

State-to-state differential cross sections from photoinitiated bulb reactions

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Received 19 April 1993; in final form 21 May 1993

We consider a mixture of a diatomic photolytic precursor AX and a reagent BC that undergoes the photoinitiated reaction $AX+h\nu\rightarrow A+X$ followed by $A+BC\rightarrow AB+C$. In the limit that AX is stationary relative to BC , we show that the three-dimensional velocity distribution of the AB product in a specified quantum state can be related to the differential cross section of the $A+BC$ reaction by a simple, invertible, closed-form expression. With a favorable choice of kinematics, we demonstrate that it is possible to extract the full state-to-state differential cross section from a measurement of the velocity distribution of the AB product in the laboratory frame.

1. Introduction

The measurement of differential cross sections from state-to-state reactions promises to offer new insight into how elementary reactions occur. At the simplest level of interpretation, differential cross sections distinguish between classes of reaction dynamics, such as stripping, rebound, and insertion [1]. State-to-state differential cross sections should reveal with an unprecedented degree of clarity the mechanism of a chemical reaction. For example, state-to-state differential cross sections of the $H+H_2$ reaction should provide very stringent tests of the dramatic effects of quantum resonances [2] and the geometric phase [3]. Although detailed state-to-state differential cross sections would add an entirely new dimension to our understanding of a long list of reactions, only a few measurements of product-state-resolved differential cross sections have been made to date.

The most intuitive way of measuring a differential cross section is by crossing two beams of reactants and measuring the products as a function of the angle into which they scatter [4]. Although this technique has been successful in the measurement of differential cross sections that are averaged over reagent and product internal quantum states [5], only a handful of differential cross sections have been mea-

sured with product state resolution. These include studies of the $Ba+LiCl\rightarrow BaCl+Li$ [6], $Ba+KCl\rightarrow BaCl+K$ [7], $F+H_2\rightarrow HF+F$ [8], $F+I_2\rightarrow IF+I$ [9], $H+NO_2\rightarrow OH+NO$ [10] $D+H_2\rightarrow HD+H$ [31] and $H+D_2\rightarrow HD+D$ [11] reactions. Only the studies of the $D+H_2$ $H+D_2$ reactions have resulted in a differential cross section for a single state-to-state reaction [11,31]. A primary challenge of these measurements has been the experimental difficulty of having only a minuscule amount of product expected in a given rovibrational state scattered into a given element of solid angle.

In recent years great strides have been taken to overcome the small expected signal from crossed-beam experiments. These include the development of ion imaging techniques [12,13] as well as the use of Rydberg-atom time-of-flight (TOF) spectroscopy [11]. Another approach directed toward obtaining state-to-state differential cross sections has been to abandon crossed beams and to attempt to learn about differential cross sections from hot-atom reactions under bulb conditions [14–22], which tend to provide much more signal. Here the word bulb is used loosely. By “photoinitiated bulb reaction”, we mean an experiment in which a precursor, AX (normally a diatomic), is combined with a reactant, BC , in a single gas stream and allowed to enter into a reaction chamber via some means, such as an effusive or

pulsed expansion. The precursor molecule AX is then photodissociated to initiate the reaction sequence



From measurements of the velocity distribution of the AB product, the zeroth- and second-order moments of the differential cross section have been determined [14,17,22]. A possible misconception is that only these two moments of the differential cross section can be extracted from a photoinitiated bulb experiment. As we show, if the kinematics are favorable, the complete differential cross section can be deduced from the velocity distribution of the AB product, and, in principle, a direct inversion of product velocity data is possible to obtain the differential cross section. Brouard et al. [20] have calculated laboratory-frame velocity distributions for the OH product of the reaction of O(¹D) with CH₄ from assumed forms of the differential cross section, and have demonstrated that isotropic scattering in the center-of-mass frame is most consistent with their experimental OH velocity data. For the reaction of O(¹D) with N₂O, the same workers [18] were able to demonstrate that the vibrationally excited NO product is forward scattered by comparing their data to the predictions of a stripping mechanism. The general strategy for obtaining a differential cross section from a photoinitiated bulb experiment is similar to the strategy used by McCaffery and co-workers [23] in their Doppler-resolved double resonance experimental studies of inelastic scattering.

