Cross-Section Theorem

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A cross-section theorem is derived for systems consisting of several identical particles. The total cross section for all processes; elastic, inelastic, and ionization is given in terms of the imaginary part of a linear combination of direct and exchange forward amplitudes.

IN a recent paper[1] the total cross section for the scattering of unpolarized low-energy electrons by hydrogen was estimated. This estimation was accomplished by using the relation

$$Q_1=\frac{4\pi}{k_0}\operatorname{Im} f_0(0)=\int d\Omega[|f_0(\theta,\phi)|^2+|g_0(\theta,\phi)|^2],\quad (1)$$

in which formula $k_0^2\hbar^2/2m$ is the energy of the incident electrons, f_0 and g_0 are the direct and exchange amplitudes for ground state scattering, and $d\Omega$ is the element of solid angle.

One of the early forms of the cross-section theorem was derived by Feenberg[2] for the case that exchange does not occur; the physical statement being that the integrated flux of current vanishes for steady state processes, the existence of sources and sinks being excluded as well as spin-dependent forces. It is easy to extend this conservation law for systems that include several identical particles, the electron-hydrogen problem being presented as the first application.

The antisymmetrical wave function is constructed from the unsymmetrized solutions of Schrödinger's equation and is

$$\Psi=(\psi_{12}-\psi_{21})\chi_S+(\psi_{12}+\psi_{21})\chi_A,\quad (2)$$

with χ_S and χ_A the symmetrical and antisymmetrical spin functions, respectively, and the asymptotic coordinate functions are:

$$\psi_{12}(r_1\rightarrow\infty)=e^{ik_0\mathbf{n}_0\cdot\mathbf{r}_1}\phi_0(\mathbf{r}_2)+\sum_n r_1^{-1}e^{ik_nr_1}\phi_n(\mathbf{r}_2)f_n(\theta_1,\phi_1),$$

$$\psi_{12}(r_2\rightarrow\infty)=\sum_n r_2^{-1}e^{ik_nr_2}\phi_n(\mathbf{r}_1)g_n(\theta_2,\phi_2),$$

$$\psi_{21}(r_2\rightarrow\infty)=e^{ik_0\mathbf{n}_0\cdot\mathbf{r}_2}\phi_0(\mathbf{r}_1)+\sum_n r_2^{-1}e^{ik_nr_2}\phi_n(\mathbf{r}_1)f_n(\theta_2,\phi_2),$$

$$\psi_{21}(r_1\rightarrow\infty)=\sum_n r_1^{-1}e^{ik_nr_1}\phi_n(\mathbf{r}_2)g_n(\theta_1,\phi_1).$$

ϕ_n are the hydrogen functions, $\mathbf{n}_0$ is the unit vector in the direction of incidence, and $\sum_n$ means a sum over all discrete states and an integration over the continuum.

One calculates the three-dimensional current $\mathbf{j}$ given by

$$\mathbf{j}=\operatorname{Im}(\hbar/m)\sum_{\text{spin}}\left(\int d\mathbf{r}_2\Psi^*\nabla_1\Psi+\int d\mathbf{r}_1\Psi^*\nabla_2\Psi\right),\quad (3a)$$

and requires that the integrated flux over spheres of infinite radius be zero; that is,

$$\operatorname{Im}\left(\int d\mathbf{r}_2\int \mathbf{j}\cdot d\mathbf{s}_1+\int d\mathbf{r}_1\int \mathbf{j}\cdot d\mathbf{s}_2\right)=0.\quad (3b)$$

The sum over the spin is effected to get

$$\operatorname{Im}\int d\mathbf{r}_2\int d\mathbf{s}_1\cdot[\psi_{12}^*\nabla_1\psi_{12}+\psi_{21}^*\nabla_1\psi_{21} -\tfrac{1}{2}(\psi_{12}^*\nabla_1\psi_{21}+\psi_{21}^*\nabla_1\psi_{12})]=0,\quad (3c)$$

the term $\int d\mathbf{r}_1\int\mathbf{j}\cdot d\mathbf{s}_2$ providing an identical contribution. The asymptotic forms of the wave functions are employed in (3c) to get

$$\int d\Omega\sum_n\frac{k_n}{k_0}[|f_n|^2+|g_n|^2-\tfrac{1}{2}|f_n^*g_n+f_ng_n^*)]$$
$$+\operatorname{Im}\int d\Omega r^2\Big\{ik_0\cos\theta+e^{ik_0r(1-\cos\theta)}\left(\frac{ik_0}{r}-\frac{1}{r^2}\right)$$
$$\times[f_0(\theta,\phi)-\tfrac{1}{2}g_0(\theta,\phi)]+\frac{ik_0}{r}\cos\theta[f_0^*(\theta,\phi)$$
$$-\tfrac{1}{2}g_0^*(\theta,\phi)]e^{-ik_0r(1-\cos\theta)}\Big\}=0.\quad (4)$$

