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MOMENTUM TRANSFER THEOREM FOR INELASTIC PROCESSES

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E. GERJUOY

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Momentum Transfer Theorem for Inelastic Processes

E. Gerjuoy

University of Pittsburgh, Pittsburgh, Pennsylvania

ABSTRACT

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Recently it has been shown that for potential scattering, the well known optical theorem--relating the total cross section to the imaginary part of the forward scattering amplitude--can be generalized to yield a "momentum transfer cross section theorem." The present paper further generalizes the previous potential scattering result. Specifically, it appears that the momentum transfer cross section theorem is valid also for many-particle systems, wherein inelastic processes occur. Although this last assertion probably holds quite generally, a proof is given only for the collisions of electrons with atomic hydrogen. The proof takes into account electron indistinguishability, as well as the possibility that the incident electron ionizes the atom, but assumes the forces are not spin-dependent.

Author

I. Introduction and Summary

Recently¹ I have shown that for potential scattering, the momentum transfer cross section

$$\sigma_d = \int d\mathbf{n}' (1 - \mathbf{n} \cdot \mathbf{n}') |A(\mathbf{n} \rightarrow \mathbf{n}')|^2 \quad (1)$$

can be expressed in the form

$$\sigma_d = \frac{1}{2E} \int d\mathbf{r} \Psi^* \frac{\partial V}{\partial z} \Psi \quad (2)$$

In the above equations: $A(\mathbf{n} \rightarrow \mathbf{n}')$ is the amplitude for elastic scattering from initial direction \mathbf{n} to final direction \mathbf{n}' ; $E = \hbar^2 k^2 / 2m$ is the kinetic energy; the Hamiltonian is

$$H = T + V = \frac{-\hbar^2}{2m} \nabla^2 + V(\mathbf{r}); \quad (3)$$

the potential $V(\mathbf{r})$ is not necessarily spherically symmetric, i.e., $V(\mathbf{r})$ need not equal $V(r)$; the wave function Ψ satisfies

$$(H - E)\Psi = 0 \quad (4)$$

subject to the boundary condition (when \mathbf{n} is along the z-direction)

$$\Psi = e^{ikz} + \phi(\mathbf{r}) \quad (5)$$

where

$$\lim_{r \rightarrow \infty} \phi = A(\mathbf{n} \rightarrow \mathbf{n}') \frac{e^{ikr}}{r}; \quad (6)$$

when \mathbf{n} is not parallel to z, $\partial V / \partial z$ in Eq. (2) is replaced by $\mathbf{n} \cdot \text{grad } V$.

For potential scattering the result (2) is a generalization of the optical theorem

$$\sigma = \int d\mathbf{n}' |A(\mathbf{n} \rightarrow \mathbf{n}')|^2 = \frac{4\pi}{k} \text{Im } A(\mathbf{n} \rightarrow \mathbf{n}). \quad (7)$$

It is known, however, that the optical theorem remains valid in many-particle collisions involving inelastic processes. Similarly, it appears that the momentum transfer cross section theorem (2) remains valid even when inelastic processes can occur. Of course, some modification of the right side of (2) is necessary in a many-particle collision. Also, one must generalize the definition (1) of the momentum transfer cross section σ_d .

Because a proof of the momentum transfer cross section theorem for arbitrarily complicated colliding systems would be awkward and hard to follow (mainly because the notation gets correspondingly complicated), I shall content myself here with carrying out the proof for the simple case of e-H scattering. In this case the momentum transfer theorem has the form

$$\sigma_d = \frac{1}{2E_0} \int d\mathbf{r} \psi^* \frac{\partial V}{\partial z_1} \psi \quad (8)$$

where $E_0 = \hbar^2 k_0^2 / 2m$ is the incident kinetic energy; z_1 is the z-coordinate of the two electrons in the system; and the quantities V , ψ , σ_d are defined respectively by Eqs. (12), (14) and (56) below. This proof for e-H scattering makes it fairly obvious that a similar momentum transfer theorem holds for electron scattering by more complicated atoms, and makes it plausible that a corresponding momentum transfer theorem continues to hold for collisions between more complex aggregates of fundamental particles, e.g., for molecule-molecule scattering.

In connection with the above paragraph, the following remarks, concerning assumptions made in the proof, shall be noted. The proof includes the effects of particle indistinguishability and electron exchange, i.e., the wave function is antisymmetric under exchange of electron space and spin coordinates. However, the spin-dependent part of the wave function is factored out, i.e., it is assumed that all components of the total spin are separately conserved, which in turn implies that the Hamiltonian is

spin-independent. There is little doubt that a momentum transfer theorem remains valid for spin-dependent interactions, but carrying through the proof would require taking into account the properties of the eigenfunctions under time-reversal; considering only the spatially dependent part of the wave function, as is done here, avoids this complication. Another complication which is ignored in the following proof of (8) is the effects of Coulomb forces on the asymptotic behavior of the continuum wave function solving the many-particle Schrodinger equation. More precisely, although ionization is included in the possible inelastic processes contributing to momentum transfer, it is assumed that the Hamiltonian is effectively a free-particle Hamiltonian when the particles are infinitely separated. It is easily seen that this assumption is inconsequential for (8) when the free-particle plane waves can be replaced by Coulomb functions as, e.g., in excitation of H^- by electrons, or ionization of H^- by a neutral particle. In more complex situations, e.g., ionization of H^- or H by electrons, there is no reason to think the momentum transfer theorem fails, but it must be admitted that the detailed asymptotic behavior of the wave function has not been examined in circumstances such as these, where two or more charged particles go out to infinity in the center of mass system. Finally, the proof wholly ignores radiative processes.