Shafer [16] and Aoiz et al. [24] have given integral expressions for the velocity distribution of the AB product under conditions where the thermal motion of the reagents is significant, and Hall [15] has used Monte Carlo calculations to determine the one-dimensional projection of the velocity distribution onto a single axis. An invertible expression for the velocity distribution as a function of the differential cross section, however, has yet to be published. In this Letter we suppose that the AX, BC gas mixture is stationary, i.e. the translational temperature of the gas is cooled to 0 K before the photoinitiated reaction occurs. By making this approximation, we are able to obtain a simple relationship between the AB product velocity and the differential cross section.

The equations of Shafer [16] and of Aoiz et al. [24] collapse to the equations presented here if the approximation of a stationary photolysis precursor AX and a stationary target molecule BC is made. We then discuss the conditions necessary to obtain the differential cross section from a bulb experiment. We compare the expected velocity distribution from our simple analysis with that obtained from a Monte Carlo calculation that includes the effect of temperature. In a companion Letter [25] we illustrate the results of this analysis by determining the state-to-state differential cross section for HCl from the reaction $\text{Cl} + \text{CH}_4(\nu_3=1, J=1) \rightarrow \text{CH}_3 + \text{HCl}(v'=1, J')$.

2. The velocity distribution of product molecules from a stationary photoinitiated reaction

Even in the limit of a stationary AX, BC gas mixture, the velocity distribution of the AB product from the reactions given in eqs. (1) and (2) can be a highly averaged quantity. The photolysis of AX by a monochromatic light source normally leads to a range of photoproduct states. This range in turn leads to a spectrum of A translational energies, E_A , determined by the difference between the photon energy, $h\nu$, and the endothermicity, ΔE_A , of individual photodissociation channels:

$$E_A = \left(\frac{m_X}{m_A + m_X} \right) (h\nu - \Delta E_A). \quad (3)$$

The velocity distribution of the AB product will therefore be a sum of velocity distributions that arise from reactions at several different collisional energies.

An additional degree of averaging occurs because of the possible internal-state combinations of the reactants and products. Single state-to-state reactions can be studied, however, by careful choice of the precursor AX and the photodissociation wavelength, cooling or laser-induced state preparation of the BC reactant, and selective detection of the AB product [26]. If the velocity distribution of the detected AB product of such a system were to be measured, it could be expressed as a single summation over the state-to-state velocity distributions from the individual internal states of C. Often C is con-

strained to have a narrow range of internal energies. This constraint can occur either when C acts as a spectator to the reaction or when C has no energetically accessible excited states. In this case the velocity distribution of the detected AB molecule is determined by a single reaction pathway. In the following treatment we only consider the velocity distribution from a single state-to-state reaction. The extension of our analysis to the more general case is straightforward and therefore omitted.

Because the internal states of the reactants and products are defined by the reaction pathway, the speed of the AB product in the center-of-mass frame, u_{AB} , can be deduced by conservation of energy and momentum, as is shown in the Appendix,

$$u_{AB} = \frac{m_C}{M} \left(\frac{2(E_A \mu / m_A - \Delta E)}{\mu'} \right)^{1/2}. \quad (4)$$

Here m_A , m_{BC} , μ , m_C , and μ' are the masses and reduced masses of the reactants and products, $M = m_A + m_{BC} = m_{AB} + m_C$, and ΔE is the difference between the potential energy of the products and reactants. The speed of the AB product in the laboratory frame, v_{AB} , is determined by the speed of the center of mass, u , the speed of AB in the center-of-mass frame, u_{AB} , and the scattering angle of the reaction, θ_r ,

$$v_{AB} = u + u_{AB}, \quad (5)$$

$$v_{AB}^2 = u^2 + u_{AB}^2 + 2uu_{AB} \cos \theta_r, \quad (6)$$

where the speed of the center of mass is given by

$$u = \frac{m_A}{M} \left(\frac{2E_A}{m_A} \right)^{1/2}. \quad (7)$$

Eq. (6) is intriguing; the only variable needed to determine the speed of AB in the laboratory frame is the scattering angle. Alternatively, if we measure the speed of AB we have determined the three speeds v_{AB} , u_{AB} , and u that make up the sides of a triangle (fig. 1). From the law of cosines we can determine the cosine of scattering angle, $\cos \theta_r$, as a function of the speed of the AB product, v_{AB} ,

$$\cos \theta_r = \hat{u}_{AB} \cdot \hat{u} = \frac{v_{AB}^2 - u^2 - u_{AB}^2}{2uu_{AB}}. \quad (8)$$

