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A PROBABILITY DENSITY FUNCTION FOR REFLECTED BEAM MOLECULES

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16. Abstract

Some ten years ago Nocilla proposed a theoretical model for the angular distribution of reflected molecules which often, although not always, yields adequate descriptions of observed distributions. An improvement is obtained in the present paper through the use of a more flexible probability density function whose definition issues from an argument on the scattering of the random speeds generated in the reflection process. The theoretical distribution derived from it was put to task with four experimental point groupings, two of which could not be reproduced satisfactorily by the older approach. The results being encouraging, it seemed warranted to extend the work to include the determination of the aerodynamic force exerted by reflected molecules on an elemental surface.

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A PROBABILITY DENSITY FUNCTION FOR REFLECTED BEAM MOLECULES

SUMMARY

A speculative probability density function is constructed on the basis of what would be reasonably expected of the probabilities for the thermal speed components of molecules that are ejected from an elemental surface struck by a molecular beam. It contains five free parameters. Three combinations of them occur in the general distribution function derivable for molecules moving in the plane of incidence and render the law more adaptable than Nocilla's earlier version which provides only two. A proper choice of the parameter combinations will usually cause it to agree with measured distributions. Pertinent methods are developed, and four sample adaptations are described in some detail. To determine the five probability parameters themselves the number distribution in a second plane must be available and, in addition, the heat flux to the surface must be measured. Also one has to stipulate that all the incoming molecules and no others are ejected from the elemental surface. The pressure on it and the shear stress in it can then be numerically computed, so that the aerodynamic force acting on it is known insofar as it originates with the reflection process.

I. INTRODUCTION

A plentiful supply of documentation on the intensity flux measured in locally reflected molecule ensembles has long revealed the fact that the number of beam molecules returned in the several directions cannot always be described, as a simplest approach recommends, by a sphere touching the elemental surface impacted, when it would be proportional to the cosine of the angle made by an outgoing direction and the surface normal. The speeds of such molecules rarely obey a Maxwellian equilibrium distribution with perfect accommodation to the surface temperature (completely diffuse reflection*). Experimental work usually operates with a molecular beam generated in a high vacuum chamber and often counts only those molecules which leave in the plane of incidence.

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*The evidence for largely specular reflection seems more scanty still, if not virtually absent.

If the numbers observed in selected directions are graphically represented by proportionate lengths of radius vectors drawn from the point of impact (origin), the vector tips occasionally trace out a nearly circular curve. In the great majority of cases they point to a roughly elliptical ("lobular") shape which is often tilted toward the surface. The particular form suggested by a data set depends on the impacting material and on that impacted, on the surface structure and contamination, on the angle of incidence, and on the energy in the incident stream. A rather bewildering variety of forms ensues from these concurring conditions.

A molecular beam will be acting on a surface element when it is moving through a rarefied gas. The experimental evidence then indicates that the cosine law of reflection is not in general applicable in free flight and should not be employed as a matter of course in calculating the aerodynamic force attacking a vehicle in the uppermost reaches of the atmosphere.

Since in a beam every molecule possesses, in addition to its random speed components, a directed ("macroscopic" or "mass") velocity, it seems natural to conjecture that a similar mass velocity may also be present after reflection. In reference 1 Nocilla, who introduced that idea, was indeed able to approximate, in a satisfactory manner, many (but not all) of the experimental point arrays obtained by Hurlbut [2]. However, he was forced in several instances to postulate the reflected mass flow as approaching the surface element, instead of leaving it as would seem appropriate. This queer circumstance is apt to throw some doubt on the actual existence of a superimposed directed velocity after reflection.

A probability density function for reflected molecules, without leaning on that notion and yet without giving up Nocilla's accomplishments, can be constructed on the strength of two broad assumptions regarding the probabilities for the occurrence of the thermal (random) speed components ξ_1, ξ_2, ξ_3. Whether or not the function generated in this manner is a solution of Boltzmann's equation is left an open question; very likely it is not. But if it can reproduce many experimental point groupings, especially those not amenable to the interpretation of reference 1, as in fact it can, one may live with it. It may then be considered a bona fide semi-empirical approximation to a rigorous solution.

II. CONSTRUCTION OF THE FUNCTION

Since Nocilla was able to accommodate a number of experimental patterns, it stands to reason that the general form of his approximating expression is suitably chosen for obtaining closed curves such as are indicated by the observations. It seems therefore advisable to start out, as he does, with Maxwell's distribution function excluding, however, the mass flow terms. The probability of finding, in any given volume of physical space, a thermal velocity in the differential range

$$<\xi_i,\ \xi_i + d\xi_i> \quad (i = 1,2,3)$$

may then be written as

$$Ae^{-\kappa^2(\xi_1^2+\xi_2^2+\xi_3^2)}\, d\xi_1 d\xi_2 d\xi_3, \tag{1}$$

where A is a constant of proportionality, and

$$\kappa^2 = \frac{1}{2RT} \tag{2}$$

(R = specific gas constant; T = gas temperature). With completely diffuse reflection the molecular velocities are assumed to have adapted to the surface ("wall") temperature: $T = T_w$. Expressions (1) and (2) then lead to the cosine law which cannot adequately describe the angular distribution of re-emitted beam molecules.

More specifically, the probability of finding a molecule with the ξ_1-component of the thermal velocity between a fixed value ξ_1 and $\xi_1 + d\xi_1$ emerges as

$$Ae^{-\kappa^2\xi_1^2}\, d\xi_1 \int_{-\infty}^{+\infty} e^{-\kappa^2\xi_2^2}\, d\xi_2 \int_{-\infty}^{+\infty} e^{-\kappa^2\xi_3^2}\, d\xi_3 = A\,\frac{\pi}{\kappa^2}\, e^{-\kappa^2\xi_1^2}\, d\xi_1.$$

The analogous probabilities for fixed components ξ_2 and ξ_3 are

$$A \frac{\pi}{\kappa^2} e^{-\kappa^2 \xi_2^2} d\xi_2, \quad A \frac{\pi}{\kappa^2} e^{-\kappa^2 \xi_3^2} d\xi_3.$$

With equal values of ξ_1, ξ_2, ξ_3, these probabilities are equal, a fact that characterizes purely diffuse reflection where κ^2 is a common constant. Clearly, one must relinquish this equality in beam reflection processes or, phrased differently, adaptation to wall temperature should no longer be upheld. Preserving the form of Maxwell's expression as far as possible one may define a probability density function as

$$A e^{-(\kappa_1^2 \xi_1^2 + \kappa_2^2 \xi_2^1 + \kappa_3^2 \xi_3^2)} \tag{3}$$

giving, for fixed values of ξ_1, ξ_2, ξ_3, the probabilities

$$A \frac{\pi}{\kappa_2 \kappa_3} e^{-\kappa_1^2 \xi_1^2} d\xi_1, \quad A \frac{\pi}{\kappa_3 \kappa_1} e^{-\kappa_2^2 \xi_2^2} d\xi_2, \quad A \frac{\pi}{\kappa_1 \kappa_2} e^{-\kappa_3^2 \xi_3^2} d\xi_3, \tag{4}$$

which, if the κ_i differ, are evidently not equal for equal values of the components.

For a still closer look at the reflection process we first introduce three physical axes x_1, x_2, x_3 parallel to the axes ξ_1, ξ_2, ξ_3 in velocity space and, following reference 1, define the beam as arriving in the (x_3,x_1)-plane, striking the elemental (x_1,x_2)-surface at the origin. Any thermal speed component, ξ_2, of the reflected molecules is normal to that plane and may be expected to be quite as probable as its negative counterpart, so that the second of the expressions (4) seems adequate. Not the same can be said a priori of the components ξ_1 and ξ_3. On the contrary, since some of the incoming molecules certainly will not dive into the surface, being repelled by the very first surface molecule they encounter, an initial irregularity in the distribution of these components arises which is likely to persist even if there are subsequent collisions among the reflected molecules.*

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*In such wall reflection modes, ξ_2 and $-\xi_2$ still may be considered equally likely to occur.

