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New quantum numbers in collision theory. III. Symmetries of the scattering geometry

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Scattering geometries are represented by tensorial parameters classified according to symmetry under permutations P and Q: P changes a base set of wave functions into its Hermitian conjugate and Q interchanges the directions of incidence and scattering. These parameters interlink initial and final states of projectile and target, a linkage mediated by the angular momentum $\mathbf{j}_t$ transferred in the collision. Collision cross sections and expectation values of the observables are constructed as sums of geometrical parameters with different symmetries, weighted by dynamical parameters.

I. INTRODUCTION

Earlier papers of this series,[1,2] referred to in the following as I and II, have replaced orbital quantum numbers of collision theory with an alternative set $\{\sigma,\tau,\zeta,\eta\}$ appropriate to a symmetry analysis of the scattering geometry. The present paper recasts the scattering geometry in a tensorial form that displays its symmetries and selects relevant combinations of the (unsymmetric) dynamical parameters.

Papers I and II dealt explicitly with the prototype process

$$e+\mathrm{He}(1s^2\,{}^1S)\rightarrow e+\mathrm{He}(1snp\,{}^1P)\ . \tag{1}$$

The present paper has a broader scope, largely independent of the restricted set of quantum numbers in process (1). Its notation will nevertheless refer for simplicity to electron-atom collisions, disregarding the influence of electron spins, of electron exchange, and hence of spin reorientation. Modifications of the treatment, required to broaden its scope further, will be indicated where appropriate.

Main elements of a scattering geometry are the momenta $\{\mathbf{p}_a,\mathbf{p}_b\}$ of the projectile before and after collision. These momenta combine to yield the following scalars and tensors symmetric under reflection through the plane $(\mathbf{p}_a,\mathbf{p}_b)$: (1) the momentum $\mathbf{p}_a-\mathbf{p}_b$ transferred to a target, which is most relevant to the Born approximation and to target alignment; (2) the vector product $\mathbf{p}_a\times\mathbf{p}_b$, which defines the axis of target orientation induced by the collision; (3) the product $\hat{\mathbf{p}}_a\cdot\hat{\mathbf{p}}_b=\cos\theta$, the variable of the projectile's angular distribution; and (4) the dyadic $\mathbf{p}_a\mathbf{p}_a+\mathbf{p}_b\mathbf{p}_b+3(\mathbf{p}_a\times\mathbf{p}_b)(\mathbf{p}_a\times\mathbf{p}_b)$. Additional base elements of collision geometry are the multipole moments of the target—and of the projectile, if any—before and after the collision. (Regarding $\{\mathbf{p}_a,\mathbf{p}_b\}$ as projectile momenta is correct only in the limit of infinite target mass. These momenta pertain actually to the *relative* motion of projectile and target or, more generally, of any two fragments of a collision complex.)

The role of observable momenta $\{\mathbf{p}_a,\mathbf{p}_b\}$ as building blocks of scattering geometry contrasts with the role of unobserved orbital (or other angular) momentum states as base sets for exploiting the invariance of collision dynamics under space rotations. Base eigenstates of $\{\mathbf{p}_a,\mathbf{p}_b\}$ and of $\{l_a,l_b\}$ are connected by standard partial-wave expansions, but the multiplicity of these expansions—for eigenstates and for their Hermitian conjugates—leads to the complications of collision theory [see, e.g., paper I, Eqs. (12)–(17)]. To manage this complication, paper I introduced the quantum numbers

$$\begin{aligned}
\sigma&=\tfrac{1}{2}(l_a+l_b+l_a'+l_b'),\quad P\sigma=\sigma,\quad Q\sigma=\sigma\ ,\\
\tau&=\tfrac{1}{2}(l_a+l_b-l_a'-l_b'),\quad P\tau=-\tau,\quad Q\tau=\tau\ ,\\
\zeta&=\tfrac{1}{2}(l_a-l_b+l_a'-l_b'),\quad P\zeta=\zeta,\quad Q\zeta=-\zeta\ ,\\
\eta&=\tfrac{1}{2}(l_a-l_b-l_a'+l_b'),\quad P\eta=-\eta,\quad Q\eta=-\eta\ ,
\end{aligned}\tag{2}$$

with characteristic parities under the Hermitian conjugation P and under the permutation Q of $\{\mathbf{p}_a,\mathbf{p}_b\}$. The same goal will be pursued here by tensorial analysis of the scattering geometry along the lines of Wigner-Racah algebra developed long ago for nuclear collisions,[3] which are compatible with the (P,Q) symmetry analysis.