The possible utility of (8) has been discussed previously.¹ Bearing on its utility, and relevant also to the discussion of the preceding paragraph, is the fact that the right side of (8) apparently diverges whenever electrons are incident on ions, e.g., H^- . The source of the divergence can be understood by examining elastic scattering in a fixed Coulomb potential $V = C/r$. Substituting (5) in (2), which now is applicable, one sees that integration over angles annihilates the matrix element of $\partial V/\partial z = -C \cos\theta/r^2$ between e^{ikz} and e^{-ikz} . The matrix element of $\partial V/\partial z$ between e^{-ikz} and ϕ need not vanish, however, and in this

matrix element the integral over r is divergent at $r = \infty$. Moreover, this divergence is to be expected, because for Coulomb scattering, directly from the fundamental definition (1)

$$\sigma_d \sim \int_0^\pi \sin\theta (1 - \cos\theta) \csc^4(\theta/2) \quad (9)$$

diverges logarithmically at $\theta = 0$.

The following remarks are also worth noting. The proof of (8) given here indicates that in a sense the momentum transfer cross section theorem is a generalization--to continuum eigenfunctions--of the so-called hypervirial theorems.² In fact the proof of (8) is based on a wholly time-independent (wherein transition probabilities are never explicitly introduced) treatment³ of many particle collisions involving rearrangement. In this treatment the cross section is computed, using Green's theorem, from the flow of probability current across the surface at infinity in the $3n$ -dimensional space spanned by $\underline{r}_1, \dots, \underline{r}_n$, where the collision involves n particles in all, and \underline{r}_i is the position vector of the i th particle. Consequently, to derive the theorem (8) via the more conventional operator techniques--which are based on a time-dependent transition probability formalism wherein contributions from the wave function at infinite distances are taken into account implicitly rather than explicitly--would require a very different approach; in fact, it probably will be necessary to essentially redo the Lippmann-Schwinger⁴ or related derivations⁵ of the scattering amplitude, starting as those derivations start, but examining the time-evolution of the momentum transport as well as of the total wave amplitude.

II. Review of Time-Independent Formalism

Especially when ionization can occur, to make the proof of the momentum transfer theorem understandable, it is desirable to review some results of the time-independent treatment. As explained above, I confine my attention to the scattering of electrons by atomic hydrogen in the ground $1s$ state ϕ_0 . The atomic hydrogen eigenfunction $\phi_j(\mathbf{r})$, of energy ϵ_j , obeys

$$\left(\frac{-\hbar^2}{2m} \nabla^2 - \frac{e^2}{r} \right) \phi_j = \epsilon_j \phi_j. \quad (10)$$

The spatially dependent part of the total wave function describing the collision is $\Psi(\mathbf{r}_1, \mathbf{r}_2)$, which satisfies Eq. (4) with

$$H = \frac{-\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{2m} \nabla_2^2 + V(\mathbf{r}_1, \mathbf{r}_2) \quad (11)$$

$$V = \frac{-e^2}{r_1} - \frac{e^2}{r_2} + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (12)$$

and obeys

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \pm \Psi(\mathbf{r}_2, \mathbf{r}_1) \quad (13)$$

The upper sign in Eq. (13) applies to singlet scattering; the lower sign to triplet scattering. In what follows I shall use the plus sign only, but it is easily verified that the proof can be just as readily carried through for triplet scattering.

Outgoing Current and the Total Cross Section

Ignoring the long-range character of the potential, the singlet Ψ can be written in the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = e^{i\mathbf{k}_0 \cdot \mathbf{r}_1} \phi_0(\mathbf{r}_2) + e^{i\mathbf{k}_0 \cdot \mathbf{r}_2} \phi_0(\mathbf{r}_1) + \phi(\mathbf{r}_1, \mathbf{r}_2) \quad (14)$$

where $\phi(\underline{r}_1, \underline{r}_2)$ is everywhere outgoing and obeys

$$\phi(\underline{r}_1, \underline{r}_2) = \phi(\underline{r}_2, \underline{r}_1). \quad (15)$$

The everywhere outgoing property implies

$$\lim_{r_1 \rightarrow \infty} \int d\underline{r}_2 \phi_j^*(\underline{r}_2) \phi(\underline{r}_1, \underline{r}_2) = A_j(\underline{n} \rightarrow \underline{n}') \frac{e^{ik_j r_1}}{r_1} \quad (16)$$

where

$$E = \frac{\hbar^2 k_0^2}{2m} + \epsilon_0 = \frac{\hbar^2 k_j^2}{2m} + \epsilon_j \quad (17)$$

It is easily seen that, as one expects for singlet scattering,

$$A_j = f_j + g_j \quad (18)$$

where f_j and g_j are respectively the ordinary and exchange amplitudes for collisions leaving the atom in the state ϕ_j .