Obviously, this irregularity is brought about by something akin to specular reflection experienced by a certain fraction of the incoming molecules. To account for it and to achieve a difference required by it in the probabilities of oppositely equal components, two more probability parameters, λ_1 and λ_3, may be employed by writing, in analogy to the Maxwellian mass flow terms, $(\xi_1-\lambda_1)^2$ and $(\xi_3-\lambda_3)^2$ for ξ_1^2 and ξ_3^2 in the first and third of the expressions (4).* As a consequence, $\xi_1 = \lambda_1$ and $\xi_3 = \lambda_3$ rather than $\xi_1 = 0$ and $\xi_3 = 0$ are the most probable values of these components in the reflected gas.

The modified expression (4) can be set into still another form. The probability for a molecule to have any thermal speed is unity and can most readily be computed from the second formula (4):

$$1 = A \frac{\pi}{\kappa_3\kappa_1} \int_{-\infty}^{+\infty} e^{-\kappa_2^2\xi_2^2}\, d\xi_2 = A \frac{\pi^{3/2}}{\kappa_1\kappa_2\kappa_3} . \tag{5}$$

In removing the constant A from the set (4) we may write its modified form as

$$\frac{\kappa_1}{\sqrt{\pi}} e^{-\kappa_1^2(\xi_1-\lambda_1)^2}\, d\xi_1, \quad \frac{\kappa_2}{\sqrt{\pi}} e^{-\kappa_2^2\xi_2^2}\, d\xi_2, \quad \frac{\kappa_3}{\sqrt{\pi}} e^{-\kappa_3^2(\xi_3-\lambda_3)^2}\, d\xi_3. \tag{6}$$

It is useful to notice that

$$\kappa_i > 0, \tag{7}$$

as probabilities are positive quantities. With the method of reference 1 where

$$A = \frac{1}{(2\pi RT_r)^{3/2}}, \quad \kappa_i = \frac{1}{\sqrt{2RT_r}}$$

relation (5) is identically satisfied.

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[*] With surfaces far from smooth, one may be forced also to alter ξ_2^2 into $(\xi_2-\lambda_2)^2$.

The final expression for the density function proposed becomes

$$\frac{\kappa_1\kappa_2\kappa_3}{\pi^{3/2}}\, e^{-[\kappa_1^2(\xi_1-\lambda_1)^2+\kappa_2^2\xi_2^2+\kappa_3^2(\xi_3-\lambda_3)^2]}. \tag{8}$$

The probabilities (6) can be derived from it. With $\kappa_1 = \kappa_2 = \kappa_3$ the function (8) assumes the form adopted in reference (1) where the quantities λ_1 and λ_3 are indeed seen as the components of a reflected mean velocity lying in the (x_3,x_1)-plane. The physical oddity occasionally encountered with this view did not appear when the angular distribution law derivable from the function (8) was applied to four data plots selected more or less at random: the mass flow was always directed away from the elemental surface, even in two cases where it was approaching it in reference 1. Taking this as a general rule, one may at last interpret the modifiers λ_1 and λ_3 both ways: either as probability parameters or as mass flow components.

III. ANGULAR DISTRIBUTION OF REFLECTED MOLECULES

In deriving the reflection law it is advisable to use spherical coordinates in the velocity space with the point of impact at the origin and the (ξ_1,ξ_2)-plane coinciding with that of the elemental surface, i.e., with the (x_1,x_2)-plane. The azimuthal angle, or longitude, ϕ, is counted from the positive ξ_1-axis, running from zero to 2π. The co-latitude, θ, counted from the positive ξ_3-axis, varies between 0 and $\pi/2$ in reflection processes, from 0 to π in the reflected gas outside the surface. If v denotes the magnitude of the thermal speed,

$$\xi_1 = v \cos \phi \sin \theta$$

$$\xi_2 = v \sin \phi \sin \theta$$

$$\xi_3 = v \cos \theta$$

where v goes from zero to infinity. The exponential bracket in expression (8) assumes the form

$$a^2v^2 - 2bv + c^2 = (av - Q)^2 + c^2 - Q^2$$

with

$$\begin{cases} a^2 = (\kappa_1^2 \cos^2\phi + \kappa_2^2 \sin^2\phi) \sin^2\theta + \kappa_3^2 \cos^2\theta \\ b = \kappa_1^2\lambda_1 \cos\phi \sin\theta + \kappa_3^2\lambda_3 \cos\theta \\ c^2 = \kappa_1^2\lambda_1^2 + \kappa_3^2\lambda_3^2 \\ Q = \frac{b}{a}\,. \end{cases} \tag{9}$$

If dS denotes the area of the elemental surface and n_r is the number density in the reflected gas, there will be

$$n_r \, dS \, v \cos\theta \, dt$$

molecules of a given speed component ξ_3 returned by the surface during the time differential dt.

The volume element in spherical coordinates being

$$v^2 dv \sin\theta \, d\theta \, d\phi \equiv v^2 \, dv \, d\Omega,$$

the total number of molecules reflected in dt seconds in the direction of the solid angle $d\Omega$ is then indicated by the expression

$$n_r \frac{\kappa_1\kappa_2\kappa_3}{\pi^{3/2}} \, dS \cos\theta \, dt \, d\Omega \, e^{Q^2-c^2} \int_0^\infty e^{-(av-Q)^2} v^3 dv \tag{10}$$

where the probability density function (8) has been employed. The evaluation of the improper integral (and others of its kind) can be carried out with the aid of reference 3, where a list of basic such quadratures is supplied on p. 195/196. One finds its value as

$$\frac{1}{2a^4} \left[(1+Q^2)e^{-Q^2} + Q\sqrt{\pi}\left(\frac{3}{2} + Q^2\right)(1 + \operatorname{erf} Q)\right]. \tag{11}$$

The number (10) and therefore the intensity of the molecular flux in the elemental solid angle $d\Omega$ is thus proportional to

$$\frac{\cos\theta}{a^4} \left[(1+Q^2) + Q\sqrt{\pi}\left(\frac{3}{2} + Q^2\right)(1 + \operatorname{erf} Q)e^{Q^2}\right] \tag{12}$$

where

$$\operatorname{erf} Q = \frac{2}{\sqrt{\pi}} \int_0^Q e^{-x^2}\, dx.$$

Note that by the system (9) a^2 depends both on $\emptyset$ and θ while e^{-c^2} is a constant which may be taken into the factor of proportionality.

In order to examine the relationship of expressions (10) and (12) with the corresponding results of reference 1, we remark at first that there we have

$$\kappa_1^2 = \kappa_2^2 = \kappa_3^2 \equiv \kappa^2 = \frac{1}{2RT_r} . \tag{13}$$

It follows that

$$a^2 = \kappa^2, \qquad b^2 = \kappa^4(\lambda_1 \cos \emptyset \sin \theta + \lambda_3 \cos \theta)^2$$

$$Q = \frac{b}{a} = \kappa(\lambda_1 \cos \emptyset \sin \theta + \lambda_3 \cos \theta).$$

Formulas (13) and (16) of reference 1 show that Q is identical with the quantity X_r which, by the further expressions (14) and (2), is defined as

$$X_r = s_r(\sin \theta_r \cos \emptyset \sin \theta + \cos \theta_r \cos \theta)$$

with

$$s_r = \frac{U_r}{\sqrt{2RT_r}} = \kappa U_r .$$

Thus

$$\begin{cases} \lambda_1 = U_r \sin \theta_r \\ \lambda_3 = U_r \cos \theta_r , \end{cases} \tag{14}$$

so that λ_1 and λ_3 indeed emerge as the components of the postulated mass velocity U_r. Furthermore,

$$c^2 = \kappa_1^2 \lambda_1^2 + \kappa_3^2 \lambda_3^2 = \kappa^2 (\lambda_1^2 + \lambda_3^2) = \kappa^2 U_r^2 = s_r^2 . \tag{15}$$

By this relation and our formula (10) the factor $e^{-s_r^2}$ enters Nocilla's expression (13) for the intensity flux. The presence there of the denominator $\pi X(\sigma_r)$ can also be derived from the result (10). To show this is somewhat laborious and may be left to the reader if so minded.

