Exclusion of Parity Unfavored Transitions in Forward Scattering Collisions

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Functions $\mathcal{Y}_{ll'LM}(\hat{k},\hat{k}')$ of the directions of incidence and scattering are considered which transform like spherical harmonics Y_{LM} and are linear combinations of products $Y_{lm}(\hat{k})Y_{l'm'}(\hat{k}')$. When they are parity unfavored ($l+l'-L$ odd), these functions vanish for $\hat{k}\cdot\hat{k}=\pm1$. This property accounts for selection rules pointed out previously for particular types of collision.

It has been pointed out by Becker and Dahler[1] that the helium atom cannot be excited from its ground state to its (still unobserved) $2p^2\,{}^3P$ state by electron-atom collisions if the outgoing electron emerges at 0° (or 180°) from the direction of incidence. This prediction has been recently verified in that the line corresponding to excitation to $2p^2\,{}^3P$ failed to appear in a forward scattering experiment which revealed other optically forbidden double excitations (e.g., to $2s^2\,{}^1S$ and $2s2p\,{}^3P$).[2] The relevant property of excitation to $2p^2\,{}^3P$ consists of the uptake of one unit of orbital angular momentum without any change of parity with respect to space inversion. Transitions with $\Delta J+\Delta\pi$ odd (ΔJ=angular momentum transfer, $\Delta\pi=(0,1)$=parity transfer) are called "parity unfavored." The exclusion of parity unfavored transitions in forward scattering experiments has emerged also in the study of nuclear collisions.[3]

Becker and Dahler's remark was justified initially in terms of a Born-Oppenheimer approximation which is not dependable under the relevant circumstances; a later proof removed this limitation but involved nevertheless a consideration of the special form of wave function appropriate to electron-helium collisions.[1] On the nuclear side, the role of the parity-unfavored character of a transition does not appear to have been disentangled from that of other symmetry considerations.[3] Therefore, it seems worthwhile to single out in the present paper what appears to be the essential relationship between forward scattering and parity unfavoredness.

Consider a collision in which $\hat{k}$ and $\hat{k}'$ indicate the directions of an incident and of an outgoing particle and i and f indicate the quantum numbers of the initial and final states of the scatterer—i.e., of the helium atom in the Becker-Dahler problem. The transition amplitude of this collision can be indicated by

$$(f|T|i). \tag{1}$$

The transition operator T, which is a function of $\hat{k}$ and $\hat{k}'$ and possibly of other variables, is independent of any system of coordinates and, therefore, invariant under rotation or space inversion of such a system. On the other hand, the quantum numbers i and f must be defined, in general, with reference to a coordinate system.

The dependence of T on $\hat{k}=(\theta,\varphi)$ and $\hat{k}'=(\theta',\varphi')$ can be expanded into spherical harmonics,

$$T=\sum_{lml'm'}T_{lml'm'}Y_{lm}(\hat{k})Y_{l'm'}(\hat{k}'). \tag{2}$$

The coefficients $T_{lml'm'}$ and the spherical harmonics are now dependent on the choice of a system of polar coordinates. The spherical harmonics may be regarded as parity favored operators since multiplication of a function by Y_{lm} contributes an angular momentum $\Delta J=l$ and a parity change $\Delta\pi=l$ (mod 2).

The products of spherical harmonics in (2) can be replaced by functions

$$\mathcal{Y}_{ll'LM}(\hat{k},\hat{k}')=\sum_{mm'}(ll'LM|lml'm')Y_{lm}(\hat{k})Y_{l'm'}(\hat{k}') \tag{3}$$

each of which transforms under coordinate rotations as a single harmonic Y_{LM}. [The coefficients on the right of (3) are Clebsch-Gordan-Wigner coefficients.] Equation (2) becomes now

$$T=\sum_{ll'LM}T_{ll'LM}\mathcal{Y}_{ll'LM}(\hat{k},\hat{k}'), \tag{4}$$

with

$$T_{ll'LM}=\sum_{mm'}(ll'LM|lml'm')T_{lml'm'}. \tag{5}$$

The function $\mathcal{Y}_{ll'LM}$ has parity $(-1)^{l+l'}$ and may be regarded as an operator that transfers L units of angular momentum. Therefore, it may be said to constitute an operator that is parity favored or parity unfavored depending on whether $l+l'-L$ is even or odd.[4] The coefficients $T_{ll'LM}$ must be similarly favored or unfavored because the whole T is invariant (i.e., of even parity).

