\psi}^*_{12\mathrm{f}} V_{12}\hat{g}_F V_{12}\hat{g}_F V_{12} \overline{\psi}_{12\mathrm{i}} + \ldots. \tag{212 d}$$

Equation (212 *d*) can be represented diagrammatically by



(213)

where the rules for constructing the matrix element counterpart to any individual diagram on the right side of (213) are obvious; it only is necessary to remember that between any pair of successive vertical lines connecting 1 and 2 the particles propagate freely, i.e. in each matrix element the free particle propagator $\hat{g}_F$ separates successive interactions V_{12}. Placing the initial state on the right and the final state on the left, as in the matrix elements (212 *d*) themselves, minimizes possible confusion in interpreting the diagrams; in other words, we suppose the system evolves from right to left as indicated by the arrows. The bubble diagram on the left denotes the sum of the diagrams on the right; equivalently, the bubble diagram denotes the matrix element of $t_{12}(r_{12}; r'_{12})$ itself.

Similarly, in the three-particle system (again dropping the bars), where

$$T = V + V\hat{G}V, \tag{214 a}$$

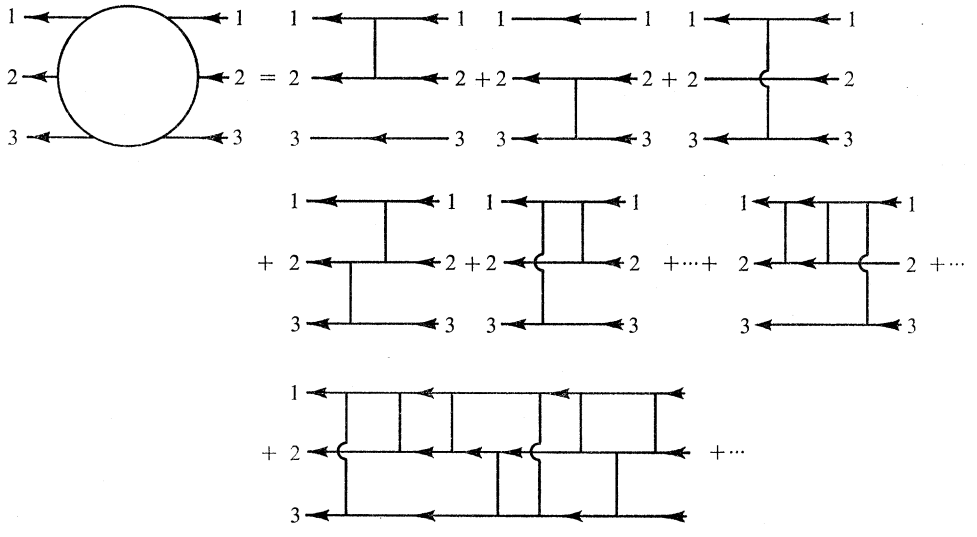
using

$$\hat{G} = \hat{G}_F + \hat{G}_F V\hat{G}, \tag{214 b}$$

obviously leads to

$$T = V_{12} + V_{23} + V_{31} + V_{23}\hat{G}_F V_{12} + V_{31}\hat{G}_F V_{12} + \ldots + V_{12}\hat{G}_F V_{12}\hat{G}_F V_{31} + \ldots$$
$$+ V_{31}\hat{G}_F V_{12}\hat{G}_F V_{12}\hat{G}_F V_{23}\hat{G}_F V_{31}\hat{G}_F V_{12}\hat{G}_F V_{23}\hat{G}_F V_{12} + \ldots. \tag{214 c}$$

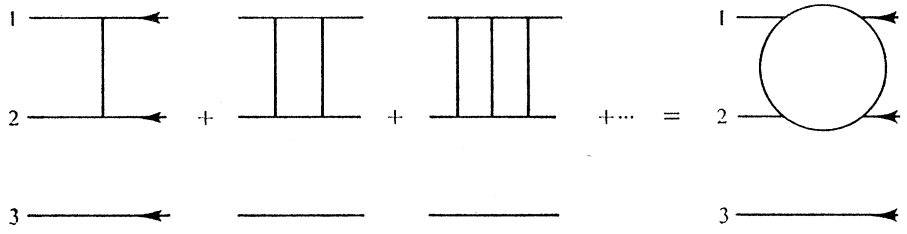
That is to say, every possible sequence (with repeats) of the three interactions V_{12}, V_{23}, V_{31} occurs in the iteration of T. Correspondingly we have the diagrammatic representation



(215)

where the super-bubble in (215) denotes $\langle f|\, \boldsymbol{T}\,|i\rangle$, and where on the right side of (215) there occurs every possible diagram constructed from successive vertical lines V_{12}, V_{23} or V_{31} connecting pairs of the horizontal lines 1, 2, 3. Actually (215) has been drawn so that the individual diagrams therein are the counterparts of the particular terms included in (214 *c*).

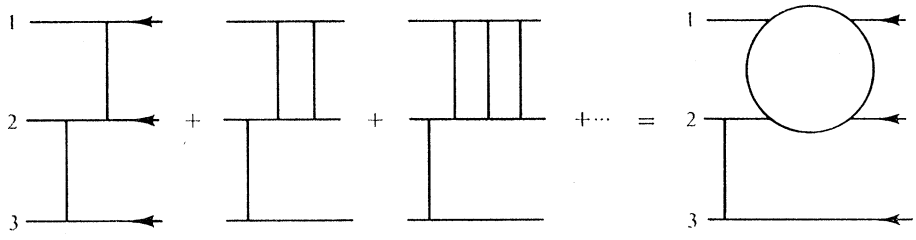
Now consider the first diagram on the right side of (215), representing the matrix element $\langle f|\, V_{12}\,|i\rangle$. Evidently this diagram is the first in a whole sequence of diagrams on the right side of (215), each of which is composed solely of interactions V_{12}. In other words, on the right side of (215) I can single out the sum of diagrams