In (4) terms in r^{-l} with $l>2$ are dropped. A partial integration is effected on the second integral of (4) to give the result

$$Q=(4\pi/k_0)\operatorname{Im}[f_0(0)-\tfrac{1}{2}g_0(0)],\quad (5)$$

with Q the total cross section for all processes: elastic, inelastic, and ionization, Q being given by the first integral of (4).

Equation (1) is obtained by omitting the cross terms in (3c), or the equivalent way by using $\Psi=\psi_{12}$ and omitting the spin summation in (3b), low-energy electrons being assumed.

For energies sufficiently low to insure purely elastic scattering, (5) takes a familiar form in terms of phase

[1] Howard Boyet and Sidney Borowitz, Phys. Rev. 93, 1225 (1954).
[2] Eugene Feenberg, Phys. Rev. 40, 40 (1932).

shifts as now demonstrated.

$$f_0(\theta)+g_0(\theta)=\frac{1}{2ik_1}\sum_{l=0}^{\infty}(2l+1)[\exp(i2\eta_l^+)-1]P_l(\cos\theta),$$

$$f_0(\theta)-g_0(\theta)=\frac{1}{2ik_0}\sum_{l=0}^{\infty}(2l+1)[\exp(i2\eta_l^-)-1]P_l(\cos\theta).$$

Consequently, from (5) Q becomes a well-known form:

$$Q=\frac{\pi}{k_0^2}\sum_{l=0}^{\infty}(2l+1)[3\sin^2\eta_l^-+\sin^2\eta_l^+]. \tag{6}$$

The derivation of (5) assumed infinite nuclear mass, consequently, (5) is only approximate. That this result is true for a nucleus of finite mass is now sketched for the scattering of protons by hydrogen, the result for electron scattering will then follow by the appropriate changes in charge and mass.

Let $\mathbf{r}_P$ and $\mathbf{r}_N$ be the proton coordinates and $\mathbf{r}_1$ the electron coordinate, all with respect to a fixed coordinate system. The following coordinate transformations are used[3,4]:

$$\xi_i=\mathbf{r}_1-\mathbf{r}_N,\quad \xi_f=\mathbf{r}_1-\mathbf{r}_P,$$

$$\mathbf{Z}=\frac{m\mathbf{r}_1+m(\mathbf{r}_P+\mathbf{r}_N)}{2M+m},$$

$$\gamma_i=\mathbf{r}_P-\frac{M\mathbf{r}_N+mr_1}{M+m},\quad \gamma_f=\mathbf{r}_N-\frac{M\mathbf{r}_P+m\mathbf{r}_1}{M+m},$$

$$\gamma_f=-\frac{\mu_1}{m}\gamma_i-\frac{\mu_1}{\mu_2}\xi_i,\quad \xi_f=-\gamma_i+\frac{\mu_1}{m}\xi_i,$$

$$\gamma_i=-\frac{\mu_1}{m}\gamma_f-\frac{\mu_1}{\mu_2}\xi_f,\quad \xi_i=-\gamma_f+\frac{\mu_1}{m}\xi_f,$$

$$\mu_1=\frac{mM}{M+m},\quad \mu_2=\frac{M(M+m)}{2M+m},$$

where m = electron mass and M = proton mass.

The transformed Hamiltonian becomes

$$H-T_Z=T_{\gamma i}+H_i+V_i=T_{\gamma f}+H_f+V_f,$$

with

$$T_Z=-\frac{\hbar^2}{2(2M+m)}\nabla_Z^2,\quad T_{\gamma i}=-\frac{\hbar^2}{2\mu_2}\nabla_{\gamma i}^2,$$

$$H_i=-\frac{\hbar^2}{2\mu_1}\nabla_{\xi i}^2-\frac{e^2}{\xi_i},$$

$$V_i=-\frac{e^2}{|\gamma_i-(\mu_1/m)\xi_i|}+\frac{e^2}{|\gamma_i+(\mu_1/M)\xi_i|},$$

$$T_{\gamma f}=-\frac{\hbar^2}{2\mu_2}\nabla_{\gamma f}^2,\quad H_f=-\frac{\hbar^2}{2\mu_1}\nabla_{\xi f}^2-\frac{e^2}{\xi_f},$$

$$V_f=\frac{-e^2}{|\gamma_f-(\mu_1/m)\xi_f|}+\frac{e^2}{|\gamma_f+(\mu_1/M)\xi_f|}.$$