We can also determine the cosine of the angle be-

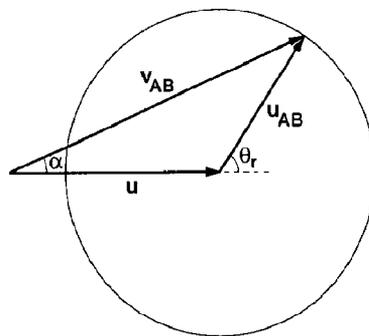


Fig. 1. Velocity diagram for the $A + BC$ reaction in which the BC molecule is stationary. The velocity of the center of mass, u , lies parallel to the velocity of A. The laboratory frame and center-of-mass frame velocities of the AB product are denoted by v_{AB} and u_{AB} , respectively.

tween the center-of-mass velocity and laboratory-frame velocity of the AB product, $\cos \alpha$, as a function of v_{AB} ,

$$\cos \alpha = \hat{v}_{AB} \cdot \hat{u} = \frac{v_{AB}^2 + u^2 - u_{AB}^2}{2v_{AB}u}. \quad (9)$$

These relationships imply a simple relationship must exist between the product velocity distribution $f(v_{AB})$ and the distribution of scattering angles given by the normalized differential cross section, $(1/\sigma)d\sigma/d\Omega$. In the Appendix we show that for a state-to-state photoinitiated bulb reaction, the velocity distribution of the AB products is related to the differential cross section by the expression

$$f(v_{AB}) = \frac{1}{2v_{AB}uu_{AB}} \frac{1}{\sigma} \frac{d\sigma}{d\Omega} \times [1 + \beta P_2(\hat{v}_{AB} \cdot \hat{u}) P_2(\hat{v}_{AB} \cdot \hat{\epsilon})],$$

$$v_{\min} < v_{AB} < v_{\max},$$

$$f(v_{AB}) = 0,$$

$$v_{AB} < v_{\min} \text{ OR } v_{AB} > v_{\max}, \quad (10)$$

Here

$$v_{\min} = |u - u_{AB}|, \quad (11)$$

$$v_{\max} = |u + u_{AB}|, \quad (12)$$

$\hat{\epsilon}$ is the direction of the electric vector of the photodissociation laser, which is assumed to be linearly polarized, β is the anisotropy parameter for the pho-

photodissociation, and $f(v_{AB})$ is normalized to unity,

$$\int f(v_{AB}) dv_{AB} = 1. \quad (13)$$

We note that $f(v_{AB})$ depends on the direction of v_{AB} only through the term $P_2(\hat{v}_{AB} \cdot \hat{\epsilon})$. The quantity $(1/\sigma)d\sigma/d\Omega$ is evaluated at the value of $\hat{u}_{AB} \cdot \hat{u}$ given by eq. (8) and $\hat{v}_{AB} \cdot \hat{u}$ is a function of v_{AB} which is given by eq. (9).

Eq. (10) is a remarkable result; the differential cross section for a state-to-state reaction can be directly obtained from a measurement of the three-dimensional velocity distribution of the product of a photoinitiated bulb reaction. This conclusion requires some qualification. The range of possible product velocities given by eqs. (11) and (12) must be large enough to be measured and to survive the effect of thermal averaging. This condition in turn requires that the speed of the center of mass, u , must be neither much smaller nor much larger than the speed of the product in the center-of-mass frame, u_{AB} . For example, if DI is photodissociated at 242 nm to produce a D atom with 2.0 eV of energy and the D atom is allowed to react with $H_2(v=1, J=1)$ to produce HD($v'=1, J'=7$), the forward-scattered HD will have a laboratory-frame velocity of 10600 m/s whereas the backward-scattered HD will have a laboratory-frame velocity of 3300 m/s. This velocity difference is readily measured. On the other hand, if these D atoms were instead allowed to react with ground-state HI to form HD($v'=0, J'=0$) + $I(^2P_{3/2})$, the forward-scattered HD product would have a velocity of 14900 m/s, whereas the backward-scattered HD would have a velocity of 14500 m/s. Clearly, care must be taken to choose a system with kinematics that lead to a range in the product velocity,

