The kinematic apse and jz-preserving propensities for nonreactive, dissociative, and reactive polyatomic collisions

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Abstract
We consider the generalization of the kinematic apse to nonreactive polyatom–polyatom impulsive collisions, dissociative atom–molecule impulsive collisions, and (partially) impulsive reactive atom–diatom collisions. Appropriate generalizations of the kinematic apse are obtained along which there is a classical propensity for preserving the projection of the total intrinsic spin. In the case of reactive scattering, we discuss several different situations for which such a propensity occurs. For reactive systems in which no such propensity exists, the analysis may still provide a basis for classifying reactions.

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Comments
The kinematic apse and $j_z$-preserving propensities for nonreactive, dissociative, and reactive polyatomic collisions

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We consider the generalization of the kinematic apse to nonreactive polyatom-polyatom impulsive collisions, dissociative atom-molecule impulsive collisions, and (partially) impulsive reactive atom-diatom collisions. Appropriate generalizations of the kinematic apse are obtained along which there is a classical propensity for preserving the projection of the total intrinsic spin. In the case of reactive scattering, we discuss several different situations for which such a propensity occurs. For reactive systems in which no such propensity exists, the analysis may still provide a basis for classifying reactions.

I. INTRODUCTION

It has long been known that a feature of $l$ labeling in certain versions of the CS approximation is that it leads to a $\Delta m = 0$ selection or propensity rule in nonreactive, atom-diatom collisions for an appropriate choice of quantization axis.\(^1\) Thus, $\Delta m = 0$ if $I = I_{\text{initial}}$, and the quantization axis is the final relative momentum and, similarly, $\Delta m = 0$ if $I = I_{\text{final}}$ and the quantization axis is the initial relative momentum. (Here $I$ is the choice of the orbital angular momentum parameter used in a particular version of $l$ labeling in the CS approximation.) This feature of conservation of the azimuthal quantum number along an appropriately chosen quantization axis has come to be referred to as $j_z$ preservation. Since the above conservation laws are, in fact, not observed in accurate CC calculations when the quantization axis is the initial or final relative momentum (except trivially demanded by kinematic constraints), it has been widely believed that the preservation of azimuthal quantum number is simply an artifact of the CS approximation, without dynamical significance.

It is true that these conservation laws are only obeyed exactly for $I_{\text{initial}}$ or $I_{\text{final}}$ labeling in the CS. However, Khare et al.\(^1\) have recently demonstrated that there is a propensity for $j_z$ preservation (but not exact conservation) in the $I_{\text{final}} = \frac{1}{2}(I_{\text{initial}} + I_{\text{final}})$ version of the approximation. The quantization axis for which this propensity is observed is the so-called geometric apse $\bar{A}_z = (\bar{k}_r - \bar{k}_f)/|\bar{k}_r - \bar{k}_f|$, where $\bar{k}_r$ and $\bar{k}_f$ are unit vectors along the initial and final directions of the relative linear momentum. This version of the CS has the formal advantage that it preserves time reversal symmetry and the practical advantage that it is usually more accurate than other $l$-labeling procedures.

However, a point of even greater significance in the work of Khare et al. is that they were able to show by a very simple argument that conservation of the component of angular momentum along a particular quantization axis is an exact dynamical result for a rigid sphere-rigid ovaloid system in classical mechanics (ignoring chattering collisions). This axis, which they call the kinematic apse ($\bar{A}_z = (\bar{k}_r - \bar{k}_f)/|\bar{k}_r - \bar{k}_f|$) lies along the direction of the impulse, i.e., the collisional change of the relative linear momentum. Obviously, there is only a difference between the kinematic apse and the geometric apse for inelastic collisions where $|\bar{k}_f| < |\bar{k}_i|$. This difference is usually unimportant except for extremely inelastic collisions and/or for small angle scattering.

The significant feature of the rigid ovaloid potential is that the colliding molecules suffer impulsive collisions. That is, the configuration variables do not have time to change over the duration of a collision. It is this restriction which implies the neglect of chattering collisions. However, it is important to point out that molecular collisions can be impulsive with respect to some coordinates and not others. This is, in fact, the basis of different sudden approximations, a topic which will be explored in more detail in a later communication. For present purposes it should be remarked that $j_z$ preservation, as discussed above, requires only “impulsiveness” with respect to the relative separation vector and this condition can hold even for certain chattering collisions. The concept that a collision can be impulsive in some, but not all, of its coordinate variables plays an important role in the present study.