The essential point to be made in this paper stems from the observation that each *parity unfavored* $\mathcal{Y}$ *vanishes* when $\hat{k}$ and $\hat{k}'$ are parallel or antiparallel. In a coordinate system with its polar axis parallel to $\hat{k}$ and

[1] P. M. Becker and J. S. Dahler, Phys. Rev. Letters **10**, 491 (1963); Phys. Rev. (to be published).

[2] J. A. Simpson, S. R. Mielczarek and J. W. Cooper, J. Opt. Soc. Am. **54**, 269 (1964).

[3] See, in particular, K. Alder and A. Winther, Nucl. Phys. **37**, 194 (1962). Some inconsistency has occurred in the description of the relevant coordinate systems utilized in this reference. Thanks are due to Professor L. C. Biedenharn for a discussion of parity unfavored transitions in nuclear physics and for directing the author's attention to relevant literature.

[4] In the simplest example where $l=l'=L=1$, the spherical harmonics Y_{lm}, $Y_{l'm'}$, $\mathcal{Y}_{ll'LM}$ represent, respectively, components of the vectors $\hat{k}$, $\hat{k}'$, $\hat{k}\times\hat{k}'$. The vector product $\hat{k}\times\hat{k}'$ may be regarded as the prototype of a parity unfavored operator.

with its zero-azimuth plane through $\hat{k}'$, we have

$$Y_{lm}(\hat{k})=[(2l+1)/4\pi]^{1/2}\delta_{m0},$$
$$Y_{l'm'}(\hat{k}')=[(2l'+1)/4\pi]^{1/2}P_{l'm'}(\hat{k}\cdot\hat{k}'), \quad (6)$$

where $\delta_{m0}=0$ or 1 for $m\neq 0$ or $m=0$ and where $P_{l'm'}$ is an associated Legendre function. This function contains a factor

$$[1-(\hat{k}\cdot\hat{k}')^2]^{(1/2)|m'|}, \quad (7)$$

and therefore vanishes, for $m'\neq 0$, when $\hat{k}$ and $\hat{k}'$ are parallel or antiparallel. In this coordinate system (3) becomes

$$\mathcal{Y}_{ll'LM}(\hat{k},\hat{k}')=(ll'LM|l0l'M)[(2l+1)^{1/2} \times(2l'+1)^{1/2}/4\pi]P_{l'M}(\hat{k}\cdot\hat{k}'). \quad (8)$$

Now, the coefficient $(ll'LM|l0l'M)$ vanishes for $M=0$ and $l+l'-L$ odd because the Clebsch-Gordan-Wigner coefficients have parity $(-1)^{l+l'-L}$ under sign reversal of m, m', and M. Therefore, the entire expression (8) vanishes for $l+l'-L$ odd and $\hat{k}\cdot\hat{k}'=\pm 1$. (Note also that the parity unfavored $\mathcal{Y}_{ll'LM}$ are odd under permutation of $\hat{k}$ and $\hat{k}'$ so that they obviously vanish for $\hat{k}=\hat{k}'$.)[4a]

The application of this remark to specific collisions is straightforward when the incident and outgoing particles are spinless, as in the example of α particle scattering considered by Alder and Winther.[3] In this event, the entire dependence of T on the direction of the incident and outgoing particles is represented by the functions $\mathcal{Y}_{ll'LM}$ in (4), whereas the coefficients $T_{ll'LM}$ of (4) represent operators that depend only on variables of the scatterer and on radial distances of the other particles. Therefore, if the scatterer's transition $i\rightarrow f$ is parity unfavored, the matrix elements $(f|T_{ll'LM}|i)$ vanish unless $T_{ll'LM}$ is itself unfavored, i.e., unless $l+l'-L$ is odd. We have then

$$(f|T|i)=\sum_{ll'LM}(f|T_{ll'LM}|i)\mathcal{Y}_{ll'LM}(\hat{k},\hat{k}')=0 \quad \text{for} \quad (\hat{k}\cdot\hat{k}')^2=1 \quad (9)$$

because the first factor of each term of the sum vanishes for $l+l'-L$ even and the second one for $l+l'-L$ odd. More specifically, under the circumstances considered here, L coincides with the angular momentum ΔJ taken up by the scatterer in the $i\rightarrow f$ transition and therefore $\Delta\pi$ coincides with $l+l'-L$ (mod 2).