Eq. (16) yields no information about the behavior of ϕ when r_1, r_2 each become infinite. However, the everywhere outgoing property also implies³

$$\lim_{\substack{r_1 \rightarrow \infty \\ r_2 \rightarrow \infty \\ r_1/r_2 = q = \text{constant}}} \phi(\underline{r}_1, \underline{r}_2) = A(\underline{n} \rightarrow \underline{k}_1', \underline{k}_2') \frac{e^{iKr}}{r^{5/2}} \quad (19)$$

where

$$E = \frac{\hbar^2 K^2}{2m} = \frac{\hbar^2 k_1'^2}{2m} + \frac{\hbar^2 k_2'^2}{2m} \quad (20)$$

$$r = (r_1^2 + r_2^2)^{1/2} = r_1(1+q^2)^{1/2} \quad (21)$$

$$\underline{k}_1' = \frac{Kr_1 \underline{n}_1'}{r} = K(1+q^2)^{-1/2} \underline{n}_1' \quad (22)$$

$$\underline{k}_2' = \frac{Kr_2 \underline{n}_2'}{r} = Kq(1+q^2)^{-1/2} \underline{n}_2'$$

The total cross section, including ionization as well as excitation, is³

$$\sigma = \frac{m}{2\hbar k_0} \int_{\infty} dS \underline{v} \cdot \underline{J} \quad (23)$$

integrated over the surface of the six dimensional sphere at infinity in $\underline{r}_1, \underline{r}_2$ space, where the six-dimensional current vector \underline{J} has components

$$\begin{aligned} \underline{J}_1 &= \frac{\hbar}{2mi} (\phi^* \nabla_1 \phi - \phi \nabla_1 \phi^*) \\ \underline{J}_2 &= \frac{\hbar}{2mi} (\phi^* \nabla_2 \phi - \phi \nabla_2 \phi^*) \end{aligned} \quad (24)$$

In (24) \underline{J}_1 represents the three components of \underline{J} along $\underline{i}_1, \underline{j}_1, \underline{k}_1$, i.e., along the usual right-handed basis defining the \underline{r}_1 subspace of $\underline{r}_1, \underline{r}_2$ space.

Similarly \underline{J}_2 represents the three components of \underline{J} along $\underline{i}_2, \underline{j}_2, \underline{k}_2$. Correspondingly, in (23) the outward drawn six-dimensional normal to the sphere at infinity has components

$$\begin{aligned} \underline{v}_1 &= \frac{\underline{r}_1}{r} = \frac{r_1}{r} \underline{n}'_1 \\ \underline{v}_2 &= \frac{\underline{r}_2}{r} = \frac{r_2}{r} \underline{n}'_2 \end{aligned} \quad (25)$$

Excitation and Ionization Cross Sections

The result (23) is basic to the time-independent treatment of many-particle collisions, and is not evident. In fact, Eq. (23) amounts to accepting the postulate that (24) represents the current operator conserving probability flux in many-particle collisions, just as the usual formula (7) for the total cross section in potential scattering implies acceptance of the usual one-particle current operator [of which Eq. (24) is the obvious generalization]. Nevertheless the correctness of (23) is not in question, since it can be shown that the accepted expressions for the rates of excitation and ionization follow from (23).

To amplify this last assertion, note that on the sphere at infinity the surface elements dS (and corresponding \underline{y}) are of two essentially different types, namely: surface elements dS where one of r_1, r_2 is infinite, but not the other; and those dS forming a manifold of higher dimensionality than the first type, where r_1 and r_2 are each infinite. It has been proved³ that the contribution to (23) from surface elements of the first type, with $r_1 \rightarrow \infty$ and r_2 finite, reduces to

$$\frac{m}{2\hbar k_0} \sum_j \int_{S_1} dS_1 \underline{n}' \cdot \underline{J}_j' \quad (26)$$

integrated over the surface S_1 of the three-dimensional sphere at infinity in r_1 -space, where

$$\underline{J}_j' = \frac{\hbar}{2mi} (Z_j^* \nabla_1 Z_j - Z_j \nabla_1 Z_j^*) \quad (27)$$

and

$$Z_j(\underline{r}_1) = \int d\underline{r}_2 \phi_j^*(\underline{r}_2) \Phi(\underline{r}_1, \underline{r}_2) \quad (28)$$

integrated over all \underline{r}_2 . Of course in (26) \underline{n}' is the normal to dS_1 , and $\underline{J}_j'(\underline{r}_1)$ is evaluated at infinite $\underline{r}_1 = r_1 \underline{n}'$. Using (16), therefore, (26) yields

$$\sum_j \frac{k_j}{2k_0} \int d\underline{n}' |A_j(\underline{n} \rightarrow \underline{n}')|^2 = \frac{1}{2} \sigma_{ex} \quad (29)$$

where σ_{ex} obviously is the total cross section for excitation, including elastic scattering ($j = 0$). The left side of (29) is only half σ_{ex} because (26) has not included the contribution to (23) from surface elements with $r_2 \rightarrow \infty$ and r_1 finite; by virtue of (15) the contributions from $r_1 \rightarrow \infty$, r_2 finite and $r_2 \rightarrow \infty$, r_1 finite must be equal. Correspondingly, one sees that the right side of (23), which must represent the total outgoing current divided by the incident current per unit area is correctly multiplied by $(2\hbar k_0/m)^{-1}$, because each of the first two terms on the right side of (14) corresponds to an incident current density $\hbar k_0/m$.

