The Symmetry of the S Matrix

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It is proven that any Heisenberg S matrix is symmetric for an appropriate choice of arbitrary phases in a representation in which the square and one component of the total angular momentum are diagonal. The consequences of this symmetry for the complex phases of the matrix elements are discussed.

I. THE SYMMETRY OF THE S-MATRIX

WIGNER and Eisenbud[1] have shown that the collision matrix for simple nuclear reactions is symmetric, provided arbitrary phases in the nuclear wave functions are chosen appropriately. This symmetry is a consequence of the time reversal invariance of the quantum-mechanical formalism. The proof of Wigner and Eisenbud applies only to reactions in which there are two heavy fragments in the initial and final states.

It is the purpose of this note to prove that any Heisenberg S matrix[2] is symmetric for an appropriate choice of arbitrary phases in a representation in which the square and one component of the total angular moment $\mathbf{J}$ are diagonal. This proof will be developed by combining the theory of time reversal in quantum mechanics given by Wigner[3] with the methods of transformation theory.

Time reversal for a classical system can be defined by stating the transformation properties of a complete set of dynamical variables: velocities, momenta, angular momenta, and the electromagnetic vector potential change their sign as $t\rightarrow -t$. Position coordinates and energies remain unchanged. This determines the transformation property of any dynamical variable Q: $Q(t)\rightarrow Q^\tau(-t)$ as $t\rightarrow -t$ (e.g., $\mathbf{v}^\tau=-\mathbf{v}$, $\mathbf{x}^\tau=\mathbf{x}$). The operator of time reversal in quantum mechanics K must then satisfy for every Q and every state $\psi(t)$ the requirement

$$(K\psi(t), QK\psi(t))=(\psi(-t), Q^\tau\psi(-t)). \tag{1}$$

According to Wigner,[3] this operator takes the form

$$K\psi(t)=U\psi^*(-t), \tag{2}$$

where U is a unitary operator determined by the requirement (1). In a Schrödinger representation Q and U will be time independent, and from (1) it follows that

$$U^+QU=\tilde{Q}^\tau, \tag{3}$$

where $\tilde{Q}$ is Q transposed. If $Q^\tau=Q$, we call Q invariant under time reversal. The Hamiltonian of any system is invariant in this sense. The invariance of the S matrix is the mathematical expression of the principle of detailed balance. It can be shown to follow from the time reversal invariance of the Hamiltonian.[4]

A change in representation affects U in the following manner. Let ψ and ψ' be two representations of the same state related by the unitary transformation T:

$$\psi'=T\psi, \quad (K\psi)'=TK\psi. \tag{4}$$

From (2) and

$$(K\psi(t))'=U'\psi'^*(-t), \tag{5}$$

one finds with (4) that

$$U'=TU\tilde{T}.^5 \tag{6}$$

For a system consisting of any number of particles (including photons), we specify the states by the quantum numbers J, M of the total angular momentum and other quantum numbers collectively denoted by A, $B\cdots$. Since $\mathbf{J}^2$ is invariant under time reversal,

$$U^+\mathbf{J}^2U=\mathbf{J}^{2*}. \tag{7}$$

Hence, U must be diagonal in the quantum number J. The quantum numbers A, $B\cdots$ are chosen such that they label the eigenvalues of time reversal invariant operators, for instance, the squares of the angular momenta of parts of the system. U must therefore also be diagonal in A. The M dependence of U can be determined from the condition

$$U^+\mathbf{J}U=-\mathbf{J}^*. \tag{8}$$

With the help of the known matrix representation[6] for J, one finds from (8), with some simple algebra,

$$(J'M'A'|U|JMA)=\delta_{A'A}\delta_{J'J}\delta_{-M'M}e^{i\pi[\alpha(J,A)+M]}, \tag{9}$$

where $\alpha(J, A)$ is an undetermined real function of J and A. The fact that U is unitary has, of course, also been used in the derivation of (9). α is, however, not only undetermined but completely arbitrary: we may always change the phases of the wave function by operating with the unitary matrix,

$$(J'M'A'|T|JMA)=\delta_{J'J}\delta_{M'M}\delta_{A'A}e^{-i\pi\beta(J,A)}. \tag{10}$$

[1] E. P. Wigner and L. Eisenbud, Phys. Rev. **72**, 29 (1947).
[2] W. Heisenberg, Z. Physik **120**, 513, 673 (1943).
[3] E. P. Wigner, Gött. Nach. **31**, 546 (1932).
[4] F. Coester, Phys. Rev. **84**, 1259 (1951).
[5] It is easy to generalize this for time dependent transformations $T(t)$, where

$$U'(t)=T(t)U\tilde{T}(-t).$$

With this equation one can show that U is time independent in any interaction representation in which H_0 is real.
[6] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, Cambridge, 1951), p. 48.