The deviations from the relations of reference (1) center about the quantity a^2 which is no longer a constant, but has become a variable incorporated, e.g., in expression (12), both explicitly and implicitly (by way of Q^2). Experimental evidence is as a rule established in the plane of incidence where $\emptyset = 0$ (the incoming beam being located in the (x_3, x_1)-plane). A simplification ensues:

$$\begin{cases} a^2 = \kappa_1^2 \sin^2 \theta + \kappa_3^2 \cos^2 \theta \\ Q = \dfrac{\kappa_1^2 \lambda_1 \sin \theta + \kappa_3^2 \lambda_3 \cos \theta}{\sqrt{\kappa_1^2 \sin^2 \theta + \kappa_3^2 \cos^2 \theta}} . \end{cases} \tag{16}$$

The probability parameter κ_2 is absent now in a^2; it has no bearing on the return in the plane of incidence. The four remaining parameters can be reduced to essentially three:

$$\begin{cases} \delta = \dfrac{\kappa_1^2}{\kappa_3^2} - 1 \\ \bar{\mu}_1 = \kappa_3 \lambda_1 (\delta + 1) \\ \mu_3 = \kappa_3 \lambda_3 \end{cases} \tag{17}$$

which transform the set (16) into

$$\begin{cases} a^2 = \kappa_3^2(1 + \delta \cos^2\varphi) \\[2ex] Q = \dfrac{\bar{\mu}_1 \cos \varphi + \mu_3 \sin \varphi}{\sqrt{1 + \delta \cos^2\varphi}} \end{cases} \tag{18}$$

where at the same time the co-latitude θ has been replaced by the polar angle

$$\varphi = \frac{\pi}{2} - \theta \tag{19}$$

in the (x_3, x_1)-plane. The second coordinate in this plane, i.e., the radius vector, when ascribed a length proportional to the number of molecules returned in given directions, will enter into a relationship with φ which, on the strength of expressions (12) and (18), may be written as

$$L = \frac{\beta}{(1 + \delta \cos^2\varphi)^2} \left[(1+Q^2) + Q \sqrt{\pi} \left(\frac{3}{2} + Q^2\right)(1 + \operatorname{erf} Q) e^{Q^2}\right] \tag{20}$$

where Q is given in the set (18) and the constant $1/\kappa_3^4$ has been absorbed in the factor, β, of proportionality. The latter's magnitude is essentially determined by the scale chosen for plotting the measured flux data.

The function $L(\varphi)$ represents a general angular distribution law for molecules reflected in the plane of incidence. It is more flexible than the law proposed in reference 1 where the parameter δ always has the value zero. This can be seen by relations (13) and (17).

Similar but somewhat more complex laws can be written down when measurements are to be interpreted, made in planes $\emptyset = \emptyset_c \neq 0$, or, for that matter, in planes of constant co-latitude ($\theta = \theta_c$) where the longitude $\emptyset$ is variable rather than θ. A plane of the latter kind is considered in section V.

IV. CURVE ADAPTATION

To fit the curve $L(\varphi)$ to a plotted point set, suitable values must be found for the parameters β, δ, $\bar{\mu}_1$, μ_3 of which the last three are intimately interlocked in expression (20). As a consequence, the normal equations arising with the least square approach are unwieldy to a degree rendering the solution for the four parameters all but forbidding except perhaps with the use of high-speed computers (which was counterindicated for a number of reasons). Less precise, but better manageable, means were substituted for Gauss' method. The adaptations are therefore not the best obtainable. It is hoped, notwithstanding, that the four cases reported on later do suggest sufficient flexibility of the function $L(\varphi)$ in general, so that the probability density function from which it is derived recommends itself as a workable proposition.

The four specimens dealt with here, and many more of measured point arrays, permit us to locate, with some certainty, that particular point of the otherwise still unknown curve fit which is farthest away from the origin. Quantities related to that maximum of $L(\varphi)$ are denoted by an asterisk. The condition

$$\left.\frac{d(\log L)}{d\varphi}\right|_{\varphi=\varphi^*} = 0$$

takes the explicit form

$$(1 + 3\sin^2\varphi^*)\, W^{*2} + \mu_3 G^* \sin\varphi^* \cdot W^* - (Q^*G^*+4)\sin^2\varphi^* = 0 \qquad (21)$$

where, for any value of φ,

$$\begin{cases} W = \sqrt{1 + \delta \cos^2\varphi} \\[2ex] G = \dfrac{Q(5 + 2Q^2) + \sqrt{\pi}\,[\frac{3}{2} + Q^2(6 + 2Q^2)](1 + \operatorname{erf} Q)e^{Q^2}}{(1 + Q^2) + Q\sqrt{\pi}\,(\frac{3}{2} + Q^2)(1 + \operatorname{erf} Q)e^{Q^2}} \end{cases} . \qquad (22)$$

The function G depends on φ through the variable Q and has the form of a logarithmic differential quotient (the numerator being the Q-derivative of the denominator*). It grows beyond all bounds when $Q \to \infty$, but as can be shown with the use of the asymptotic expansion** of 1 - erf x, tends to zero when $Q \to -\infty$. Its values around Q = 0 are moderately large as appears from the following table.

TABLE I

The Function G in $|Q| \leqq 1$

Q	-1.0	-.9	-.8	-.7	-.6	-.5	-.4	-.3	-.2	-.1	0
G	1.897	1.959	2.024	2.092	2.163	2.237	2.314	2.395	2.479	2.567	2.659

Q	0	.1	.2	.3	.4	.5	.6	.7	.8	.9	1.0
G	2.659	2.754	2.853	2.955	3.061	3.171	3.285	3.482	3.523	3.467	3.775

The second differences being nearly equal in this row of G-values, the function can be approximated by the quadratic expression

$$G \approx 2.659 + 0.937 + 0.177\, Q^2$$

which in fact is not bad even somewhat beyond $|Q| = 1$.

---

[*] One observes that, curiously enough, the denominator itself, which is the bracket in expression (20), may be written as

$$\frac{\sqrt{\pi}}{8} \frac{d^3}{dQ^3} (1 + \text{erf } Q) e^{Q^2} .$$

Which advantages (if any) might be gained from this fact has not been explored yet.

[**] See, for example, reference 4, p. 24.

Suitable measures of φ^* and L^* can be read off the given point plot. If in addition tentative values are placed both on μ_3 and Q^*, the positive solution W^* of equation (21) defines the three parameters

$$\left\{\begin{aligned} \delta &= \frac{W^{*2} - 1}{\cos^2\varphi^*} \\ \bar{\mu}_1 &= \frac{Q^*W^* - \mu_3 \sin\varphi^*}{\cos\varphi^*}, \text{ and} \\ \beta &= \frac{L^*W^{*4}}{\sin\varphi^*[1 + Q^{*2} + Q^*\sqrt{\pi}\,(\frac{3}{2} + Q^*)(1 + \operatorname{erf} Q^*)e^{Q^{*2}}]} . \end{aligned}\right. \tag{23}$$

A table of the error function is supplied in reference 4, p. 24. The validity of the two guesses must be checked with further information to be drawn from the experimental evidence. After selecting two more points (φ,L), preferably far away from the curve's tip on both sides of it, one computes the two theoretical values (20) of L from φ and the above three parameters (μ_3 has been chosen beforehand). If they don't agree with the experimental lengths, one has to resort to different guesses. By diligently operating in this manner one should be able as a rule to reach satisfactory agreement. This trial and error procedure has been employed with the last two of our four examples (figures 3 and 4). It is surprising and gratifying that, merely using the maximum condition, the maximum length, and two further points, one is able to construct a rather well adapted curve, a fact that speaks for the suitability of the expression L.