The contribution to (23) from surface elements dS where r_1 and r_2 are each infinite must be the ionization cross section σ_{ion} . In fact, for K real [$E > 0$ in (17) and therefore capable of ionizing the atom], this contribution is, using Eqs. (19) and (21) - (25)

$$\sigma_{ion} = \frac{1}{2k_0} \int \frac{dS}{r^5} K |A(\underline{n} \rightarrow \underline{k}'_1, \underline{k}'_2)|^2 \quad (30a)$$

$$= \frac{1}{2k_0} \int dk_2' dn_{\underline{m}1}' dn_{\underline{m}2}' \frac{k_2'^2 k_1'}{K^3} |A(\underline{n} \rightarrow \underline{k}'_1, \underline{k}'_2)|^2 \quad (30b)$$

where I have used³

$$dS = \frac{r^{5q^2}}{(1+q^2)^3} dq dn_{\underline{m}1}' dn_{\underline{m}2}' \quad (31)$$

The right side of Eq. (30b), which still is subject to Eq. (20), is not altered in value if one multiplies by $\delta(E'-E)$, and then integrates over an infinitesimal range dE' about $E' = E$. Thus, using Eq. (20) to find dE' in terms of dk_1' , Eq. (30b) becomes

$$\sigma_{ion} = \frac{1}{2k_0} \frac{\hbar^2}{mK^3} \int dk_1' dk_2' \delta(E'-E) |A(\underline{n} \rightarrow \underline{k}'_1, \underline{k}'_2)|^2 \quad (32)$$

where now $\underline{k}'_1, \underline{k}'_2$ range over all real values, with E' defined by the right side of Eq. (20).

Eq. (32) is the desired expression for σ_{ion} . When the symmetry requirements of particle indistinguishability are ignored, e.g., when the second term on the right side of (14) is dropped in the definition of Ψ , it can be seen that³

$$A(\underline{n} \rightarrow \underline{k}'_1, \underline{k}'_2) = \left(\frac{2m}{\hbar^2}\right)^3 \frac{e^{-3i\pi/4}}{2\sqrt{E}} \left(\frac{\sqrt{E}}{2\pi\sqrt{\frac{2m}{\hbar^2}}}\right)^{5/2} T(\underline{n} \rightarrow \underline{k}'_1, \underline{k}'_2) \quad (33)$$

where T is the usual transition amplitude

$$T(i \rightarrow f) = \int \psi_f^{(-)*} V_i \psi_i \quad (34)$$

from initial to final states. In this unsymmetrized case, therefore, realizing that the factor 1/2 must be dropped because now the incident current density is only $\hbar k_0/m$, Eq. (32) takes the familiar form

$$\sigma_{\text{ion}} = \frac{m}{\hbar k_0} \frac{2\pi}{\hbar} \frac{1}{(2\pi)^6} \int d\underline{k}_1' d\underline{k}_2' \delta(E'-E) |T(\underline{n} \rightarrow \underline{k}_1', \underline{k}_2')|^2 \quad (35)$$

In the symmetrized case, where all terms in Eq. (14) are retained, one also can retain Eq. (33), in which event Eq. (35) again holds provided 1/2 is restored. The expression (34) for $T(i \rightarrow f)$ is not valid in the symmetrized case however.

III. Proof of Momentum Transfer Theorem

With the foregoing results in hand, the desired momentum transfer cross section theorem can be derived. As in the simpler case of potential scattering¹

$$- \int d\tilde{r} (H\Psi)^* p_{1z} \Psi + \int d\tilde{r} \Psi^* p_{1z} H\Psi = 0 \quad (36)$$

where: $\Psi(\underline{r}_1, \underline{r}_2)$ is the function defined by Eqs. (14) and (15); Eq. (11) defines H ; $p_{1z} = (\hbar/i)\partial/\partial z_1$ is the z -component of the momentum of particle 1; the z -direction now is supposed to coincide with the incident direction \underline{n} ; and $d\tilde{r} \equiv d\underline{r}_1 d\underline{r}_2$ signifies integration over all $\underline{r}_1, \underline{r}_2$. Again as previously,¹ to keep the integrals in (36) convergent, the integration volume may at first be supposed to equal the interior of a six-dimensional sphere (in $\underline{r}_1, \underline{r}_2$ space) of finite though very large radius. Whatever the integration volume, Eq. (36) is true because Ψ satisfies Eq. (4).

Using (11), Eq. (36) becomes

$$\frac{-\hbar^2}{2m} \int d\tilde{r} \left\{ \Psi^* (\nabla_1^2 + \nabla_2^2) \frac{\partial \Psi}{\partial z_1} - [(\nabla_1^2 + \nabla_2^2) \Psi]^* \frac{\partial \Psi}{\partial z_1} \right\} + \int d\tilde{r} \Psi^* \frac{\partial V}{\partial z_1} \Psi = 0 \quad (37)$$

with V given by (12). The next step is to substitute (14) into the first integral of Eq. (37), thereby obtaining eighteen independent pairs of terms under the integral sign. Most of these pairs vanish, however.