The three-dimensional current is

$$\mathbf{j}=\hbar\,\mathrm{Im}\sum_{\mathrm{spin}}\left(\frac{1}{2M+m}\int d\gamma_i\int d\xi_i\Psi^*\nabla_Z\Psi\right.$$
$$\times\frac{1}{\mu_1}\int d\mathbf{z}\int d\gamma_i\Psi^*\nabla_{\xi i}\Psi$$
$$\left.+\frac{1}{\mu_2}\int d\mathbf{z}\int d\xi_i\Psi^*\nabla_{\gamma i}\Psi\right), \tag{6a}$$

and the conservation of integrated flux is

$$\mathrm{Im}\sum_{\mathrm{spin}}\left(\frac{1}{2M+m}\int d\gamma_i\int d\xi_i\int d\mathbf{s}_Z\cdot\Psi^*\nabla_Z\Psi\right.$$
$$+\frac{1}{\mu_1}\int d\mathbf{z}\int d\gamma_i\int d\mathbf{s}_{\xi i}\cdot\Psi^*\nabla_{\xi i}\Psi$$
$$\left.+\frac{1}{\mu_2}\int d\mathbf{z}\int d\xi_i\int d\mathbf{s}_{\gamma i}\cdot\Psi^*\nabla_{\gamma i}\Psi\right)=0. \tag{6b}$$

The asymptotic form of the wave functions are

$$\begin{aligned}\psi_{NP}(\gamma_i\to\infty)&=e^{ik_0\mathbf{n}_0\cdot\gamma_i}\phi_0(\xi_i)+\sum_n\gamma_i^{-1}e^{ik_n\gamma_i}f_n(\theta_i,\phi_i)\phi_n(\xi_i),\\ \psi_{NP}(\gamma_f\to\infty)&=\sum_n\gamma_f^{-1}e^{ik_n\gamma_f}g_n(\theta_f,\phi_f)\phi_n(\xi_f),\\ \psi_{PN}(\gamma_f\to\infty)&=e^{ik_0\mathbf{n}_0\cdot\gamma_f}\phi_0(\xi_f)+\sum_n\gamma_f^{-1}e^{ik_n\gamma_f}f_n(\theta_f,\phi_f)\phi_n(\xi_f),\\ \psi_{PN}(\gamma_i\to\infty)&=\sum_n\gamma_i^{-1}e^{ik_n\gamma_i}g_n(\theta_i,\phi_i)\phi_n(\xi_i),\end{aligned} \tag{6c}$$

by noting that (γ_i,ξ_i) are transformed into (γ_f,ξ_f) upon interchanging proton coordinates. As in (2) the antisymmetric wave function is

$$\Psi=[(\psi_{PN}-\psi_{NP})\chi_S+(\psi_{PN}+\psi_{NP})\chi_A]\exp(i\mathbf{k}'\cdot\mathbf{z}). \tag{6d}$$

The first integral in (6b) gives no contribution since $\mathbf{Z}$ only appears as a plane wave coordinate. The second integral $(\xi_i\to\infty)$ likewise gives no contribution. In fact, by the use of the integral equation formulation as in the paper by Borowitz and Friedman[5] it can be shown that this integral gives no contribution. Consequently

[3] J. D. Jackson and H. Schiff, Phys. Rev. **89**, 359 (1953).

[4] Edwin C. Kemble, *Fundamental Principles of Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1937), p. 64.

[5] S. Borowitz and B. Friedman, Phys. Rev. **89**, 441 (1953).

if (6d) is inserted in (6b), (6b) becomes

$$\mathrm{Im}\int d\mathbf{z}\int d\xi_i\int ds_{\gamma i}\cdot[\psi_{PN}^*\nabla_{\gamma i}\psi_{PN}+\psi_{NP}^*\nabla_{\gamma i}\psi_{NP}$$
$$-\tfrac{1}{2}(\psi_{PN}^*\nabla_{\gamma i}\psi_{NP}+\psi_{NP}^*\nabla_{\gamma i}\psi_{PN})]=0, \quad (6e)$$

and using (6c) ($\gamma_i\to\infty$) leads to (5) for the total cross section. That this, likewise, is valid for the electron-hydrogen problem follows immediately. (One could use the $[Z,\gamma_f,\xi_f]$ system with the corresponding functions from (6c) but the results are identical.)

