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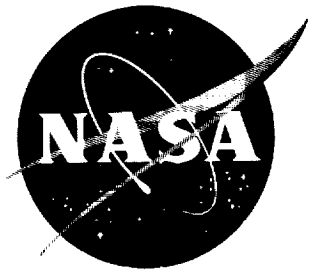

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SUMMARY

This report presents a new derivation of the generalized reciprocity theorem of quantum mechanics.

In most branches of physics, reciprocity refers to a symmetry condition on a Green's function, whereas in quantum mechanics the term is used to denote a condition on scattering amplitude or on the S-matrix. The derivation given here relates these two points of view by first deriving a generalized symmetry condition on the quantum mechanical Green's function, and from it obtaining a condition on the scattering amplitude. The reciprocity condition on the scattering amplitude is given by

$$\mu_i f^{it,js}(-\hat{r}_i,\hat{r}_j) = \mu_j f^{j\bar{s},i\bar{t}}(-\hat{r}_j,\hat{r}_i)$$

The quantity $f^{it,js}$ is the amplitude for the reaction in which there is a collision between two bound systems i in internal states t whose reduced mass is μ_i and whose centers of mass are separated by the vector $\hat{r}_i$. This results in two new bound systems j in internal states s. The state $\bar{s}$ is the state reciprocal to s; if the Hamiltonian is time-reversal invariant, $\bar{s}$ is the time reverse of the state s.

INTRODUCTION

The term reciprocity usually denotes a symmetry condition on a Green's function (ref. 1). In electrostatics, for example, the symmetry has a simple physi-

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cal interpretation because the Green's function is just the potential due to a point charge under a specific boundary condition. The reciprocity symmetry ensures that the potential is the same if the source and field point are reversed.

In quantum mechanics, reciprocity is usually thought of as connected with a symmetry condition on scattering amplitudes (ref. 2). It is readily shown (ref. 3) that, if the Hamiltonian is both Hermitian and time-reversal invariant, the system is reciprocal. There are, however, systems that are neither Hermitian nor time-reversal invariant that nevertheless display reciprocity. For example, the scattering from a complex optical model potential is reciprocal. A more general reciprocity relation, which includes both this example and the usual theorem as special cases, has been discussed by several workers (refs. 4 and 5).

In this report it is shown that reciprocity symmetry of the Green's function leads directly to reciprocity of the reaction matrix. First, a generalized reciprocity condition on the Green's function is obtained from the invariance properties of the Hamiltonian. Since the Green's function is a wave function due to a point source, it is seen that, when the source is infinitely distant from the interaction region, the wave emerging from the source is plane in the vicinity of the interaction. In the asymptotic region ($r \to \infty$), the scattering amplitude can be identified as the amplitude of the outgoing wave function. (Symbols are defined in appendix A.) Thus, the reciprocity symmetry relation for the Green's function is shown to lead to a reciprocity condition on the reaction-matrix elements. A physical interpretation is, of course, that the reciprocity symmetry assures equality of the scattering amplitude when source and detector are reversed.

In appendix B an alternative derivation of the reciprocity theorem is given that makes use of formal scattering theory.

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SYMMETRY OF THE GREEN'S FUNCTION (SPECIAL CASE - POTENTIAL SCATTERING)

It might be said that a system is reciprocal if a source located at A produces the same signal at B as would be produced at A by that source if it were located at B. This definition will now be applied to a nonrelativistic one-body quantum mechanical system characterized by the Hamiltonian

$$H = \frac{p^2}{2\mu} + V(\vec{r}) \tag{1}$$

where $p^2/2\mu$ is the kinetic-energy operator and $V(\vec{r})$, the potential energy, is a multiplicative operator. In order to make the argument as simple as possible, a spin-independent interaction is used. It is further assumed that $V(\vec{r}) = 0$ for $r > R$ (clearly, this is the conventional choice for the location of the origin of the coordinate system). For convenience, only steady-state conditions are considered so that it is possible to use the time-independent form of the Schrödinger equation

$$H\Psi(\vec{r}) - E\Psi(\vec{r}) = 0 \tag{2}$$

If there is a point source at $\vec{r} = \vec{r}_A$, the Schrödinger equation becomes

$$H\Psi(\vec{r}_A,\vec{r}) - E\Psi(\vec{r}_A,\vec{r}) = \delta(\vec{r} - \vec{r}_A) \tag{3}$$

where the wave function $\Psi(\vec{r}_A,\vec{r})$ is a function of $\vec{r}$ and depends parametrically on the location of the source $\vec{r}_A$. Similarly, a source of the same strength located at $\vec{r}_B$ will give rise to the Schrödinger equation

$$H\Psi(\vec{r}_B,\vec{r}) - E\Psi(\vec{r}_B,\vec{r}) = \delta(\vec{r} - \vec{r}_B) \tag{4}$$

Equation (3) or (4) is the equation satisfied by the Green's function corresponding to equation (2). Occasionally $\Psi(\vec{r}_1,\vec{r}_2)$ will be referred to as a Green's function.

Multiplying equation (3) by $\Psi(\vec{r}_B,\vec{r})$ and equation (4) by $\Psi(\vec{r}_A,\vec{r})$, taking the difference of the resulting two equations, and integrating over all space yields

$$\int \left[\Psi(\vec{r}_B,\vec{r})H\Psi(\vec{r}_A,\vec{r}) - \Psi(\vec{r}_A,\vec{r})H\Psi(\vec{r}_B,\vec{r})\right] d\tau = \left[\Psi(\vec{r}_B,\vec{r}_A) - \Psi(\vec{r}_B,\vec{r}_A)\right] \tag{5}$$

Thus, if the left side of equation (5) vanishes,

$$\Psi(\vec{r}_B,\vec{r}_A) = \Psi(\vec{r}_A,\vec{r}_B) \tag{6}$$

which is the reciprocity relation. In other words, it may be said that reciprocity implies symmetry of the Green's function with respect to the interchange of the coordinates, which clearly implies that the wave function at $\vec{r}_A$ due to a point source at $\vec{r}_B$ is equal to the wave function at $\vec{r}_B$ due to a source of the same strength at $\vec{r}_A$.