For example,

$$\int d\tilde{r} \left\{ e^{-ik_0 \underline{n} \cdot \underline{r}_1} \phi_0^*(\underline{r}_2) \nabla_1^2 \frac{\partial}{\partial z_1} e^{ik_0 \underline{n} \cdot \underline{r}_1} \phi_0(\underline{r}_2) - \left[\frac{\partial}{\partial z_1} e^{ik_0 \underline{n} \cdot \underline{r}_1} \phi_0(\underline{r}_2) \right] \nabla_1^2 e^{-ik_0 \underline{n} \cdot \underline{r}_1} \phi_0^*(\underline{r}_2) \right\} = 0$$

because

$$(\nabla_1^2 + k_0^2) e^{\pm ik_0 \underline{n} \cdot \underline{r}_1} = 0. \quad (38)$$

Also, holding \underline{r}_2 fixed and employing Green's Theorem in the three-dimensional \underline{r}_1 -space, one sees that

$$\int d\underline{r}_1 d\underline{r}_2 \left\{ e^{-ik_0 \underline{n} \cdot \underline{r}_2} \phi_0^*(r_1) \nabla_1^2 \frac{\partial}{\partial z_1} e^{ik_0 \underline{n} \cdot \underline{r}_1} \phi_0(r_2) - \left[\frac{\partial}{\partial z_1} e^{ik_0 \underline{n} \cdot \underline{r}_1} \phi_0(r_2) \right] \nabla_1^2 e^{-ik_0 \underline{n} \cdot \underline{r}_2} \phi_0^*(r_1) \right\} = 0$$

because $\phi_0(r_1)$ is exponentially decreasing as $r_1 \rightarrow \infty$; similarly, pairs of terms involving ∇_2^2 and $\phi_0(r_2)$ are seen to vanish after employing Green's Theorem in \underline{r}_2 -space.

In this fashion, Eq. (37) yields

$$\begin{aligned} & \int d\underline{r} \left\{ \phi^* \nabla_1^2 \frac{\partial}{\partial z_1} e^{ik_0 \underline{n} \cdot \underline{r}_1} \phi_0(r_2) - \left[\frac{\partial}{\partial z_1} e^{ik_0 \underline{n} \cdot \underline{r}_1} \phi_0(r_2) \right] \nabla_1^2 \phi^* \right\} \\ & + \int d\underline{r} \left\{ e^{-ik_0 \underline{n} \cdot \underline{r}_1} \phi_0^*(r_2) \nabla_1^2 \frac{\partial \phi}{\partial z_1} - \frac{\partial \phi}{\partial z_1} \nabla_1^2 e^{-ik_0 \underline{n} \cdot \underline{r}_1} \phi_0^*(r_2) \right\} \\ & + \int d\underline{r} \left\{ \phi^* \nabla_2^2 \frac{\partial}{\partial z_1} e^{ik_0 \underline{n} \cdot \underline{r}_2} \phi_0(r_1) - \left[\frac{\partial}{\partial z_1} e^{ik_0 \underline{n} \cdot \underline{r}_2} \phi_0(r_1) \right] \nabla_2^2 \phi^* \right\} \\ & + \int d\underline{r} \left\{ e^{-ik_0 \underline{n} \cdot \underline{r}_2} \phi_0^*(r_1) \nabla_2^2 \frac{\partial \phi}{\partial z_1} - \frac{\partial \phi}{\partial z_1} \nabla_2^2 e^{-ik_0 \underline{n} \cdot \underline{r}_2} \phi_0^*(r_1) \right\} \\ & + \int d\underline{r} \left\{ \phi^* (\nabla_1^2 + \nabla_2^2) \frac{\partial \phi}{\partial z_1} - \frac{\partial \phi}{\partial z_1} (\nabla_1^2 + \nabla_2^2) \phi^* \right\} - \frac{2m}{\hbar^2} \int d\underline{r} \psi^* \frac{\partial V}{\partial z_1} \psi = 0. \end{aligned} \quad (39)$$

Reduction to Surface Integrals

Green's theorem in \underline{r}_1 -space can be employed in the first integral of Eq. (39). Thus, using (16), this first term reduces to

$$\begin{aligned} & \int d\underline{r}_2 \int dS_1 \cdot \left\{ \phi^* \nabla_1 \frac{\partial}{\partial z_1} e^{ik_0 \underline{n} \cdot \underline{r}_1} \phi_0(r_2) - \left[\frac{\partial}{\partial z_1} e^{ik_0 \underline{n} \cdot \underline{r}_1} \phi_0(r_2) \right] \nabla_1 \phi^* \right\} \\ & = \int dS_1 \cdot \left\{ A_0^*(\underline{n} \rightarrow \underline{n}') \frac{e^{-ik_0 r_1}}{r_1} \nabla_1 \frac{\partial}{\partial z_1} e^{ik_0 \underline{n} \cdot \underline{r}_1} - \left[\frac{\partial}{\partial z_1} e^{ik_0 \underline{n} \cdot \underline{r}_1} \right] \nabla_1 A_0^*(\underline{n} \rightarrow \underline{n}') \frac{e^{-ik_0 r_1}}{r_1} \right\} \end{aligned} \quad (40)$$

where $dS_1 = r_1^2 d\underline{n}'$ is the surface element on the sphere at infinity in 3-dimensional \underline{r}_1 -space. Similarly, the second term in (39) reduces to

$$\int d\tilde{S}_1 \cdot \left\{ e^{-ik_0 \tilde{n} \cdot \tilde{r}_1} \nabla_1 \frac{\partial}{\partial z_1} A_0(\tilde{n} \rightarrow \tilde{n}') \frac{e^{ik_0 r_1}}{r_1} - \left[\frac{\partial}{\partial z_1} A_0(\tilde{n} \rightarrow \tilde{n}') \frac{e^{ik_0 r_1}}{r_1} \right] \nabla_1 e^{-ik_0 \tilde{n} \cdot \tilde{r}_1} \right\} \quad (41)$$