$$v_{\text{range}} = |u + u_{AB}| - |u - u_{AB}|, \quad (14)$$

that can be measured. We can write

$$\begin{aligned} v_{\text{range}} &= 2u\gamma, & \gamma < 1, \\ v_{\text{range}} &= 2u, & \gamma > 1, \end{aligned} \quad (15)$$

where γ is the ratio of the speed of the AB product in the center-of-mass frame to the speed of the center of mass,

$$\begin{aligned} \gamma &= u_{AB}/u \\ &= \frac{m_C}{m_A} \left(\frac{\mu E_A - m_A \Delta E}{\mu' E_A} \right)^{1/2}. \end{aligned} \quad (16)$$

For $\Delta E=0$, eq. (16) reduces to

$$\gamma = \left(\frac{m_C m_{BC}}{m_A m_{AB}} \right)^{1/2}. \quad (17)$$

If m_B is much greater than the masses of the other particles, most of the kinetic energy will be transferred to the C product, and the AB product velocity will not be large enough to be measured. If m_B is not much greater than m_C or m_A , the quantity γ determines the amount of information that can be extracted from a photoinitiated bulb reaction. Consider three limiting cases: (1) $u_{AB} \ll u$ ($\gamma \ll 1$), (2) $u_{AB} \gg u$ ($\gamma \gg 1$), and (3) $u_{AB} \approx u$ ($\gamma \approx 1$). For case (1), no information about the differential cross section can be deduced from the velocity distribution of the AB product; for case (2), only the second-order moment of the differential cross section can be obtained; whereas for case (3), the entire differential cross section can be extracted from the velocity distribution of the AB product. In sections 2.1–2.3, we consider each of these cases.

2.1. Case (1): $u_{AB} \ll u$ ($\gamma \ll 1$)

When a heavy A reacts with a light molecule BC, γ is small. The center-of-mass velocity dominates the kinematics so that the velocity of the AB product is close to the center-of-mass velocity, regardless of whether it is forward or backward scattered. Thus, in the limit that γ approaches zero, nothing about the differential cross section can be deduced from the velocity distribution of the AB product.

2.2. Case (2): $u_{AB} \gg u$ ($\gamma \gg 1$)

When a light A reacts with a heavy molecule BC, γ is large. In this case the center-of-mass speed becomes insignificant, and the product velocity in the laboratory frame takes on the same value as the product velocity in the center-of-mass frame. Because u_{AB} is fixed by the kinematics of the state-to-state reaction, the speed of the product in the laboratory frame, v_{AB} , is also fixed. The only dynami-

cally significant component to the product velocity distribution is the angular anisotropy. For photoinitiated bulb reactions, this angular anisotropy is limited by the angular anisotropy of the reactant A. Thus, in the limit that γ becomes large, only the zero- and second-order moments of the differential cross section can be determined.

2.3. Case (3): $u_{AB} \approx u$ ($\gamma \approx 1$)

The optimal reaction systems for measurement of a differential cross section in a bulb are those for which $\gamma \approx 1$. For thermoneutral reactions, this situation occurs when $m_A \approx m_C$. When $\gamma \approx 1$ the range of product speeds for different scattering angles is significant. Because of this range, the product speed distribution is sensitive to the differential cross section. Unlike for $\gamma \gg 1$, the measurable information is no longer limited by the degree of anisotropy of the photofragments: instead it is limited by the sharpness of the distribution of speeds of the hot-atom reagent A. For a monoenergetic photoproduct A and a stationary reactant BC, the sensitivity of the AB speed distribution to the differential cross section is not restricted. We conclude that bulb experiments are well suited to the measurement of differential cross sections from state-to-state reactions of A with BC where $m_A \approx m_C$ and m_B is not much greater than m_A . Ideal reactions include that of $H+H_2$ and its isotopomers, and $X+HY$ hydrogen-transfer reactions in which m_X and m_Y are similar masses.