The adaptation in figures 1 and 2 was attained in a somewhat different manner. The given points here permit an estimate of what the slope of the curves should be when they intersect with the vertical axis ($\varphi = \pi/2$). Since

$$\mu_3 = Q(\tfrac{\pi}{2}),$$

quantities related to that point will be identified by the subscript 3, so that, e.g., $Q(\pi/2) = Q_3$. One finds by straightforward differentiation that

$$\tan\chi_3 = -\left.\frac{d(\log L)}{d\varphi}\right|_{\varphi=\frac{\pi}{2}} = \bar{\mu}_1 G_3$$

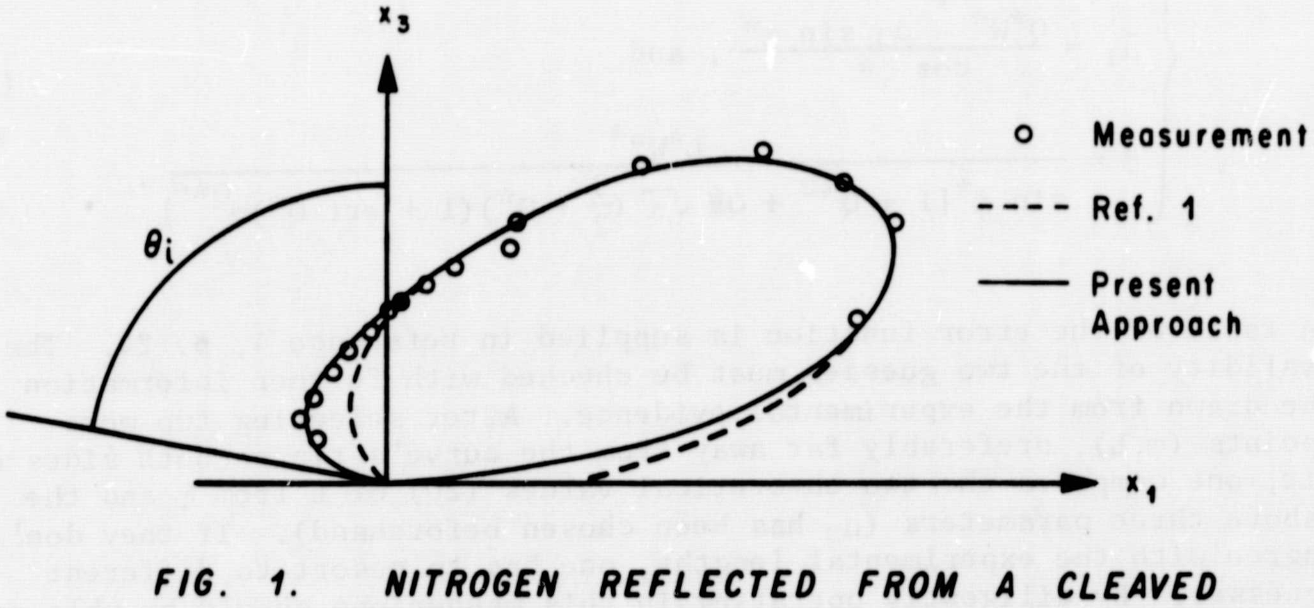

FIG. 1. NITROGEN REFLECTED FROM A CLEAVED LITHIUM FLUORIDE CRYSTAL. $\theta_i = -79.9°$

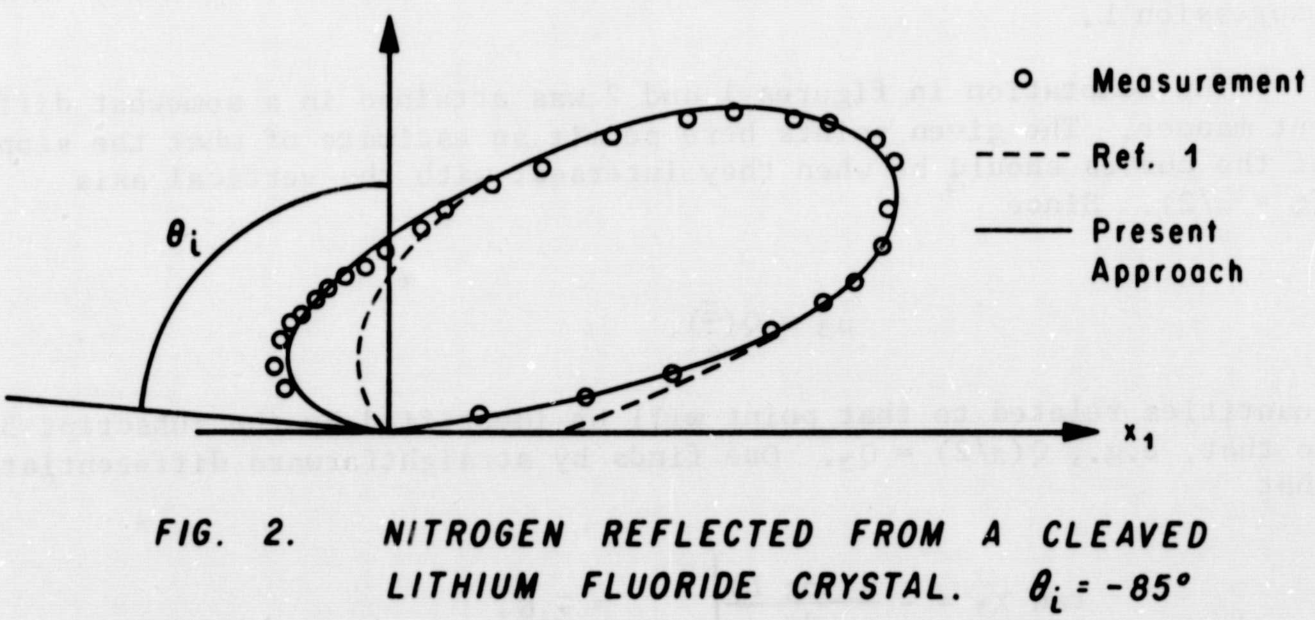

FIG. 2. NITROGEN REFLECTED FROM A CLEAVED LITHIUM FLUORIDE CRYSTAL. $\theta_i = -85°$

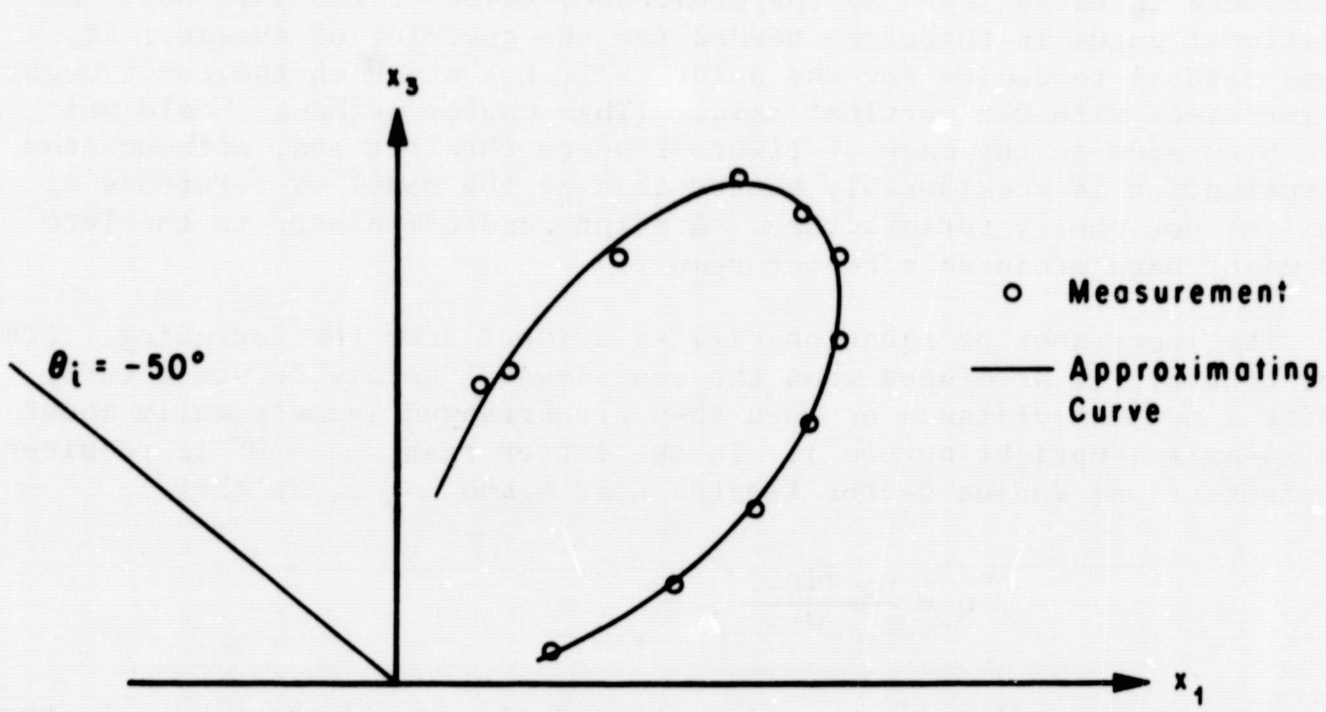

FIG. 3. ARGON SCATTERED FROM SILVER.
INCIDENT ENERGY = 0.064 eV

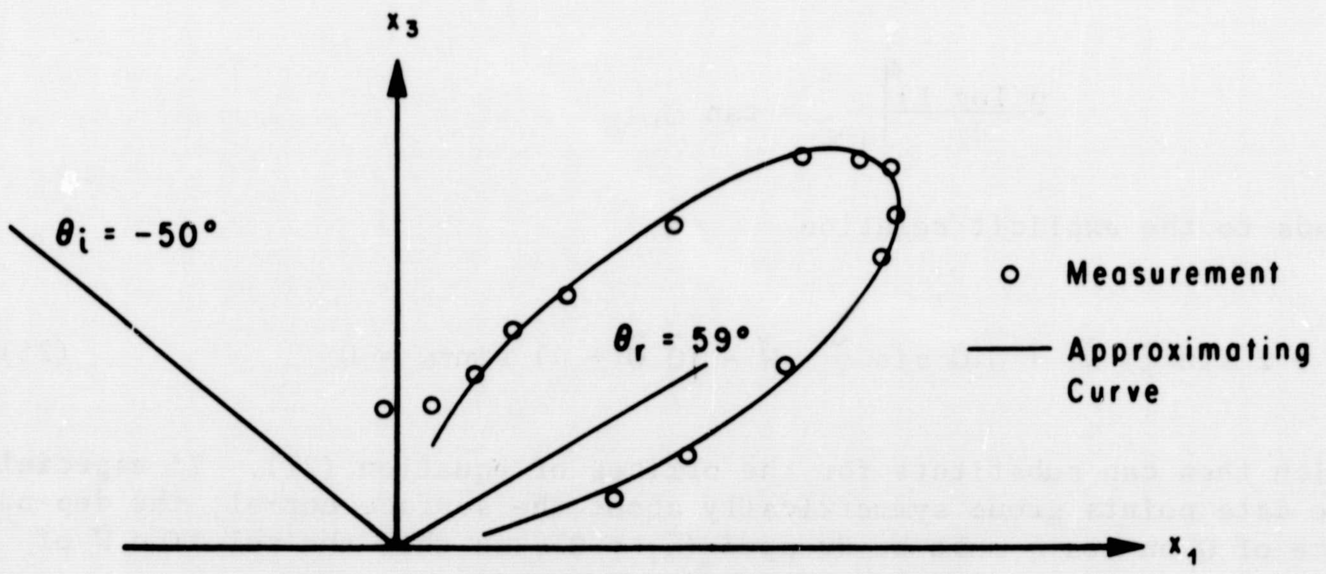

FIG. 4. ARGON SCATTERED FROM SILVER.
INCIDENT ENERGY = 4.35 eV

where χ_3 is the angle of inclination at $\varphi = \pi/2$. Thus a relation between parameters is established by the prescribed value of tan χ_3. Only one additional point is therefore needed for the checking of guesses; it seems natural to decide for the point $(\pi/2, L_3)$ at which the curve ought to intersect with the vertical axis. (This choice perhaps should not have been made in the case of figure 2 where the left end, although the approximation is considerably better than by the model of reference 1, still is not wholly satisfactory. A point read off nearer to the left end might have produced a better result.)

The importance of equation (21) is evident from the foregoing. Its use, however, is precluded when the experimental points do not clearly define a maximum distance or when they are arranged symmetrically about the x_3-axis ("upright curves"). In the latter case, $\bar{\mu}_1 = 0$* is required to ensure equal radius vector lengths L at φ and $\pi - \varphi$, so that

$$Q = \frac{\mu_3 \sin \varphi}{W} .$$

Since the maximum distance here is attained at $\varphi = \pi/2$ where $W^* = 1$, the value of Q related to it becomes $Q^* = \mu_3$. Equation (21) then reduces to the identity 0 = 0 and is rendered useless.

In such circumstances it may be feasible to operate with the location $(\tilde{\varphi}, \tilde{L})$ of a vertical tangent's point of contact. The general condition for infinite slope,

$$\left.\frac{d(\log L)}{d\varphi}\right|_{\varphi=\tilde{\varphi}} = \tan \tilde{\varphi},$$

leads to the explicit relation

$$(1 + 2 \sin^2\tilde{\varphi})\, \tilde{W}^2 + \mu_3\tilde{G} \sin \tilde{\varphi} \cdot \tilde{W} - (\tilde{Q}\, \tilde{G} + 4) \sin^2\tilde{\varphi} = 0 \tag{25}$$

which then can substitute for the offices of equation (21). If especially the data points group symmetrically about the surface normal, the dependence of Q on cos φ must be dropped $(\bar{\mu}_1 = 0)$, so that the solution $\tilde{W}$ of

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[*] By expressions (17) and (14) this is equivalent to $\theta_r = 0$ in reference 1.