Using Green's Theorem in \tilde{r}_2 -space, the third integral in (39)

becomes

$$\int d\tilde{r}_1 \int d\tilde{S}_2 \cdot \sum_j \left\{ \phi_j^*(\tilde{r}_1) A_j^*(\tilde{n}') \frac{e^{-ik_j r_2}}{r_2} \frac{\partial \phi_0(r_1)}{\partial z_1} \nabla_2 e^{ik_0 \tilde{n} \cdot \tilde{r}_2} - \frac{\partial \phi_0(r_1)}{\partial z_1} e^{ik_0 \tilde{n} \cdot \tilde{r}_2} \phi_j^*(\tilde{r}_1) \nabla_2 A_j^*(\tilde{n}') \frac{e^{-ik_j r_2}}{r_2} \right\} \quad (42)$$

where $d\tilde{S}_2 = r_2^2 d\tilde{n}'$. The quantity $A_j(\tilde{n}')$ in (42) is identical with $A_j(\tilde{n} \rightarrow \tilde{n}')$ defined in (16) because

$$\begin{aligned} \lim_{\substack{r_2 \rightarrow \infty \\ r_2 = \rho}} \int d\tilde{r}_1 \phi_j^*(\tilde{r}_1) \phi(\tilde{r}_1, \tilde{r}_2) &= \lim_{\substack{r_1 \rightarrow \infty \\ r_1 = \rho}} \int d\tilde{r}_2 \phi_j^*(\tilde{r}_2) \phi(\tilde{r}_2, \tilde{r}_1) \\ &= \lim_{\substack{r_1 \rightarrow \infty \\ r_1 = \rho}} \int d\tilde{r}_2 \phi_j^*(\tilde{r}_2) \phi(\tilde{r}_1, \tilde{r}_2) = A_j(\tilde{n} \rightarrow \tilde{n}') \frac{e^{ik_j \rho}}{\rho} \end{aligned} \quad (43)$$

The first equality in (43) simply interchanges the labeling on \tilde{r}_1, \tilde{r}_2 ; the second equality makes use of (15). I now observe that when $k_j \neq k_0$ the integral in (42) oscillates infinitely rapidly at infinite r_2 , and gives no net contribution when averaged over any small range of incident energies.

Hence the terms $k_j \neq k_0$ are inconsequential, and can be dropped from (42).

But the remaining term $k_j = k_0$ vanishes after integration over \tilde{r}_1 , because $\partial/\partial z_1$ has odd parity. Thus the expression (42), which equals the third integral in (39), vanishes. Similarly, the fourth integral in (39) vanishes.

The fifth integral in (39) is evaluated using Green's Theorem in \tilde{r}_1, \tilde{r}_2 space. As explained in connection with Eq. (23), the surface elements at infinity in \tilde{r}_1, \tilde{r}_2 -space are of the following different types:

(a) $r_1 \rightarrow \infty$, r_2 remains finite; (b) $r_2 \rightarrow \infty$, r_1 remains finite; (c) both

$r_1, r_2 \rightarrow \infty$. Then, as in Eqs. (26)-(29), the contribution from surface elements of type (a) to the fifth integral in (39) is

$$\int d\mathbf{r}_2 \int dS_1 \cdot \sum_{j, \ell} \left\{ \phi_j^*(\mathbf{r}_2) A_j^*(\mathbf{n}') \frac{e^{-ik_j r_1}}{r_1} \nabla_1 \phi_\ell(\mathbf{r}_2) \frac{\partial}{\partial z_1} A_\ell(\mathbf{n}') \frac{e^{ik_\ell r_1}}{r_1} \right. \\ \left. - [\phi_\ell(\mathbf{r}_2) \frac{\partial}{\partial z_1} A_\ell(\mathbf{n}') \frac{e^{ik_\ell r_1}}{r_1}] \nabla_1 \phi_j^*(\mathbf{r}_2) A_j^*(\mathbf{n}') \frac{e^{-ik_j r_1}}{r_1} \right\} \quad (44a)$$

$$= \int dS_1 \cdot \sum_j \left\{ A_j^*(\mathbf{n}') \frac{e^{-ik_j r_1}}{r_1} \nabla_1 \frac{\partial}{\partial z_1} A_j(\mathbf{n}') \frac{e^{ik_j r_1}}{r_1} \right. \\ \left. - [\frac{\partial}{\partial z_1} A_j(\mathbf{n}') \frac{e^{ik_j r_1}}{r_1}] \nabla_1 A_j^*(\mathbf{n}') \frac{e^{-ik_j r_1}}{r_1} \right\}. \quad (44b)$$

The expression (44a) is simply the contribution to the fifth integral of (39) made by the terms involving ∇_1^2 . The expression (44b) equals (44a) by virtue of the orthonormality of the $\phi_j(\mathbf{r}_2)$. Even if $\phi_j(\mathbf{r}_2)$ were not an orthogonal set, however, the terms $k_j \neq k_\ell$ in (44) would be inconsequential, just as in Eq. (42).