When the incident and/or outgoing particles carry a nonzero spin, the coefficients $T_{ll'LM}$ still depend on their spin orientation and further analysis of this dependence is required. This analysis is still straightforward in the case of electron-helium collisions, because spin-orbit coupling has an altogether negligible influence on the excitation of atoms of very low atomic number. Under this circumstance the dependence of the probability amplitude $(f|T|i)$ upon all spin coordinates can be treated separately, so that $(f|T|i)$ is reduced to a linear combination of unsymmetrized amplitudes $(\bar{f}|\bar{T}|\bar{\imath})$ which depend only on orbital variables.[5] The result derived above for the collisions of spinless particles applies to each $(\bar{f}|\bar{T}|\bar{\imath})$.

The vanishing of the parity unfavored harmonics $\mathcal{Y}_{ll'LM}(\hat{k},\hat{k}')$ for $\hat{k}\cdot\hat{k}'=\pm 1$ and other symmetry properties of these functions have presumably additional applications. A coordinate system with polar axis parallel to $\hat{k}$ was utilized in (8), but other systems may be appropriate for other purposes. For example, a choice of the polar axis perpendicular to both $\hat{k}$ and $\hat{k}'$ emphasizes the symmetry of $\mathcal{Y}_{ll'LM}$ with respect to these variables. With this choice of axis, the products $Y_{lm}Y_{l'm'}$ in (3) vanish unless both $l-m$ and $l'-m'$ are even, so that nonvanishing parity unfavored harmonics $\mathcal{Y}_{ll'LM}$ occur only for odd values of $L-M$. The excitation of $2p^2\,{}^3P$ in helium corresponds to $L=1$ (and hence to $l'=l$); therefore, it must be mediated by the operators $\bar{T}_{ll10}$, with $M=0$ along the axis $\hat{k}\times\hat{k}'$. This implies that the final ${}^3P$ state has zero orbital magnetic quantum number with respect to this axis.

[4a] *Note added in proof.* Prof. Racah kindly points out that $\mathcal{Y}_{ll'LM}(\hat{k},-\hat{k})=(-1)^{l'}\mathcal{Y}_{ll'LM}(\hat{k},\hat{k}')$, owing to the definition (3) and to $Y_{l'm'}(-\hat{k}')=(-1)^{l'}Y_{l'm'}(\hat{k}')$. Therefore, $\mathcal{Y}_{ll'LM}(\hat{k},-\hat{k}')$ vanishes whenever $\mathcal{Y}_{ll'LM}(\hat{k},\hat{k}')$ does. This observation, together with the permutation property

$$\mathcal{Y}_{ll'LM}(\hat{k}',\hat{k})=(-1)^{l+l'-L}\mathcal{Y}_{ll'LM}(\hat{k},\hat{k}'),$$

replaces the proof based on Eqs. (6), (7), and (8).

[5] In the excitation of He to $2p^2\,{}^3P$ by electron collision, the total spin quantum number of the three electrons remains $S=\frac{1}{2}$, which results from the vector addition of $S_{\text{He}}=0$ and $s=\frac{1}{2}$ before the collision and $S_{\text{He}}=1$ and $s=\frac{1}{2}$ after the collision. By working which results from the vector addition of $S_{\text{He}}=0$ and $s=\frac{1}{2}$ before the collision and $S_{\text{He}}=1$ and $s=\frac{1}{2}$ after the collision. By working out the recoupling of spins, one finds that $(f|T|i)=\sqrt{3}\times(\bar{f}(2,3)|\bar{T}(\hat{k}_1',\hat{k}_3)|\bar{\imath}(1,2))$, where the indices 1, 2 pertain to the electrons that belong to He before the collision and 3 to the incident electron.