equation (25) is the same whether the angle $\tilde{\varphi}$ is used or its supplement $\pi - \tilde{\varphi}$. It should indeed make no difference which one of the two vertical tangents one chooses to consider.

With upright curves there are but three unknown probability parameters (δ, μ_3, β). It is tempting to try $\delta = 0$ first (Nocilla's approach). With this provision,

$$\tilde{Q} = \mu_3 \sin \tilde{\varphi},$$

and relation (25) reduces to the equation

$$\mu_3 \tilde{G} = \frac{2 \sin^2 \tilde{\varphi} - 1}{\sin \tilde{\varphi} \cos^2 \tilde{\varphi}}$$

which can be solved directly for μ_3 because $\tilde{G}$ depends on $\tilde{Q}$ alone. The last remaining parameter, β, may be computed, e.g., from the axis length L^* associated with $\varphi^* = \pi/2$:

$$\beta = \frac{L^*}{(1 + \mu_3^2) + \mu_3 \sqrt{\pi}\, (\frac{3}{2} + \mu_3^2)(1 + \operatorname{erf} \mu_3) e^{\mu_3^2}},$$

as $Q^* = \mu_3$ with a symmetric setup. If the numerical values of μ_3 and β lead to the proper length $\tilde{L}$, the assumption $\delta = 0$ is justified. Otherwise, the more cumbersome trial and error procedure involving equation (25) must be initiated.

A spot check of equation (26) was made with the "upright" figure 13 of reference 1 which is characterized there by $\theta_r = 0$, $s_r = 1/2$. As $\lambda_1 = 0$ here, formulas (15) and (17) give

$$s_r^2 = \kappa_3^2 \lambda_3^2 = \mu_3^2,$$

so that $\mu_3 = 1/2$. The above equation is then satisfied with $\tilde{\varphi} = 56.5°$. The top distance of the figure, $L^* = 3$ cm, gives $\beta = 0.701$ and $\tilde{L} = 1.92$ cm. Inspection shows that the pair, $\tilde{\varphi}$, $\tilde{L}$ very nearly defines a point of infinite slope. As a consequence, curve (13) in reference 1 should be closely reproduced by the expression*

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*No such representations are given in the referenced article.

$$L = 0.701 \sin \varphi \left[1 + Q^2 + Q\sqrt{\pi}\left(\frac{3}{2} + Q^2\right)(1 + \operatorname{erf} Q)e^{Q^2}\right],$$

where

$$Q = \frac{1}{2} \sin \varphi.$$

All those curves of reference 1 that provide a satisfactory fit can be represented in a similar manner.* Our concern is with figures (17) and (18) where Hurlbut's [2] measurements are rather poorly approximated.** The results when applying the second method outlined above are depicted in our figures 1 and 2. Major assumptions and the four probability parameters are given in Table II.

TABLE II

Significant Quantities for Figures 1 and 2

	φ^*	L^*	tan χ_3	L_3	β	δ	$\bar{\mu}_1$	μ_3
Fig. 1	27°50'	7.4 cm	0.85	2.3 cm	0.398	-0.605	0.280	0.373
Fig. 2	27°50'	7.4 cm	0.724	2.5 cm	0.51	-0.605	0.243	0.324

The values in the last four columns specify the expressions (20) and (18) for L and Q so that the pertaining curves can be plotted. Several entries are equal, reflecting a general resemblance of the measured point arrays which are both obtained by shooting a molecular beam on cleaved lithium fluoride crystals. Merely the beam angles are somewhat different ($\theta_i = -79.9°$ and $\theta_i = -85°$, respectively). The almost glancing incidence is perhaps responsible for the strong inclination of the data "axis." As broadly indicated by the values of tan χ_3, it is even larger in the second case than in the first.