The predicted conservation laws have been tested using accurate CC calculations for a number of atom-diatom systems and have been verified, not only for integral state-to-state cross sections,\(^2\) but also for angle resolved transitions.\(^3\) Furthermore, observations consistent with $j_z$ preservation along the geometric apse have recently been made in Na$_2$-He scattering experiments.\(^4\)
The purpose of the present communication is to extend the results of Khare et al. in several important ways. In Sec. II we further analyze the case of nonreactive scattering, by considering the form of \( j_\nu \) preservation for a general impulsive collision of two structured molecules. In Sec. III we extend the concept of the kinematic apse to atom–polyatom collision induced dissociation reactions. In Sec. IV we consider atom–diatom exchange reactions and discuss the conditions under which a kinematic apse provides a convenient quantization axis. More generally, we comment on the possibility of obtaining information about the reaction geometry from observations on \( j_\nu \) transitions. Finally, in Sec. V, we give our conclusions.

II. NONREACTIVE, IMPULSIVE COLLISIONS OF POLYATOMIC MOLECULES

The classical analysis of \( j_\nu \) preservation for nonreactive impulsive atom–diatom collisions by Khare et al. may be applied immediately to impulsive polyatom–polyatom collisions. The derivation is exactly parallel to that for atom–diatom systems. We define the total angular momentum \( \mathbf{J} \) by

\[
\mathbf{J} = \mathbf{r} \times \mathbf{p} + J_1 + J_2 ,
\]

where \( \mathbf{r} \) is the separation between the centers of mass of the two polyatoms, \( \mathbf{p} \) is the corresponding relative Jacobi momentum, and \( J_i, i=1,2 \) are the intrinsic total spins of the polyatomic molecules. The change in \( \mathbf{J} \) during the collision is zero and one therefore has

\[
0 = \Delta \mathbf{J} = \Delta \mathbf{r} \times \mathbf{p} + \Delta (J_1 + J_2) .
\]

If the collision is impulsive in \( \mathbf{r} \), then \( \Delta \mathbf{r} \) is zero and one has

\[
\mathbf{r} \times \Delta \mathbf{p} = - \Delta (J_1 + J_2) .
\]

It immediately follows that the component of \( J_1 + J_2 \) along \( \Delta \mathbf{p} \) is preserved in the collision. With suitable interpretation, this argument (though classical) also holds even if \( J_1 \) and \( J_2 \) include electronic contributions.

It is appropriate here to remark on the quantum mechanical form of \( j_\nu \) preservation for these systems. Since \( j_\nu \) commutes with the Hamiltonian of a polyatomic molecule, its eigenvalue \( \nu \) can be chosen as a state label. Let us now consider \( T \)-matrix elements for polyatom–polyatom scattering for a particular choice of precollisional \( \mathbf{k}_1 \) and postcollisional \( \mathbf{k}_2 \) relative Jacobi momenta (in the center of mass frame). Here we choose the \( \epsilon \)-quantization axis in the direction of \( \Delta \mathbf{K} = \mathbf{k}_2 - \mathbf{k}_1 \), i.e., of the kinematic apse. Let \( m_i, i=1,2 \), be the corresponding \( j_\nu \) quantum numbers for the two polyatoms. Then only \( T \)-matrix elements where \( m_1 + m_2 \) is conserved are nonzero if quantum \( j_\nu \) preservation holds along the kinematic apse. Quantum mechanical calculations in support of such a propensity for \( \text{H}_2 \text{--H}_2 \) (diatom–diatom) scattering can be found in Ref. 5.

III. IMPULSIVE, COLLISION INDUCED DISSOCIATION

It is natural to extend the analysis of classical, nonreactive \( j_\nu \) preservation to cases where the collision is still impulsive but dissociation is possible. We consider here atom–molecule, dissociative collisions. Let \( \mathbf{k}_i \) (\( \mathbf{k}_f \)) be the relative Jacobi momentum between the atom and the center of mass of the molecule (molecular fragments) before (after) collision. The kinematic apse \( \hat{\mathbf{a}}_\nu \) is again defined as the unit vector in the direction of \( \mathbf{k}_f - \mathbf{k}_i \). Let \( \mathbf{j} \) denote the intrinsic total spin of the molecule prior to collision and the sum of the orbital and intrinsic spin angular momenta of the molecular fragments after collision (corresponding to the total intrinsic angular momentum of the molecule dissociating).