The remaining system containing two identical particles that is easily treated is the two-body problem. The result is

$$Q=(8\pi/k_0)\,\mathrm{Im}[f(0)-\tfrac{1}{2}f(\pi)]. \quad (7a)$$

(The additional factor of 2 arises from the fact that in this problem there are two particles per unit area, i.e., one particle per unit area in each beam on the *same* surface.)[6] The cross section Q, for this case, is

$$Q=\int d\Omega[\tfrac{3}{4}|f(\theta,\phi)-f(\pi-\theta,\,\pi+\phi)|^2$$
$$+\tfrac{1}{4}|f(\theta,\phi)+f(\pi-\theta,\,\pi+\phi)|^2], \quad (7b)$$

It is perhaps interesting to conclude the applications of this conservation theorem by considering a three-electron problem; *viz.*, the scattering of electrons from helium for unpolarized incident electrons as before.

First, the initial state of the target is selected to be a singlet state. It is convenient to select the following eight orthonormal spin functions[7]:

$$\alpha(1)\alpha(2)\alpha(3),\quad \beta(1)\beta(2)\beta(3),$$
$$\frac{1}{\sqrt{3}}[\alpha(1)\alpha(2)\beta(3)+\alpha(1)\beta(2)\alpha(3)+\beta(1)\alpha(2)\alpha(3)],$$
$$\frac{1}{\sqrt{3}}[\beta(1)\beta(2)\alpha(3)+\beta(1)\alpha(2)\beta(3)+\alpha(1)\beta(2)\beta(3)],$$
$$\frac{1}{\sqrt{6}}[\alpha(1)\alpha(2)\beta(3)+\alpha(1)\beta(2)\alpha(3)-2\beta(1)\alpha(2)\alpha(3)], \quad (8a)$$
$$\frac{1}{\sqrt{6}}[\beta(1)\beta(2)\alpha(3)+\beta(1)\alpha(2)\beta(3)-2\alpha(1)\beta(2)\beta(3)],$$
$$\frac{1}{\sqrt{2}}\alpha(1)[\alpha(2)\beta(3)-\alpha(3)\beta(2)],$$
$$\frac{1}{\sqrt{2}}\beta(1)[\beta(2)\alpha(3)-\beta(3)\alpha(2)].$$

The first six of these spin functions are symmetrical in the coordinates and 2 and 3, while the last two are antisymmetrical in 2 and 3. The total wave function is constructed as

$$\Psi=\psi^{S,A}(123)\chi^{A,S}(123)+\psi^{S,A}(231)\chi^{A,S}(231)$$
$$+\psi^{S,A}(312)\chi^{A,S}(312), \quad (8b)$$

where the superscripts label the type of symmetry of the last two indices. χ are the spin functions given by (8a) and ψ are the asymptotic form for the wave functions on a sphere at infinity as given in (8c):

$$\psi^S(123)\underset{r_1\to\infty}{=}\exp(ik_0{}^S\mathbf{n}_0\cdot\mathbf{r}_1)\psi_0{}^S(2,3)$$
$$+\sum_n r_1{}^{-1}e^{ik_nr_1}\psi_n{}^S(2,3)f_n{}^S(\theta_1,\phi_1),$$
$$\psi^S(231)\underset{r_1\to\infty}{=}\sum_n r_1{}^{-1}\exp(ik_n{}^Sr_1)\psi_n{}^S(3,2)g_n{}^S(\theta_1,\phi_1),$$
$$\psi^S(312)\underset{r_1\to\infty}{=}\sum_n r_1{}^{-1}\exp(ik_n{}^Sr_1)\psi_n{}^S(3,2)g_n{}^S(\theta_1,\phi_1), \quad (8c)$$
$$\psi^A(123)=0,$$
$$\psi^A(231)\underset{r_1\to\infty}{=}\sum_n r_1{}^{-1}\exp(ik_n{}^Ar_1)\psi_n{}^A(3,2)g_n{}^A(\theta_1,\phi_1),$$
$$\psi^A(312)\underset{r_1\to\infty}{=}\sum_n r_1{}^{-1}\exp(ik_n{}^Ar_1)\psi_n{}^A(3,2)g_n{}^A(\theta_1,\phi_1).$$

In (8c) $\psi_n{}^S(3,2)=\psi_n{}^S(2,3)$ and $\psi_n{}^A(3,2)=-\psi_n{}^A(2,3)$, these coordinate wave functions being solutions of Schrödinger's equation for helium. The direct and exchange amplitudes f_n and g_n, as well as the propagation numbers k_n, are distinguished by superscripts in order to associate them with the proper helium wave functions; e.g., $f_n{}^S$, $g_n{}^S$, and $k_n{}^S$ belong to $\psi_n{}^S$. It is assumed that $\psi_n{}^S$, and $\psi_n{}^A$ form complete orthogonal sets of symmetrical and antisymmetrical solutions to the helium wave equation, and $\sum_n$ represents a summation over discrete states and integration over the continuum as before.

