On the Motion of Small Spheres in Gases

I. General Theory

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We have developed a global scattering kernel which describes the scattering of gas atoms by spherical particles which are small compared with a mean free path in the gas. The global kernel, which is analogous in many ways to the thermal neutron scattering kernel employed in neutron thermalization studies, is given in terms of the gas-surface scattering law for the particle. Thus the global kernel can be studied as a function of specular reflection and incomplete accommodation. The recent model of Kuščer and of Cercignani is used for the latter investigation and we find that on the average the angular distribution of the scattered gas atoms depends sensitively on the tangential momentum accommodation coefficient but only very weakly on the energy coefficient. However, the phenomenon is strongly dependent on the speed of the approaching gas atom and, for low speed gas atoms, the sensitivity to energy accommodation becomes much more important.

The net scattering rate is obtained and put in a form convenient for later calculations to be described in a series of companion papers.

1. Introduction

The motion in gases of spherical particles that are small compared with a mean free path has long been of scientific interest [1, 2]. A knowledge of the behaviour of such particles is required in, (1) the theory of aerosols (thermo-phoresis and diffusiophoresis), (2) the calculation of drag forces and heat transfer from satellites in the upper atmosphere, (3) the mobility of charged particles in neutral gases and (4) in the calculation of effective diffusion coefficients for the porous membranes employed in isotope separation.

In the past, these problems have been treated in an isolated manner with either none, or very little, of the common basic theory from which they stem, pointed out. It may be shown, however, that the evaluation of the physically interesting parameters of the problems mentioned above all depend upon a knowledge of the net collision rate of gas atoms with the surface of the particle. In this introductory paper, therefore, we consider the general problem of calculating the "global" scattering kernel [3] $\sigma(\boldsymbol{v}' \to \boldsymbol{v})$, directly from the experimentally available gas-surface kernel [4] $P(\boldsymbol{v}' \to \boldsymbol{v})$. To be more precise, $\sigma(\boldsymbol{v}' \to \boldsymbol{v})\, \mathrm{d}\boldsymbol{v}$ is the reaction rate for a gas atom of velocity $\boldsymbol{v}'$ striking the particle *anywhere* to be scattered from it with a new velocity in the range $(\boldsymbol{v}, \boldsymbol{v} + \mathrm{d}\boldsymbol{v})$. On the other hand, $P(\boldsymbol{v}' \to \boldsymbol{v})\, \mathrm{d}\boldsymbol{v}$ is the probability that a gas atom of velocity $\boldsymbol{v}'$ striking the sphere at a *particular* point S will be reflected from that point with velocity in the range $(\boldsymbol{v}, \boldsymbol{v} + \mathrm{d}\boldsymbol{v})$. From symmetry then $\sigma(\boldsymbol{v}' \to \boldsymbol{v})$ will depend only on v, v' and the angle between $\boldsymbol{v}$ and $\boldsymbol{v}'$; this is in contrast to $P(\boldsymbol{v}' \to \boldsymbol{v})$ which depends upon the angles made by $\boldsymbol{v}$ and $\boldsymbol{v}'$ with the surface normal.

Knowing $\sigma(\boldsymbol{v}' \to \boldsymbol{v})$ we can obtain the net collision rate and, in the subsequent part of this paper (II), we calculate the important integral parameters associated with the problems discussed above.

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2. The Global Scattering Kernel

The purpose of this section is to perform the purely geometrical calculation of averaging the gas-surface kernel over the surface of the sphere to obtain the physically, and analytically, more convenient global scattering kernel.

Figure 1 illustrates the situation. A molecule of velocity $\boldsymbol{v}'$ strikes the particle at point S and is reflected according to the law $P(\boldsymbol{v}' \to \boldsymbol{v})$ with velocity $\boldsymbol{v}$. The unit vector normal to the surface at S is $\boldsymbol{\varepsilon}$. The net scattering rate $(\partial f/\partial t)_{\text{coll}}$ is given by the difference between two terms,

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \left(\frac{\partial f}{\partial t}\right)_{\text{in}} - \left(\frac{\partial f}{\partial t}\right)_{\text{out}} . \qquad (1)$$

By considering Fig. 1 and integrating the flux of gas atoms over the surface of the sphere for both incident and reflected particles, we find that

$$(\partial f/\partial t)_{\text{out}} = -\int_{\boldsymbol{n}\cdot\boldsymbol{\varepsilon}<0} \boldsymbol{n}\cdot\boldsymbol{\varepsilon}\, \mathrm{d}S\, v\, f(\boldsymbol{v}, \boldsymbol{r}) \qquad (2)$$