If the wave function obeys homogeneous boundary conditions on some bounding surface S, then the left side of equation (5) vanishes:

$$\begin{aligned} L &\equiv \int \left[\Psi(\vec{r}_B,\vec{r})H\Psi(\vec{r}_A,\vec{r}) - \Psi(\vec{r}_A,\vec{r})H\Psi(\vec{r}_B,\vec{r})\right] d\tau \\ &= \frac{-\hbar^2}{2\mu} \int \left[\Psi(\vec{r}_B,\vec{r})\nabla^2\psi(\vec{r}_A,\vec{r}) - \psi(\vec{r}_A,\vec{r})\nabla^2\psi(\vec{r}_B,\vec{r})\right] d\tau \\ &= \frac{-\hbar^2}{2\mu} \int \left[\Psi(\vec{r}_B,\vec{r})\nabla\Psi(\vec{r}_A,\vec{r}) - \Psi(\vec{r}_A,\vec{r})\nabla\Psi(\vec{r}_B,\vec{r})\right] \cdot d\vec{S} \end{aligned} \tag{7}$$

where the integration is performed over the bounding surface.

Since homogeneous boundary conditions mean that at the bounding surface

$$\alpha\Psi + \beta \frac{\partial\Psi}{\partial n} = 0 \tag{8}$$

where $\partial\Psi/\partial n$ is the derivative in the direction of the outward normal to the surface, it follows immediately that L in equation (7) vanishes, and, therefore, that equation (6) holds.

RECIPROCITY OF THE SCATTERING AMPLITUDE

(SPECIAL CASE - POTENTIAL SCATTERING)

Equation (6) expresses the reciprocity relation in terms of the Green's function. From equation (6), however, it is easy to obtain a corresponding symmetry property that must be obeyed by the scattering amplitude. The Green's function of interest in the present case must be of the form

$$\Psi(\vec{r}_A,\vec{r}) = X \frac{e^{ik|\vec{r}-\vec{r}_A|}}{|\vec{r} - \vec{r}_A|} + \Psi_{scatt}(\vec{r}_A,\vec{r}) \tag{9}$$

where $k = \sqrt{2\mu E/\hbar^2}$ and Ψ_{scatt} is everywhere regular. The singular term represents the spherical wave emanating from the source. Direct integration of equation (3) over an infinitesimal volume containing the point $\vec{r} = \vec{r}_A$ shows that

$$X = 2\mu/4\pi\hbar^2 \tag{10}$$

Asymptotically, for large values of r, $\Psi_{scatt}(\vec{r}_A,\vec{r})$ must have the form of an outgoing spherical wave emanating from the scattering center (which has been chosen to be at the origin); that is, for $r \gg R$

$$\Psi_{scatt} \to \mathcal{F}(-\vec{r}_A,\hat{r}) \frac{e^{ikr}}{r} \tag{11}$$

where $\hat{r}$ is the unit vector $\vec{r}/r$. Thus, for large r

$$\Psi(\vec{r}_A,\vec{r}) \to (2\mu/4\pi\hbar^2) \frac{e^{ik|\vec{r}-\vec{r}_A|}}{|\vec{r} - \vec{r}_A|} + \mathcal{F}(-\vec{r}_A,\hat{r}) \frac{e^{ikr}}{r} \quad (r \gg R) \tag{12}$$

The expressions analogous to equations (9) to (12) for the source at $\vec{r}_B$ are self-evident.

If it is assumed, for convenience, that the bounding surface is a sphere whose radius ρ is very large compared with R (the range of the force), r_A, and r_B, then, from equation (12)

$$\left(\frac{1}{\Psi}\frac{\partial\Psi}{\partial r}\right)_{r=\rho} \xrightarrow[\rho\to\infty]{} ik \tag{13}$$

so that L in equation (7) vanishes in the present case, and the reciprocity relation, equation (6), must hold.

In the usual idealization of the scattering experiment, the source is taken to be an infinite distance from the scattering center. The result for this special case is easily obtained from equation (12). If $r_A \gg r \gg R$, equation (12) becomes

$$\Psi(\vec{r}_A,\vec{r}) = (2\mu/4\pi\hbar^2)\,\frac{e^{ikr_A}}{r_A}\left\{e^{-ik\hat{r}_A\vec{r}} + \left[(2\mu/4\pi\hbar^2)\,\frac{e^{ikr_A}}{r_A}\right]^{-1}\mathcal{T}(-\vec{r}_A,\hat{r})\,\frac{e^{ikr}}{r}\right\} \tag{14}$$

This limiting form of the wave function $\Psi(\vec{r}_A,\vec{r})$ satisfies the same differential equation with the same boundary conditions as the usual wave function of time-independent scattering theory, except for the overall factor $(2\mu/4\pi\hbar^2)(e^{ikr_A}/r_A)$. Thus, for $r_A,\ r \gg R$,

$$\left[(2\mu/4\pi\hbar^2)\,\frac{e^{ikr_A}}{r_A}\right]^{-1}\mathcal{T}(-\vec{r}_A,\hat{r}) = f(-\hat{r}_A,\hat{r}) \tag{15}$$

where f is the usual scattering amplitude. It is noted that the validity of equation (14) required that $r_A \gg r \gg R$. The restriction $r_A \gg r$ applies only to the source term of equation (14) and is not required for equation (15) (see appendix C). It is necessary only to require that the source term be a plane wave within the range of the force in order that equation (15) hold; that is, in equation (15) it is permissible that $r_A \approx r$.