(216 *a*)

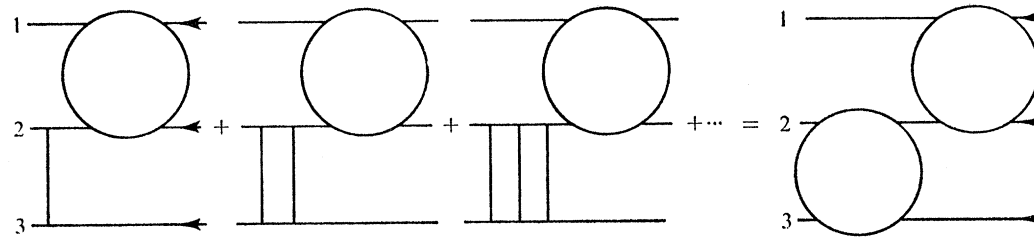
where the bubble on the right side of (216 *a*) now denotes the matrix element $\psi_f^*\, \boldsymbol{T}_{12}\, \psi_i$. This bubble must be identified with the matrix element of the three-particle $\boldsymbol{T}_{12}$ of (77 *a*)—rather than with the two-particle $\boldsymbol{t}_{12}$ of (131*f*) and the bubble in (213)—because in (214 *a*) $\boldsymbol{V}_{12}(\boldsymbol{r};\boldsymbol{r}')$ is proportional to the three-particle $\delta(\boldsymbol{r}-\boldsymbol{r}')$ of (27 *e*), rather than merely to the two-particle $\delta(\boldsymbol{r}_{12}-\boldsymbol{r}'_{12})$ of (131*f*); correspondingly, the matrix element counterparts of the diagrams in (216 *a*) involve the three-particle free space propagator $\hat{G}_F = -G_F$ we have used throughout, and are taken between the three-particle plane wave states ψ_f, ψ_i of (100 *c*), (21 *a*) respectively.

Next consider, for example, the fourth diagram on the right side of (215). Then on the right side of (215) I first can single out the sum of diagrams



(216 *b*)

followed by the sum of sums



(216 *c*)

The diagram on the right side of (216 *c*) obviously denotes a $\psi_f^*\, \boldsymbol{T}_{23}\, \hat{G}_F\, \boldsymbol{T}_{12}\, \psi_i$ contribution to the overall sum on the right side of (216 *a*). Similarly, starting with the last diagram (I will call it D) on the right side of (215), I first sum those diagrams which repeat the right-most interaction V_{12}, obtaining a sum represented by a diagram identical with D, except that $\boldsymbol{T}_{12}$ replaces V_{12} on the right. Next I sum the sums in which $\boldsymbol{T}_{12}$ has replaced V_{12} on the right side of D, but in which the

interaction V_{23} immediately to the left of T_{12} is repeated. Evidently, proceeding in this fashion, I single out in (215) a collection of diagrams associated with D whose sum represents the matrix element

$$\psi_f^* T_{31} \hat{G}_F T_{12} \hat{G}_F T_{12} \hat{G}_F T_{23} \hat{G}_F T_{31} \hat{G}_F T_{12} \hat{G}_F T_{23} \hat{G}_F T_{12} \psi_i.$$

It is now apparent that (215) yields

$$\psi_f^* T \psi_i = \psi_f^* \{T_{12} + T_{23} + T_{31} + T_{23} \hat{G}_F T_{12} + T_{23} \hat{G}_F T_{31} + T_{31} \hat{G}_F T_{23} + T_{31} \hat{G}_F T_{12} + T_{12} \hat{G}_F T_{31} + T_{12} \hat{G}_F T_{23}\} \psi_i + T^d(\boldsymbol{k}_i \to \boldsymbol{k}_f), \quad (217\,a)$$

where T^d can be thought to consist of all matrix elements corresponding to $n \geqslant 3$ successive two-body scatterings, i.e.

$$T^d(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \psi_f^* \{T_{23} \hat{G}_F T_{12} \hat{G}_F T_{31} + T_{23} \hat{G}_F T_{12} \hat{G}_F T_{23} + \ldots + T_{23} \hat{G}_F T_{12} \hat{G}_F T_{31} \hat{G}_F T_{23} + \ldots\} \psi_i. \quad (217\,b)$$

Replacing $\hat{G}_F$ in (217) by $-G_F$, and recalling (165 b) and (166 b), we see that (217 a), signs and all, is identical with (the laboratory frame version of) (187 b).

5.3.2. *Single and double scattering diagrams*

Thus far this section 5.3 has made it clear that our configuration space expressions for $\langle f| \bar{\boldsymbol{T}} |i\rangle \equiv \bar{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ agree formally with expressions for $\langle f| \bar{\boldsymbol{T}} |i\rangle$ derived via momentum space procedures, and that they should be expected to manifest such agreement. On the other hand, this assertion, important though it is, does not of itself imply that reaction rates computed using our configuration space expressions necessarily will agree with the results of reaction rate computations using momentum space expressions. In the first place, the whole possibility of demonstrating a correspondence between configuration space and momentum space formulations depends on being able to interchange order of integration and limit $\bar{\boldsymbol{r}} \to \infty$ in various integral expressions for $\bar{\Phi}_i^{(+)}$ or parts of $\bar{\Phi}_i^{(+)}$, as discussed in chapter 4; without this interchange, the configuration space results for probability current flow cannot be expressed in terms of matrix elements (such as $\bar{\psi}_f^* V \bar{\Phi}_i^{(+)}$, $\bar{\Phi}_f^{(-)*} V_{23} \bar{\Phi}_{12}^{s(+)}$, etc.) ultimately identifiable with momentum space matrix elements composing all or part of $\langle f| \bar{\boldsymbol{T}} |i\rangle$. Moreover, the aforementioned formal agreement between the configuration space and momentum space expressions for $\langle f| \bar{\boldsymbol{T}} |i\rangle$ has been established without regard to the possible influences of manipulations such as: (i) interchange of orders of integration, (ii) interchange of order of integration and limit $\epsilon \to 0$ in $\langle f| \bar{\boldsymbol{T}}(\bar{E} + i\epsilon) |i\rangle$, and (iii) Fourier transformation, i.e. transformation from the coordinate to momentum representations. Such manipulations, if not legitimate, can produce differences in the numerical values of matrix elements which are formally identical, and strict proofs of legitimacy are hard to come by; in fact, it already has been pointed out, in connexion with (51 c), (51 d) and (131 d), that the relations