and

$$(\partial f/\partial t)_{\text{out}} = -\int_{\boldsymbol{n}\cdot\boldsymbol{\varepsilon}<0} \boldsymbol{n}\cdot\boldsymbol{\varepsilon}\ \mathrm{d}S \int_{\boldsymbol{n}\cdot\boldsymbol{\varepsilon}<0} \boldsymbol{n}'\cdot\boldsymbol{\varepsilon} \cdot R(\boldsymbol{v}'\to\boldsymbol{v})\ v'\, f(\boldsymbol{v}',\boldsymbol{r}) \tag{3}$$

where $f(\boldsymbol{v},\boldsymbol{r})$ is the gas atom distribution function at the particle and we have set $\boldsymbol{v}'=\boldsymbol{n}'v'$, $\boldsymbol{v}=\boldsymbol{n}v$ and

$$\boldsymbol{\varepsilon}\cdot\boldsymbol{n}\, R(\boldsymbol{v}'\to\boldsymbol{v}) = P(\boldsymbol{v}'\to\boldsymbol{v}). \tag{4}$$

Combining Eqs. (1), (2) and (3), we find that

$$(\partial f/\partial t)_{\text{coll}} = -\int_{\boldsymbol{n}\cdot\boldsymbol{\varepsilon}<0} \boldsymbol{n}\cdot\boldsymbol{\varepsilon}\,\mathrm{d}S \int_{\boldsymbol{n}\cdot\boldsymbol{\varepsilon}<0} \boldsymbol{n}'\cdot\boldsymbol{\varepsilon} \cdot v'\, R(v',v\,|\,\boldsymbol{n}'\cdot\boldsymbol{\varepsilon}\,|\,\boldsymbol{n}\cdot\boldsymbol{\varepsilon}\,|\,\boldsymbol{n}'\cdot\boldsymbol{n}) \cdot f(\boldsymbol{v}',\boldsymbol{r})\ \mathrm{d}\boldsymbol{v}' + v\int_{\boldsymbol{n}\cdot\boldsymbol{\varepsilon}<0} \boldsymbol{n}\cdot\boldsymbol{\varepsilon}\,\mathrm{d}S\, f(\boldsymbol{v},\boldsymbol{r}) \tag{5}$$

where we have writen out the explicit dependence of $R(\ldots)$ on the various angles.

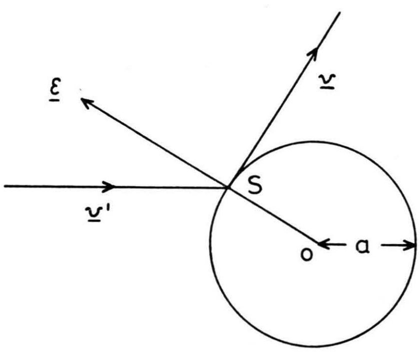

Fig. 1. S is a point on the surface of the sphere of radius a. The unit vector ε is normal to the surface at S.

Now in order to calculate $\sigma(\boldsymbol{v}'\to\boldsymbol{v})$ we can, without loss of generality, choose our system of axes such that $f(\boldsymbol{v},\boldsymbol{r}) = f(v,\boldsymbol{n}\cdot\boldsymbol{i},\boldsymbol{r})$ where $\boldsymbol{i}$ is a unit vector in the x-direction, where x is in the direction of the incident beam. This does not mean that our results for $\sigma(\boldsymbol{v}'\to\boldsymbol{v})$ will only be valid for one-dimensional problems, it merely exploits the assumed azimuthal symmetry of the scattering process. Thus, Eq. (5) becomes:

$$(\partial f/\partial t)_{\text{coll}} = -\int_{\boldsymbol{n}\cdot\boldsymbol{\varepsilon}<0} \boldsymbol{n}\cdot\boldsymbol{\varepsilon}\,\mathrm{d}S \int_{\boldsymbol{n}\cdot\boldsymbol{\varepsilon}<0} \boldsymbol{n}'\cdot\boldsymbol{\varepsilon} \cdot v'\, R(v',v\,|\,\boldsymbol{n}'\cdot\boldsymbol{\varepsilon}\ |\,\boldsymbol{n}\cdot\boldsymbol{\varepsilon}\,|\,\boldsymbol{n}'\cdot\boldsymbol{n}) \cdot f(v',\boldsymbol{n}'\cdot\boldsymbol{i},\boldsymbol{r}) + v\int_{\boldsymbol{n}\cdot\boldsymbol{\varepsilon}<0} \boldsymbol{n}\cdot\boldsymbol{\varepsilon}\,\mathrm{d}S\, f(v,\boldsymbol{n}\cdot\boldsymbol{i},\boldsymbol{r}). \tag{6}$$

However from the definition of $\sigma(\boldsymbol{v}'\to\boldsymbol{v})$ we see that the net collision rate can also be written as

$$(\partial f/\partial t)_{\text{coll}} = \int \mathrm{d}\boldsymbol{v}'\, f(v',\boldsymbol{n}'\cdot\boldsymbol{i},\boldsymbol{r})\ \sigma(\boldsymbol{v}'\to\boldsymbol{v}) - v\,\sigma\, f(v,\boldsymbol{n}\cdot\boldsymbol{i},\boldsymbol{r}). \tag{7}$$

Thus the problem is to identify $\sigma(\boldsymbol{v}'\to\boldsymbol{v})$ in Eq. (7) with the corresponding term in Equation (6).