The contribution to the fifth integral of (39) from surface elements of type (b) (described in the preceding paragraph) is simply the contribution to that integral made by the terms involving ∇_2^2 . This contribution, which also involves a double sum over j, ℓ as in (44a) vanishes because: (i) terms $k_j \neq k_\ell$ are inconsequential; (ii) the fact that $\partial/\partial z_1$ has odd parity eliminates terms $k_j = k_\ell$. There remains the contribution to the fifth integral of (39) from surface elements of type (c). As in Eq. (23), this contribution is

$$\int dS \left\{ A^* \frac{e^{-iKr}}{r^{5/2}} \frac{\partial}{\partial r} \frac{\partial}{\partial z_1} A \frac{e^{iKr}}{r^{5/2}} - [\frac{\partial}{\partial z_1} A \frac{e^{iKr}}{r^{5/2}}] \frac{\partial}{\partial r} A^* \frac{e^{-iKr}}{r^{5/2}} \right\} \quad (45)$$

where r is defined by Eq. (21); $A \equiv A(\mathbf{n} \rightarrow \mathbf{k}'_1, \mathbf{k}'_2)$ defined by Eqs. (19)-(22); dS is given by Eq. (31); and I have recognized that $\mathbf{y} \cdot \nabla = y_1 \cdot \nabla_1 + y_2 \cdot \nabla_2 = \partial/\partial r$ (\mathbf{y} as in Eqs. (23) and (25), ∇ the six-dimensional gradient operator in $\mathcal{E}_1, \mathcal{E}_2$ -space).

Surface Integrals Evaluated

The first five integrals in (39) have been reduced to (40), (41), (44b) and (45). I now shall evaluate these surface integrals. Using Eq. (12) of Reference 1, one sees (just as in the case of potential scattering) that (40) and (41) together yield

$$\int d\underline{n}' 4\pi i k_0 (\underline{n} \cdot \underline{n}') \delta(\underline{n} - \underline{n}') [A_0^*(\underline{n} \rightarrow \underline{n}') - A_0(\underline{n} \rightarrow \underline{n}')] = 8\pi k_0 \text{Im} A_0(\underline{n} \rightarrow \underline{n}). \quad (46)$$

The expression (44b) obviously reduces to

$$- \sum_j 2k_j^2 \int d\underline{n}' (\underline{n} \cdot \underline{n}') |A_j(\underline{n} \rightarrow \underline{n}')|^2. \quad (47)$$

Using (21), (22) and (31), the expression (45) is seen to equal

$$-2 \int \frac{dS}{r^5} |A|^2 K^2 \frac{z_1}{r} = -2 \int \frac{dS}{r^5} |A|^2 K^2 (\underline{n} \cdot \underline{n}_1') \frac{r_1}{r} = -2 \int \frac{dS}{r^5} |A|^2 K (\underline{n} \cdot \underline{k}_1'). \quad (48)$$

Thus, since (30a) can be put in the form (32), the right side of (48) --which equals (45)--can be expressed as

$$\frac{-2\hbar^2}{mK^3} \int d\underline{k}_1' d\underline{k}_2' \delta(E' - E) (\underline{n} \cdot \underline{k}_1') |A(\underline{n} \rightarrow \underline{k}_1', \underline{k}_2')|^2. \quad (49)$$

I next note that the definitions (22) imply the magnitudes k_1', k_2' of $\underline{k}_1', \underline{k}_2'$ obey the relations

$$\begin{aligned} k_1'(q^{-1}) &= k_2'(q) \\ k_2'(q^{-1}) &= k_1'(q) \end{aligned} \quad (50)$$

Consequently, directly from the definition (19)

$$\begin{aligned} \lim_{\substack{r_1 \rightarrow \infty || \underline{n}_2' \\ r_2 \rightarrow \infty || \underline{n}_1' \\ r_2/r_1 = q^{-1}}} \phi(\underline{r}_1, \underline{r}_2) &= A(\underline{n} \rightarrow \underline{k}_2', \underline{n}_2', \underline{k}_1', \underline{n}_1') \frac{e^{iKr}}{r^{5/2}} \end{aligned} \quad (51)$$

where k'_1, k'_2 are $k'_1(q), k'_2(q)$ of Eq. (22). Using (15), Eq. (51) can be rewritten as

$$\lim_{\substack{r_2 \rightarrow \infty \\ r_1 \rightarrow \infty \\ r_1/r_2 = q}} \phi(r_2, r_1) = A(\underline{n} \rightarrow \underline{k}'_2, \underline{k}'_1) \frac{e^{iKr}}{r^{5/2}} \quad (52)$$

Hence, because r_1, r_2 are just dummy variables in Eqs.(19) and (52), those equations imply

$$A(\underline{n} \rightarrow \underline{k}'_1, \underline{k}'_2) = A(\underline{n} \rightarrow \underline{k}'_2, \underline{k}'_1) \quad (53)$$

Obviously, with indistinguishable electrons, the actual amplitude for ionization must obey a relation like (53). It seemed desirable to show that (53) indeed does follow from the definition of A, however; moreover, the fact that (53) can be proved supports the interpretation of the many-particle current operator (discussed in section II), which interpretation led to the relations (30)-(32) between σ_{ion} and A. Relabeling the dummy variables \underline{k}'_1 and \underline{k}'_2 in (49), and using (53), one sees that (45) equals

$$\begin{aligned} & \frac{-2\hbar^2}{mK^3} \int d\underline{k}'_2 d\underline{k}'_1 \delta(E'-E)(\underline{n} \cdot \underline{k}'_2) |A(\underline{n} \rightarrow \underline{k}'_2, \underline{k}'_1)|^2 \\ & = \frac{-\hbar^2}{mK^3} \int d\underline{k}'_1 d\underline{k}'_2 \delta(E'-E)(\underline{n} \cdot \underline{k}'_1 + \underline{n} \cdot \underline{k}'_2) |A(\underline{n} \rightarrow \underline{k}'_1, \underline{k}'_2)|^2 \end{aligned} \quad (54)$$

Expressions for σ_d and σ .

