PHYSICAL REVIEW C VOLUME 23, NUMBER 1 JANUARY 1981

Reciprocity relation for multichannel coupling kernels

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(Received 2 June 1980)

Assuming time-reversal invariance of the many-body Hamiltonian, it is proven that the kernels in a general coupled-channels formulation are symmetric, to within a specified spin-dependent phase, under the interchange of channel labels and coordinates. The theorem is valid for both Hermitian and suitably chosen non-Hermitian Hamiltonians which contain complex effective interactions. While of direct practical consequence for nuclear rearrangement reactions, the reciprocity relation is also appropriate for other areas of physics which involve coupled-channels analysis.

[NUCLEAR REACTIONS Symmetry relation for multichannel coupling kernels. Non-Hermitian operators. Time-reversal invariance and reciprocity.]

In several fields of physics, increasing theoretical effort is being devoted to solving or approximately solving the general many-body scattering problem. Because of the rather formidable nature of this goal, it is quite important that all symmetry properties of the physical system be fully utilized to reduce or at least to constrain the complexity of the problem. To this end, the current work presents a proof, based upon time-reversal invariance, that the coupling kernels (interactions) in a general coupled-channels scattering problem are symmetric to within a specific spin-dependent phase. The arguments presented below are closely related to those used in establishing the reciprocity of the S matrix first discussed by Wigner and Eisenbud[1] and by Coester[2,3] as well as to the work of Rose and Biedenharn[4] concerning the reality of matrix elements for gamma correlations with mixed multipoles and also a recent paper on various coupled-channels equations by Greben and Levin.[5] The proof is a generalization of the result obtained by Ohmura *et al.*,[6] who demonstrated, using analytical methods, that the coupling kernel is symmetric for a two-channel, spin-independent three-body model of (d,p) stripping. Our result, which is valid for the many-body spin-dependent problem having an arbitrary number of channels, shows that the symmetry follows directly from time-reversal invariance and that the model Hamiltonian need not necessarily be Hermitian. Pragmatically, the reciprocity of the kernel is of important computational value. This is especially true for coupled-channels descriptions of rearrangement reactions where additional complications, such as the nonorthogonality[6-8] of the channel basis states, are present.

We begin by briefly reviewing the properties of the time-reversal operator T. Following Wigner[9] and Coester,[3] T is defined such that it transforms an arbitrary state vector ψ at time t into the time-reversed state vector ψ' at $t'=-t$,

$$\psi' \equiv T\psi, \tag{1}$$

$$\equiv U\psi^*. \tag{2}$$

Here U is a unitary operator which acts on spin and momentum variables. The time reversal operator is antilinear and also antiunitary ($T^\dagger = T^{-1}$, $T^\dagger T = TT^\dagger = 1$). For all vectors f and g we define the adjoint operator $T^\dagger$ by

$$(f,\ T^\dagger g) \equiv (Tf,\ g)^*, \tag{3a}$$

$$\equiv (g,\ Tf). \tag{3b}$$

Consider a linear, but not necessarily Hermitian, operator Q. The time-reversed operator Q', corresponding to Q, is also linear and is defined by the requirement

$$(\psi, Q\psi) = (\psi', Q'\psi'). \tag{4}$$

Use of Eqs. (1), (3), and (4) gives immediately

$$Q' = (TQT^\dagger)^\dagger, \tag{5}$$

$$= TQ^\dagger T^\dagger. \tag{6}$$

The operator Q is said to be time-reversal invariant if $Q' = Q$. This requires

$$Q = TQ^\dagger T^\dagger, \tag{7}$$

$$= TQ^\dagger T^{-1}. \tag{8}$$

More generally it can be shown that any complex function F of a time-reversal invariant operator Q is also time-reversal invariant and satisfies

$$F(Q) = TF(Q)^\dagger T^{-1}. \tag{9}$$

With these preliminaries we now address a many-body scattering problem and wish to describe the system within the framework of a coupled-channels formulation. Introduce a model Hamiltonian H which may contain complex, non-Hermitian effective interactions. The set of coupled, integrodifferential equations is obtained by diagonalizing H in a truncated model space which is a subset of the full Hilbert space for the many-body system. Let $\{\phi_\gamma\}$ represent the set of basis vectors spanning this subspace. The ϕ_γ are internal eigenfunctions of partition Hamiltonians H_γ, which correspond to specific cluster arrangements, more loosely, "channels" labeled by γ, of the many-body system. In general, the H_γ are different and therefore the ϕ_γ are not necessarily orthogonal. Consult Ref. 8 for further discussion and details. At issue in this work are the off-diagonal kernels appearing in the coupled equations connecting channels α and β,[7,8]

$$K_{\alpha\beta}(\vec{r}_\alpha, \vec{r}_\beta) \equiv (\phi_\alpha, [H-E]\phi_\beta). \tag{10}$$