2.1. *Some Special Models for Surface Scattering*

Before developing the general form of $\sigma(\boldsymbol{v}'\to\boldsymbol{v})$ from Eq. (6), we consider two special models of gas-surface interaction which are more conveniently dealt with by Eq. (6) in its present form. One of these is specular reflection [6], for which

$$\boldsymbol{n}\cdot\boldsymbol{\varepsilon}\, R(\ldots) = \frac{1}{v'^2}\,\delta(v'-v)\ \delta\big(\boldsymbol{n}'-\boldsymbol{n}+2\,\boldsymbol{\varepsilon}(\boldsymbol{\varepsilon}\cdot\boldsymbol{n})\big) \tag{8}$$

and the other backward reflection [4], where

$$\boldsymbol{n}\cdot\boldsymbol{\varepsilon}\, R(\ldots) = \frac{1}{v'^2}\,\delta(v'-v)\ \delta(\boldsymbol{n}'+\boldsymbol{n}). \tag{9}$$

Specular reflection needs no explanation; backward reflection is sometimes used as an approximation to very rough surfaces.

Noting that

$$\int_{\boldsymbol{n}\cdot\boldsymbol{\varepsilon}<0} \boldsymbol{n}\cdot\boldsymbol{\varepsilon}\,\mathrm{d}S\, f(v,\boldsymbol{n}\cdot\boldsymbol{i},\boldsymbol{r}) = -\int_{\boldsymbol{n}\cdot\boldsymbol{\varepsilon}<0} \boldsymbol{n}\cdot\boldsymbol{\varepsilon}\,\mathrm{d}S\, f(v,\boldsymbol{n}\cdot\boldsymbol{i},\boldsymbol{r}) \tag{10}$$

we find for specular reflection that

$$(\partial f/\partial t)_{\text{coll}} = v\int_{\boldsymbol{n}\cdot\boldsymbol{\varepsilon}<0} \boldsymbol{n}\cdot\boldsymbol{\varepsilon}\,\mathrm{d}S\{f(v,\boldsymbol{n}\cdot\boldsymbol{i} - 2(\boldsymbol{i}\cdot\boldsymbol{\varepsilon})(\boldsymbol{\varepsilon}\cdot\boldsymbol{n}),\boldsymbol{r}) - f(v,\boldsymbol{n}\cdot\boldsymbol{i},\boldsymbol{r})\} \tag{11}$$

and for backward reflection,

$$(\partial f/\partial t)_{\text{coll}} = v\int_{\boldsymbol{n}\cdot\boldsymbol{\varepsilon}<0} \boldsymbol{n}\cdot\boldsymbol{\varepsilon}\,\mathrm{d}S\{f(v,-\boldsymbol{n}\cdot\boldsymbol{i},\boldsymbol{r}) - f(v,\boldsymbol{n}\cdot\boldsymbol{i},\boldsymbol{r})\}. \tag{12}$$

By changing to polar coordinates and developing $f(v,\boldsymbol{n}\cdot\boldsymbol{i},\boldsymbol{r})$ in spherical harmonics, as follows,

$$f(v,\cos\vartheta,\boldsymbol{r}) = \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}\, f_l(v,\boldsymbol{r})\ P_l(\cos\vartheta) \tag{13}$$

it is not difficult to show that in the case of specular reflection

$$(\partial f/\partial t)_{\text{coll}} = \tfrac{1}{2}\,v\int_{-1}^{1}\mathrm{d}\mu'\, f(v,\mu',\boldsymbol{r}) - v\,\sigma\, f(v,\mu,\boldsymbol{r}) \tag{14}$$

where $\mu=\cos\vartheta=\boldsymbol{n}\cdot\boldsymbol{i}$.

For backward scattering, the net scattering rate becomes

$$(\partial f/\partial t)_{\text{coll}} = v\,\sigma\sum_{l=0}^{\infty}\frac{2l+1}{2}\,P_l(\mu)\,(-)^l\int_{-1}^{1}\mathrm{d}\mu' \cdot P_l(\mu')\, f(v,\mu',\boldsymbol{r}) - v\,\sigma\, f(v,\mu,\boldsymbol{r}). \tag{15}$$

Now to obtain $\sigma(\boldsymbol{v}' \to \boldsymbol{v})$ we expand as follows [4]

$$\sigma(\boldsymbol{v}' \to \boldsymbol{v}) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \sigma_l(v' \to v) \, P_l(\boldsymbol{n}' \cdot \boldsymbol{n}) . \quad (16)$$

Inserting Eqs. (13) and (16) into (17) and using the addition theorem for spherical harmonics we reduce Eq. (7) to