The analysis of Khare et al. outlined in Sec. II then immediately applies to give

\[
\Delta \mathbf{j} \cdot \hat{\mathbf{a}}_\nu = 0 ,
\]

i.e., \( j_\nu \) preservation along the kinematic apse. Thus the only change from the previous case is the more general definition of kinematic apse and interpretation of \( j \).

For the quantum mechanical discussion, again we consider \( T \)-matrix elements between states with specified \( \mathbf{k}_1 \) and \( \mathbf{k}_2 \) redefined as above. The precollisional state labels include the \( j_\nu \) quantum number \( m \) (as in Sec. II). The postcollisional fragment states are labeled by the coupled representation including a quantum number \( \mu \) for the projection of the sum of the corresponding molecular fragment orbital and intrinsic spin angular momenta also onto the space–fixed kinematic apse. Then only \( T \)-matrix elements with \( \mu = m \) are nonzero if quantum \( j_\nu \) preservation along the kinematic apse holds.

The \( T \)-matrix labeling described here is not as natural as in the nonreactive case. Consider an atom–(dissociative)diatom process. The bound diatomic state is labeled by \((v, j, m)\) where \( v \) refers to the vibrational and \( j, m \) to the spin state. The fragment state is labeled by \((k, l, \mu)\) referring to a spherical wave with wave number \( k \) (the magnitude of the relative momentum of the fragments) and orbital quantum numbers \( l, \mu \). Alternatively, and more commonly, one can use plane wave labeling \( k \) (the vector relative momentum of the fragments) for the latter.

The corresponding \( T \)-matrix elements are related by

\[
T_{j_\nu, k_f v m} = \sum_{l=0}^1 \sum_{\mu=\pm1} (-i)^j k^{-1} Y_l^\ast (\theta, \phi) T_{j_\nu, k_l v m} ,
\]

assuming normalized states and where \((\theta, \phi)\) is the orientation of \( \mathbf{k} \). If \( \theta = 0 \) corresponds to the kinematic apse and if \( j_\nu \) preservation holds, then

\[
T_{j_\nu, k_f v m} = \sum_{l=1,2} (-i)^j k^{-1} Y_l^\ast (\theta, \phi) T_{j_\nu, k_l v m} .
\]

Thus \( j_\nu \) preservation is not simply manifested in the \( k \)-labeled \( T \)'s. However, it does have practical importance in the theoretical calculation of these \( T \)'s from spherical wave labeled \( T \)'s [as seen from Eq. (6)] and in the solution of the scattering equations for the latter.

IV. CLASSICAL REACTIVE COLLISIONS

The success of the \( j_\nu \)-preservation analysis in the cases previously discussed leads naturally to the question as to whether it can be extended to atom–diatom ex-
change collisions. At the outset this might seem to be unlikely since the "atomic" and the "diatomic" species change during the course of the collision. This results in a change of the moment of inertia of the system and a concomitant change in the rotational energy. However, although the identity of the "rotor" changes over the course of the collision, the change of orbital momentum along a given reference axis must still be in integral units of $\hbar$. That is, although the quantized energy of a system varies with its moment of inertia, this is not true for the angular momentum. It is thus sensible to investigate if there is a meaningful generalization of the apse concept which ascribes special significance to $\Delta m = 0$ transitions.

The Jacobi coordinates for a three atom system are

$$ R = \sum_i m_i R_i, $$  

$$ R_a = R_a - \frac{m_a R_a + m_b R_b}{m_a + m_b}, $$  

$$ \rho_a = \rho_a - R, $$  

where $R_a$, $R_b$, and $R_c$ are the vector positions of the three atoms having masses $m_a$, $m_b$, and $m_c$, respectively, and $M = m_a + m_b + m_c$. Here $R$ is the system center of mass, $R_a$ is the position of atom $\alpha$ relative to the mass center of the $(\beta, \gamma)$ subsystem and $\rho_a$ is the position vector of atom $\beta$ relative to atom $\gamma$. This choice of coordinates treats $\alpha$ as an atom and $(\beta, \gamma)$ as a diatom; obviously $\beta$ or $\gamma$ could equally well be chosen as the atom leading to a different set of Jacobi coordinates. The inverse transformations are