$$\bar{\psi}_f^* V \bar{\Psi}_i^{(+)} = \bar{\psi}_f^* \bar{\boldsymbol{T}}(\bar{E}) \bar{\psi}_i = \lim_{\epsilon \to 0} \bar{\psi}_f^* \bar{\boldsymbol{T}}(\bar{E} + i\epsilon) \bar{\psi}_i \quad (218)$$

need not hold. However, as so often argued in this work, it is reasonable to assume that manipulations which at no step involve divergences indeed are justified.

Let me now assess the significance of (187 b) in the light of the above remarks. The discussion of (165 a) has explained that the interchange of order of integration and limit $\bar{\boldsymbol{r}} \to \infty$ yielding (165 b) is justified, except possibly along an inconsequential set of special $\bar{\boldsymbol{\nu}}_f$. Correspondingly, $\bar{T}^d(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ is composed of convergent integrals, except possibly along an inconsequential set of

special $\boldsymbol{k}_f$; moreover, because the integrals in (165 *b*) are convergent, manipulations such as those in (166 *b*) are legitimate. It follows that the quantity $\bar{T}^d(\boldsymbol{k}_i \to \boldsymbol{k}_f)$, here defined as the contribution to $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ or $\bar{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ associated with $n \geqslant 3$ successive two-body scatterings, should yield the same values whether computed in momentum space or in configuration space (except possibly along an inconsequential set of special $\boldsymbol{k}_f$). As it happens it is the carefully proved (187 *a*), rather than (187 *b*), which provides the mathematical statement of the immediately preceding assertion concerning $\bar{T}^d(\boldsymbol{k}_i \to \boldsymbol{k}_f)$, because in momentum space the scattering matrix elements comprised in $\langle f| \bar{\boldsymbol{T}}(\bar{E}) |i\rangle$ customarily are computed from the limit $\epsilon \to 0$ of the corresponding matrix elements in $\langle f| \bar{\boldsymbol{T}}(\bar{E}+i\epsilon) |i\rangle$. To put it differently, in the momentum space formalism the contributions to the total scattering amplitude $\bar{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ made by, for example the diagrams on the right sides of (216 *a*), (216 *c*) are respectively

$$\bar{T}_{12}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \lim_{\epsilon \to 0} \langle f| \bar{\boldsymbol{T}}_{12}(\bar{E}+i\epsilon) |i\rangle, \tag{219 a}$$

$$\bar{T}_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f) = \lim_{\epsilon \to 0} - \langle f| \bar{\boldsymbol{T}}_{23}(\bar{E}+i\epsilon)\, \bar{G}_F(\bar{E}+i\epsilon)\, \bar{\boldsymbol{T}}_{12}(\bar{E}+i\epsilon) |i\rangle, \tag{219 b}$$

where it is understood of course that for physically observable amplitudes $\bar{E} = \bar{E}_i = \bar{E}_f$. The relations (219) define the momentum space scattering amplitudes whether or not it is true that the corresponding relations

$$\lim_{\epsilon \to 0} \langle f| \bar{\boldsymbol{T}}_{12}(\bar{E}+i\epsilon) |i\rangle = \langle f| \bar{\boldsymbol{T}}_{12}(\bar{E}) |i\rangle \tag{220 a}$$

and

$$\lim_{\epsilon \to 0} - \langle f| \bar{\boldsymbol{T}}_{23}(\bar{E}+i\epsilon)\, \bar{G}_F(\bar{E}+i\epsilon)\, \bar{\boldsymbol{T}}_{12}(\bar{E}+i\epsilon) |i\rangle = - \langle f| \bar{\boldsymbol{T}}_{23}(\bar{E})\, \bar{G}_F^{(+)}(\bar{E})\, \bar{\boldsymbol{T}}_{12}(\bar{E}) |i\rangle \tag{220 b}$$

(involving interchange of order of integration and limit $\epsilon \to 0$) hold when these matrix elements are computed in the momentum representation.

In view of the foregoing, differences between configuration space and momentum space reaction rate predictions can stem only from the behaviour of matrix elements representing single or double scattering, i.e. from matrix elements of the types written down in (219) and (220); in the remainder of this section, therefore, we confine our attention to single and double scattering contributions to the scattering amplitude. For either of these types of scattering processes it was less obvious initially than in the case of $n \geqslant 3$ scattering processes that there would be a close agreement between configuration space and momentum space results, because for integral expressions representing those parts of $\Phi_i^{(+)}$ associated with $n = 1$ and $n = 2$ scattering processes interchange of order of integration and limit $\boldsymbol{r} \to \infty$ is not justified (recall chapter 4); correspondingly, when for these $n = 1$ and $n = 2$ processes this unjustified interchange of order of integration and limit $\boldsymbol{r} \to \infty$ was performed, the configuration space matrix elements obtained were divergent, implying that the (seemingly required for agreement between configuration space and momentum space predictions) manipulations (i) to (iii) listed in the opening paragraph of this subsection would have dubious validity. Nevertheless (as is detailed below) the momentum space and configuration space results for single and double scattering processes gratifyingly turn out to be actually identical, not merely formally identical.