A wave function due to another source located at $\vec{r}_B$ will have the asymptotic form

$$\Psi(\vec{r}_B,\vec{r}) \to (2\mu/4\pi\hbar^2)\,\frac{e^{ik|\vec{r}-\vec{r}_B|}}{|\vec{r}-\vec{r}_B|} + \mathcal{T}(-\vec{r}_B,\hat{r})\,\frac{e^{ikr}}{r}, \qquad r \gg R \tag{16}$$

Application of the symmetry relation (eq. (6)) and the wave functions (eqs. (12) and (16)) when $r_A,\ r_B \gg R$ yields

$$(2\mu/4\pi\hbar^2)\,\frac{e^{ik|\vec{r}_B-\vec{r}_A|}}{|\vec{r}_B-\vec{r}_A|} + \mathcal{T}(-\vec{r}_A,\hat{r}_B)\,\frac{e^{ikr_B}}{r_B} = (2\mu/4\pi\hbar^2)\,\frac{e^{ik|\vec{r}_A-\vec{r}_B|}}{|\vec{r}_A-\vec{r}_B|} + \mathcal{T}(-\vec{r}_B,\hat{r}_A)\,\frac{e^{ikr_A}}{r_A} \tag{17}$$

or by virtue of equation (15)

$$f(\hat{k},\hat{k}') = f(-\hat{k}',-\hat{k}) \tag{18}$$

where

$$\left.\begin{aligned} \vec{k} &= -k\,\frac{\vec{r}_A}{r_A} \\ \text{and} \\ \vec{k}' &= k\,\frac{\vec{r}_B}{r_B} \end{aligned}\right\} \tag{19}$$

It is noted that the derivation of equations (17) and (18) in no way depends on whether the Hamiltonian of equation (1) is real. On the contrary, the treatment is equally valid for a complex potential. For a Hamiltonian of the form given by equation (1), all that needs to be assumed to obtain the result is that $V(r)$ is a multiplicative operator and that the boundary conditions are such as to make the surface integral in equation (7) vanish.

Since a complex potential implies a non-Hermitian Hamiltonian, it is evident that Hermiticity is not necessary in order to obtain reciprocity. This is completely analogous to the well-known result in network theory. It is quite possible for an electrical network to be dissipative and still be reciprocal. For an electrical circuit, the crucial question is not whether there is energy dissipated in a resistor, but whether there is a rectifier in the circuit. This is exactly analogous to the quantum-mechanical case treated in this section. A non-Hermitian Hamiltonian will not conserve particles, but the reciprocity theorem may hold despite this.

RECIPROCITY OF THE GREEN'S FUNCTION

The previous discussion suggests that, although Hermiticity and time-reversal invariance of the Hamiltonian are sufficient, they are not necessary for reciprocity. A more general invariance property of the Hamiltonian that will also encompass the results obtained in the previous section is sought. Consequently, more abstract arguments than the preceding appear to be necessary. Such an argument follows.

Consider the matrix eigenvalue equation

$$(H - E)\Psi = 0 \tag{20}$$

where H is the Hamiltonian matrix and Ψ is a column vector. No distinction between position coordinates and the various discrete indices that may label the states will be made. Now, consider the corresponding Green's function equation

$$(H - E)\Psi = 1 \tag{21}$$

To make equation (21) more explicit, it may be written as

$$(H_{x'x''} - E\delta_{x'x''})\Psi_{x''x} = \delta_{x'x} \tag{22}$$

The Einstein summation convention is used in equation (22). The summations are, of course, generalized in that it is possible to sum over discrete coordinates and integrate over continuous ones. Similarly, the generalized delta function in equation (22) is a Kronecker delta for discrete coordinates and Dirac delta for continuous ones.

The transpose of both sides of equation (21) is taken and the unitary matrix U is introduced to obtain[1]

$$U\Psi^{T}U^{\dagger}U(H^{T} - E)U^{\dagger} = 1 \tag{23}$$

Thus, if $\tilde{\Psi}$ is defined to be

$$\tilde{\Psi} = U\Psi^{T}U^{\dagger} = U\Psi^{\dagger *}U^{\dagger} \tag{24}$$

and $\tilde{H}$ to be

$$\tilde{H} = UH^{T}U^{\dagger} = UH^{\dagger *}U^{\dagger} \tag{25}$$

equation (23) can be rewritten as

$$\tilde{\Psi}(\tilde{H} - E) = 1 \tag{26}$$

Now, if both sides of equation (26) operate on the Green's function Ψ,

$$\tilde{\Psi}(\tilde{H} - E)\Psi = \Psi \tag{27}$$

Thus, if H has the invariance property

$$\tilde{H} = H \tag{28}$$

and equation (21) is inserted into equation (27), the result obtained is

$$\tilde{\Psi} = \Psi \tag{29}$$

This is the general form of the reciprocity theorem expressed in terms of the Green's function.

If the unitary matrix U is taken to be the identity, then the reciprocity theorem reduces to the result that symmetry of the Hamiltonian, namely,

$$H = H^{T} = H^{\dagger *} \tag{30}$$

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[1]The following notation is used: A^{T} denotes the transpose, $A^{\dagger}$ denotes the Hermitian conjugate, and A^{*} denotes the complex conjugate of A. Only two of the three symbols are needed, of course, since $A^{T} = A^{\dagger *}$.

implies symmetry of the Green's function

$$\Psi = \Psi^{T} = \Psi^{\dagger *} \tag{31}$$

or, explicitly, $H_{xx'} = H_{x'x}$ implies that

$$\Psi_{xx'} = \Psi_{x'x} \tag{32}$$

In a representation in which x and x' are space coordinates, equations (30) to (32) are recognized as the result obtained earlier in equation (6). If the Hamiltonian is a symmetric matrix, the reciprocity relation holds, as is shown in equations (31) and (32), which says that the wave function at x due to a point source of unit strength at x' is identically equal to the wave function at x' due to a point source of unit strength at x.