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\mu) \int_{-1}^{1} \mathrm{d}\mu' \, P_l(\mu') \cdot \int_0^{\infty} \mathrm{d}v' \, v'^2 \, \sigma_l(v' \to v) \, f(v', \mu', \boldsymbol{r}) - v\,\sigma\, f(v, \mu, \boldsymbol{r}) . \quad (17)$$

Comparing Eq. (14) with Eq. (17) we note that

$$\sigma_l(v' \to v) = (\sigma/v) \, \delta(v' - v) \, \delta_{l,0} \quad (18)$$

or

$$\sigma(\boldsymbol{v}' \to \boldsymbol{v}) = \frac{\sigma}{4\pi v} \delta(v' - v) . \quad (19)$$

Thus the scattering of molecules by a sphere which has a specular surface law is isotropic and elastic. This is not surprising since it is the basis of hard-sphere mechanics. On the other hand, for backward scattering, we obtained

$$\sigma_l(v' \to v) = (\sigma/v) \, (-)^l \, \delta(v' - v) \quad (20)$$

or

$$\sigma(\boldsymbol{v}' \to \boldsymbol{v}) = \delta(v' - v) \frac{\sigma}{2\pi v} \sum_{l=0}^{\infty} \frac{2l+1}{2} (-)^l \, P_l(\boldsymbol{n}' \cdot \boldsymbol{n}) . \quad (21)$$

Recognizing that $P_l(-1) = (-)^l$, we can sum Eq. (21), leading to

$$\sigma(\boldsymbol{v}' \to \boldsymbol{v}) = \frac{\sigma}{2\pi v} \delta(v' - v) \, \delta(\boldsymbol{n}' \cdot \boldsymbol{n} + 1) . \quad (22)$$

Thus backward surface reflection leads also to backward scattering for the global kernel $\sigma(\boldsymbol{v}' \to \boldsymbol{v})$.

Finally, we note that in both cases the total cross section σ, which is given by

$$\sigma = - \int_{\boldsymbol{n} \cdot \boldsymbol{\varepsilon} < 0} \boldsymbol{n} \cdot \boldsymbol{\varepsilon} \, \mathrm{d}S \quad (23)$$

is equal to πa^2 and independent of velocity. This is verified by calculating

$$v\,\sigma = \int \mathrm{d}\boldsymbol{v}' \, \sigma(\boldsymbol{v} \to \boldsymbol{v}') . \quad (24)$$

In fact it is easy to see for any form of $R(\ldots)$ that $\sigma = \pi a^2$.

2.2. General Expression for $\sigma(\boldsymbol{v}' \to \boldsymbol{v})$

Let us now consider the first term on the right hand side of Eq. (6) for a general kernel $R(\ldots)$. Inserting the expansion for f we find that we can write

$$- \sum_{l=0}^{\infty} \frac{2l+1}{2} \int_0^{\infty} \mathrm{d}v' \, v'^3 \int_{-1}^{1} \mathrm{d}\bar{\mu} \, P_l(\bar{\mu}) \, f(v', \bar{\mu}, \boldsymbol{r}) \cdot \int_{\boldsymbol{n} \cdot \boldsymbol{\varepsilon} < 0} \boldsymbol{n} \cdot \boldsymbol{\varepsilon} \, \mathrm{d}S \int_{\boldsymbol{n} \cdot \boldsymbol{\varepsilon} < 0} \mathrm{d}\boldsymbol{n}' \, \boldsymbol{n}' \cdot \boldsymbol{\varepsilon} \, R(v', v \,|\, \boldsymbol{n}' \cdot \boldsymbol{\varepsilon} \,|\, \boldsymbol{n} \cdot \boldsymbol{\varepsilon} \cdot |\, \boldsymbol{n}' \cdot \boldsymbol{n}) \, P_l(\boldsymbol{n}' \cdot \boldsymbol{i}) \quad (25)$$

where we have set $\mathrm{d}\boldsymbol{v}' = v'^2 \, \mathrm{d}v' \, \mathrm{d}\boldsymbol{n}'$.

Now considering the vector $\boldsymbol{n}'$ as arbitrary and using $\boldsymbol{n}$ as the reference direction we can write

$$\boldsymbol{n}' \cdot \boldsymbol{i} = (\boldsymbol{n} \cdot \boldsymbol{i}) \, (\boldsymbol{n}' \cdot \boldsymbol{n}) + [1 - (\boldsymbol{n} \cdot \boldsymbol{i})^2]^{1/2} \, [1 - (\boldsymbol{n}' \cdot \boldsymbol{n})^2]^{1/2} \cos(\varphi' - \varphi_i) \quad (26)$$

where φ' and φ_i are the azimuthal angles subtended by the projections of $\boldsymbol{n}'$ and $\boldsymbol{i}$ on the tangent plane at S in Figure 1. Using the addition theorem for spherical harmonics for $P_l(\boldsymbol{n}' \cdot \boldsymbol{i})$ and noting that f does not depend on the azimuthal angle φ_i, we can average the term (25) over $\varphi_i(0, 2\pi)$ to get