To this end the geometrical parameters of projectile and target will be cast initially into separate multipole moments covariant under space rotations and then combined into scalar products (Sec. II). These multipole moments will then be classified according to their symmetry under the permutations P and Q, thus determining the symmetry of their products as well (Sec. III). The theoretical expressions for cross sections and for other observables consist of summed contributions from scalar products of geometrical multipole moments with alternative quantum numbers, each of them weighted by a corresponding dynamical parameter.

The expectation value of a collision observable is bilinear in the scattering matrix S for the relevant process and in its Hermitian conjugate $S^\dagger$, as noted in I; it thus depends linearly on the elements of the *direct product matrix* $S^\dagger\times S$. This dependence will be analyzed in Sec. IV with reference to each group of four elements of this matrix that are transformed into one another by the permutations of quantum numbers P,Q, and PQ. The coefficients of four such elements are geometrical parameters, even or odd under each permutation, thus differing only by factors ± 1. The dynamical parameters of the theory are thus identified as *sums of the four elements* of each group weighted by ± 1. The variation of these parameters under P and Q will be discussed in the final Sec. V. A subsequent paper by Lee will analyze the dependence of the target orientation in process (1) on its dynamical parameters.

II. SEPARATION OF GEOMETRICAL ELEMENTS FOR TARGET AND PROJECTILE

The scattering matrix S for a collision is usually expressed in the representation of the total angular momentum J of the projectile and target. Its invariance under space rotations is shown by expanding it into products of an invariant dynamical parameter and of two Wigner coefficients, according to the Wigner-Eckart theorem,

$$(L_B M_B l_b m_b \mid S \mid L_A M_A l_a m_a) = \sum_{J,M} (L_B M_B l_b m_b \mid JM)$$
$$(L_B l_b \mid S(J) \mid L_A l_a)(JM \mid L_A M_A l_a m_a) , \quad (3)$$

where the capital L and M denote the target angular momentum and its magnetic quantum number and small letters l and m apply to the projectile; the labels (A,B) and (a,b) apply to the initial and final states, respectively.

An alternative representation that separates the target and projectile indices is obtained[4] by recoupling the Wigner coefficients in (3) by a standard formula [Eqs. (1.1) and (2.19) of Ref. 5]:

$$\sum_M (L_B M_B l_b m_b \mid JM)(JM \mid L_A M_A l_a m_a)$$
$$= (2J+1) \sum_{j_t, m_t} (-1)^{J+j_t+M_A-m_b} \begin{Bmatrix} l_a & L_A & J \\ L_B & l_b & j_t \end{Bmatrix} (L_B\, M_B\, L_A\, -M_A \mid j_t m_t)(j_t m_t \mid l_b\, -m_b\, l_a\, m_a) . \quad (4)$$

Equation (3) thus transforms into

$$(L_B M_B l_b m_b \mid S \mid L_A M_A l_a m_a)$$
$$= \sum_{j_t, m_t} (-1)^{j_t+M_A-m_b} (L_B M_B L_A - M_A \mid j_t m_t)$$
$$\times (L_A L_B \mid S(j_t) \mid l_a l_b)(j_t m_t \mid l_b - m_b l_a m_a) , \quad (5)$$

where

$$(L_A L_B \mid S(j_t) \mid l_a l_b) = \sum_J (-1)^J (2J+1) \begin{Bmatrix} l_a & L_A & J \\ L_B & l_b & j_t \end{Bmatrix}$$
$$\times (L_b l_b \mid S(J) \mid L_A l_a) . \quad (6)$$

This transformation corresponds to regrouping the addition of angular momenta,

$$\mathbf{J} = \mathbf{L}_A + \boldsymbol{l}_a = \mathbf{L}_B + \boldsymbol{l}_b , \quad (7)$$

into the equation of angular momentum transfer

$$\mathbf{j}_t = \mathbf{L}_B - \mathbf{L}_A^* = \boldsymbol{l}_a - \boldsymbol{l}_b^* . \quad (8)$$

The asterisk has been inserted in (8) to specify that commutation rules for the components of $\mathbf{L}_A^*$ and $\mathbf{l}_b^*$ involve $-i$ instead of i, to preserve the standard rule for the components of $\mathbf{j}_t$.[6] With this proviso, the ket $\mid (l_a l_b) j_t m_b)$ represents an eigenstate of $\mid \mathbf{j}_t \mid^2$. The proviso also implies that this ket is constructed from the product of the ket $\mid l_a m_a)$ with the bra $(-1)^{l_a - m_a}(l_a m_a \mid$ renormalized by the phase factor $(-1)^{l_a-m_a}$ which also appears in the transformation formulas (4) and (5). In vector symbols, this construction is represented by

$$\mid (l_a l_b) j_t m_t) = [\, \mid l_a) \times U^{[l_b]} (l_b \mid \,]_{m_t}^{(j_t)} . \quad (9)$$

[The usage of parentheses and brackets in the superscript of (9) as well as the symbol $U^{[l_b]}$ for the matrix $U^{[l_b]}_{-m_b m_b'} = (-1)^{l_b - m_b} \delta_{m_b m_b'}$ follow conventions of Ref. 3.]