Consider first the typical single scattering process represented by the diagram (216 *a*), whose contribution to the scattering amplitude is computed in momentum space via (219 *a*). I shall show that the formula (219 *a*) leads to precisely the same result for $\bar{T}_{12}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ as was obtained in § 4.1.2, wherein $\bar{T}_{12}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ was inferred for purely real energies ($\epsilon = 0$) via admittedly

mathematically incorrect relations such as (126 *a*) or (131 *b*). In effect, therefore, I am going to demonstrate that (220 *a*) really does hold. By definition (recalling also (33 *b*), (40 *b*) and (77 *a*))

$$\begin{aligned}\langle \mathrm{f}|\,\bar{\boldsymbol{T}}_{12}(\bar{E}_\mathrm{i}+\mathrm{i}\epsilon)\,|\mathrm{i}\rangle &= \int \mathrm{d}\bar{\boldsymbol{r}}\,\mathrm{d}\bar{\boldsymbol{r}}'\exp\{-\mathrm{i}(\boldsymbol{k}_{12\mathrm{f}}\cdot\boldsymbol{r}_{12}+\boldsymbol{K}_{12\mathrm{f}}\cdot\boldsymbol{q}_{12})\}\,\overline{T}_{12}(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}';\bar{E}_\mathrm{i}+\mathrm{i}\epsilon)\\ &\qquad\times\exp\{\mathrm{i}(\boldsymbol{k}_{12\mathrm{i}}\cdot\boldsymbol{r}'_{12}+\boldsymbol{K}_{12\mathrm{i}}\cdot\boldsymbol{q}'_{12})\}\\ &= \int \mathrm{d}\bar{\boldsymbol{r}}\,\mathrm{d}\bar{\boldsymbol{r}}'\overline{\psi}^*_\mathrm{f}(\bar{\boldsymbol{r}};\boldsymbol{k}_\mathrm{f})\,[V_{12}(\boldsymbol{r}_{12})\,\delta(\boldsymbol{r}_{12}-\boldsymbol{r}'_{12})\,\delta(\boldsymbol{q}_{12}-\boldsymbol{q}'_{12})\\ &\qquad-V_{12}(\boldsymbol{r}_{12})\,\bar{G}_{12}(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}';\bar{E}_\mathrm{i}+\mathrm{i}\epsilon)\,V_{12}(\boldsymbol{r}'_{12})]\,\overline{\psi}_\mathrm{i}(\bar{\boldsymbol{r}}';\boldsymbol{k}_\mathrm{i}).\end{aligned} \tag{221 a}$$

But
$$\begin{aligned}&\int \mathrm{d}\boldsymbol{r}_{12}\,\mathrm{d}\boldsymbol{q}_{12}\,\mathrm{d}\boldsymbol{r}'_{12}\,\mathrm{d}\boldsymbol{q}'_{12}\exp\{-\mathrm{i}(\boldsymbol{k}_{12\mathrm{f}}\cdot\boldsymbol{r}_{12}+\boldsymbol{K}_{12\mathrm{f}}\cdot\boldsymbol{q}_{12})\}V_{12}(\boldsymbol{r}_{12})\,\delta(\boldsymbol{r}_{12}-\boldsymbol{r}'_{12})\,\delta(\boldsymbol{q}_{12}-\boldsymbol{q}'_{12})\\ &\qquad\times\exp\{\mathrm{i}(\boldsymbol{k}_{12\mathrm{i}}\cdot\boldsymbol{r}'_{12}+\boldsymbol{K}_{12\mathrm{i}}\cdot\boldsymbol{q}'_{12})\}\\ &= (2\pi)^3\,\delta(\boldsymbol{K}_{12\mathrm{f}}-\boldsymbol{K}_{12\mathrm{i}})\int \mathrm{d}\boldsymbol{r}_{12}\,\mathrm{d}\boldsymbol{r}'_{12}\exp\{-\mathrm{i}\boldsymbol{k}_{12\mathrm{f}}\cdot\boldsymbol{r}_{12}\}V_{12}(\boldsymbol{r}_{12})\,\delta(\boldsymbol{r}_{12}-\boldsymbol{r}'_{12})\\ &\qquad\times\exp\{\mathrm{i}\boldsymbol{k}_{12\mathrm{i}}\cdot\boldsymbol{r}'_{12}\}.\end{aligned} \tag{221 b}$$

Also, using the appropriate analogue of (53 *a*) (see § D. 1), the integral involving $\bar{G}_{12}$ in (221 *a*) becomes

$$\begin{aligned}&-\frac{1}{(2\pi)^3}\int \mathrm{d}\boldsymbol{r}_{12}\,\mathrm{d}\boldsymbol{q}_{12}\,\mathrm{d}\boldsymbol{r}'_{12}\,\mathrm{d}\boldsymbol{q}'_{12}\exp\{-\mathrm{i}(\boldsymbol{k}_{12\mathrm{f}}\cdot\boldsymbol{r}_{12}+\boldsymbol{K}_{12\mathrm{f}}\cdot\boldsymbol{q}_{12})\}\exp\{\mathrm{i}(\boldsymbol{k}_{12\mathrm{i}}\cdot\boldsymbol{r}'_{12}+\boldsymbol{K}_{12\mathrm{i}}\cdot\boldsymbol{q}'_{12})\}\\ &\qquad\times V_{12}(\boldsymbol{r}_{12})\,V_{12}(\boldsymbol{r}'_{12})\int \mathrm{d}\hat{\boldsymbol{K}}_{12}\exp\{\mathrm{i}\hat{\boldsymbol{K}}_{12}\cdot(\boldsymbol{q}_{12}-\boldsymbol{q}'_{12})\,g_{12}\Big(\boldsymbol{r}_{12};\boldsymbol{r}'_{12};\bar{E}_\mathrm{i}-\frac{\hbar^2\hat{K}^2_{12}}{2\mu_{3R}}+\mathrm{i}\epsilon\Big)\\ &= -(2\pi)^3\,\delta(\boldsymbol{K}_{12\mathrm{i}}-\boldsymbol{K}_{12\mathrm{f}})\int \mathrm{d}\boldsymbol{r}_{12}\,\mathrm{d}\boldsymbol{r}'_{12}\exp\{-\mathrm{i}\boldsymbol{k}_{12\mathrm{f}}\cdot\boldsymbol{r}_{12}\}V_{12}(\boldsymbol{r}_{12})\,g_{12}\Big(\boldsymbol{r}_{12};\boldsymbol{r}'_{12};\frac{\hbar^2k^2_{12\mathrm{i}}}{2\mu_{12}}+\mathrm{i}\epsilon\Big)\\ &\qquad\times V_{12}(\boldsymbol{r}'_{12})\exp\{\mathrm{i}\boldsymbol{k}_{12\mathrm{i}}\cdot\boldsymbol{r}'_{12}\}\end{aligned} \tag{221 c}$$