If we transform U with (10) according to (6), we get

$$(J'M'A'|U'|JMA)=\delta_{J'J}\delta_{M'M}\delta_{A'A}e^{i\pi(\alpha-2\beta+M)}. \quad (11)$$

β is arbitrary; we may therefore choose α conveniently in the first place. The choice

$$(J'M'A'|U|JMA)=\delta_{A'A}\delta_{J'J}\delta_{-M'M}e^{i\pi(J+M)} \quad (12)$$

makes U real and has the following advantage: Consider two systems, respectively, described by the quantum numbers $J_1M_1A_1$ and $J_2M_2A_2$; $\mathbf{J}_1+\mathbf{J}_2=\mathbf{J}$. The matrix U for the combined system in a $JMJ_1J_2A_1A_2$ representation can be obtained by taking the outer product of the U's for the separate systems and transforming according to (6) with the Clebsch-Gordan coefficient $(J_1J_2M_1M_2|JM)$. We assume (12) for the individual systems. Since the conventional Clebsch-Gordan coefficients are real and satisfy the symmetry relation[7]

$$(J_1J_2-M_1-M_2|J-M)=(-1)^{J_1+J_2-J}(J_1J_2M_1M_2|JM), \quad (13)$$

we again find (12) for the combined system if A is understood to stand for $J_1J_2A_1A_2$. No additional phase transformation is needed.

The time reversal invariance of the S matrix is, according to (3), expressed in the form

$$U^+SU=\tilde{S}. \quad (14)$$

Since S is invariant under rotations of the coordinate system, it is diagonal in J and M and independent of M. It can therefore be written in the form $(B|S_J|A)$. From (12) and (14) it follows that

$$(B|S_J|A)=(A|S_J|B). \quad (15)$$

This establishes the symmetry of the S matrix which we set out to prove.

II. THE PHASES OF REACTION MATRIX ELEMENTS

If we substitute in (14) and (15) for S any invariant Hermitian operator, the matrix elements must be real. This is important in those cases where perturbation theory is applicable.[8] Whenever perturbation theory is applicable, the matrix elements are real. In general, the phases of the elements of S are not determined by (15), but for reactions involving the formation of a compound nucleus further conclusions can be drawn.

For resonance reactions elements of a certain finite submatrix of $R=S-1$ are large compared to all other elements. The picture of the compound nucleus suggests that all large elements belong to the same J. Neglecting small terms, we have a finite unitary and symmetric matrix $(B|S|A)$ to consider.[9] Any such matrix can be written in the form

$$S=(1+i\pi K)^{-1}(1-i\pi K), \quad (16)$$

where K is a real symmetric matrix. K and consequently S can be diagonalized by a real unitary matrix $T_{\lambda A}$. If K_λ are the eigenvalues of K, we have

$$R_\lambda=-2\pi iK_\lambda/(1+i\pi K_\lambda). \quad (17)$$

Assuming that $|K_\lambda|\gg 1$ at resonance for some values of λ, one finds

$$(B|R|A)=-2\sum_\lambda{}' T_{\lambda B}T_{\lambda A}, \quad (18)$$

where $\sum_\lambda{}'$ indicates summation over those values of λ for which $|K_\lambda|\gg 1$.

More can be said if the picture of the compound nucleus is further exploited. We describe the initial ensemble of particles capable of forming a compound nucleus of spin J by the density matrix[10] $(AJM|\rho_0|BJM')$. The ensemble of decay products of the compound nucleus is described by $(CJM|\rho_f|DJM')$. Since $(1/2\pi)|(B|R|A)|^2$ is the probability per unit time for the transition $A\to B$, ρ_0 and ρ_f are related by[11]

$$(CJM|\rho_f|DJM')=\text{const}\sum_{AB}(C|R|A)(AJM|\rho_0|BJM')(B|R^+|D). \quad (19)$$

The picture of the compound nucleus suggests that ρ_f should be independent of the way in which the compound nucleus is formed. That means it should be independent[12] of ρ_0. This requirement is satisfied if and only if R is proportional to a projection operator P which projects all states into a one-dimensional subspace. That means R has only one nonvanishing eigenvalue. $\sum_\lambda{}'$ in (18) reduces then to one term. The reality of $(B|R|A)$ in (18) is, however, independent of the assumption just discussed. On the other hand, off resonance the compound nucleus assumption formulated above gives us

$$(B|R|A)=-\frac{2\pi i\kappa}{1+i\pi\kappa}T_{\lambda B}T_{\lambda A}, \quad (20)$$

where κ is the nonvanishing eigenvalue of K. Since $T_{\lambda B}$ is real, this means that the matrix elements for all reactions which go through the same compound nucleus have the same phase. To what extent the basic assumption is valid must be decided ultimately by experiment. A resonance in the cross section is not sufficient to guarantee its validity. It rests at present mainly on its plausibility.

[7] G. Racah, Phys. Rev. **62**, 438 (1942).

[8] S. P. Lloyd has shown [Phys. Rev. **81**, 161 (1951)] that the relative phase of the matrix elements for multipole emission is either 0 or π. This result is a special case of our theorem.

[9] We drop the subscript J here for the sake of simplicity.

[10] For a definition of the density matrix and discussion of its formal properties see for instance R. C. Tolman, *The Principles of Statistical Mechanics* (Clarendon Press, Oxford, 1938), Chap. IX.

[11] This follows directly in a representation in which both ρ_0 and ρ_f are diagonal; if ρ_f and ρ_0 do not commute, they can both be diagonal if A, B and C, D refer respectively to different coordinate systems in Hilbert space. Equation (19) itself is then obtained by appropriate change of the representation. See also L. Wolfenstein and J. Ashkin, Phys. Rev. **85**, 947 (1952).

[12] T. D. Newton, Can. J. Phys. **30**, 53 (1952). See in particular assumption (A), p. 57.