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* The not quite commendable adaptations in figures (15) and (16) are likely to improve with $\delta \neq 0$.

** One will notice that Nocilla's curve fits generally deteriorate with increasing "major axis" inclination which is particularly large in these two figures. From this observation it was inferred earlier that $\delta = 0$ might be a good guess with upright configurations.

By the value of δ we have

$$\frac{\kappa_1^2}{\kappa_3^2} \equiv \delta + 1 = 0.395$$

so that $\kappa_1 < \kappa_3$. Furthermore, expressions (17) and the result (7) show that λ_1 and λ_3 are both positive. As opposed to reference 1[*], the mass velocity, if one chooses to interpret the λ as their components (14), is directed away from the surface, since θ_r has to be an acute angle ($\tan \theta_r \approx 1.9$, or $\theta_r \approx 62.3°$ in both figures).

For further examination of the method two angular distributions were selected given in figures 4 and 5 of reference 5 (where the point connections shown no doubt have been drawn in with the use of french curves). Both depict argon scattering from silver.[**] Since a value of the angle χ_3 cannot be ascertained here, one has to employ the first of the methods sketched above. The results are given by our figures 3 and 4. The approximations are virtually as good as those by the empirical curves excepting two deviating points in the second example which could not be reproduced. The abrupt change in curvature they indicate is, however, a quite unusual feature attributable perhaps to some freakish surface peculiarity. Underlying numerical values are given in Table III.

TABLE III

Significant Quantities Related to Figures 3 and 4

	φ^*	L^*	φ_1	L_1	φ_2	L_2	β	δ	$\bar{\mu}_1$	μ_3
Fig. 3	50°	8.3 cm	30°	6.0 cm	70°	5.8 cm	0.362	2.13	2.5597	0
Fig. 4	38°	8.2 cm	20°	4.0 cm	60°	3.4 cm	0.003128	0	1.7268	1.03833

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[*] Here, θ_r is given as 120° in both cases.

[**] Since the angle of incidence is the same (50°), they demonstrate, incidentally, that the shape of the reflected curve depends on the incident energy (0.064 eV and 4.35 eV, respectively.) Unfortunately, free flight energies have not yet been realized experimentally. It is most desirable that future efforts correct for this deficiency.

The two zero values had suggested themselves in the course of the trial-and-error calculations. The first one entails that $\lambda_3 = 0$ while

$$\lambda_1 = \frac{\bar{\mu}_1}{\kappa_3(\delta + 1)}$$

remains a positive quantity, because $\kappa_3 > 0$ by the result (7). Thus, the numerator of the Q-expression contains the cosine term only. Its presence causes the shape to be tilted.

The second zero ($\delta = 0$) means that $\kappa_1 = \kappa_3$ and shows that Nocilla's approach would do nicely with the distribution of figure 4. Since $\bar{\mu}_1$ and μ_3 are both positive, the reflected mass flow again would turn away from the elemental surface. From the formulas (17) one sees that

$$\frac{\lambda_1}{\lambda_3} = \frac{\bar{\mu}_1}{\mu_3} = \tan \theta_r,$$

so that, with the last two figures in the lower row of Table III, the angle θ_r would be 59° equivalent to $\varphi_r = 31°$, while $\varphi^* = 38°$. Furthermore, relation (15) shows that, when $\delta = 0$,

$$s_r^2 = \kappa_3^2(\lambda_1^2 + \lambda_3^2) = \bar{\mu}_1^2 + \mu_3^2 = 4.06.$$

Owing perhaps to the slenderness of figure 4, the directed speed of the returned molecules thus is surprisingly high; it comes out more than twice as large as their most probable thermal speed, whereas in reference 1 the ratio was at most unity.

The above two methods proved to be the relatively most pliable of the many one can think of. All of them require four bits of information furnished by the raw data. For instance, one may consider the horizontal tangent, its point of contact and two more points, or, with tilted curves, two vertical tangents and their points of contact, or simply four points. Whenever possible, it seems advisable to include L* and the maximum condition (21).

V. THE PROBABILITY PARAMETERS

The function (20) can be expected to be adaptable to a large number of experimental point sets including all that can be handled by the method of reference 1. However, the numerical values it yields in a given case are too few to completely characterize the probability behavior (8) in the reflected gas.

In the first place, the three parameters (17) that can be elicited from data measured in the plane $\varnothing = 0$ evidently do not suffice for the determination of κ_1, κ_3, λ_1, λ_3. A hope to improve on the situation by additional observation in a vertical plane $\varnothing = \varnothing_c \neq 0$* or in a horizontal plane $\theta = \theta_c$ was found abortive. To illustrate this point let us look into the second case (where for good resolution we might choose $\theta_c = \theta^* = \frac{\pi}{2} - \varphi^*$). If

$$\epsilon = \frac{\kappa_2^2}{\kappa_1^2} - 1 \tag{27}$$

the first and last of the expressions (9) may be written as

$$\left\{\begin{aligned} a^2 &= \kappa_3^2[(\delta + 1)(1 + \epsilon \sin^2\varnothing) \sin^2\theta_c + \cos^2\theta_c] \\ Q &= \frac{\bar{\mu}_1 \cos \varnothing \sin \theta_c + \mu_3 \cos \theta_c}{\sqrt{(\delta + 1)(1 + \epsilon \sin^2\varnothing) \sin^2\theta_c + \cos^2\theta_c}} . \end{aligned}\right. \tag{28}$$

One gathers from the Q-formula where the parameter combinations $\bar{\mu}_1$ and μ_3 are already known that an approximation of the "horizontal" plot by $L(\varnothing)$ will not grant more than a value for $(1 + \epsilon)$ which like $(1 + \delta)$ is a ratio, to be sure, this time involving the parameter κ_2 for which so far no information was available.**

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*The symmetry existing about $\varnothing = 0$ with the random speed components ξ_2 and $-\xi_2$ taken as equally probable should lead to the same results when observing in $\varnothing = -\varnothing_c$. Otherwise, one would have to introduce the probability parameter λ_2; see footnote on p. 5.

**If a satisfactory value of ϵ cannot be determined, the ξ_2-probabilities are not equal on both sides of the plane of incidence and one must resort to $\lambda_2 \neq 0$. The set (9) then becomes more complicated.

When measurements in a plane $\emptyset = \emptyset_c$ are evaluated, the expression for Q also exhibits but one additional parameter configuration including κ_2. An analogous difficulty evolves with the approach of reference 1, in which $\delta = \epsilon = 0$ so that the expression (28) for Q is useless for parameter identification and the set (17) reduces to $\bar{\mu}_1 = \kappa\lambda_1$, $\mu_3 = \kappa\lambda_3$ leaving the three quantities κ, λ_1, λ_3 indeterminate.

To overcome the impasse we will first assume that all the gas molecules striking the elemental surface in dt seconds are re-emitted and that no others leave the surface. Let us further stipulate that the incoming gas obeys Maxwell's velocity distribution law with the superimposed macroscopic velocity components

$$V_1 = V_i \sin \theta_i$$

$$V_3 = V_i \cos \theta_i .$$

If n_i is the number density, we have the familiar expression

$$N_i dtdS = n_i \sqrt{\frac{RT_i}{2\pi}}\, dtdS \, [e^{-S_3^2} + \sqrt{\pi}\, S_3(1 + \text{erf } S_3)] \qquad (29)$$

where N_i is the number of molecules striking per unit time and area, T_i is the gas temperature, and

$$S_3 = \frac{V_3}{\sqrt{2RT_i}} .$$

With the aid of the probability function (8) the corresponding number, N_r, of molecules reflected per unit time and area becomes

$$N_r = n_r \frac{\kappa_1\kappa_2\kappa_3}{\pi^{3/2}} \int_{\xi_1=-\infty}^{+\infty} e^{-\kappa_1^2(\xi_1-\lambda_1)^2} d\xi_1 \int_{\xi_2=-\infty}^{+\infty} e^{-\kappa_2^2\xi_2^2} d\xi_2 \int_{\xi_3=0}^{\infty} \xi_3 e^{-\kappa_3^2} d\xi_3 ,$$

or

$$N_r = \frac{n_r}{2\sqrt{\pi}\,\kappa_3} [e^{-\mu_3^2} + \sqrt{\pi}\, \mu_3 \, (1 + \text{erf } \mu_3)] . \qquad (30)$$

Equating N_i and N_r yields the ratio

$$\frac{n_r}{\kappa_3} = n_i \sqrt{2RT_i} \; \frac{e^{-S_3^2} + \sqrt{\pi}\, S_3(1 + \text{erf } S_3)}{e^{-\mu_3^2} + \sqrt{\pi}\, \mu_3(1 + \text{erf } \mu_3)} \,, \tag{31}$$

which, n_r being unknown, still does not specify a value for κ_3. A further measurement obviously is called for. That of the heat flux

$$q = e_i - e_r \tag{32}$$

will be shown to supply the necessary information.