Formally, this kernel is a matrix element of vectors in the model Hilbert space and is labeled by the channel labels α, β and channel coordinates $\vec{r}_\alpha$, $\vec{r}_\beta$. We wish to relate $K_{\alpha\beta}(\vec{r}_\alpha, \vec{r}_\beta)$ to $K_{\beta\alpha}(\vec{r}_\beta, \vec{r}_\alpha)$. Letting $Q=H-E$, we have from above

$$K_{\alpha\beta}(\vec{r}_\alpha, \vec{r}_\beta) = (\phi_\alpha, T^\dagger TQT^\dagger T\phi_\beta), \tag{11}$$

$$= (T\phi_\alpha, TQT^\dagger T\phi_\beta)^*, \tag{12}$$

$$= (\phi'_\alpha, Q'^\dagger\phi'_\beta)^*, \tag{13}$$

$$= (Q'^\dagger\phi'_\beta, \phi'_\alpha), \tag{14}$$

$$= (\phi'_\beta, Q'\phi'_\alpha), \tag{15}$$

$$= (\phi'_\beta, [H-E]\phi'_\alpha), \tag{16}$$

$$\equiv K_{-\beta-\alpha}(\vec{r}_\beta, \vec{r}_\alpha), \tag{17}$$

where the notation $-\gamma$ indicates time-reversed basis states. Notice the last step follows if, and only if, H is time-reversal invariant (i.e., $H=TH^\dagger T^\dagger$). The complex interactions appearing in typical coupled channel analysis satisfy this condition. To proceed further, the phase of the basis states must be specified. In the simplest case in which spin is neglected and the basis states can be taken real, we have $\phi'_\gamma=\phi_\gamma$, giving

$$K_{\alpha\beta}(\vec{r}_\alpha, \vec{r}_\beta) = (\phi_\beta, [H-E]\phi_\alpha), \tag{18}$$

$$= K_{\beta\alpha}(\vec{r}_\beta, \vec{r}_\alpha). \tag{19}$$

More generally, including angular momenta will introduce phase factors. For example, in the channel spin representation having total spin S_γ, projection M_γ, we have $\phi_\gamma \rightarrow \phi_{S_\gamma M_\gamma}$ and the phase is usually chosen such that

$$\phi'_{S_\gamma M_\gamma} = (-1)^{S_\gamma - M_\gamma}\phi_{S_\gamma - M_\gamma}, \tag{20}$$

which gives

$$K_{S_\alpha M_\alpha, S_\beta M_\beta}(\vec{r}_\alpha, \vec{r}_\beta) = (-1)^{S_\alpha - M_\alpha + S_\beta - M_\beta} K_{S_\beta - M_\beta, S_\alpha - M_\alpha}(\vec{r}_\beta, \vec{r}_\alpha). \tag{21}$$

Further, in a total angular momentum representation J, M involving a partial-wave decomposition the phase exactly cancels from angular momentum conservation yielding

$$K^{JM}_{\alpha\beta}(r_\alpha, r_\beta) = K^{JM}_{\beta\alpha}(r_\beta, r_\alpha). \tag{22}$$

This clearly establishes the symmetry relation connecting the two channels.

As a final comment we stress the importance of distinguishing between Hermitian and non-Hermitian operators when discussing antilinear transformations such as time reversal. If, as is usually the case, a physical system possesses time-reversal symmetry, all computed observables (i.e., probabilities and expectation values) must be invariant under the time-reversal transformation T. Equation (4) therefore completely specifies the principle of time-reversal invariance and along with Eq. (3) defines the correct time-reversed operator given by Eq. (6).

Often one deals with Hermitian operators ($Q = Q^\dagger$) in which case Eq. (6) trivially reduces to the more familiar form

$$Q' = TQT^\dagger, \tag{23}$$

which applies to linear, unitary transformations. However, Eq. (23) certainly is not appropriate for the complex, non-Hermitian interaction used in model calculations of scattering and reaction problems. These model interactions, we maintain, should be chosen so as to satisfy the more general Eq. (7). The exact Hamiltonian $\mathcal{H}$ is Hermitian and usually is required to be invariant under time reversal, so that $\mathcal{H}' = \mathcal{H}$. An effective Hamiltonian is defined to act within a truncated Hilbert space so as to give observables computed in that space that are identical to those generated by the exact Hamiltonian in the full space. This condition leads to complicated, non-Hermitian operators; nonetheless, Eq. (6) still defines their time reverses. In practice we introduce model Hamiltonians H which are intended as approximations to the exact, effective Hamiltonians. However, it is natural to demand that the model interactions continue to embody the physical symmetries contained in the underlying exact Hamiltonian. In particular, we demand that $H' = H$ where H' is the time-reversed operator defined by Eq. (6), or

$$TH^\dagger T^\dagger = H. \tag{24}$$

Such a condition, ensures, for example, the model scattering matrix will be symmetric. It has also been used[10] to establish the acceptable types of spin-orbit-coupling operator for particles of spin one.

Equation (24) is certainly satisfied by the usual complex optical potential which describes elastic scattering even though it contains an imaginary part V_I which is often referred to as being "odd under time reversal." This reference simply means that this part has the property $TV_IT^\dagger = -V_I$. However, we see that this is somewhat misleading; the correct criterion of invariance under time reversal is that $V' = V$, where V' is given by Eq. (6), $V' = TV^\dagger T^\dagger$. This is satisfied by V_I and leads to an optical model Hamiltonian which is also invariant under time reversal. This discussion will be further developed elsewhere.[11]

In summary, the symmetry of the channel coupling kernels follows directly from the time-reversal invariance of the coupling interactions and parallels the reciprocity relation for the S matrix. From a practical standpoint this relation is quite useful and important since in detailed numerical calculations only half of the kernels need be computed and stored. For applications requiring large numbers of channels the benefits readily become apparent.

The authors are grateful to the Summer Institute in Theoretical Physics at the University of Washington, Seattle, Washington for providing the environment for this research. In addition, one of us (S.C.) wishes to acknowledge informative discussions with F. Coester and C. M. Vincent. Research support was provided in part by the U. S. Department of Energy.

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