SYMMETRY OF THE MATRIX ELEMENTS

For the general case when U is not unity, conditions on the matrix elements of H can be determined. If Ψ^{α} and Ψ^{β} are two particular state vectors, $H_{\alpha\beta}$ and $\Psi_{\alpha\beta}$ are defined as

$$H_{\alpha\beta} \equiv (\psi^{\alpha})^{\dagger} H \psi^{\beta} \equiv (\psi^{\alpha})^{*}_{x} H_{xx'} (\psi^{\beta})_{x'} \tag{33}$$

and

$$\Psi_{\alpha\beta} \equiv (\psi^{\alpha})^{\dagger} \Psi \psi^{\beta} \equiv (\psi^{\alpha})^{*}_{x} \Psi_{xx'} (\psi^{\beta})_{x'} \tag{34}$$

Equation (33) may be rewritten to read[2]

$$H_{\alpha\beta} = (\psi^{\beta})^{\dagger *} H^{\dagger *} (\psi^{\alpha})^{*} = (U\psi^{\beta *})^{\dagger} (UH^{\dagger *}U^{\dagger})(U\psi^{\alpha *}) = (\psi^{\overline{\beta}})^{\dagger} \tilde{H} \psi^{\overline{\alpha}} = \tilde{H}_{\overline{\beta}\overline{\alpha}} \tag{35}$$

where U is a unitary matrix, $\tilde{H}$ is as defined in equation (25), and

$$\psi^{\overline{\alpha}} = U\psi^{\alpha *} \tag{36}$$

Thus, if the Hamiltonian obeys the symmetry relation (eq. (28)), then

$$H_{\alpha\beta} = H_{\overline{\beta}\overline{\alpha}} \tag{37}$$

Similarly,

$$\Psi_{\alpha\beta} \equiv (\psi^{\alpha})^{\dagger} \Psi (\psi^{\beta}) = (\psi^{\overline{\beta}})^{\dagger} \Psi \psi^{\overline{\alpha}} \equiv \tilde{\Psi}_{\overline{\beta}\overline{\alpha}} \tag{38}$$

---

[2]The first equality in equation (35) is a consequence of the fact that ψ is a column vector, so that $(\psi^{\alpha})^{\dagger} H (\psi^{\beta})$ is a scalar and is, therefore, equal to its transpose.

which according to equation (29) yields

$$\Psi_{\alpha\beta} = \Psi_{\overline{\beta\alpha}} \tag{39}$$

if $H = \tilde{H}$.

Equation (36) will be recognized as the general definition of an antiunitary transformation. Familiar examples of antiunitary transformations are the time-reversal and charge-conjugation transformations. The antiunitary transformation that maps the state ψ^{α} into $\psi^{\overline{\alpha}}$ as defined in equation (36) will map the Hamiltonian H into $\overline{H}$, where $\overline{H}$ is defined as

$$\overline{H} = UH^{*}U^{\dagger} \tag{40}$$

Therefore, the reciprocity theorem is expressed as follows. Given an antiunitary transformation that maps a state ψ^{α} into $\psi^{\overline{\alpha}}$ and transforms an operator $\mathcal{O}$ into $\overline{\mathcal{O}}$, then, if the Hamiltonian has the invariance property $H = \overline{H}^{\dagger}$, the Green's function will possess the reciprocity symmetry $\Psi_{\alpha\beta} = \Psi_{\overline{\beta\alpha}}$.

It should be noted that the definition of an antiunitary transformation (unlike that of a unitary transformation) is not independent of the representation (ref. 5). To see this, it is noted that for a unitary transformation

$$\psi = U\varphi \tag{41}$$

where U is unitary and ψ and φ are column vectors. Under a change of representation generated by the unitary matrix Y, it can be seen that

$$\psi' = U'\varphi' \tag{42}$$

where

$$\psi' = Y\psi \tag{43}$$

$$\varphi' = Y\varphi \tag{44}$$

and

$$U' = YUY^{\dagger} \tag{45}$$

On the other hand, an antiunitary transformation

$$\psi = U\varphi^{*} \tag{46}$$

under a change of representation generated by the unitary matrix Y, becomes

$$\psi' = (YUY^{\dagger *})\varphi'^{*} \neq U'\varphi'^{*} \tag{47}$$

and hence, is representation dependent. Thus, in using equations (36) and (40), it must be remembered that the choice of representation is of some significance.

If in one representation, however,

$$H = \overline{H}^{\dagger} = UH^{\dagger *}U^{\dagger} \tag{48}$$

then in the new representation

$$H' = WH'^{\dagger *}W^{\dagger} \tag{49}$$

where

$$W = YUY^{\dagger *} \tag{50}$$

and the previous results, equations (33) to (40), hold with the unitary matrix U replaced by the unitary matrix W of equation (50).

RECIPROCITY OF THE REACTION MATRIX

In order to obtain the reciprocity condition on the reaction matrix, it is necessary first to rewrite the results of the section RECIPROCITY OF THE GREEN'S FUNCTION for the case where the unit matrix is in space-spin coordinates with the space-coordinate dependence of the wave function shown explicitly. The Green's function equation is

$$(H - E)\Psi(\xi,\xi') = \delta(\xi - \xi')\underset{\sim}{1} \tag{51}$$

where $\underset{\sim}{1}$ is the unit matrix in spin space. The reciprocity symmetry condition can be written

$$H^{T}(\xi',\xi)U^{\dagger} = U^{\dagger}H(\xi,\xi') \tag{52}$$

and

$$\Psi^{T}(\xi',\xi)U^{\dagger} = U^{\dagger}\Psi(\xi,\xi') \tag{53}$$

The unitary matrix $U^{\dagger}$ is restricted here to operate only on the spin components of H and Ψ as is the transpose operation. The symbol ξ represents the space coordinates of the system.