An important aspect of this introduction of the angular momentum transfer lies in the range of the quantum number j_t which is *limited* by the amount of angular momentum that the target can absorb in a transition of interest, $j_t \leq L_A + L_B$. This limitation contrasts with the range of the total angular momentum $J \leq \min[L_A + l_a, L_B + l_b]$ which is *unrestricted* as projectile angular momenta range to infinity.

The representation in terms of j_t also affords separate analysis of the observables of target and projectile. Let us consider an experiment where (1) target and projectile are prepared with density matrices ρ_A and ρ_a, respectively, and (2) final target and projectile states with density matrices ρ_B and ρ_b are observed through the responses of detectors D_B and D_b, respectively.[3] For example, in a collision where an electron beam is prepared with momentum $\mathbf{p}_a$ and the scattered electron is detected with momentum $\mathbf{p}_b$, we have $\rho_a = \mid \mathbf{p}_a)(\mathbf{p}_a \mid$ and $D_b = \mid \mathbf{p}_b)(\mathbf{p}_b \mid$. The expectation value of the joint detector operator $D_B D_b$ is represented by

$$\langle D_B D_b \rangle = \mathrm{tr}(\rho_B \rho_b D_B D_b) = \mathrm{tr}(S \rho_A \rho_a S^{-1} D_B D_b) , \quad (10)$$

where S denotes the scattering matrix.

Instead of considering the joint detector matrix $D_B D_b$ and the joint initial density matrix $\rho_A \rho_a$, we now consider their alternative combinations $\rho_A D_B$ and $\rho_a D_b$. In the angular momentum transfer representation, Eq. (10) can be written as

$$\langle D_B D_b \rangle = \sum_{l_a,l_b,l'_a,l'_b} \sum_{j_t,j'_t} (L_A L_B | S(j_t) | l_a l_b)(L_A L_B | S(j'_t) | l'_a l'_b)^* \sum_{m_t,m'_t} [((L_A L_B) j'_t m'_t | \rho_A D_B | (L_A L_B) j_t m_t) \times ((l_a l_b) j_t m_t | \rho_a D_b | (l'_a l'_b) j'_t m'_t)] , \quad (11)$$

thus separating the geometrical elements of the system into those of target and projectile. The separate matrix elements of $\rho_A D_B$ and $\rho_a D_b$ in (11) can be reduced under space rotations,

$$\langle D_B D_b \rangle = \sum_{l_a,l_b,l'_a,l'_b} \sum_{j_t,j'_t} (L_A L_B | S(j_t) | l_a l_b)(L_A L_B | S(j'_t) | l'_a l'_b)^* \sum_{K_t,Q_t} [((L_A L_B) j'_t | \rho_A D_B | (L_A L_B) j_t)]^{(K_t)}_{Q_t} \times [((l_a l_b) j_t | \rho_a D_b | (l'_a l'_b) j'_t)]^{(K_t)}_{-Q_t} (-1)^{Q_t} . \quad (12)$$

This reduction introduces a *new tensorial parameter*, namely, the 2^{K_t}*-pole moment* of the angular momentum transfer between projectile and target,

$$(K_t Q_t | = \sum_{m_t,m'_t} (-1)^{j_t - m_t} (K_t Q_t | j'_t m'_t j_t - m_t) | j_t m_t)(j'_t m'_t | . \quad (13)$$

The value of K_t is restricted by the triangular condition $| j_t - j'_t | \le K_t \le j_t + j'_t$ and thus implicitly by the target properties.

The density and detector matrices of the target can also be expressed in terms of the measurable multipole moments[3] of the target states, by recoupling the tensorial set

$$[((L_A L_B) j_t | \times U^{[j'_t]} | (L_A L_B) j'_t)]^{(K_t)}$$

into

$$[((L_A L_A) K_A | \times U^{[K_B]} | (L_B L_B) K_B)]^{(K_t)}$$

as in Eq. (3.9) of Ref. 5,

$$[((L_A L_B) j_t | \rho_A D_B | (L_A L_B) j'_t)]^{[K_t]}_{Q_t} = \sum_{K_A,K_B} [(2j_t+1)(2j'_t+1)(2K_A+1)(2K_B+1)]^{1/2} \begin{Bmatrix} L_A & L_B & j_t \\ L_A & L_B & j'_t \\ K_A & K_B & K_t \end{Bmatrix} \times [[(L_B | D_B | L_B)]^{[K_B]} \times U^{(K_A)} [(L_A | \rho_A | L_A)]^{(K_A)}]^{[K_t]}_{Q_t} . \quad (14)$$

Equation (14) shows how K_t represents the rank of the multipole moment transferred to the target. The transfer obviously satisfies the triangular condition $| K_B - K_A | \le K_t \le K_A + K_B$. The set of multipole moments $\{ [(L_A | \rho_A | L_A)]^{(K_A)}_{Q_A}; Q_A = -K_A, \ldots, K_A \}$ represents the coordinates of ρ_A in the Liouville representation[7] where the operators ρ_A are treated as vectors. The quantity in the bracket in Eq. (14) represents the multipole moment transferred to or from the target through the operator relation $\mathbf{K}_t = \mathbf{K}_B - \mathbf{K}^*_A$.