In the present e-H scattering problem, using (29) and (32), the total cross section is

$$\sigma = \sum_j \frac{k_j}{k_0} \int d\underline{n}' |A_j(\underline{n} \rightarrow \underline{n}')|^2 + \frac{1}{2k_0} \frac{\hbar^2}{mK^3} \int d\underline{k}'_1 d\underline{k}'_2 \delta(E'-E) |A(\underline{n} \rightarrow \underline{k}'_1, \underline{k}'_2)|^2 \quad (55)$$

Correspondingly, the definition (1) of the momentum transfer cross section generalizes to

$$\begin{aligned} \sigma_d = & \frac{1}{k_0} \sum_j \frac{k_j}{k_0} \int d\mathbf{n}' [k_0 - k_j (\mathbf{n}' \cdot \mathbf{n})] |A_j(\mathbf{n} \rightarrow \mathbf{n}')|^2 \\ & + \frac{1}{k_0} \frac{1}{2k_0} \frac{\hbar^2}{mK^3} \int d\mathbf{k}'_1 d\mathbf{k}'_2 \delta(E' - E) [k_0 - \mathbf{k}'_1 \cdot \mathbf{n} - \mathbf{k}'_2 \cdot \mathbf{n}] |A(\mathbf{n} \rightarrow \mathbf{k}'_1, \mathbf{k}'_2)|^2 \end{aligned} \quad (56)$$

When multiplied by the incident velocity $\hbar k_0/m$, the first term on the right side of (56) obviously represents the rate (in units of the initial momentum $\hbar k_0$, to keep the dimensions of σ_d equal to length squared) with which momentum along the incident direction \mathbf{n} is being transferred in excitation processes, including elastic scattering. Similarly, the last term in (56) obviously represents the momentum transfer by ionization, recognizing that when ionization occurs both electrons simultaneously carry away momentum.

The generalization of (7) to the present problem is

$$\sigma = \frac{4\pi}{k_0} \operatorname{Im} A_0(\mathbf{n} \rightarrow \mathbf{n}) \quad (57)$$

where σ is given by (55), and A_0 as always is the elastic forward scattering amplitude. In other words, although the particles are indistinguishable and A involves both ordinary and exchange amplitudes via (18), the optical theorem has exactly the same form as if the particles were distinguishable. If a proof of (57) is desired, it can be obtained by starting from

$$- \int d\mathbf{r} (H\Psi)^* \Psi + \int d\mathbf{r} \Psi^* H\Psi = 0 \quad (58)$$

instead of (36), and then reducing (58) to surface integrals along the lines employed earlier in this section.

Returning now to Eq. (39), the first five integrals in (39) have been reduced to the sum of (46), (47) and (54). Therefore, using (57), Eq. (39) yields

$$2k_0^2 \sigma - \sum_j 2k_j^2 \int d\underline{n}' (\underline{n} \cdot \underline{n}') |A_j(\underline{n} + \underline{n}')|^2$$

$$\frac{-\hbar^2}{mK^3} \int d\underline{k}_1' d\underline{k}_2' \delta(E' - E) (\underline{k}_1' \cdot \underline{n} + \underline{k}_2' \cdot \underline{n}) |A(\underline{n} + \underline{k}_1', \underline{k}_2')|^2 = \frac{2m}{\hbar^2} \int d\underline{r} \psi^* \frac{\partial V}{\partial z_1} \psi \quad (59)$$

Using (55) to eliminate σ , and dividing by $2k_0^2$, one sees that Eq. (59) implies Eq. (8).

There remains one point to be discussed before concluding this paper, namely the effect of including Coulomb functions rather than plane waves in (14). Using Coulomb functions in (14) means the asymptotic form of (16) must be modified by inclusion of an extra factor⁷, proportional to $\exp(-in_j \ln k_j r_1)$, where n_j is proportional to k_j^{-1} . Once this factor is included, the proof which has been given goes through essentially as in the plane wave case, except that one must include derivatives of $\exp(-in_j \ln k_j r_1)$ at infinity. But these derivatives, like the derivatives of r_1^{-1} itself, are of higher order in r_1^{-1} and so can be neglected at infinite r_1 . This justifies the assertion, in section I, that the momentum transfer theorem should apply, e.g., to excitation of H^- by electrons. The argument in this paragraph also suggests the momentum transfer theorem will remain valid in, e.g., ionization of H^- by electrons; for a more definitive statement, however, it is necessary to know how Eq. (19) must be modified when two electrons go out to infinity in the field of the proton (fixed at the origin). The reader is reminded, moreover, of the remark in section I that the right side of (8) apparently diverges for $e-H^-$ collisions. In electron-ion collisions, therefore, Eq. (8) (whether or not it is essentially valid) is not likely to be very useful without imposition of suitable cutoffs.

References

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