The complete Hamiltonian can be broken up in a number of ways corresponding to various groupings of the particles:

$$H = H_i + T_i + V_i = H_j + T_j + V_j \tag{54}$$

where H_i is the Hamiltonian for the internal motion of two groups of particles whose centers of mass are separated by the vector $\vec{r}_i$, T_i is the operator for the relative kinetic energy, and V_i is the interaction between them. It is assumed that H_i, H_j, etc. are Hermitian, although H itself need not be. The wave equation for the internal motion is

$$(H_i - E_t)\varphi_{it}(\xi_i) = 0 \tag{55}$$

where ξ_i includes all coordinates ξ except $\vec{r}_i$ and t is the state of internal motion.

Multiplying the Green's function (eq. (51)), on the right by the internal function $\varphi_{it}(\xi_i)$ and integrating over ξ_i give the result

$$(H - E)X_{it}(\xi,r_i') = \delta(\vec{r}_i - \vec{r}_i')\varphi_{it}(\xi_i) \tag{56}$$

where

$$X_{it}(\xi,\vec{r}_i') = \int d\xi_i' \, \Psi(\xi,\xi')\varphi_{it}(\xi_i') \tag{57}$$

The wave function X_{it} plays the same role here as the Green's function $\Psi(\vec{r}_A,\vec{r})$ introduced earlier. Equation (56) describes the motion of the system with a point source in channel i.

From equation (56) an integral equation for X_{it} can be obtained by expanding it in the complete orthonormal set, $e^{i\vec{k}\cdot\vec{r}_i}\varphi_{it'}(\xi_i)$, of eigenfunctions of $H_i + T_i$. For $r_i' \gg r_i \gg R$ the integral equation has the asymptotic form (see appendix D):

$$X_{it}(\xi,\vec{r}_i') \to (2\mu_i/4\pi\hbar^2)\frac{\exp(ik_{it}r_i')}{r_i'}\exp(-ik_{it}\hat{r}_i'\cdot\vec{r}_i)\varphi_{it}(\xi_i)$$

$$-\sum_{t'}\varphi_{it'}(\xi_i)\frac{\exp(ik_{it'}r_i)}{r_i}F^{it,it'}(-\vec{r}_i',\hat{r}_i) \tag{58}$$

Equation (58) has the form of an incident plane wave plus scattered waves in all excited internal states. Because the normalization of the plane wave is not unity,

$$f^{it,it'} \equiv \frac{F^{it,it'}}{(2\mu_i/4\pi\hbar^2)\dfrac{e^{ik_{it}r_i'}}{r_i'}} \tag{59}$$

is interpreted as the scattering amplitude for the process $it \to it'$.

In order to study a reaction from the channel represented by i to a different channel j, X_{it} is expanded in terms of eigenstates of $H_j + T_j$, $e^{i\vec{k}\cdot\vec{r}_j}\varphi_{js}(\xi_j)$. The asymptotic form is

$$X_{it}(\xi,\vec{r}_i') = \sum_{s'} \frac{e^{ik_{js'}r_j}}{r_j} \varphi_{js'}(\xi_j) \left\{ 2\mu_j/4\pi\hbar^2 \right.$$

$$\left. \times \left[\int d\xi'' \exp(-ik_{js'}\hat{r}_j \cdot \vec{r}_j'') \delta(\vec{r}_i'' - \vec{r}_i') \varphi_{js'}^{\dagger}(\xi_j'') \varphi_{it}(\xi_i'') \right] - F^{it,js'}(-\vec{r}_i', \hat{r}_j) \right\} \qquad (60)$$

(see appendix D). The second term in the braces gives the scattered wave in the j channel. The first term, which is due to the source, vanishes for all bound internal states s' if the state t is also bound, since the product $\delta(\vec{r}_i'' - \vec{r}_i')\varphi_{js'}^{\dagger}(\xi_j'')\varphi_{it}(\xi_i'')$ then decays exponentially with $\vec{r}_i''$. Since the plane-wave term of equation (58) does not have unit amplitude,

$$f^{it,js'} = \frac{F^{it,js'}}{\frac{e^{ik_{it}r_i'}}{r_i'}(2\mu_i/4\pi\hbar^2)} \qquad (61)$$

is interpreted as the reaction amplitude for the process $it \to js'$. Arguments similar to those made in the section RECIPROCITY OF THE SCATTERING AMPLITUDE (SPECIAL CASE - POTENTIAL SCATTERING) show that the amplitudes $f^{it,it'}$ and $f^{it,js'}$ are each independent of r_i', and the quantities $F^{it,it'}$ and $F^{it,js'}$ therefore depend on r_i' through the overall constant $e^{ik_{it}r_i'}/r_i'$.

In order to obtain the reciprocity relation for the reaction matrix it is necessary to multiply both sides of the reciprocity symmetry relation (eq. (51)) by a pair of bound state internal functions - on the left by $\varphi_{it}^{T}(\xi_i)$ and on the right by[3] $\varphi_{j\bar{s}}(\xi_j')$ - and to integrate over ξ_i and ξ_j'. From the definition of X in equation (57), it follows that

$$\int d\xi_j' \, X_{it}^{T}(\xi',\vec{r}_i) U^{\dagger} \varphi_{j\bar{s}}(\xi_j') = \int d\xi_i \varphi_{it}^{T}(\xi_j) U^{\dagger} X_{j\bar{s}}(\xi,\vec{r}_j') \qquad (62)$$

With the asymptotic forms for X_{it} and $X_{j\bar{s}}$ appropriate for large r_i, r_j', equation (62) becomes

[3]The wave function $\varphi_{j\bar{s}}(\xi_j')$ is the reciprocal state defined in equation (36).

$$\int d\xi_j' \left[-\sum_{s'} \frac{e^{ik_{js'}r_j'}}{r_j'} F^{it,js'}(-\hat{r}_i,\vec{r}_j')\varphi^T_{js'}(\xi_j') \right] U^\dagger \varphi_{j\bar{s}}(\xi_j')$$

$$= \int d\xi_i \, \varphi^T_{it}(\xi_i) U^\dagger \left[-\sum_{t'} \varphi_{i\bar{t}'}(\xi_i) \frac{e^{ik_{it'}r_i}}{r_i} F^{j\bar{s},i\bar{t}'}(-\vec{r}_j',\hat{r}_i) \right] \tag{63}$$