Usual experiments can be viewed as special cases of Eqs. (10)–(14). If an initially unpolarized target is excited by collision, we have

$$[(L_A | \rho_A | L_A)]^{(K_A)}_{Q_A} = \delta_{K_A 0} \delta_{Q_A 0} (2L_A + 1)^{-1/2}$$

and the geometry of the final target state, specified by $| K_B Q_B)$, will simply follow that of the multipole moment transfer, i.e., $K_B = K_t$ and $Q_B = Q_t$. In a superelastic collision,[8] where the initial target state is prepared by laser with a multipole moment $| K_A Q_A)$, but the final target state is not observed, the multipole transfer $| K_t Q_t)$, with $K_t = K_A$ and $Q_t = Q_A$, will pass on to the geometry of the projectile.

A formula analogous to (14) represents the 2^{K_t}-pole moment of the angular momentum transfer in terms of projectile parameters,

$$[((l_a l_b) j_t | \rho_a D_b | (l'_a l'_b) j'_t)]^{(K_t)}_{Q_t} = \sum_{k_a,k_b} [(2j_t+1)(2j'_t+1)(2k_a+1)(2k_b+1)]^{1/2} \begin{Bmatrix} l_a & l_b & j_t \\ l'_a & l'_b & j'_t \\ k_a & k_b & K_t \end{Bmatrix} \times [[(l_a | \rho_a | l'_a)]^{(k_a)} \times U^{[k_b]} [(l'_b | D_b | l_b)]^{[k_b]}]^{(K_t)}_{Q_t} . \quad (15)$$

Our restriction to experiments on electrons colliding with targets inelastically, which prepare or observe momentum eigenstates of the electron, $|\mathbf{p}_a)$ and $|\mathbf{p}_b)$, without reference to spin polarization, yields the explicit formulas

$$[(l_a\,|\,\rho_a\,|\,l_a')]_{q_a}^{(k_a)}=(4\pi)^{-1/2}i^{l_a-l_a'}(l_a\|C^{[k_a]}\|l_a')Y^*_{k_aq_a}(\hat{\mathbf{p}}_a)\;,$$
$$[(l_b'\,|\,D_b\,|\,l_b)]_{q_b}^{[k_b]}=(4\pi)^{-1/2}i^{-l_b+l_b'}(l_b\|C^{[k_b]}\|l_b')^*Y_{k_bq_b}(\hat{\mathbf{p}}_b)\;. \tag{16}$$

Equation (3.14) of Ref. 5 gives the explicit expression of the tensorial product in Eq. (15),

$$[((l_al_b)j_t\,|\,D_b\rho_a\,|\,(l_a'l_b')j_t')]_{Q_t}^{(K_t)}=(4\pi)^{-1}i^{l_a-l_b-l_a'+l_b'}\sum_{k_a,k_b}((l_al_b)j_t\|[C^{[k_a]}(\hat{\mathbf{r}}_a)\times U^{(k_b)}C^{[k_b]\dagger}(\hat{\mathbf{r}}_b)]^{[K_t]}\|(l_a'l_b')j_t')$$
$$\times\left[\frac{(2k_a+1)(2k_b+1)}{2K_t+1}\right]^{1/2}Y_{Q_t}^{(K_t)}(k_a\hat{\mathbf{p}}_a,k_b\hat{\mathbf{p}}_b)\;, \tag{17}$$

with the two-vector harmonic defined by

$$Y_{Q_t}^{(K_t)}(k_a\hat{\mathbf{p}}_a,k_b\hat{\mathbf{p}}_b)=\sum_{q_a,q_b}(-1)^{k_b-q_b}(K_tQ_t\,|\,k_aq_ak_b-q_b)Y^*_{k_aq_a}(\hat{\mathbf{p}}_a)Y_{k_bq_b}(\hat{\mathbf{p}}_b)\;. \tag{18}$$

III. SYMMETRIES OF GEOMETRICAL ELEMENTS

The geometrical parameters introduced in the last section, e.g., the multipoles (14) and (15), have definite parities under the operators (P,Q) which are determined by the structure of angular momentum algebra. These properties, described below, will select in Sec. IV the combinations of unsymmetrical dynamical parameters which occur in cross sections and other observables. This selection results from the summation over the indices $\{l_a,l_a',l_b,l_b',j_t,j_t',k_a,k_b\}$ which are permuted by P and Q.