3. Experimental factors that affect velocity distribution measurements

A number of experimental methods can be used to measure the AB velocity distribution or its projection onto a line or a plane. Two possible factors that can affect the measurements are the temperature of the target gas, BC, and the spatial anisotropy of rotational angular momentum vectors, both of which should be considered in the analysis of AB velocity data.

3.1. The effect of temperature on the velocity distribution

As in a beam experiment, if the gas in a bulb experiment is not cold enough, information about the cross section is lost. To illustrate the extent of this loss, we consider the reaction $D+H_2(v=1, J=1) \rightarrow HD(v'=1, J'=7) + H$ at a total energy of 1.8 eV. The differential cross section for this reaction predicted by Kuppermann and Wu [27] is particularly interesting because it shows a strong influence of the geometric phase. We wish to determine if this cross section, shown in fig. 2a, can be extracted from a bulb experiment that starts with a DI, H_2 gas mixture that has not been cooled to a translational temperature of 0 K.

The DI is photodissociated at 242 nm to produce D atoms that react with the H_2 with 1.0 eV of collision energy. A collision energy of 1.0 eV corresponds to the 1.8 eV of total energy used by Kuppermann and Wu in their calculation. In figs. 2b–2d, the distribution of speeds of the $HD(v'=1, J'=7)$ product from a stationary gas is then calculated from eq. (10) and compared with a Monte Carlo calculation of the speed distribution from gases with translational temperatures of 5, 100, and 300 K, respectively. At 5 K, which is achievable by a pulsed expansion of the gas, the agreement between the analytical and the Monte Carlo calculation is quantitative. Even at 300 K, the obtained velocity distribution has indications of each of the main features of the differential cross section. We conclude that the AX, BC gas mixture must be cooled to extract detailed information about the differential cross section. If the temperature of the AX, BC gas mixture is known, however, it may be possible to extract the overall form of the differential cross section by deconvolution provided that the signal-to-noise ratio is high and the form of the differential cross section is smooth.

3.2. Sensitivity to the angular momentum anisotropy of AB

Almost all methods available to measure velocity distributions, such as sub-Doppler laser-induced fluorescence (LIF), resonance-enhanced multiphoton ionization (REMPI), and time-of-flight mass spec-