$$- \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\mu) \int_0^{\infty} \mathrm{d}v' \, v'^3 \int_{-1}^{1} \mathrm{d}\bar{\mu} \, P_l(\bar{\mu}) \, f(v', \bar{\mu}, \boldsymbol{r}) \cdot \int_{\boldsymbol{n} \cdot \boldsymbol{\varepsilon} < 0} \boldsymbol{n} \cdot \boldsymbol{\varepsilon} \, \mathrm{d}S \int_{\boldsymbol{n} \cdot \boldsymbol{\varepsilon} < 0} \mathrm{d}\boldsymbol{n}' \, \boldsymbol{n}' \cdot \boldsymbol{\varepsilon} \, P_l(\boldsymbol{n}' \cdot \boldsymbol{n}) \cdot R(v', v \,|\, \boldsymbol{n}' \cdot \boldsymbol{\varepsilon} \,|\, \boldsymbol{n} \cdot \boldsymbol{\varepsilon} \,|\, \boldsymbol{n}' \cdot \boldsymbol{n}) \quad (27)$$

Comparing (27) with the same term in Eq. (17), we find that

$$\sigma_l(v' \to v) = -v' \int_{\boldsymbol{n} \cdot \boldsymbol{\varepsilon} < 0} \boldsymbol{n} \cdot \boldsymbol{\varepsilon} \, \mathrm{d}S \int_{\boldsymbol{n} \cdot \boldsymbol{\varepsilon} < 0} \mathrm{d}\boldsymbol{n}' \, \boldsymbol{n}' \cdot \boldsymbol{\varepsilon} \cdot P_l(\boldsymbol{n}' \cdot \boldsymbol{n}) \, R(\ldots) . \quad (28)$$

To cast this in a more convenient form we write

$$P_l(\boldsymbol{n}' \cdot \boldsymbol{n}) \, R(\ldots \,|\, \boldsymbol{n}' \cdot \boldsymbol{n}) = \sum_{l'=0}^{\infty} \frac{2l'+1}{2} \cdot g_{ll'}(v', v \,|\, \boldsymbol{n}' \cdot \boldsymbol{\varepsilon} \,|\, \boldsymbol{n} \cdot \boldsymbol{\varepsilon}) \, P_{l'}(\boldsymbol{n}' \cdot \boldsymbol{n}) \quad (29)$$

from which

$$g_{ll'}(\ldots) = \int_{-1}^{1} P_{l'}(\mu_0) \, P_l(\mu_0) \, R(\ldots \,|\, \mu_0) \, \mathrm{d}\mu_0 . \quad (30)$$

Inserting (29) into (28) and changing to polar-coordinates we find that

$$\sigma_l(v' \to v) = -a^2 v \int_0^{2\pi} \mathrm{d}\varphi \int_0^1 \mu \, \mathrm{d}\mu \int_{-1}^{0} \mu' \, \mathrm{d}\mu' \int_0^{2\pi} \mathrm{d}\varphi' \cdot \sum_{l'=0}^{\infty} \frac{2l'+1}{2} g_{ll'}(v', v \,|\, \mu' \,|\, \mu) \, P_l(\boldsymbol{n}' \cdot \boldsymbol{n}) \quad (31)$$

where we have set $\boldsymbol{n}' \cdot \boldsymbol{\varepsilon} = \mu'$ and $\boldsymbol{n} \cdot \boldsymbol{\varepsilon} = \mu$.

Using the addition theorem of spherical harmonics and integrating over φ and φ' we finally obtain

$$\sigma_l(v' \to v) = 4\pi\sigma v' \sum_{l'=0}^{\infty} \frac{2l'+1}{2} (-)^{l'} \int_0^1 \mu \, d\mu \int_0^1 \mu' \, d\mu' \, P_{l'}(\mu) \, P_{l'}(\mu') \, g_{ll'}(v', v \mid -\mu' \mid \mu). \quad (32)$$

Thus given $R(\ldots)$, we may calculate $\sigma_l(v' \to v)$ quite readily.