The spherical harmonics $C_q^{[k]}(\hat{\mathbf{r}})$, which act as elements of a set of Hermitian tensorial operators,[3] are related to their adjoints by

$$C_q^{[k]\dagger}(\hat{\mathbf{r}})=(-1)^qC_{-q}^{[k]}(\hat{\mathbf{r}})\;. \tag{19}$$

The corresponding property of their tensor products in Eq. (16) is

$$[C^{[k_a]}(\hat{\mathbf{r}}_a)\times U^{(k_b)}C^{[k_b]\dagger}(\hat{\mathbf{r}}_b)]_{Q_t}^{[K_t]\dagger}=(-1)^{k_a+k_b+K_t}(-1)^{Q_t}[C^{[k_a]}(\hat{\mathbf{r}}_a)\times U^{(k_b)}C^{[k_b]\dagger}(\hat{\mathbf{r}}_b)]_{-Q_t}^{[K_t]}\;. \tag{20}$$

According to this formula the tensor products are Hermitian or anti-Hermitian depending on the parity of $k_a+k_b+K_t$. The reduced matrix elements $(l\|C^{[k]}\|l')$ (Refs. 4 and 5) are real and their parity under the permutation P equals the parity of $l+l'$. They are subject to the selection rule

$$l+l'+k=\text{even}\;. \tag{21}$$

The reduced matrix elements of their tensor product (20) transform under P as

$$((l_a'l_b')j_t'\|[C^{[k_a]}\times U^{(k_b)}C^{[k_b]\dagger}]^{[K_t]}\|(l_al_b)j_t)=(-1)^{j_t+j_t'+k_a+k_b+K_t}((l_al_b)j_t\|[C^{[k_a]}\times U^{(k_b)}C^{[k_b]\dagger}]^{[K_t]}\|(l_a'l_b')j_t')^*\;, \tag{22}$$

where the parity of $k_a+k_b+j_t+j_t'+K_t$ represents the combined parity of $(l_a\|C^{[k_a]}\|l_a')$, of $(l_b\|C^{[k_b]}\|l_b')$, and of the permutation of two rows of the $9j$ coefficient in (15). Corresponding formulas apply to the geometrical elements of the target.

The permutation Q interchanges the factors of the tensor product in (21) and (22), and hence the corresponding indices of the relevant Wigner coefficients. Its combined effect amounts to an interchange of the two columns of indices of the $9j$ coefficient in (15) bearing the labels a and b. The parity of this interchange equals that of the sum of the $9j$ indices.

The harmonics $Y_{Q_t}^{(K_t)}$ of the two projectile directions $(\hat{\mathbf{p}}_a,\hat{\mathbf{p}}_b)$ are neither even nor odd under the permutations P and Q in general. The general implications of this circumstance require further studies but cause no problem for the treatment of process (1) and of its analogs where $Y_{Q_t}^{(K_t)}$ takes a simple form in a particular coordinate system. We lay the z axis in the direction of projectile incidence $\hat{\mathbf{p}}_a$, leading to

$$Y_{k_aq_a}(\hat{\mathbf{p}}_a)=[(2k_a+1)/4\pi]^{1/2}\delta_{q_a0} \tag{23}$$

in (18), and hence to $q_b=-Q_t$. Choosing further the zero azimuthal plane (zx) to coincide with the scattering plane $(\hat{\mathbf{p}}_a,\hat{\mathbf{p}}_b)$ also simplifies $Y_{Q_t}^{(K_t)}$ through

$$Y_{k_b -Q_t}(\hat{\mathbf{p}}_b)=\left[\frac{(2k_b+1)(k_b-Q_t)!}{4\pi(k_b+Q_t)!}\right]^{1/2} P_{k_b Q_t}(\theta),\quad \cos\theta=\hat{\mathbf{p}}_a\cdot\hat{\mathbf{p}}_b \ , \tag{24}$$

with the associate Legendre function defined by Eq. 2.5.10 of Ref. 9. Equation (18) thus reduces to

$$Y_{Q_t}^{(K_t)}(k_a\hat{\mathbf{p}}_a,k_b\hat{\mathbf{p}}_b)=(-1)^{k_b-Q_t}(K_tQ_t\mid k_a0k_bQ_t)\left[\frac{(2k_a+1)(2k_b+1)(k_b-Q_t)!}{(k_b+Q_t)!}\right]^{1/2} P_{k_bQ_t}(\cos\theta)/4\pi \ . \tag{25}$$