Thus
$$\langle \mathrm{f}|\,\bar{\boldsymbol{T}}_{12}(\bar{E}_\mathrm{i}+\mathrm{i}\epsilon)\,|\mathrm{i}\rangle = (2\pi)^3\,\delta(\boldsymbol{K}_{12\mathrm{f}}-\boldsymbol{K}_{12\mathrm{i}})\,\langle \mathrm{f}|\,\boldsymbol{t}_{12}(E_{12\mathrm{i}}+\mathrm{i}\epsilon)\,|\mathrm{i}\rangle, \tag{222 a}$$

so that, recalling the remarks following (131 *e*), the definition (219 *a*) implies the momentum space contribution to $\overline{T}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f})$ made by the diagram (216 *a*) is

$$\overline{T}_{12}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) = (2\pi)^3\,\delta(\boldsymbol{K}_{12\mathrm{f}}-\boldsymbol{K}_{12\mathrm{i}})\,\langle \mathrm{f}|\,\boldsymbol{t}_{12}(E_{12\mathrm{i}})\,|\mathrm{i}\rangle, \tag{222 b}$$

where the matrix element on the right side of (222 *b*) is defined as in (131 *e*). Obviously (222 *b*) is identical with (130 *c*), recognizing that the left side of (130 *a*) is the configuration space expression for $\overline{T}_{12}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f})$.

Next consider the typical double scattering process represented by the diagram (216 *c*). Computed in momentum space the matrix element on the right side of (219 *b*) is, by definition

$$\frac{1}{(2\pi)^{12}}\int \mathrm{d}\boldsymbol{k}_{12}\,\mathrm{d}\boldsymbol{K}_{12}\,\mathrm{d}\boldsymbol{k}'_{12}\,\mathrm{d}\boldsymbol{K}'_{12}\langle \boldsymbol{k}_\mathrm{f}|\,\bar{\boldsymbol{T}}_{23}(\bar{E}_\mathrm{i}+\mathrm{i}\epsilon)\,|\boldsymbol{k}\rangle\,\langle \boldsymbol{k}|\,\bar{G}_F(\bar{E}_\mathrm{i}+\mathrm{i}\epsilon)\,|\boldsymbol{k}'\rangle\langle \boldsymbol{k}'|\,\bar{\boldsymbol{T}}_{12}(\bar{E}_\mathrm{i}+\mathrm{i}\epsilon)\,|\boldsymbol{k}_\mathrm{i}\rangle, \tag{223 a}$$

where the matrix elements of $\bar{\boldsymbol{T}}_{\alpha\beta}$ are given by (221) and (222), and where, again by definition,

$$\langle \boldsymbol{k}|\,\bar{G}_F(\bar{E}_\mathrm{i}+\mathrm{i}\epsilon)\,|\boldsymbol{k}'\rangle = \int \mathrm{d}\bar{\boldsymbol{r}}\,\mathrm{d}\bar{\boldsymbol{r}}'\overline{\psi}^*_\mathrm{f}(\bar{\boldsymbol{r}};\boldsymbol{k})\,\bar{G}_F(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}';\bar{E}_\mathrm{i}+\mathrm{i}\epsilon)\,\overline{\psi}_\mathrm{i}(\bar{\boldsymbol{r}}';\boldsymbol{k}'). \tag{223 b}$$

Using the expansion

$$\begin{aligned}\bar{G}_F(\bar{\boldsymbol{r}};\bar{\boldsymbol{r}}';\bar{E}_\mathrm{i}+\mathrm{i}\epsilon) &= \frac{1}{\bar{T}-\bar{E}_\mathrm{i}-\mathrm{i}\epsilon}\\ &= \frac{1}{(2\pi)^6}\int \mathrm{d}\hat{\boldsymbol{k}}_{12}\,\mathrm{d}\hat{\boldsymbol{K}}_{12}\,\frac{\exp\{\mathrm{i}[\hat{\boldsymbol{k}}_{12}\cdot(\boldsymbol{r}_{12}-\boldsymbol{r}'_{12})+\hat{\boldsymbol{K}}_{12}\cdot(\boldsymbol{q}_{12}-\boldsymbol{q}'_{12})]\}}{(\hbar^2\hat{k}^2_{12}/2\mu_{12})+(\hbar^2\hat{K}^2_{12}/2\mu_{3R})-\bar{E}_\mathrm{i}-\mathrm{i}\epsilon}.\end{aligned} \tag{224 a}$$

Equation (223 b) becomes

$$\langle \boldsymbol{k}|\, \bar{G}_F(\bar{E}_1+\mathrm{i}\epsilon)\,|\boldsymbol{k}'\rangle = (2\pi)^6\delta(\boldsymbol{k}_{12}-\boldsymbol{k}'_{12})\,\delta(\boldsymbol{K}_{12}-\boldsymbol{K}'_{12})\,\frac{1}{(\hbar^2k_{12}^2/2\mu_{12})+(\hbar^2K_{12}^2/2\mu_{3R})-\bar{E}_1-\mathrm{i}\epsilon}. \quad (224\,b)$$