$$ r_a = R + \left(\frac{m_b + m_c}{M}\right) R_a, $$  

$$ r_b = R - \frac{m_a m_b}{m_a + m_b} R_a + \frac{m_b}{m_a + m_b} \rho_a, $$  

$$ r_c = R - \frac{m_a m_c}{m_a + m_c} R_a - \frac{m_c}{m_a + m_c} \rho_a. $$

The classical momenta conjugate to $R$, $R_a$, and $\rho_a$ are

$$ P = M \dot{R}, $$  

$$ P_a = \mu_{\alpha(\beta \gamma)} \dot{R}_a, $$  

$$ \Pi_a = \mu_{\beta \gamma} \dot{\rho}_a, $$

respectively, where

$$ \mu_{\alpha(\beta \gamma)} = \frac{m_a (m_b + m_c)}{M} $$

is the reduced mass of the atom-"diatom" system and

$$ \mu_{\beta \gamma} = \frac{m_b m_c}{m_a + m_b} $$

is the reduced mass of the diatom. The total angular momentum of the system is given by

$$ J = r_a \times P_a + r_b \times P_b + r_c \times P_c = R \times P + R_a \times P_a + \rho_a \times \Pi_a. $$

Let us now consider the exchange reaction

$$ \alpha + (\beta \gamma) = \beta + (\alpha \gamma). $$

It follows from elementary mechanics that

$$ \frac{dJ}{dt} = \frac{d}{dt}(R \times P) = 0 $$

and hence that

$$ 0 = R_b \times P_a - R_a \times P_a + \Delta j, $$

where

$$ \Delta j = \rho_b \times \Pi_a - \rho_a \times \Pi_a, $$

is the change in "rotor" angular momentum, $R_a$, $P_a$, $\rho_a$, and $\Pi_a$ are the Jacobi coordinates and momenta for the $\alpha(\beta \gamma)$ decomposition of the system at some time prior to collision, and $R_b$, $P_b$, $\rho_b$, and $\Pi_b$ are the Jacobi coordinates and momenta for the $\beta(\alpha \gamma)$ decomposition of the system at some time after the collision.

We now make the natural restriction on the choice of "kinematic apse" to vectors lying in the collision plane. Consequently, we define the auxiliary vectors

$$ P_{\alpha \beta} = a_{\alpha} P_a + a_{\beta} P_b $$

and $R_{\alpha \beta} = a_{\alpha} R_a + a_{\beta} R_b$. In terms of these, Eq. (14) can be written as

$$ P_{\alpha \beta} \cdot \Delta j = R_{\alpha \beta} \cdot (P_a \times P_b), $$

or equivalently

$$ \Delta j = \frac{|P_a|}{|P_{\alpha \beta}|} \sin \theta \cdot R_{\alpha \beta}, $$

where $\Delta j = P_{\alpha \beta} / |P_{\alpha \beta}|$ is the generalized kinematic apse, $\theta = (P_a \times P_b) / |P_a \times P_b|$, and $\theta$ is the scattering angle. Thus, forward ($\theta = 0$) and backward ($\theta = \pi$) scattering collisions are $j_z$ preserving provided $P_{\alpha \beta} \neq 0$. In general one can choose $a_{\alpha}$, $a_{\beta}$ to cancel the component of $R_{\alpha \beta}$ in the direction of $P_a \times P_b$ demonstrating $j_z$ preservation in the direction of this $P_{\alpha \beta}$. However, such a choice depends on a detailed knowledge of the geometry of individual collisions, e.g., on impact parameters, orientations etc., which, in general, are not known. Consequently we confine our attention to simply implemented choices of $P_{\alpha \beta}$ which depend only on kinematic quantities such as the masses.

It should be pointed out that Eq. (18) is a quite general result, depending only on angular momentum conservation, and does not make use of the "impulsiveness" of the collision. For this equation to be useful for our present purposes it is required that the collision be impulsive in some, but not necessarily all, coordinates. Several cases are now considered.

A. Atom transfer involving one light and two heavy atoms

In this subsection, the coordinates appearing in $R_a$, $R_b$, and $R_{\alpha \beta}$ corresponding to the heavy particles are taken to be impulsive and thus chosen as those at the "point" of reaction (corresponding to both pre- and postcollisional variables). Those of the light particle are chosen as immediately pre- (post-) collisional in $R_a$ ($R_b$). The latter are distinguished by primes. Here we naturally consider choices of $a_{\alpha}$ and $a_{\beta}$ for which $R_{\alpha \beta}$ does not depend strongly on the (nonimpulsive) coordinates of the light particle. Observations on $j_z$ tran-
sitions for these various kinematic apse quantization axes could lead to an understanding of the impulsive reaction geometry. Here we focus our attention on the choices which optimize \( j_z \)-conserving propensity for two important special cases:

1. Light atom transfer (HL)H → H(LH)

Here \( m_r < m_A, m_B \). Then since

\[
R_a = (r_a - r_R) + \frac{m_r}{m_A}(r_B - r_R) + O\left(\frac{m_r^2}{m_A^2}\right)
\]

and

\[
R_B = (r_B - r_B) + \frac{m_B}{m_A}(r_a - r_R) + O\left(\frac{m_B^2}{m_A^2}\right)
\]

it is clear that \( R_a \approx -R_a \approx r_a - r_R \) and that \( R_{as} \) depends only weakly on \( r_a \) for any choice of \( a_a, a_B \). It is natural to choose \( a_a = a_B = 1 \), so that

\[
P_{as} = P_a + P_B
\]

and

\[
R_{as} = \frac{m_r}{m_A}(r_a - r_R) + \frac{m_B}{m_A}(r_B - r_B) + O\left(\frac{m_r^2}{m_A^2}\right)
\]

where \( m_r, m_B = O(m) \). From Eqs. (18) and (21) it is immediate that the small mass ratio will greatly restrict the range of allowed \( j_z \) transitions. (Estimates of the size of this range without mass weighting are given in the next subsection.)

Reactions involving the transfer of a hydrogen atom between two heavy halogens should be good candidates for restricted \( j_z \) transitions with respect to a quantization axis in the direction of \( P_a + P_B \) (provided the kinetic energy is sufficiently high that the interaction of the halogens is impulsive). Observation of \( j_z \)-transition behavior for any other choice of quantization axis (in the collision plane) carries information about the halogen separation vector \( (r_a - r_R) \) at the "point" of reaction. We return to this point later.

To compare this choice of kinematic apse with those of previous sections, it is natural to trivially define \( \hat{P}_a = -P_a \), i.e., the postcollisional momentum of the center of mass of the diatomic containing atom \( \alpha \) relative to atom \( \beta \). Then \( P_a + P_B = P_a - \hat{P}_a \) analogous (except for a sign) to the nonreactive choice of apse.

2. Light atom attack L(HH) → (LH)H

Here \( m_A = m_A, m_B \). From Eq. (8), \( R_{as} \) depends strongly on the light atom coordinates \( r_a \), but

\[
R_a = (r_a - r_R) + \frac{m_A}{m_A}(r_B - r_R) + O\left(\frac{m_A^2}{m_A^2}\right)
\]

Thus it is clear that only the choice \( a_B = 0 \) yields \( R_{as} \) weakly dependent on \( r_a \). With \( a_a = 1 \),

\[
P_{as} = P_a, \quad R_{as} = R_a \approx r_a - r_R
\]

During "light atom capture" in the reactions

\[
D + X + D + X, \text{ where } X = I, \text{ Cl or Br},
\]

the two heavy atoms do not move much and finally "dissociate" roughly in the direction of their bond

\[
r_a - r_R
\]

The observation that \( R_{as} \) and \( P_{as} \) are nearly parallel, leads to the conclusion, from Eq. (17), that the range of \( j_z \) transitions (relative to a quantization axis in the direction of \( P_{as} \)) will be greatly restricted.

B. Atom transfer impulsive with respect to all atoms

We consider the case where the reactive collision is completed with virtually no change in the positions of all three atoms. Here all coordinates appearing in \( R_{as} \), \( R_B \), and \( P_{as} \) correspond to those at the point of reaction. Substituting for \( R_{as} \), \( R_B \) in terms of \( r_a, r_B, r_R \), it is readily shown that the choice

\[
P_{as} = \frac{m_a + m_r}{M} P_a - \frac{m_B + m_r}{M} P_B
\]

\[
\times \left( a_a = \frac{m_a + m_r}{M}, -a_B = \frac{m_B + m_r}{M} \right)
\]

leads to

\[
R_{as} = r_a - r_R = \Delta r
\]

so now

\[
\Delta j \cdot \Delta \mathbf{R}_s = \frac{|P_a|}{|P_{as}|} \sin \hat{n} \cdot \Delta \mathbf{R}
\]

We describe \( \Delta \mathbf{R} \) as the "atomic-identity transfer vector" (i.e., \( \alpha \) is the atom before, and \( \beta \) after, the collision). Thus, from Eq. (26), the range of allowed \( j_z \) transitions in the direction of \( P_{as} \) depends on the extent to which the atomic-identity transfer vector \( \Delta \mathbf{R} \) is out of the collision plane at the point of reaction. Consequently, in-plane collisions are \( j_z \) preserving. Note that if \( m_a = m_A, P_{as} \) is in the direction of \( P_a - P_B = P_a - \hat{P}_a \) where, again, \( \hat{P}_a \) is the postcollisional momentum of the center of mass of the diatomic containing atom \( \alpha \) (relative to atom \( \beta \)). Consequently this choice of kinematic apse is not analogous to the nonreactive case.