The symmetry of (25) under the transformations P and Q will be discussed in the applications to the process (1).[10]

IV. SELECTION OF DYNAMICAL PARAMETERS

Consider now the combined implications of the parity of geometrical parameters and of the invariance of observables under the permutation P. Each observable includes the product (22) of reduced matrix elements of the projectile and of its analog for the target. The parity of $j_t+j_t'+K_t$ cancels out when projectile and target elements combine to form the scalar product in (12). The resulting parity of the geometrical parameters is then

$$(-1)^{k_a+k_b+K_A+K_B} \ . \tag{26}$$

The matrix elements of $S^\dagger\times S$,

$$(L_AL_B\mid S(j_t')\mid l_a'l_b')^*(L_AL_B\mid S(j_t)\mid l_al_b) \ , \tag{27}$$

are changed into their complex conjugates under P. These parameters will then occur in the expressions of observables in the combinations

$$(S^\dagger\times S)+(-1)^{k_a+k_b+K_A+K_B}(S^\dagger\times S)^* \ , \tag{28}$$

that is, as

$$\begin{aligned} &\mathrm{Re}(S^\dagger\times S),\quad \text{when } k_a+k_b+K_A+K_B=\text{even}\\ &\mathrm{Im}(S^\dagger\times S),\quad \text{when } k_a+k_b+K_A+K_B=\text{odd} \ . \end{aligned} \tag{29}$$

This important result has been utilized repeatedly in the past;[11] its present derivation has fuller generality.

Now let us consider the corresponding implications of the parity of the geometrical elements under the permutation Q, recalling that this permutation only interchanges terms that are summed over in the formulation of observables. The net effect of Q reduces to permuting two columns of the $9j$ coefficient in (15), since the reduced matrix elements with indices a and b appear together in each term of the summation. The parity of $9j$ coefficients equals the parity of the sum of all its indices, that is, of $j_t+j_t'+K_t$ since $l_a+l_a'+k_a$ and $l_b+l_b'+k_b$ are even. Owing to this parity, the expressions of observables consist of sums over combinations of matrix elements of $S^\dagger\times S$ and of $9j$ indices:

$$[(L_AL_B\mid S(j_t')\mid l_a'l_b')^*(L_AL_B\mid S(j_t)\mid l_al_b)+(-1)^{j_t+j_t'+K_t}(L_AL_B\mid S(j_t')\mid l_b'l_a')^*(L_AL_B\mid S(j_t)\mid l_bl_a)]\begin{Bmatrix} l_a & l_b & j_t\\ l_a' & l_b' & j_t'\\ k_a & k_b & K_t\end{Bmatrix} , \tag{30}$$

multiplied by coefficients invariant under Q. (The presence of the two-vector harmonics $Y_{Q_t}^{(K_t)}$ is disregarded here in view of the remark at the end of Sec. III.)

The symmetric quantum numbers defined by (2) enable us to condense the important result (30) into a more compact notation. Recalling that (σ,τ) are even and (ζ,η) odd under the permutation Q, we rewrite (30) in the condensed form

$$\{[S^\dagger(j_t')\times S(j_t)]_{\sigma,\tau,\zeta,\eta}+(-1)^{j_t+j_t'+k_t}[S^\dagger(j_t')\times S(j_t)]_{\sigma,\tau,-\zeta,-\eta}\}\begin{Bmatrix} l_a & l_b & j_t\\ l_a' & l_b' & j_t'\\ k_a & k_b & K_t\end{Bmatrix} . \tag{31}$$

The separation of projectile and target parameters and the tensorial analysis in Sec. II have shown that the geometrical information on projectile and target in (12), (14), and (15) is condensed into the rotationally invariant products of four tensors:

$$\sum_{Q_t}(-1)^{Q_t}[(L_B\mid D_B\mid L_B)^{(K_B)}\times U^{[K_A]}(L_A\mid\rho_A\mid L_A)^{[K_A]}]_{Q_t}^{(K_t)}[[(l_a\mid\rho_a\mid l_a')]^{[k_a]}\times U^{(k_b)}[(l_b'\mid D_b\mid l_b)]^{(k_b)}]_{-Q_t}^{(K_t)} \ . \tag{32}$$

This formula can represent both the preparation of target and projectile in specified geometries and their joint detection after collision in similarly specified geometries. Limited specification of these geometries causes one or more of the indices $\{K_A, K_B, k_a, k_b\}$ to vanish. In this event, the coefficients that multiply (32) are simplified, but the information on dynamical parameters provided by the experiment is accordingly reduced.

The structure of (32), symmetric in the target and projectile geometries, permits one to view a collision equally as transmitting anisotropy from the projectile to the target or from the target to the projectile. The representation in terms of angular momentum transfer has been used in the past[4] mainly for the case of $K_t=0$ and $j_t=j_t'$, where no anisotropy is transferred. Its extended use in this paper is apparently new.