Inserting (224 b) and (222 a) into (223 a) yields

$$\langle \mathrm{f}|\, \bar{\boldsymbol{T}}_{23}(\bar{E}_1+\mathrm{i}\epsilon)\,\bar{G}_F(\bar{E}_1+\mathrm{i}\epsilon)\,\bar{\boldsymbol{T}}_{12}(\bar{E}_1+\mathrm{i}\epsilon)\,|\mathrm{i}\rangle = \int \mathrm{d}\boldsymbol{k}_{12}\,\mathrm{d}\boldsymbol{K}_{12}\,\delta(\boldsymbol{K}_{23\mathrm{f}}-\boldsymbol{K}_{23})\,\delta(\boldsymbol{K}_{12}-\boldsymbol{K}_{12\mathrm{i}})$$
$$\times\,\frac{\langle \boldsymbol{k}_{23\mathrm{f}}|\, \boldsymbol{t}_{23}([\hbar^2k_{23\mathrm{f}}^2/2\mu_{23}]+\mathrm{i}\epsilon)\,|\boldsymbol{k}_{23}\rangle\,\langle \boldsymbol{k}_{12}|\, \boldsymbol{t}_{12\mathrm{i}}([\hbar^2k_{12\mathrm{i}}^2/2\mu_{12}]+\mathrm{i}\epsilon)\,|\boldsymbol{k}_{12\mathrm{i}}\rangle}{\bar{E}(\boldsymbol{k})-\bar{E}_1-\mathrm{i}\epsilon} \quad (225)$$

which can be seen to be equivalent to the result quoted on p. 59 of Watson & Nuttall (1967). In (225), $\bar{E}(\boldsymbol{k})$ is given by either the 1, 2 or the 2, 3 analogues of (35), as one chooses. Hence, because of the $\delta(\boldsymbol{K}_{12}-\boldsymbol{K}_{12\mathrm{i}})$ factor in the integrand, the denominator in (225) can be written as

$$\bar{E}(\boldsymbol{k})-\bar{E}_1-\mathrm{i}\epsilon = \frac{\hbar^2k_{12}^2}{2\mu_{12}}-\frac{\hbar^2k_{12\mathrm{i}}^2}{2\mu_{12}}-\mathrm{i}\epsilon. \quad (226\,a)$$

also, from (29 d)

$$\boldsymbol{k}_{23} = -\left(\boldsymbol{K}_{12}+\frac{m_3}{m_2+m_3}\boldsymbol{K}_{23}\right), \quad (226\,b)$$

$$\boldsymbol{k}_{12} = \boldsymbol{K}_{23}+\frac{m_1}{m_1+m_2}\boldsymbol{K}_{12}. \quad (226\,c)$$

Equation (226 c) further implies that (for fixed $\boldsymbol{K}_{12}$) $\mathrm{d}\boldsymbol{k}_{12} = \mathrm{d}\boldsymbol{K}_{23}$, i.e. in (225)

$$\mathrm{d}\boldsymbol{k}_{12}\,\mathrm{d}\boldsymbol{K}_{12} = \mathrm{d}\boldsymbol{K}_{23}\,\mathrm{d}\boldsymbol{K}_{12}. \quad (226\,d)$$

Using (226 d), the integrations in (225) are immediately performed, with the quantities $\boldsymbol{k}_{23}$, $\boldsymbol{k}_{12}$ being given by (226 b), (226 c) respectively after making the replacements $\boldsymbol{K}_{23} = \boldsymbol{K}_{23\mathrm{f}}$, $\boldsymbol{K}_{12} = \boldsymbol{K}_{12\mathrm{i}}$. Recalling (171 a), we now see that (219 b) and (225) imply the momentum space amplitude

$$\bar{T}_{2312}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) = -\lim_{\epsilon\to 0}\frac{\langle \boldsymbol{k}_{23\mathrm{f}}|\, \boldsymbol{t}_{23}(E_{23\mathrm{f}}+\mathrm{i}\epsilon)\,|-\boldsymbol{B}\rangle\,\langle \boldsymbol{A}|\, \boldsymbol{t}_{12}(E_{12\mathrm{i}}+\mathrm{i}\epsilon)\,|\boldsymbol{k}_{12\mathrm{i}}\rangle}{(\hbar^2A^2/2\mu_{12})-(\hbar^2k_{12\mathrm{i}}^2/2\mu_{12})-\mathrm{i}\epsilon}. \quad (227)$$

For $A^2 \neq k_{12\mathrm{i}}^2$, the limit in (227) can be performed immediately, and obviously yields

$$\bar{T}_{2312}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) = -\frac{2\mu_{12}}{\hbar^2}\frac{\langle \boldsymbol{k}_{23\mathrm{f}}|\, \boldsymbol{t}_{23\mathrm{f}}\,|-\boldsymbol{B}\rangle\,\langle \boldsymbol{A}|\, \boldsymbol{t}_{12\mathrm{i}}\,|\boldsymbol{k}_{12\mathrm{i}}\rangle}{A^2-k_{12\mathrm{i}}^2}. \quad (228\,a)$$

For $A^2 = k_{12\mathrm{i}}^2$, the limit $\epsilon\to 0$ in (227) does not really exist, but in momentum space procedures it is customary (Brenig & Haag 1963) to make the interpretation

$$\lim_{\epsilon\to 0}\frac{1}{w-\mathrm{i}\epsilon} = \mathrm{i}\pi\delta(w)+P\frac{1}{w}, \quad (228\,b)$$

where P again signifies the principal part (after integration). According to (228 b), at $A^2 = k_{12\mathrm{i}}^2$, (227) should yield

$$\bar{T}_{2312}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) = -\frac{2\mu_{12}\pi\mathrm{i}}{\hbar^2}\langle \boldsymbol{k}_{23\mathrm{f}}|\, \boldsymbol{t}_{23\mathrm{f}}\,|-\boldsymbol{B}\rangle\,\langle \boldsymbol{A}|\, \boldsymbol{t}_{12\mathrm{i}}\,|\boldsymbol{k}_{12\mathrm{i}}\rangle\,\delta(A^2-k_{12\mathrm{i}}^2). \quad (228\,c)$$