The internal portions of the energy fluxes follow from the internal energy associated with a single molecule which in reference 6, pp. 189/191 is given as*

$$\frac{1}{2}\,\frac{5 - 3\gamma}{\gamma - 1}\, mRT \tag{33}$$

where γ is the ratio of specific heats in the gas. While the incident temperature, T_i, can be taken as known, the temperature, T_r, in the reflected gas must be calculated from the mean translational energy in it:

$$\frac{m}{2}\,\frac{\kappa_1\kappa_2\kappa_3}{\pi^{3/2}} \iiint_{-\infty}^{+\infty} (\xi_1^2+\xi_2^2+\xi_3^2)\, e^{-[\kappa_1^2(\xi_1-\lambda_1)^2+\kappa_2^2\xi^2+\kappa_3^2(\xi_3-\lambda_3)^2]}\, d\xi_1 d\xi_2 d\xi_3 =$$

$$= \frac{m}{2}\left(\frac{1}{2\kappa_1^2} + \frac{1}{2\kappa_2^2} + \frac{1}{2\kappa_3^2} + \lambda_1^2 + \lambda_2^2\right).$$

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*It is written there as $\frac{3}{2}\, mRT\beta$, where $\beta = \frac{5 - 3\gamma}{3(\gamma - 1)}$.

The sum of the first three terms here is equal to the mean value of the squared random velocity, $3RT_r$, so that

$$RT_r = \frac{1}{6\kappa_1^2}\left(1 + \frac{\kappa_1^2}{\kappa_2^2} + \frac{\kappa_1^2}{\kappa_3^2}\right) = \frac{2 + \delta + (1 + \epsilon)^{-1}}{6\kappa_1^2} . \tag{34}$$

The internal portion of the reflected flux then becomes

$$(e_r)_{int.} = \frac{m}{12} N_i \frac{5 - 3\gamma}{\gamma - 1} \frac{2 + \delta + (1 + \epsilon)^{-1}}{\kappa_1^2} , \tag{35}$$

since the assumption $N_r = N_i$ was made. Everything is known at right excepting the quantity κ_1^2. Experimentation in a plane $\theta = \theta_c$ is needed to obtain a value for ϵ.

The translational energy flux of the re-emitted molecules follows from the integral expression

$$(e_r)_{tr.} = \frac{m}{2} n_r \frac{\kappa_1\kappa_2\kappa_3}{\pi^{3/2}} \iint_{-\infty}^{+\infty} \int_{\xi_3=0}^{\infty} \xi_3(\xi_1^2+\xi_2^2+\xi_3^2) e^{-[\kappa_1^2(\xi_1-\lambda_1)^2+\kappa_2^2\xi_2^2+\kappa_3^2(\xi_3-\lambda_3)^2]} \cdot d\xi_1 d\xi_2 d\xi_3 .$$

After some lengthy evaluation this becomes

$$(e_r)_{tr.} = \frac{m\, n_r}{4\sqrt{\pi}\,\kappa_3}\left\{\left(\frac{1}{2\kappa_1^2} + \frac{1}{2\kappa_2^2} + \frac{3}{2\kappa_3^2} + \lambda_1^2 + \lambda_3^2\right)\left[e^{-\mu_3^2} + \sqrt{\pi}\,\mu_3(1 + \operatorname{erf}\mu_3)\right] - \frac{1}{2\kappa_3^2} e^{-\mu_3^2}\right\} .$$

Since by the formulas (17)

$$\lambda_1^2 + \lambda_3^2 = \frac{\bar{\mu}_1^2}{\kappa_3^2(\delta + 1)^2} + \frac{\mu_3^2}{\kappa_3^2} ,$$

the expression may be set into the form

$$\left\{\begin{aligned} (e_r)_{tr.} &= \frac{m}{4\sqrt{\pi}} \frac{n_r}{\kappa_3 \kappa_1^2} P(\delta, \epsilon, \bar{\mu}_1, \mu_3), \text{ where} \\ P &= \left[\frac{4+3\delta+(1+\epsilon)^{-1}}{2} + \frac{\bar{\mu}_1^2}{\delta+1} + (\delta+1)\mu_3^2\right][e^{-\mu_3^2} + \sqrt{\pi}\,\mu_3(1+\text{erf } \mu_3)] - \frac{\delta+1}{2} e^{-\mu_3^2}. \end{aligned}\right. \tag{36}$$

Again κ_1^2 is the only unknown parameter, as n_r/κ_3 is available through relation (31). Thus, we may write

$$(e_r)_{tot.} = \frac{m}{4\kappa_1^2}\left[N_i \frac{5 - 3\gamma}{\gamma-1} \frac{2 + \delta + (1 + \epsilon)^{-1}}{3} + \frac{1}{\sqrt{\pi}} \frac{n_r}{\kappa_3} P\right].$$

By the quantity (33) and the known expression for the translational energy flux of the incident molecules, the total flux of incident energy becomes

$$(e_i)_{tot.} = \frac{N_i}{2} \frac{5 - 3\gamma}{\gamma-1} mRT_i + mN_i RT_i [(2+S^2)e^{-S_3^2} + \sqrt{\pi}\, S_3(\frac{5}{2} + S^2)(1 + \text{erf } S_3)]$$

where

$$S = \frac{V_i}{\sqrt{2RT_i}}$$

is the molecular speed ratio.

With the use of the measured heat (32) being transferred in unit time to the unit area, it follows that

$$\kappa_1^2 = \frac{1}{2RT_i} \frac{\frac{1}{2} \frac{5-3\gamma}{\gamma-1} \frac{2+\delta+(1+\epsilon)^{-1}}{3} + P[e^{-\mu_3^2} + \sqrt{\pi}\,\mu_3(1 + \text{erf } \mu_3)]^{-1}}{\frac{1}{2} \frac{5-3\gamma}{\gamma-1} + (2+S^2)e^{-S_3^2} + \sqrt{\pi}\, S_3(\frac{5}{2} + S^2)(1 + \text{erf } S_3) - q(mN_i RT_i)^{-1}}. \tag{37}$$

In cancelling N_i the aggregate

$$\frac{n_r}{\kappa_3} \frac{1}{N_i}$$

has been computed here from expressions (31) and (29). The first terms in the numerator and denominator vanish for monatomic gases (which have no internal degrees of freedom). The quantity κ_1^2 has a definite value even when $q = 0$, or is put equal to zero, as one might be tempted to do in default of a measurement.

The numerical values of the remaining four probability parameters are found from the definitions (19) and (27):

$$\kappa_2^2 = \kappa_1^2(1 + \epsilon) \qquad \lambda_1 = \frac{\mu_1}{\kappa_1 \sqrt{1 + \delta}}$$

$$\kappa_3^2 = \kappa_1^2(1 + \delta)^{-1} \qquad \lambda_3 = \frac{\mu_3 \sqrt{1 + \delta}}{\kappa_1} . \tag{38}$$

If one measures the molecular fluxes in a plane $\phi = \phi_c \neq 0$ rather than in a plane $\theta = \theta_c$ in order to arrive at an expression for κ_2, some quantity ϵ' will have to be defined instead of ϵ and the result (37) will assume a different form.

In concluding we recall that the energy accommodation coefficient

$$\alpha = \frac{q}{e_i - e_w}$$

can be determined from the measured value for q, provided that, when operating with polyatomic gases, the wall temperature, T_w, is known which enters through the quantity (33).