A second novelty of the present treatment lies in the use of symmetries under the permutations P and Q to identify the combinations (29) and (31) of dynamical parameters that are more directly accessible to experimental determination. The coefficients that combine the tensor products (32) with the dynamical parameters (29) and (31) in the expressions of observables are provided by angular momentum algebra.

V. SYMMETRIES OF DYNAMICAL PARAMETERS

Dynamical parameters have generally no symmetry under the permutations P and Q as noted above. On the other hand, they are calculated from matrix elements of the interaction between projectile and target, each of which generally has a definite parity. This parity depends on whether the interaction connects multipole moments of charge or current distributions. It applies directly to some dynamical parameters, for example, in the first Born approximations, but is mixed in higher approximations that combine effects of charge and current distributions.

Unlike the geometrical parameters, the magnitudes of dynamical parameters depend on the energy differences of the projectile and of the target in their initial and final states. This dependence may be enhanced or, instead, compensated by the difference of centrifugal potentials which accompanies changes of angular momenta. These combined effects yield "propensity rules"[12] governing the magnitude of dynamical parameters, which will be discussed below and are analyzed through their combinations (31).

A. Symmetry under P

Dynamical parameters have a definite parity under P when they are real or imaginary. In the notation of $\{\sigma,\tau,\zeta,\eta\}$ with (σ,ζ) even and (τ,η) odd under P, their parity emerges from the relation analogous to (32):

$$P(S^\dagger \times S)_{\sigma,\tau,\zeta,\eta} = (S^\dagger \times S)^*_{\sigma,\tau,\zeta,\eta} = (S^\dagger \times S)_{\sigma,-\tau,\zeta,-\eta} \ . \tag{33}$$

A definite parity, to within irrelevant phase normalization, obtains in the first Born approximation, as we have noted. The first Born approximation holds particularly for large impact parameters, that is, for large values of the orbital quantum numbers and, especially, of the new σ. This approximation also contributes to the dynamical parameters $S^\dagger \times S$ when it holds for large l contributions to S or $S^\dagger$ only; in this event the value of σ need not be large but the value of τ is comparable to it.

On the other hand, higher-order perturbation expansions include integrations over the energy of intermediate states. The integrals consist generally of two terms 90° out of phase, namely, the resonant term from intermediate states that conserve energy and the principal-part integral over states of different energies. Each of these terms has a definite parity under P to within phase normalization but P changes their sum into its complex conjugate. Approximate parity of the dynamical parameters emerges only when either term predominates over the other.

Regardless of perturbation expansions, the complex character of the scattering matrix emerges from its representation in terms of the real reaction matrix K:[13]

$$S = \frac{1+iK}{1-iK} \ . \tag{34}$$

The equation for the K matrix contains only principal-part integrals, but the resonance contributions are related to the principal parts by dispersion relations and are implied by the analytic structure of (34).

Note finally that the occurrence of charge and current interactions with opposite parity P emerges in the dynamical parameters $S^\dagger \times S$ only through the interference of cross terms in the expression of their bilinear structure. Terms of $S^\dagger \times S$ quadratic in the charge or current interactions are, of course, real. Current interactions generally contribute to dynamical parameters only weakly at nonrelativistic energies.

B. Symmetry under Q: Propensity rules

The correlated variations of the projectile energy E and orbital momentum l during a collision influence the magnitude of the relevant S matrix element as anticipated at the beginning of this section. The permutation Q of l_a with l_b will thus generally alter the magnitude of $(L_A L_B | S(j_t) | l_a l_b)$ since the energy change $E_a - E_b$ remains equal to the excitation energy of the target.

Specifically, the permutation of l_a and l_b affects the overlap of the projectile's radial wave functions, $\phi_{E_a l_a}(r)\phi_{E_b l_b}(r)$, whenever $l_a \neq l_b$. This overlap is optimized, with a resulting boost of matrix elements, when the wavelengths of $\phi_{E_a l_a}$ and $\phi_{E_b l_b}$ are nearly equal in the range of r that contributes mostly to S. Since the wavelength decreases with increasing E but increases with increasing centrifugal potential, overlap is enhanced when the differences $E_a - E_b$ and $l_a - l_b$ have the same sign.[12] S-matrix elements for target excitation, which require $E_a - E_b > 0$, will thus be larger when $l_a > l_b$ and will be reduced by the permutation Q. This is the essence of a propensity rule which depends but little on other aspects of the collision.