The right sides of (228 a) and (206) are identical; the right sides of (228 c) and (191 a) are identical. Therefore, recalling also (209 a), we see that (228 a) and (228 c) taken together show the momentum space value for $\bar{T}_{2312}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f})$ is identical with the configuration space value for

$$\bar{T}_{2312}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) = \bar{T}^{t}_{2312}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f})+\bar{T}^{a}_{2312}(\boldsymbol{k}_\mathrm{i}\to\boldsymbol{k}_\mathrm{f}) \quad (229)$$

for all A^2, where the configuration space amplitudes on the right side of (229) are defined by and computed from (175 *b*) and (176 *b*). In effect, I have shown that (220 *b*) holds for all $A^2 - k_{12i}^2$ when the right side of (220 *b*) is identified with the configuration space amplitude defined by the divergent integral (170 *a*), provided (173) is used to interpret the non-convergent parts of (170 *a*), and provided (228 *b*) is used to interpret the limit $\epsilon \to 0$ in (227).

5.3.3. *Off-shell double scattering*

Section 4.2 makes it obvious that, whether arrived at via momentum space procedures or via the configuration space approach of § 4.1, the single scattering transition amplitude of (222 *a*) or (130 *c*) must not be included in $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$. In other words, for the purpose of deciding whether or not single scattering contributes to the true three-body part of the total transition operator $\boldsymbol{T}$, configuration space and momentum space procedures are equally useful. For double scattering processes, on the other hand, the situation is somewhat different. The preceding paragraph has shown that the momentum space and configuration space double scattering contributions to the *total* $\bar{\boldsymbol{T}}$ are the same; however, the momentum space considerations, e.g. the diagrammatic derivation of (216 *c*) in § 5.3.1, do not very convincingly indicate what part of $\bar{T}_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ should be included in $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$. Again, § 4.2 makes it obvious that, whether arrived at via momentum space procedures or via the configuration space approach of § 4.1, the quantity (228 *c*) giving $\bar{T}_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ at $A^2 = k_{12i}^2$, must be excluded from $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$; otherwise the inferred three-body elastic scattering rate will have an anomalous $\tau^{\frac{4}{3}}$ dependence on the volume τ. But to decide whether (228 *a*), the value of $\bar{T}_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ at $A^2 \neq k_{12i}^2$, should or should not be excluded from $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$, it seems necessary to fall back on our configuration space arguments, which (via the definition of $\bar{\Phi}_i^{t(+)}$ in the opening paragraphs of chapter 4) provide a formal basis for this decision, although admittedly the physical interpretation of the off-shell double scattering contributions to $\bar{\boldsymbol{T}}^t$ given in the latter portion of the present subsection is so convincing that having such a formal decision basis appears almost irrelevant.

Actually, once (175 *b*) has been reduced to (206), the conclusion that it indeed represents a contribution to $\bar{\boldsymbol{T}}^t$—i.e. the conclusion that (228 *a*) should not be excluded from $\bar{\boldsymbol{T}}^t$—apparently can be inferred merely from the rules at the end of § 4.1.3. Along most directions $\boldsymbol{\nu}_f$ in the nine-dimensional configuration space, the scattered part $\Phi_i^{(+)}(\boldsymbol{r})$ decreases asymptotically like $\rho^{-5/2}$; these are the directions corresponding to those $\boldsymbol{k}_f$ for which the experimentalist expects to count truly three-body scattering events. Correspondingly, in general the allowed $\boldsymbol{k}_f$ for given $\boldsymbol{k}_i$ form a five-dimensional manifold (conservation of total momentum and total energy imposes four conditions on the otherwise arbitrary nine numbers specifying $\boldsymbol{k}_{1f}$, $\boldsymbol{k}_{2f}$, $\boldsymbol{k}_{3f}$). Now for specified $\boldsymbol{k}_i$, $\boldsymbol{k}_f$, the quantities $\boldsymbol{A}$, $\boldsymbol{B}$ are uniquely determined by (171 *a*), without imposition of any additional conditions; therefore, for physically allowed $\boldsymbol{k}_f$ consistent with given $\boldsymbol{k}_i$, the double scattering processes whose contributions are evaluated by (228 *a*) are associated with the full five-dimensional manifold of final $\boldsymbol{k}_f$. Consequently, in general (228 *a*) represents a contribution to $\bar{T}_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ along directions $\boldsymbol{k}_f$ corresponding to truly three-particle scattering, i.e. in general (228 *a*) should be included in $\bar{\boldsymbol{T}}^t$. Because of (177), the result (228 *a*) can be interpreted as resulting from a pair of successive purely two-body scatterings, each of which conserves momentum but not energy (though of course conservation of total energy in the overall transition from $\boldsymbol{k}_i \to \boldsymbol{k}_f$ is guaranteed, because $\boldsymbol{k}_f$ is presumed to lie on the total energy shell). The extra condition that energy shall be conserved in the individual two-body scattering events can be satisfied only on a four-dimensional manifold of final directions $\boldsymbol{k}_f$, along which § E. 3 shows

$\Phi_i^{(+)}(\boldsymbol{r})$ decreases asymptotically as ρ^{-2} (consistent with the fact that a $\delta(A^2-k_{12i}^2)$ factor turns up in (228 *c*)); consequently the double scattering contributions (228 *a*) along directions $A^2 = k_{12i}^2$ should be excluded from $\overline{T}^t$.