To ascertain whether we can expect \( j_z \)-conserving propensity for any of these collision systems, it is instructive to examine the condition of Eq. (26) for a worst case situation. Here we suppose that

\[
\sin \theta \approx 1, \quad |\mathbf{n} \cdot \Delta \mathbf{R}| \approx |\Delta \mathbf{R}|
\]

and

\[
|P_a| \approx |P_{as}| \approx |P_{as}| = O(hk)
\]

Then changes \( \Delta m \) of \( m \) in \( j_z \) transitions are restricted to

\[
|\Delta m| \leq k|\Delta \mathbf{R}|
\]

The minimum relative kinetic energy for which impulsive collision behavior is anticipated would roughly correspond to a small multiple (say twice) the well depth of the attractive part of the interaction. This corresponds to

\[
|\Delta m| \leq 30(E_{ev}m_{atm})^{1/2} |\Delta \mathbf{R}_{a,b}|
\]

where \( E_{ev} \) is the well depth in eV's and \( m_{atm} \) the reduced mass of the atom–diatom system in atomic units. (Note that such choices of \( k \) typically imply that, if \( \tau_{coll} \) is the collision time and \( \tau_{rot} \) the period for internal rotations, then \( \tau_{coll}/\tau_{rot} \ll 1 \).)

Thus for heavy/large atom systems the worst case
range of $\Delta m$ is in the hundreds. Note that often for the direct reactions of interest here (where the “time of interaction” is less than, say, one rotational period), the angular scattering distribution is often strongly biased towards the forward direction (e.g., a stripping mode) or the backward direction (e.g., a rebound mechanism), so we expect at least $\sin \theta < \frac{1}{2}$ for angles with significant scattering. This further restricts the $\Delta m$ range. More pertinent to the discussion here is the case where $\Delta m$ is almost in plane, i.e., $\hat{n} \cdot \Delta r \ll 1$ which would greatly restrict the range of possible $j_+^L$ transitions. One such case is where the atom $\gamma$ only slightly perturbs the spherical symmetry of the interaction potential between $a$, $\phi$ and $\beta$ (i.e., for classical impulsive collisions, the size of atom $\gamma$ is small compared with $a$, $\phi$). Clearly $\hat{n} \cdot \Delta r$ will be limited by the “size” of $\gamma$ (noting that $\Delta r$ is in-plane for two colliding spherical atoms). One might anticipate such behavior in processes involving hydrogen transfer between two “large” halogens. But then, from the analysis of the preceding subsection, for any in-plane choice of kinematic apse, $R_{\alpha \beta}$ is a linear combination of a nearly in-plane atomic-identity transfer vector and a small mass weighted term. That is, all choices of apse should exhibit somewhat restricted $j_+^L$ transitions.

Finally we remark on situations where there is no propensity for $j_+^L$-conservation/in-planeness of $\Delta r$. Equation (26) could still be useful in elucidating the impulsive reaction geometry. For example, if at a given scattering angle $\theta$ and for a fixed beam momentum $P_\alpha$, one observes one predominant value of $|\Delta m|$ and $|P_\beta|$, it follows that most collisions occur for a particular value of $\hat{n} \cdot \Delta r$.

V. CONCLUSIONS

The treatments of nonreactive polyatom–polyatom collisions, and even dissociative collisions, given here are obvious extensions of the previous classical analysis of $j_+^L$ preservation. In the latter case, however, the physical dissociation amplitudes are not labeled by the angular momentum projection quantum number $m$. They can however be obtained as linear combinations of such quantities which, for impulsive collisions, exhibit $j_+^L$-conserving propensity.

The results of the analysis for reactive systems are particularly interesting. Even though, in general, one does not expect $j_+^L$-preserving propensity, we have noted that two important processes where this may still occur are light atom transfer $(HL)H \rightarrow H(LH)$ and light atom attack $L(HH) \rightarrow (LH)H$. This is anticipated even if the interaction dynamics of the light atom is not impulsive during reaction. Finally for impulsive reactions, we have indicated the possibility of elucidating some aspects of the collision geometry from observation of $j_+^L$ transitions (even without $j_+^L$-preserving propensity).