The continuum terms due to the source appearing in equation (60) vanish because of orthogonality of the φ's. On the left of equation (63) there is the integral

$$\int \varphi^T_{js'} U^\dagger \varphi_{j\bar{s}} \, d\xi_{j'} = \int \varphi^T_{js'} \varphi^*_{js} = \delta_{ss'} \tag{64}$$

and on the right

$$\int d\xi_i \, \varphi^T_{it} U^\dagger \varphi_{i\bar{t}'} = \int d\xi_i \, \varphi^\dagger_{i\bar{t}'} \varphi_{i\bar{t}'} = \delta_{\bar{t}\bar{t}'} \tag{65}$$

From equations (63) to (65) it follows that

$$\frac{e^{ik_{js}r_j}}{r_j} F^{it,js}(-\vec{r}_i,\hat{r}_j') = \frac{e^{ik_{i\bar{t}}r_i'}}{r_i'} F^{j\bar{s},i\bar{t}}(-\vec{r}_j',\hat{r}_i) \tag{66}$$

which along with equation (61) gives the result

$$\mu_i f^{it,js}(-\hat{r}_i,\hat{r}_j') = \mu_j f^{j\bar{s},i\bar{t}}(-\hat{r}_j',\hat{r}_i) \tag{67}$$

It can easily be shown by using equation (58) that equation (67) also holds for scattering.

It has been shown that a generalized reciprocity relation on the reaction matrix follows directly from the reciprocity symmetry of the Green's function. The conditions under which it holds are that (1) the Hamiltonian has the reciprocity symmetry (eq. (28)), (2) the channel Hamiltonians are both Hermitian, and (3) the internal states of the two colliding systems before and after the collision are bound.

Lewis Research Center
National Aeronautics and Space Administration
Cleveland, Ohio, June 10, 1963

APPENDIX A

SYMBOLS

E	energy
$F^{it,it'}$	angle dependent amplitude of it' component of scattered wave
$f^{it,it'}$	scattering amplitude for process $it \rightarrow it'$
G	complete Green's function
H	Hamiltonian
$\hbar$	$h/2\pi$
k,k'	wave numbers for E
L	surface integral
m	mass
$\mathcal{O}$	arbitrary operator
p	momentum operator
R	distance beyond which potential is zero
r	length of radius vector from origin to some field point
S	bounding surface
s,t	internal states
T	part of H describing relative motion of system when broken into two noninteracting parts
$\mathcal{T}$	angle dependent part of scattered wave function
U,W,Y	unitary matrices
V	channel interaction potential
X	source strength
X_{it}	wave function; Green's function for single-channel source
α,β	coefficients of homogeneous boundary condition

δ generalized δ function: Kronecker δ for discrete coordinates and Dirac δ for continuous coordinates

ϵ energy of an internal state

μ reduced mass

ξ space coordinates of system

ρ radius of bounding sphere

τ element of volume

φ state vector

Ψ solution of Schrödinger equation; wave function; Green's function

ψ state vector

$\mathbb{1}$ unit matrix

Subscripts:

i,j,k channels

scatt scattered part

Superscripts:

i,j,k channel subscripts

T transpose operation

$\rightarrow$ vector

$\hat{}$ unit vector

$\bar{}$ reciprocal

$\dagger$ Hermitian conjugate operation

$*$ complex conjugate operation

APPENDIX B

DERIVATION OF THE RECIPROCITY THEOREM BY MEANS OF FORMAL SCATTERING THEORY

The reciprocity theorem can readily be derived by using the results and methods of formal scattering theory.

Let H be the Hamiltonian of the system. The channel Hamiltonians are denoted by H_i, H_j, . . . , and the channel interaction potentials by V_i, V_j, ... Thus,

$$H = H_i + V_i = H_j + V_j = \cdots \tag{B1}$$

Next, the eigenfunctions of the various Hamiltonians are defined as

$$(E - H)\psi = 0 \tag{B2}$$

and

$$(E - H_k)\varphi_k = 0 \tag{B3}$$

and the corresponding outgoing Green's functions

$$(E - H)G = 1 \tag{B4}$$

and

$$(E - H_k)G_k = 1 \tag{B5}$$

A well-known result of formal scattering theory is the following expression for the scattering amplitude:

$$T_{ij} = \langle \varphi_i | V_i + V_i G V_j | \varphi_j \rangle \tag{B6}$$

T_{ij} is the amplitude for scattering from state φ_j to state φ_i. An alternative expression for the scattering amplitude is

$$T_{ij} = \langle \varphi_i | V_j + V_i G V_j | \varphi_j \rangle \tag{B7}$$

The system under discussion will be said to be reciprocal if the scattering amplitude has the property

$$T_{ij} = T_{\overline{ji}} \tag{B8}$$

where the state $\varphi_{\overline{i}}$ is related to the state φ_i by the antiunitary transformation

$$\varphi_i = U\varphi_i^* \tag{B9}$$

with

$$U^{\dagger} = U^{-1} \tag{B10}$$

To determine under what circumstances the system is reciprocal, it is necessary to make use of the following result:

$$\langle \varphi_i | A | \varphi_j \rangle = \langle \varphi_j^* | A^{\dagger *} | \varphi_i^* \rangle = \langle \varphi_{\overline{j}} | UA^{\dagger *}U^{\dagger} | \varphi_{\overline{i}} \rangle \tag{B11}$$