As an example of our formalism, consider the case of diffuse reflection[6] for which

$$R(\ldots) = \frac{2}{\pi} \left(\frac{m}{2kT}\right)^2 v \exp\left\{-\frac{m v^2}{2kT}\right\}. \quad (33)$$

Then we find without difficulty that

$$\sigma_l(v' \to v) = 8\sigma \left(\frac{m}{2kT}\right)^2 v v' (-)^l \exp\left\{-\frac{m v^2}{2kT}\right\} \cdot \left\{\int_0^1 d\mu \, \mu \, P_l(\mu)\right\}^2. \quad (34)$$

Similarly, for Lambert's law[5] of scattering

$$R(\ldots) = \frac{1}{\pi v^2} \delta(v' - v) \quad (35)$$

we find

$$\sigma_l(v' \to v) = \frac{4\sigma}{v} (-)^l \delta(v' - v) \left\{\int_0^1 d\mu \, \mu \, P_l(\mu)\right\}^2. \quad (36)$$

Finally, we can apply our formalism to the synthetic surface kernel developed by KUŠČER et al.[7] and CERCIGNANI[8] (see also WILLIAMS[9]). In that case $R(\ldots)$ depends upon two arbitrary parameters Δ_0 and Δ both of which may be related to the various accommodation coefficients. The form of $R(\ldots)$ is

$$R(v', v \mid \mu' \mid \mu \mid \mu_0) = \frac{2}{\pi} \left(\frac{m}{2kT}\right)^2 \frac{v \, e^{c'^2}}{(1-\Delta^2)(1-\Delta_0^2)} \exp\left\{-\frac{(c^2+c'^2)}{1-\Delta_0^2}\right\} \exp\left\{-\frac{(\Delta^2-\Delta_0^2)}{(1-\Delta^2)(1-\Delta_0^2)} (c^2\mu^2 + c'^2\mu'^2)\right\} \cdot \exp\left\{-\frac{2\Delta_0}{1-\Delta_0^2} c c' \mu \mu'\right\} I_0\left(\frac{2\Delta}{1-\Delta^2} c c' \mu \mu'\right) \exp\left\{\frac{2\Delta_0}{1-\Delta_0^2} c c' \mu_0\right\} \quad (37)$$

where $c^2 = m v^2 / 2kT$ and $c'^2 = m v'^2 / 2kT$.

It is interesting to observe the detailed balance condition

$$v' e^{-c'^2} R(v', v \mid \mu' \mid \mu \mid \mu_0) = v \, e^{-c^2} R(v, v' \mid \mu \mid \mu' \mid \mu_0) \quad (38)$$

which is obeyed by this and indeed all kernels of physical interest.

Clearly, for $\Delta = \Delta_0 = 0$, this model reduces to that of Equation (33). KUŠČER et al.[7] have shown that Δ and Δ_0 are related to the conventional accommodation coefficients, the most convenient form for Δ^2 and $\Delta_0^2 \ll 1$ being that $(1 - \alpha_{\|}) = \Delta_0$ and $(1 - \alpha_{\perp}) \approx \Delta^2$ or $(1 - \alpha_{\mathrm{E}}) \approx \frac{1}{2} \Delta^2$. Here, $\alpha_{\|}$ and $\alpha_{\perp}$ are the tangential and normal occommodation coefficients, respectively, and α_{E} is the energy accommodation coefficient. This model will prove particularly useful since it indicates how the global kernel is influenced by the surface conditions of the spherical particle.

We have not been able to evaluate analytically any of the $\sigma_l(v' \to v)$ for the synthetic kernel in all its generality; however, we have considered the case when Δ and Δ_0 are small compared with unity. We have then expanded $R(\ldots)$ in powers of Δ_0 and Δ^2 [i. e. $(1 - \alpha_{\|})$ and $(1 - \alpha_{\mathrm{E}})$ small], and obtained

$$R(\ldots) \cong \frac{2}{\pi} \left(\frac{m}{2kT}\right)^2 v \, e^{-c^2} \{1 + 2\Delta_0 c c' (\mu_0 - \mu \mu') + \Delta^2 (c^2 \mu^2 - 1)(c'^2 \mu'^2 - 1)\}. \quad (39)$$

We then find from (32) that, with the abbreviation

$$T_{nl} = \int_0^1 d\mu \, \mu^n P_l(\mu),$$

$$\sigma_l(v' \to v) = 8\sigma v v' \left(\frac{m}{2kT}\right)^2 e^{-c^2} (-)^l \cdot \left(T_{1l}^2 + \Delta^2 \{T_{3l} c^2 - T_{1l}\} \{T_{3l} c'^2 - T_{1l}\} + 2\Delta_0 c c' \left\{T_{2l}^2 - \frac{l+1}{2l+1} T_{1,l+1}^2 - \frac{l}{2l+1} T_{1,l-1}^2\right\}\right). \quad (40)$$

Specifically,

$$\sigma_0(v' \to v) = 2\sigma v v' e^{-c^2} \left(\frac{m}{2kT}\right)^2 \cdot \{1 + \tfrac{1}{4} \Delta^2 (c^2 - 2)(c'^2 - 2)\} \quad (41)$$

and

$$\sigma_1(v' \to v) = -\frac{8}{9} \sigma v v' e^{-c^2} \left(\frac{m}{2kT}\right)^2 \cdot \left\{1 - \frac{9}{16} \Delta_0 c c' + \frac{9}{25} \Delta^2 (c^2 - \tfrac{5}{3})(c'^2 - \tfrac{5}{3})\right\}. \quad (42)$$

It is interesting to note that $\sigma_0(v' \to v)$ depends on the energy accommodation coefficient, whereas $\sigma_1(v' \to v)$ which is the dominant angular term, depends mainly on the tangential momentum accommodation coefficient. We shall see this effect in a more direct manner when the various physical problems are considered in later papers.