The factor $(A^2-k_{12i}^2)^{-1}$ in the right side of (206) means that $\overline{w}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ of (3) will diverge when integrated over all final $\boldsymbol{k}_f$ consistent with $A^2 \neq k_{12i}^2$. This result, for the elastic scattering processes here being discussed, can be interpreted along the lines of § 4.2.2. Although the diagram (216 *c*) corresponds to a pair of purely two-body scatterings, nevertheless this diagram's off-shell contributions (206) or (228 *a*) cannot occur unless all three particles somehow simultaneously interact; if particle 3 is infinitely far from the pair 1, 2, then the pair 1, 2 can only make a collision which conserves energy as well as momentum. To put it differently, after the first collision in (216 *c*) the particles 1, 2 are in a state which lasts only a time Δt until particle 2 collides with 3. The magnitude of Δt is given by

$$\Delta t \sim \frac{X}{v_2'} \tag{230 a}$$

where X is the distance travelled by particle 2 between its collisions with 1 and with 3, and $\boldsymbol{v}_2' = \hbar \boldsymbol{k}_2'/m_2$ is the velocity of particle 2 after its first collision. But the magnitude ΔE of the departure from energy conservation in the intermediate state is

$$\Delta E = \frac{\hbar^2}{2\mu_{12}}(A^2-k_{12i}^2) \sim \frac{\hbar}{\Delta t}, \tag{230 b}$$

yielding

$$X \sim \frac{\hbar v_2'}{\Delta E}. \tag{230 c}$$

Now, as in § 4.2.2, suppose the volume τ contains precisely one particle of each species, 1 2, 3. The rate of double scatterings in which a collision between 1, 2 is followed by a collision between 2, 3 during the time for particle 2 to travel a distance X is (compare (159 *a*))

$$\sim \left\langle \left(\frac{\overline{w}_{12}^{(2)}}{\tau}\right)\left(\frac{X\overline{\sigma}_{23}}{\tau}\right)\right\rangle_{\text{av}}. \tag{231 a}$$

Therefore the rate of double scatterings in which the scattering between 2, 3 takes place after particle 2 has travelled a distance between X and $X+\mathrm{d}X$ is

$$\sim \left\langle \frac{\overline{w}_{12}^{(2)}}{\tau}\frac{\overline{\sigma}_{23}}{\tau}\right\rangle_{\text{av}} \mathrm{d}X. \tag{231 b}$$

But, from (230 *c*),

$$\mathrm{d}X \sim \frac{\hbar v_2'}{(\Delta E)^2}\mathrm{d}(\Delta E) \tag{231 c}$$

so that, still with one particle of each species in τ, the rate of double scatterings in which energy conservation in the intermediate state fails by an amount between ΔE and $\Delta E+\mathrm{d}(\Delta E)$ is (using (152 *b*))

$$\hat{w}'_{\Delta E}(1,2;2,3) \cong \left\langle \frac{\overline{w}_{12}^{(2)}}{\tau}\frac{\overline{\sigma}_{23}}{\tau}\hbar v_2'\right\rangle_{\text{av}} \frac{\mathrm{d}(\Delta E)}{(\Delta E)^2} \tag{232 a}$$

$$\cong C'\frac{\overline{\sigma}_{12}\overline{\sigma}_{23}}{\tau^2}\frac{\mathrm{d}(\Delta E)}{(\Delta E)^2}, \tag{232 b}$$

where C' here is independent of the shape of the scattering region τ, and represents an average (over scattering directions and velocities) of the various primarily velocity-dependent factors in

(232 *a*) not explicitly included in (232 *b*). The corresponding rate with $\hat{N}_\alpha$ particles of each species in τ is

$$\hat{w}_{\Delta E}(12;23) = \hat{N}_1 \hat{N}_2 \hat{N}_3 \hat{w}'_{\Delta E}(12,23) \cong N_1 N_2 N_3 \tau \frac{C' \overline{\sigma}_{12} \overline{\sigma}_{23}}{(\Delta E)^2} \mathrm{d}(\Delta E). \qquad (232\,c)$$

Except for the factor C', the result (232 *c*) has precisely the form obtained when the contribution $|\overline{T}^t_{2312}(\boldsymbol{k}_1 \to \boldsymbol{k}_\mathrm{f})|^2$ from (206) is substituted into equations (2) and (3), remembering that $\overline{\sigma}_{12}$ is proportional to $|\langle \mathrm{f}|\, \boldsymbol{t}_{12\mathrm{i}}\, |\mathrm{i}\rangle|^2$, and that $\mathrm{d}\boldsymbol{k}_{1\mathrm{f}}$, $\mathrm{d}\boldsymbol{k}_{2\mathrm{f}}$, $\mathrm{d}\boldsymbol{k}_{3\mathrm{f}}$ in (3) can be re-expressed in terms of $\mathrm{d}(\Delta E)$ and other $\boldsymbol{k}$-dependent differentials. The fact that (232 *c*) is proportional to τ once again indicates that the expression (206) must be included in the physical three-body scattering amplitude; the fact that (232 *c*) is non-integrable at $\Delta E \to 0$, corresponding to collisions at distances $X \to \infty$ in (230 *c*), accounts for the divergence of (3) when integrated over final $\boldsymbol{k}_\mathrm{f}$.

I believe the above qualitative largely geometrical argument is basically consistent with the arguments of Iagolnitzer (1965),† who has examined the interpretability of a propagator pole in the scattering amplitude. He finds that the pole can be understood to represent a pair of successive real two-body collisions, but his analysis holds only in the limit that the distance X between the collisions is very large. It is to be noted that the geometrical argument in this subsection differs in one important aspect from those given in § 4; in § 4 it always was presumed that each individual collision under discussion (e.g. the individual two-body processes considered in the derivation of (159 *a*)) was an actually occurring event, i.e. was consistent with energy and momentum conservation. Finally, I close this, the last section of the main text, with the remark that despite the consistency and interpretability of our result (206) for the contribution to $\overline{\boldsymbol{T}}^t$ made by double scattering processes, it still would be desirable to confirm our conclusions via a configuration space calculation of $\overline{T}^t_{2312}(\boldsymbol{k}_\mathrm{i} \to \boldsymbol{k}_\mathrm{f})$ which somehow avoids having to reinterpret singular integrals, as we were unable to avoid doing in deriving (175).

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