Exactly as before, one constructs the three-dimensional current vector and sets the total integrated flux equal to zero. This leads to the following results for the total cross section.

$$Q=(\pi/k_0{}^S)\,\mathrm{Im}[f_0{}^S(0)-g_0{}^S(0)], \quad (9a)$$

with

$$Q=\tfrac{1}{4}Q_{S\leftarrow S}+\tfrac{3}{4}Q_{T\leftarrow S},$$

and

$$Q_{S\leftarrow S}=\sum_n(k_n{}^S/k_0{}^S)\int d\Omega|f_n{}^S-g_n{}^S|^2,$$

for singlet-singlet transitions;

$$Q_{T\leftarrow S}=3\sum_n(k_n{}^A/k_0{}^S)\int d\Omega|g_n{}^A|^2$$

for singlet-triplet transitions.[8]

[6] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, London, 1950), p. 100.

[7] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), p. 229.

[8] Bates, Fandaminsky, and Massey, Trans. Roy. Soc. (London) **A243**, 111 (1950).

Similarly, for the initial state a triplet state (of helium) the coordinate functions are obtained by changing superscripts in (8c). The results of this case becomes

$$Q=(3\pi/k_0{}^A)\,\mathrm{Im}[f_0{}^A(0)-g_0{}^A(0)], \quad (9b)$$

with

$$Q=\tfrac{3}{4}Q_{T\leftarrow T}+\tfrac{1}{4}Q_{S\leftarrow T},$$

and

$$Q_{T\leftarrow T}=\sum_n (k_n{}^A/k_0{}^A)\int d\Omega\{|f_n{}^A-g_n{}^A|^2+2|g_n{}^A|^2\},$$

for triplet-triplet transitions, and

$$Q_{S\leftarrow T}=\sum_n (k_n{}^S/k_0{}^A)\int d\Omega|g_n{}^S|^2$$

for triplet-singlet transitions.

From the examples considered, it is seen that the total cross section is given by an integral of interference terms consisting of plane and spherical waves; thus, the general structure can be displayed as

$$Q=(4\pi/k_0)\,\mathrm{Im}A(0)$$
$$=-2\pi\,\mathrm{Re}\int_0^\pi r^2\sin\theta d\theta(1+\cos\theta)A(\theta)e^{ikr(1-\cos\theta)},$$

with $A(\theta)$ some linear combination of direct and exchange amplitudes. It is instructive to transform the variable of integration by the substitution

$$u=r(1-\cos\theta),$$

and pass to the limit $r\rightarrow\infty$. Then, Q becomes

$$Q=-4\pi\,\mathrm{Re}A(0)\int_0^\infty due^{iku}.$$

Consider the quantity I defined by

$$I=-4\pi\,\mathrm{Re}A(0)\int_0^{\lambda/2} due^{iku}$$

with $\lambda=2\pi/k$. Transform this integral by the change of variable $u=v-r_0$ to obtain

$$I=-4\pi\,\mathrm{Re}A(0)e^{-ikr_0}\int_{r_0}^{r_0+\lambda/2} dve^{ikv}.$$

The integral that appears as a factor in I is of the same type (apart from angular dependence) that appears in the Kirchoff formulation of Huygen's principle.[9] This integral would then correspond to an integration over the first Fresnel zone (of a plane or spherical surface). An evaluation of I shows that $I=2Q$ and in scalar optics the integral over the first Fresnel zone is also twice the total contribution. Moreover, the phase of the contribution of the integral in I is shifted by $\pi/2$ with respect to the phase of the contribution from the center of the first zone, also as in scalar optics. Since $\cos(ku)$ is odd and $\sin(ku)$ is even on the range $0\leq u\leq\lambda/2$, it is clear why only $\mathrm{Im}A(0)$ appears in the expressions for Q.

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[9] Max Born, *Optik* (Edwards Brothers, Inc., Ann Arbor, 1943), pp. 144–151.