One final point to be noted is that $\sigma(\boldsymbol{v}' \to \boldsymbol{v})$ satisfies the detailed balance condition provided the particle surface temperature and the temperature of the equilibrium gas atom distribution function are the same, viz.:

$$e^{-m v'^2/2kT} \sigma(\boldsymbol{v}' \to \boldsymbol{v}) = e^{-m v^2/2kT} \sigma(\boldsymbol{v} \to \boldsymbol{v}').$$

This relation is not true, however, if the surface temperature of the sphere is different from the undisturbed gas. We shall see that this fact is of importance in calculations of heat transfer and drag.

3. Angular Distribution of Global Kernel

We have already seen from Eq. (19) that specular surface reflection leads to isotropic scattering for the global effect. Also, we observed that backward surface scattering led to backward global scattering. These are useful results which need no further discussion. On the other hand, the global kernel for diffuse scattering and Lambert's law [i. e. Eqs. (34) and (35)], both have the same angular distribution; although not the same energy spectrum. This is not surprising since they both assume a cosine re-emission law from the surface. It was not possible to sum analytically the $\sigma_l(v' \to v)$ for these two cases, but we have obtained the form of the scattering law by summing the series for $\sigma(\boldsymbol{v}' \to \boldsymbol{v})$ numerically. Thus we note that both diffuse and Lambert laws lead to a global scattering function whose angular part is proportional to

$$F(\mu_0) = \sum_{l=0}^{\infty} \frac{2l+1}{2} (-)^l T_{1,l}^2 P_l(\mu_0). \quad (43)$$

in the range $-1 \leqq \mu_0 \leqq 1$ where $\mu_0 = \cos \vartheta_0$, ϑ_0 being the angle between $\boldsymbol{v}'$ and $\boldsymbol{v}$.

It may be shown, using properties of spherical harmonics, that $T_{1,0} = \frac{1}{2}$, $T_{1,1} = \frac{1}{3}$, $T_{1,l} = 0$ for $l = 3, 5, 7, \ldots$ etc., and

$$T_{1,l} = \tfrac{1}{3} [\tfrac{3}{2} (\tfrac{3}{2} - 1)(\tfrac{3}{2} - 2) \ldots (\tfrac{3}{2} - \tfrac{1}{2} l)/(\tfrac{1}{2} l + 1)! \quad (44)$$

for $l = 2, 4, 6, 8$, etc.

With these matrix elements, (43) is summed and the result displayed in Figure 2. The marked backscattering is self-evident and, indeed, as we shall see below, the mean cosine of scattering is equal to $-4/9$, which corresponds to an average scattering angle of about 117°. Numerical values of $F(\mu_0)$ are given in Table 1.

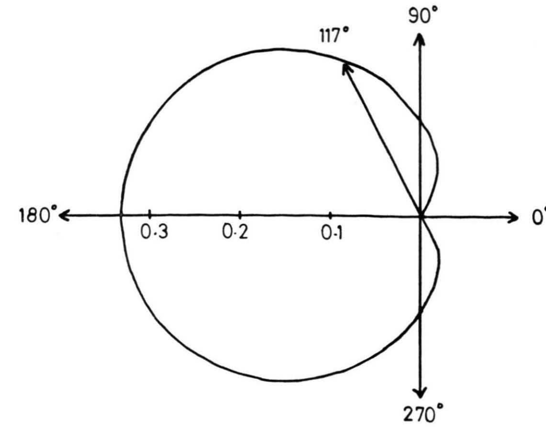

Fig. 2. The angular distribution of scattered atoms by a massive sphere which has a surface emission proportional to the cosine of the angle that the scattered atom makes with the normal.

Table 1. Numerical values of the angular distribution, F of atoms reflected from a diffusely scattering sphere.

μ_0	$F(\mu_0)$	μ_0	$F(\mu_0)$
−1.0	0.3333	0.1	0.08997
−0.9	0.3032	0.2	0.07490
−0.8	0.2757	0.3	0.06091
−0.7	0.2500	0.4	0.04805
−0.6	0.2258	0.5	0.03633
−0.5	0.2030	0.6	0.02585
−0.4	0.1814	0.7	0.01670
−0.3	0.1609	0.8	0.00904
−0.2	0.1416	0.9	0.00318
−0.1	0.1233	1.0	0.00000