If this expression is compared with equations (B6) and (B7), it can be seen that the system will be reciprocal if

$$U(V_i + V_i G V_j)^{\dagger *} U^{\dagger} = \begin{cases} V_{\overline{i}} + V_{\overline{j}} G V_{\overline{i}} \\ \text{or} \\ V_{\overline{j}} + V_{\overline{j}} G V_{\overline{i}} \end{cases} \tag{B12}$$

By definition, however,

$$U(V_i + V_i G V_j)^{\dagger *} U^{\dagger} = \tilde{V}_i + \tilde{V}_j \tilde{G} \tilde{V}_i \tag{B13}$$

where

$$\tilde{A} \equiv UA^{\dagger *}U^{\dagger} \tag{B14}$$

Thus, sufficient conditions for reciprocity are

$$\left.\begin{aligned} \tilde{V}_i &= V_{\overline{i}} \\ \tilde{V}_j &= V_{\overline{j}} \\ \tilde{G} &= G \end{aligned}\right\} \tag{B15}$$

and

Conditions (B15) on the Green's function and the channel interaction potentials are readily translated into requirements on H, H_i, and H_j. From equations (B4) and (B14),

$$\tilde{G}(E - \tilde{H}) = 1 \tag{B16}$$

so that

$$\tilde{G}(E - \tilde{H})G = G \tag{B17}$$

A comparison of equations (B17) and (B4) shows that $\tilde{H} = H$ implies that $\tilde{G} = G$.

For the channel potentials,

$$\tilde{V}_i - V_{\bar{i}} = (\tilde{H} - H_i) - (H - H_{\bar{i}})$$

$$= H_{\bar{i}} - H_{\bar{i}}^{\dagger} \tag{B18}$$

where, in accordance with equations (B3) and (B9),

$$H_{\bar{i}} = UH_i^{*}U^{\dagger} \tag{B19}$$

Thus, the requirement $\tilde{V}_i = V_{\bar{i}}$ is equivalent to the requirement[4]

$$H_{\bar{i}} = H_{\bar{i}}^{\dagger} \tag{B20}$$

It is concluded that a system is reciprocal with respect to an antiunitary transformation $\varphi \rightarrow U\varphi^{*}$ if the Hamiltonian of the system is invariant under the transformation $H \rightarrow UH^{\dagger *}U^{\dagger}$ and the scattering connects channel states that are eigenstates of Hermitian Hamiltonians (in agreement with the results of the section RECIPROCITY OF THE REACTION MATRIX).

[4]It should be noted that the equality of equations (6) and (7) already requires the condition of equation (B20).

APPENDIX C

DEPENDENCE OF THE SCATTERED WAVE ON SOURCE DISTANCE

The following is an elaboration on the discussion that permitted the removal of the restriction $r_A \gg r$ from equation (15), which is required for the validity of equation (14).

Adapting equation (D5) to the special case of potential scattering gives an integral equation for $\psi(\vec{r}_A,\vec{r})$:

$$\psi(\vec{r}_A,\vec{r}) = \frac{2\mu}{4\pi\hbar^2}\left[\frac{e^{ik|\vec{r}-\vec{r}_A|}}{|\vec{r}-\vec{r}_A|} - \int d\vec{r}' \; \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}')\psi(\vec{r}_A,\vec{r}')\right]$$

$$\xrightarrow[r_A>>r>>R]{} \frac{2\mu}{4\pi\hbar^2}\left[\left(\frac{e^{ikr_A}}{r_A} e^{-ik\hat{r}_A\cdot\vec{r}}\right) - \frac{e^{ikr}}{r}\int d\vec{r}' \; e^{-ik\hat{r}\cdot\vec{r}'} V(r')\psi(\vec{r}_A,\vec{r}')\right] \qquad (C1)$$

Comparing equations (14) and (C1) yields

$$T(-\vec{r},\hat{r}) = -\frac{2\mu}{4\pi\hbar^2}\int d\vec{r}' \; e^{-ik\hat{r}\cdot\vec{r}'} V(\vec{r}')\psi(\vec{r}_A,\vec{r}') \qquad (C2)$$

If a Born series expansion is valid in equation (C2), equations (C1) and (C2) yield

$$T(\vec{r},\hat{r}) = -\frac{2\mu}{4\pi\hbar^2}\left[\int d\vec{r}' \; e^{-ik\vec{r}\cdot\vec{r}'} V(\vec{r}')\left(\frac{2\mu}{4\pi\hbar^2}\frac{e^{ik|\vec{r}'-r_A|}}{|\vec{r}'-\vec{r}_A|}\right) + \int dr'' \; e^{-ik\hat{r}\cdot r''} V(r'')\right.$$

$$\left. \times \int dr' \; \frac{2\mu}{4\pi\hbar^2}\frac{e^{ik|r''-r'|}}{|\vec{r}''-\vec{r}'|} V(r')\left(\frac{2\mu}{4\pi\hbar^2}\frac{e^{ik|\vec{r}'-\vec{r}_A|}}{|\vec{r}'-\vec{r}_A|}\right) + \ldots\right] \qquad (C3)$$

Provided that the source distance r_A is much larger than the range of forces R, the equation

$$\frac{e^{ik|r'-r_A|}}{|\vec{r}' - \vec{r}_A|} = \frac{e^{ikr_A}}{r_A} e^{ik\hat{r}_A \cdot \vec{r}'} \tag{C4}$$

(C4) holds within the region of integration because r_A is taken to be much larger than any value of r' contributing significantly to the integral. With the equality (C4) in equation (C3), it is possible to factor out $(2\mu/4\pi\hbar^2)e^{ikr_A}/r_A$, which is common to each term. The other factor is just the Born series for the scattering amplitude in time-independent scattering theory. Thus, equation (C3) reduces to

$$T(-\vec{r}_A,\hat{r}) = \frac{2\mu}{4\pi\hbar^2} \frac{e^{ikr_A}}{r_A} f(-\hat{r}_A,\hat{r}) \tag{C5}$$

Although the Born series expansion has been used in the calculation of equation (C5), it is by no means necessary for the proof. It is only necessary that, within the range of forces, the Green's function $\psi(\vec{r},\vec{r}_A)$ have a form that is asymptotically a plane wave plus an outgoing scattered wave. Then, since $\psi(\vec{r},\vec{r}_A)$ and the usual wave function of time-independent scattering theory also satisfy the same differential equation within the range of forces, they can differ there only by an overall constant factor. This constant is just the coefficient of the plane wave.