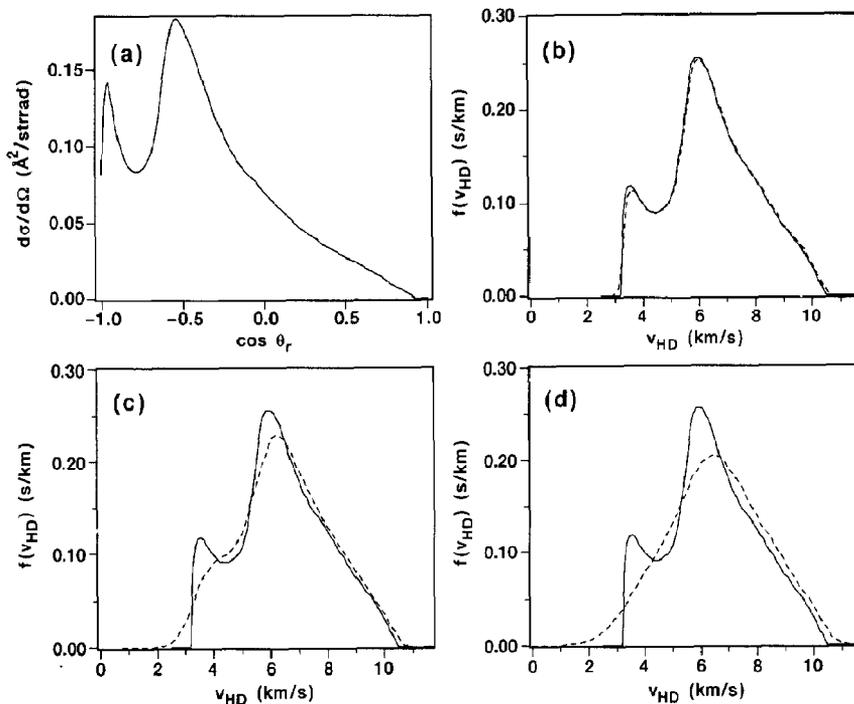


Fig. 2. A comparison of the speed distributions obtained from eq. (10) and from Monte Carlo calculations of HD molecules formed from the state-to-state photoinitiated bulb reaction sequence $\text{DI} + h\nu \rightarrow \text{D} + \text{I}$, followed by $\text{D} + \text{H}_2(v=1, J=1) \rightarrow \text{HD}(v'=1, J'=7) + \text{D}$, assuming 1.0 eV of collisional energy. The form of the differential cross section used is that calculated by Kuppermann and Wu [27] (see their fig. 5c) and is shown in (a). The dotted lines are the results of the Monte Carlo calculation for DI, H_2 translational temperatures of (b) 5 K, (c) 100 K, and (d) 300 K, which should be compared to the solid line which is the result of calculating from eq. (10) the HD speed distribution for a stationary DI, H_2 gas mixture.

trometry (TOF/MS) are also sensitive to the alignment of the AB product [28,29]. A complete discussion of the correlated velocity and angular momentum distributions is beyond the scope of this Letter, and we will consider it elsewhere. We emphasize that such effects are interesting and must be considered to obtain differential cross sections from photoinitiated bulb experiment.

4. Conclusions

For a favorable choice of masses, the full differential cross section of a state-to-state chemical reaction $\text{A} + \text{BC} \rightarrow \text{AB} + \text{C}$ can be extracted from a photoinitiated bulb experiment in which the A atom is generated with a known speed and angular distribution, and the velocity distribution of a given state

of the AB product is measured. This analysis suggests the design of a new generation of experiments that provide high-resolution, state-to-state differential cross sections for a variety of elementary chemical reactions.

Acknowledgement

We thank A. Kuppermann for providing us with calculations of the form of the differential cross section for $\text{D} + \text{H}_2(v=1, J=1) \rightarrow \text{HD}(v'=1, J'=7) + \text{H}$ at a collision energy of 1.0 eV prior to publication. WRS thanks the National Science Foundation for a predoctoral fellowship. This work is supported by the National Science Foundation under grant number NSF CHE 89-21198.

Appendix: Derivation of the relationship between the distribution of product velocities and the differential cross section

In this Appendix we calculate the velocity distribution of product molecules from a state-to-state photoinitiated bulb reaction with stationary reactants. To solve for the velocity distribution of the AB product of a state-to-state photoinitiated bulb experiment, we first review the kinematic constraints of conservation of energy and momentum:

$$\frac{1}{2}\mu v_r^2 + E = \frac{1}{2}\mu' v_r'^2 + E' + \Delta D \quad (\text{A.1})$$

and

$$m_A v_A + m_{BC} v_{BC} = m_{AB} v_{AB} + m_C v_C, \quad (\text{A.2})$$

where

$$v_r = v_A - v_{BC} \quad (\text{A.3})$$

and

$$v_r' = v_{AB} - v_C. \quad (\text{A.4})$$

Here E and E' refer to the internal energy of the reactants and products respectively, and ΔD is the difference in potential energy between the ground state products and ground state reactants. We have used the convention that the direction of the relative velocity of the reactants is given by the velocity of the slower reactant subtracted from the velocity of the faster reactant. The relative velocity of the products is defined as the velocity of the unobserved product subtracted from the velocity of the observed product.

Because the gas is assumed to be stationary, $v_{BC} = 0$, and eq. (A.2) can be rewritten as eq. (5) in section 2, where

$$\mathbf{u} = \left(\frac{m_A}{M} \right) v_A \quad (\text{A.5})$$

is the velocity of the center of mass, and

$$\mathbf{u}_{AB} = \left(\frac{m_C}{M} \right) v_r' \quad (\text{A.6})$$

is the velocity of AB in the center-of-mass frame. The magnitude of the velocity of the center of mass and of the velocity of AB in the center-of-mass frame are given by eqs. (7) and (4) of section 2, respectively.