We have seen that specular reflection leads to isotropic scattering and that a cosine reflection law from the surface leads to a marked anisotropy. The question that remains is, how does incomplete accommodation affect the result? This question may be answered for small values of Δ and Δ_0 by appealing to Equation (40). We have not summed this function, but a number of comments can be made by elementary considerations. Firstly we note that, contrary to the case of complete accommodation ($\Delta = \Delta_0 = 0$), the angular distribution is speed dependent and depends on the final and initial speeds of the gas atom. To assess this effect quantitatively we shall calculate the mean cosine of scattering [3]

$$\overline{\mu_0(v)} = \int \mathrm{d}\boldsymbol{v}' \, \boldsymbol{n} \cdot \boldsymbol{n}' \, \sigma(\boldsymbol{v} \to \boldsymbol{v}') \Big/ \int \mathrm{d}\boldsymbol{v}' \, \sigma(\boldsymbol{v} \to \boldsymbol{v}') \quad (45)$$

$$= \frac{1}{v\,\sigma} \int_0^{\infty} \mathrm{d}v' \, v'^2 \, \sigma_1(v \to v') \equiv v\,\sigma_1(v)/v\,\sigma \quad (46)$$

and its Maxwellian average

$$\langle \mu_0 \rangle = \int_0^\infty dv\, v^3\, \sigma_1(v)\, e^{-c^2} \Big/ \int_0^\infty dv\, v^3\, \sigma\, e^{-c^2}. \tag{47}$$

Inserting (42) to (46), we find that

$$\overline{\mu_0(v)} = -\frac{4}{9}\left\{1 - \frac{27\sqrt{\pi}}{64}\Delta_0 c + \frac{3\Delta^2}{25}\left(c^2 - \tfrac{5}{3}\right)\right\}. \tag{48}$$

This expression is not expected to be valid for c^2 greater than about 5 because of the limitations on the convergence of our expansion for R. Nevertheless, it gives a fairly accurate idea of the way in which gas atoms of different speeds are scattered. For example, at low speeds $c \to 0$, we see that

$$\overline{\mu_0(v)} \to -\frac{4}{9}\{1 - \tfrac{1}{5}\Delta^2\} \tag{49}$$

and therefore energy accommodation is the significant process in determining the direction of scattering from the sphere. The net effect is to make the scattering rather more isotropic than that predicted by complete accommodation. In contrast, for larger values of c the effect of incomplete accommodation causes the correction to $\overline{\mu_0(v)}$ to change sign and increase the anisotropy. However, because of the limitations on the value of c, this conclusion should not be considered definitive and it is likely that, for the general form of $R(\ldots)$, $\overline{\mu_0(\infty)}$ would tend to a finite value. A more convenient measure of the anisotropy is the Maxwellian average of $\overline{\mu_0(v)}$ as defined by Equation (47). Inserting (48) into (47) leads to

$$\langle \mu_0 \rangle = -\frac{4}{9}\left\{1 - \frac{81\,\pi}{256}\Delta_0 + \frac{1}{25}\Delta^2\right\}. \tag{50}$$

The factor $81\,\pi/256 = 0.994\ldots$ so that to a good approximation we may write Eq. (50) as

$$\langle \mu_0 \rangle = -\frac{4}{9}\{a_{\|} + 0.08(1 - a_{\mathrm{E}})\}. \tag{51}$$

From this formula we can conclude that the scattered intensity in a particular direction depends quite sensitively on the tangential momentum accommodation coefficient $a_{\|}$ but only weakly on the energy coefficient a_{E}. This is, of course, "on the average" because, as we have seen earlier, certain speed ranges are more sensitive to a_{E} than to $a_{\|}$.

The sensitivity of $\langle \mu_0 \rangle$ to $a_{\|}$ is not unexpected since reducing $a_{\|}$ tends to increase the pseudo-specular component in $R(\ldots)$. Indeed, if we considered $\langle \mu_0 \rangle$ for a mixture of specular and completely accommodated diffuse scattering, we should obtain

$$\langle \mu_0 \rangle = -\frac{4}{9} f \tag{52}$$

where $(1-f)$ is the fraction of collisions which lead to specular reflection. Thus $\langle \mu_0 \rangle$ varies from zero to $-4/9$ as $0 \leqq f \leqq 1$.

4. Conclusions and Discussion

We have developed a general method for calculating a global scattering kernel for gas atoms interacting with a small sphere with quite arbitrary surface conditions. The only limitation is that there are no polarization effects, i. e. the surface of the sphere has uniform properties. The form of this kernel has been obtained for a number of common gas-surface interaction laws and the angular distribution obtained. The effect of incomplete accommodation is studied and the various accommodation coefficients are found to have different influences on the scattered gas atom distribution.

The purpose of the study has been to obtain an expression for the net scattering rate in terms of a universal kernel, thereby obviating the need to recalculate the collision terms for different problems. The formulation so obtained is very similar to that encountered in neutron transport theory where neutrons collide with nuclei which, themselves, may be chemically bound or in thermal motion[3]. In our case, the surface law is analogous to the distribution of possible energy states that the struck nucleus can have. The power of our formulation will become evident in the following companion paper.

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