APPENDIX D

DERIVATION OF THE INTEGRAL EQUATIONS

Equation (53) can be written

$$(H_i + T_i - E)X_{it}(\xi,\vec{r}_i') = \delta(\vec{r}_i - \vec{r}_i')\varphi_{it}(\xi_i) - V_i X_{it}(\xi,r_i') \tag{D1}$$

In order to obtain an integral equation for $X_{it}(\xi,r_i')$, it is necessary to expand it in a complete set of eigenfunctions of $H_i + T_i$:

$$X_{it}(\xi,r_i') = \sum_{t'} \int d\vec{k}\, A_{t'}(\vec{k}) e^{i\vec{k}\cdot\vec{r}_i}\, \varphi_{it'}(\xi_i) \tag{D2}$$

Using this form in equation (D1) yields

$$(H_i + T_i - E)X_{it}(\xi,\vec{r}_i) = \sum_{t'} \int d\vec{k} \left(\epsilon_{t'} + \frac{\hbar^2 k^2}{2\mu_i} - E\right) A_{t'}(\vec{k}) e^{i\vec{k}\cdot\vec{r}_i}\, \varphi_{it'}(\xi_i)$$

$$= \delta(\vec{r}_i - \vec{r}_i')\varphi_{it}(\xi_i) - V_i X_{it}(\xi,\vec{r}_i') \tag{D3}$$

Because H_i is Hermitian, the following is obtained from equation (D3):

$$A_{t'}(\vec{k}) = \frac{1}{\epsilon_{t'} + \frac{\hbar^2 k^2}{2\mu_i} - E} \left[\frac{e^{-i\vec{k}\cdot\vec{r}_i}}{8\pi^3} \delta_{tt'} - \frac{1}{8\pi^3} \int d\xi\, e^{-i\vec{k}\cdot\vec{r}_i}\, \varphi_{it}^{\dagger}(\xi_i) V_i X_{it}(\xi,\vec{r}_i') \right] \tag{D4}$$

Putting this result into equation (D3) gives the equation

$$X_{it}(\xi,\vec{r}_i') = \frac{1}{8\pi^3} \int d\vec{k}\, \frac{e^{-i\vec{k}\cdot(\vec{r}_i' - \vec{r}_i)}}{\epsilon_t + \frac{\hbar^2 k^2}{2m} - E} \varphi_{it}(\xi_i)$$

$$- \int d\xi'' \sum_{t'} \frac{1}{8\pi^3} \int d\vec{k}\, \frac{e^{-i\vec{k}\cdot(\vec{r}_i'' - \vec{r}_i)}}{\epsilon_{t'} + \frac{\hbar^2 k^2}{2m} - E} \varphi_{it'}(\xi_i)\varphi_{it'}^{\dagger}(\xi_i'') V_i X_{it}(\xi'',r_i') \tag{D5}$$

The integral over $\vec{k}$ gives the free-particle Green's function:

$$\frac{1}{8\pi^3}\int d\vec{k}\,\frac{e^{-ik\cdot(\vec{r}'-\vec{r})}}{\epsilon_t + \frac{\hbar^2k^2}{2\mu_i} - E} = \frac{2\mu_i}{4\pi\hbar^2}\,\frac{e^{ik_t|\vec{r}_i'-\vec{r}_i|}}{|\vec{r}_i' - \vec{r}_i|} \tag{D6}$$

where

$$k_t = \frac{2\mu_i}{\hbar^2}(E - \epsilon_t)$$

Using this result in equation (D5) and looking at large values of r_i' yield

$$X_{it}(\xi,\vec{r}_i') = \frac{2\mu_i}{4\pi\hbar^2}\left[\frac{e^{ik_t|\vec{r}_i'-\vec{r}_i|}}{|\vec{r}_i' - \vec{r}_i|}\,\varphi_{it}(\xi_i)\right.$$

$$\left. - \sum_{t'}\frac{e^{ik_{t'}r_i}}{r_i}\,\varphi_{it'}(\xi_i)\int d\xi''\,\exp(-ik_{t'}\hat{r}\cdot\vec{r}'')\varphi^\dagger_{it'}(\xi'')V_iX_{it}(\xi'',\vec{r}_i')\right] \tag{D7}$$

A different interaction term can just as well be separated from the Hamiltonian, in which case equation (53) can be rewritten:

$$(H_j + T_j)X_{it}(\xi,\vec{r}_i') = \delta(\vec{r}_i - \vec{r}_i')\varphi_{it}(\xi_i) - V_jX_{it}(\xi,r_i') \tag{D8}$$

Expanding in eigenfunctions of $H_j + T_j$ yields

$$X_{it}(\xi,r') = \sum_{s'}B_{s'}(\vec{k})e^{i\vec{k}\cdot\vec{r}_j}\,\varphi_{js'}(\xi_j) \tag{D9}$$

Using the same procedure as before results in the alternative integral equation

$$X_{it}(\xi,r_j') = \frac{2\mu_j}{4\pi\hbar^2}\sum_s\int d\xi''\,\frac{e^{ik_s|\vec{r}_j-\vec{r}_j''|}}{|\vec{r}_j - \vec{r}_j''|}\,\varphi_{js}(\xi_j)\varphi^\dagger_{js}(\xi_j'')\left[\delta(\vec{r}_i - \vec{r}_i')\varphi_{it}(\xi_i'')\right.$$

$$\left. - V_jX_{it}(\xi'',r_i')\right] \tag{D10}$$

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