In eqs. (A.5), (A.6) and (4) and (7) from section 2, $M = m_A + m_{BC}$ and $\Delta E = E' + \Delta D - E$. Eq. (7) of section 2 implies that the center-of-mass speed takes on a fixed value, i.e. the distribution of center-of-mass speeds is a delta function. From eq. (A.5) we know $\hat{v}_A = \hat{u}$, which implies that the anisotropy of the distribution in center-of-mass velocities will be identical to that of the photofragments. The complete distribution function of the center-of-mass velocities is therefore given by

$$g(\mathbf{u}') = \frac{\delta(u' - u)}{u^2} \frac{1 + \beta P_2(\hat{u}' \cdot \hat{\epsilon})}{4\pi}. \quad (\text{A.7})$$

Eq. (4) of section 2 implies that the speed of the AB product in the center-of-mass frame takes on a fixed value. By definition, the differential cross section gives the angular distribution of the product in the center-of-mass frame. The complete distribution function of the velocity of the AB product in the center-of-mass frame is therefore

$$h(\mathbf{u}'_{AB}) = \frac{\delta(u'_{AB} - u_{AB})}{u_{AB}^2} \frac{1}{\sigma} \frac{d\sigma}{d\Omega}, \quad (\text{A.8})$$

with $d\sigma/d\Omega$ evaluated at $\hat{u}'_{AB} \cdot \hat{u}'$. By convoluting eqs. (A.7) and (A.8), we obtain the velocity distribution of the AB product in the laboratory frame,

$$\begin{aligned} f(v_{AB}) &= \int d\mathbf{u}' \int d\mathbf{u}'_{AB} g(\mathbf{u}') \\ &\quad \times h(\mathbf{u}'_{AB}) \delta^3(v_{AB} - \mathbf{u}' - \mathbf{u}'_{AB}) \\ &= \int d\mathbf{u}' g(\mathbf{u}') h(v_{AB} - \mathbf{u}') \\ &= \int u'^2 du' d(\hat{u}' \cdot \hat{v}_{AB}) d\phi_{u'} g(\mathbf{u}') h(v_{AB} - \mathbf{u}'). \end{aligned} \quad (\text{A.9})$$

In eq. (A.9) we have chosen to integrate over the variable \mathbf{u}' in a spherical coordinate system in which the z axis is chosen to be parallel to \hat{v}_{AB} . To evaluate the integral of eq. (A.9) we express the distribution functions g and h in terms of this coordinate system.

We may use the spherical harmonic addition theorem [30] to rewrite eq. (A.7) as

$$g(\mathbf{u}') = \frac{\delta(u' - u)}{4\pi u'^2} \times \left(1 + \frac{4}{3}\pi\beta \sum_{m=-2}^2 Y_{2m}^*(\theta_{u'}, \phi_{u'}) Y_{2m}(\theta_\epsilon, \phi_\epsilon) \right), \quad (\text{A.10})$$

where $\theta_{u'}$ and $\phi_{u'}$ are the coordinates of \hat{u}' and θ_ϵ and ϕ_ϵ are the coordinates of $\hat{\epsilon}$ in a spherical coordinate system with $\hat{z} = \hat{v}_{AB}$. To rewrite h in the v_{AB} coordinate system, we use the relationship

$$q(x)\delta(y(x)) = \sum_i q(x_i) \frac{\delta(x - x_i)}{|dy/dx|}, \quad (\text{A.11})$$

where

$$y(x_i) = 0, \quad (\text{A.12})$$

to obtain the expression

$$h(v_{AB} - u') = \frac{1}{u' v_{AB} v_{AB}} \delta\left(\frac{v_{AB}^2 + u'^2 - u_{AB}^2}{2u'v_{AB}} - \hat{u}' \cdot \hat{v}_{AB}\right) \times \frac{1}{\sigma} \frac{d\sigma}{d\Omega} \frac{v_{AB}^2 - u'^2 - u_{AB}^2}{2u'v_{AB}}. \quad (\text{A.13})$$

The integral that results from substituting the forms of $g(\mathbf{u}')$ and $h(\mathbf{u}'_{AB})$ given by eqs. (A.10) and (A.13) into eq. (A.9) can be evaluated in a straightforward manner to yield the laboratory frame velocity of the AB product given by eq. (10).

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