This rule is illustrated by the data of Table I for the e-He collision (1) calculated in the distorted-wave Born approximation (DWBA) as described in Ref. 10. Some

TABLE I. The modulus and phase of the radial overlap integral $R_{l_b l_a}$ [this integral determines the scattering matrix $(L_B l_b | S(j_t) | L_A l_a)$ in the calculation of Ref. 10] calculated from DWBA for the process (1) at 80-eV impact energy. Numerals in square brackets represent powers of ten.

l_a	l_b	Modulus	Phase	l_a	l_b	Modulus	Phase
1	0	0.126	0.230[+01]	0	1	0.305	−0.956
2	1	0.424	0.111[+01]	1	2	0.121	−0.206[+01]
3	2	0.456	0.634	2	3	0.187[−01]	−0.251[+01]
4	3	0.414	0.417	3	4	0.208[−01]	0.416
5	4	0.356	0.292	4	5	0.328[−01]	0.292
6	5	0.297	0.211	5	6	0.332[−01]	0.211
7	6	0.244	0.154	6	7	0.292[−01]	0.155
8	7	0.199	0.113	7	8	0.242[−01]	0.114
9	8	0.162	0.831[−01]	8	9	0.193[−01]	0.845[−01]
10	9	0.132	0.612[−01]	9	10	0.152[−01]	0.626[−01]
11	10	0.107	0.450[−01]	10	11	0.119[−01]	0.464[−01]
12	11	0.879[−01]	0.331[−01]	11	12	0.926[−02]	0.344[−01]
13	12	0.721[−01]	0.243[−01]	12	13	0.724[−02]	0.255[−01]
14	13	0.593[−01]	0.179[−01]	13	14	0.566[−02]	0.189[−01]
15	14	0.489[−01]	0.132[−01]	14	15	0.446[−02]	0.140[−01]
16	15	0.405[−01]	0.977[−02]	15	16	0.352[−02]	0.105[−01]
17	16	0.335[−01]	0.726[−02]	16	17	0.280[−02]	0.781[−02]
18	17	0.278[−01]	0.542[−02]	17	18	0.224[−02]	0.586[−02]
19	18	0.232[−01]	0.407[−02]	18	19	0.180[−02]	0.442[−02]
20	19	0.193[−01]	0.309[−02]	19	20	0.145[−02]	0.337[−02]
21	20	0.161[−01]	0.236[−02]	20	21	0.118[−02]	0.258[−02]
22	21	0.134[−01]	0.184[−02]	21	22	0.969[−03]	0.200[−02]
23	22	0.112[−01]	0.144[−02]	22	23	0.787[−03]	0.157[−02]
24	23	0.940[−02]	0.115[−02]	23	24	0.662[−03]	0.124[−02]
25	24	0.786[−02]	0.927[−03]	24	25	0.539[−03]	0.101[−02]
26	25	0.660[−02]	0.771[−03]	25	26	0.466[−03]	0.818[−03]
27	26	0.551[−02]	0.633[−03]	26	27	0.379[−03]	0.689[−03]
28	27	0.464[−02]	0.544[−03]	27	28	0.339[−03]	0.567[−03]
29	28	0.387[−02]	0.457[−03]	28	29	0.274[−03]	0.494[−03]
30	29	0.326[−02]	0.404[−03]	29	30	0.253[−03]	0.414[−03]

violations of the propensity rule are apparent for low values of l_b in the Table. In these cases the reduction of the centrifugal potential from $l_a(l_a+1)/r^2$ to $l_b(l_b+1)/r^2$ has greater effects upon the electron than the concurrent reduction of energy from E_a to E_b.

The effect of the propensity rule upon the dynamical parameters is readily seen to depend on the quantum numbers (ζ,η), at least for process (1). Four distinct combinations of the signs of l_a-l_b and $l_a'-l_b'$ occur, namely,

$$\begin{aligned}
&(l_a>l_b, l_a'>l_b'), \quad \text{(favored, favored)}, \quad \text{when } \eta=0 \text{ and } \zeta=1, \\
&(l_a>l_b, l_a'<l_b'), \quad \text{(favored, unfavored)}, \quad \text{when } \eta=1 \text{ and } \zeta=0, \\
&(l_a<l_b, l_a'>l_b'), \quad \text{(unfavored, favored)}, \quad \text{when } \eta=-1 \text{ and } \zeta=0, \\
&(l_a<l_b, l_a'<l_b'), \quad \text{(unfavored, unfavored)}, \quad \text{when } \eta=0 \text{ and } \zeta=-1 .
\end{aligned} \tag{35}$$

It is apparent from (35) that the sum of $\eta=0$ components have much larger magnitude than for $\zeta=0$. The two combinations of $\zeta=0$ with $\eta=\pm1$ appear equivalent on inspection of (32). However, a closer analysis shows a systematic dependence on η of the dynamical parameters as functions of σ, namely, $\eta=1$ prevails for small σ, and $\eta=-1$ for large σ.

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