VI. RE-EMISSION STRESSES

To calculate the force vector issuing from the action of re-emitted molecules on the elemental surface let us first introduce the unit vectors $\underline{i}$, $\underline{j}$, $\underline{k}$ in direction of the axes x_1, x_2, x_3. The momentum of a single molecule,

$$m(\underline{i}\xi_1 + \underline{j}\xi_2 + \underline{k}\xi_3),$$

leads to the sum total of the momenta carried away from the unit surface in unit time:

$$mn_r \frac{\kappa_1\kappa_2\kappa_3}{\pi^{3/2}} \iint_{-\infty}^{+\infty} \int_{\xi_3=0}^{\infty} \xi_3(\underline{i}\xi_1+\underline{j}\xi_2+\underline{k}\xi_3)e^{-[\kappa_1^2(\xi_1-\lambda_1)^2+\kappa_2^2\xi_2^2+\kappa_3^2(\xi_3-\lambda_3)^2]}d\xi_1 d\xi_2 d\xi_3. \tag{39}$$

Its negative value gives the stresses acting on the surface.

Evaluation of the $\underline{i}$-component yields the shear stress in x_1-direction:

$$\tau_{1,r} = -\frac{mn_r\,\lambda_1}{2\sqrt{\pi}\,\kappa_3}\left[e^{-\mu_3^2} + \sqrt{\pi}\,\mu_3(1 + \text{erf}\,\mu_3)\right],$$

which, by virtue of relation (31), may be written as

$$\tau_{1,r} = -\lambda_1\, mn_i \sqrt{\frac{RT_i}{2\pi}}\left[e^{-S_3^2} + \sqrt{\pi}\,S_3(1 + \text{erf}\,S_3)\right] = -\frac{\lambda_1}{V_1}\tau_i \tag{40}$$

where τ_i is the incident stress.

There is no component in the x_2-direction (the integral vanishes):

$$\tau_{2,r} = 0. \tag{41}$$

This is a consequence of the assumption that ξ_2 and $-\xi_2$ are equally likely to occur which precludes the introduction of a probability parameter $\lambda_2 \neq 0$.

It was pointed out earlier that, with an "upright" data plot, the quantity $\bar{\mu}_1$, and therefore λ_1, must be taken as zero. In such an event, reflection does not generate a shear stress at all. Nor does incidence as a rule, because it should have to be vertical ($V_1 = 0$) for a symmetrical ejection pattern to appear.

Expression (40) is the total shear stress, τ_r, when $\lambda_2 = 0$. It has been derived with the use of the probability density function (8) and permits the computation of the accommodation coefficient

$$\sigma = 1 - \frac{\tau_r}{\tau_i} = 1 + \frac{\lambda_1}{V_1} . \tag{42}$$

The numerical value of λ_1 is available from the set (38); by the result (7) it is positive with the parameter $\bar{\mu}_1$ (which was found so in the four cases dealt with here and altogether might never turn out negative). The incident motion (assigned to the quadrant where $x_3 > 0$, $x_1 < 0$) defines θ_i and $V_1 = V_i \sin \theta$ as negative. The coefficient σ will then be smaller than unity.

The k-component of the integral (39) determines the pressure

$$p_r = - \frac{m}{2\sqrt{\pi}} \frac{n_r}{\kappa_3^2} [\mu_3 e^{-\mu_3^2} + \sqrt{\pi} (\frac{1}{2} + \mu_3^2)(1 + \operatorname{erf} \mu_3)] \tag{43}$$

which, being negative, is directed toward the backside of the elemental surface. By the ratio (31) and the set (38)

$$\frac{1}{2\sqrt{\pi}} \frac{n_r}{\kappa_3^2} = \frac{1 + \delta}{\kappa_1} n_i \sqrt{\frac{RT_i}{2\pi}} \frac{e^{-S_3^2} + \sqrt{\pi} S_3(1 + \operatorname{erf} S_3)}{e^{-\mu_3^2} + \sqrt{\pi} \mu_3(1 + \operatorname{erf} \mu_3)} \tag{43a}$$

where $\kappa_1(> 0)$ can be found from expression (37).

The pressure accommodation coefficient

$$\sigma' = \frac{p_i - p_r}{p_i - p_w}$$

which is sometimes recommended for use can be calculated when the wall temperature is known. The representation in terms of speeds, temperatures, and probability parameters is rather lengthy and is not set down here.

The aerodynamic force exerted by reflected molecules on the surface element,

$$\underline{f}_r = (\underline{i}\tau_r + \underline{k}p_r)\ dS, \tag{44}$$

can be resolved into lift and drag components (which refer to a system of coordinates usually different from that affixed to the element). In using expression (44), it should be kept in mind, however, that outgassing or ingassing must be held negligible* on account of the condition $N_r = N_i$ which was a mainstay in deriving major relations, and, secondly, that the basic observations were made with reflected molecules hardly subject to collisions with incoming molecules and not at all with those reflected by adjacent surface elements. The application therefore is restricted to free-molecule or nearly free-molecule flow until the probability parameters can be obtained in some manner not relying on such observations. Even if efforts in this direction should meet with insurmountable difficulties and must be given up as hopeless, free-molecule reflection, at any rate, is better described on the basis of the function (20) and proper experimental evidence than by the cosine law.

VII. CONCLUDING REMARKS

The tentative probability density function (8) gives rise to the angular number distribution law (20) whose analytic form is rather involved, so that the trial and error processes proposed for curve fitting purposes require lengthy computations often to be repeated many times. One may expect to end up with a somewhat more easily tractable expression of the law when the plane $\emptyset = 0$ in which most observations

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*There is an opinion that in free flight they would be so.

are made is considered the fundamental plane in a cylindrical (φ,r,y)-system into which the function (8) would have to be transformed. Carrying through that idea one indeed arrives at the slightly simpler representation

$$L = \frac{\beta' \sin \varphi}{(1 + \delta \cos^2\varphi)^{3/2}} \left[\frac{2}{\sqrt{\pi}} Q + (1 + 2Q^2)(1 + \text{erf } Q)e^{Q^2} \right] \tag{45}$$

where δ and Q again have the meanings (17) and (18). There is a certain connection to expression (20) in that the bracket there is the $\sqrt{\pi}/4$ multiple of the Q-derivative of the bracket here which, incidentally, may be written as

$$\frac{1}{2} \frac{d^2}{dQ^2} (1 + \text{erf } Q)e^{Q^2}.$$

The former bracket is essentially the third-order derivative as mentioned in the footnote on page 12. It is perhaps worthwhile to inquire more deeply into all these relationships; time did not permit doing this here.

Almost certainly the distribution law (45) will lead to satisfactory approximations of measurements performed in the plane of incidence to which it is geared. A spot check was made with the data presented in figure 13 of reference 1 which, as was explained in section IV, require $\delta = 0$, $\bar{\mu}_1 = 0$, and $\mu_3 = 1/2$. A close fit then ensues with $\beta' = 0.85$. The different analytic forms notwithstanding, both the laws (20) and (45) describe the measured angular distribution adequately with the use of the same probability parameters. They ought to do so, since they claim to interpret the behavior of the same reflected gas. The formal differences are probably brought about by the imprecise handling of infinitesimal volumes usually tolerated in dealing with molecular ensembles.

For a complete (and desirable) determination of all the probability parameters a survey in a second plane is needed. Moreover, the law (45) does not lend itself to an easy comparison with the theoretical results in Nocilla's paper which uses spherical coordinates. For these reasons, although set up first, it was abandoned in favor of the law (20).

REFERENCES

1. Nocilla, Silvio, The Surface Re-emission Law in Free Molecule Flow, Rarefied Gas Dynamics, ed. J. A. Laurmann, Acad. Press, New York, Vol. 1, 1963, pp. 327-346.

2. Hurlbut, F. C., RAND Rept. 339, 21-1 (June 1959).

3. Patterson, G. N., Molecular Flow of Gases, John Wiley and Sons, Inc., New York.

4. Jahnke, Eugene and Fritz Emde, Tables of Functions, 4th Edition, 1945, Dover Publications.

5. Romney and Anderson, "Scattering of 0.05-5eV Argon from the (111) Plane of Silver," Journal of Chemistry and Physics, Vol. 51, No. 6, September 1969.

6. Jeans, J. H., The Dynamical Theory of Gases, 4th Edition, Dover Publications.

APPROVAL

A PROBABILITY DENSITY FUNCTION FOR REFLECTED BEAM MOLECULES

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The information in this report has been reviewed for security classification. Review of any information concerning Department of Defense or Atomic Energy Commission programs has been made by the MSFC Security Classification Officer. This report, in its entirety, has been determined to be unclassified.

This document has also been reviewed and approved for technical accuracy.

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