DISTRIBUTION OF DIFFUSING PARTICLES NEAR AN ABSORBING WALL

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On the basis of Boltzmann's kinetic equation we obtain and solve numerically the exact diffusion integral equation for the distribution of particles which is valid throughout the whole region of transition from macroscopic to kinetic description. It is shown that in spite of strong distortion of the angular part of the distribution function, the behavior of the density at the wall varies little by comparison with the diffusion distribution.

To describe the behavior of the particles in a neutral gas and plasma, the typical dimension L of which significantly exceeds the mean free path λ, a macroscopic diffusion equation [1] is usually used. But such equations are inappropriate in the boundary layers near the wall of thickness of the order of λ (Knudsen's λ-layer [2]), where the discrete structure of the medium becomes apparent. Strictly speaking, a kinetic description is necessary here. Similar problems in the transition from a macroscopic description in the internal region to a kinetic description in the boundary layers also occur in the theory of radiation transport in gases [3, 4].

The kinetic approach within the limits of the λ-layer is usually used to describe the fictitious macroscopic boundary conditions at the wall, for example, for the diffusion equation, the solution of which would coincide with the true solution outside the λ-layer to some degree of accuracy.

The simplest boundary condition for a plasma at the wall is Schottky's condition [5] $n_W = 0$, which was used to describe ambipolar diffusion. A similar condition was used by Tonks [6] to describe the diffusion of a plasma in a magnetic field. A more exact boundary condition, taking into account the finite ratio λ/L, was deduced by de Groot [7] and then, with a number of refinements, used by Fabrikant [8] in problems concerning radiation transport in a plasma and by Granovskii [9] to describe ionic diffusion in a positive column when there are electric fields.

But these boundary conditions, obtained in the diffusion approximation, are not exact because of the complete breakdown of the well-known criteria for the diffusion description in the neighborhood of the λ-layer. Hence, before discussing the applicability of these results when there are electric and magnetic fields, we have to obtain an answer to the fundamental question of the exactness of these boundary conditions for simple particle diffusion. To do this, we first discuss the pattern of the phenomena in the neighborhood of the λ-layer, and then, on the basis of Boltzmann's kinetic equation, we deduce and solve numerically the exact diffusion integral equation for the particle density and the particle distribution function which is valid throughout the whole transition region. Then we compare both solutions.

1. Boundary conditions and the Density Distribution in the Diffusion Approximation. We consider the simplest case of the two-dimensional stationary diffusion of particles against a fixed homogeneous background of scattering centers when there is an absorbing boundary at $x = 0$. When the flux is constant ($j(x) = -I$), the density distribution in the diffusion approximation has the form

$$n(x) = \frac{I}{D} x + n_w \tag{1.1}$$

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The boundary condition for n_w follows from the fact that the flux across the boundary of the λ-layer is equal to that at the wall, j_w [8].

The particle fluxes are usually computed by the mean free path method [1]. Its basis in Boltzmann's kinetic equation is given in the next section.

In the general case of linear or three-dimensional particle flight the directed fluxes have the form

$$j_{\pm} = \pm j_0 + {}^1/_2 j_D \qquad (j_D = -D dn/dx) \tag{1.2}$$

in which the random fluxes j_0 are, respectively, $(^1/_2)nv$ and $(^1/_4)nv$, and the diffusion coefficients are $D = \lambda v$ and $(^1/_3)\lambda v$.

It is easy to see that in this approximation the fluxes $j_{\pm}(x)$ are equal to the random fluxes at cross-sections at the distance of the mean free diffusion path λ_D (respectively, λ or $(2/3)\lambda$ [9]) from x.

By [8, 9] we can take the cross section $x = \lambda_D$ as the boundary of the λ-layer. Then, assuming the flux across this section is equal to the diffusion flux, while the flux at the wall, j_w, is directed, and ignoring the change in dn/dx over the length λ_D, at the wall we have

$$n_w = \lambda_D dn/dx \tag{1.3}$$

But, since, by the foregoing, $j_w = -j_0(\lambda_D)$, the above-mentioned matching of the fluxes is equivalent to saying that the fluxes j_0 and j_D are equal at the diffusion boundary $x = \lambda_D$, for which

$$n_\Gamma = 2\lambda_D dn/dx \tag{1.4}$$

Although (1.3) and (1.4) are equivalent in the linear approximation, as we shall see in the sequel, (1.4) more closely corresponds to the true situation since it holds at the boundary between two zones at a given distance from the wall.

Noting (1.3), (1.4), we can put (1.1) in the form

$$n^\circ(x) = 1 + \frac{x}{\lambda_D} \qquad \left(n^\circ = \frac{n}{n_w}\right) \tag{1.5}$$

Thus, in the neighborhood of the λ-layer the typical scale of the density is of the order of λ, the diffusion flux no longer being small by comparison with the random flux. The error thus committed can be determined only after comparing the distribution (1.5) with the exact kinetic solution.

2. The Kinetic Equation for the Particle Distribution in the Transition Layer. As we know [2], Boltzmann's equation

$$\frac{\partial f}{\partial t} + \mathbf{v}\frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m}\frac{\partial f}{\partial \mathbf{v}} = J_{st} \tag{2.1}$$

where

$$J_{st} = \iint (f' f_1' - f f_1) g\sigma(g, \vartheta)\, d\sigma d\mathbf{v}_1 = J_1 - f J_2$$

can be put in equivalent integral form. In the two-dimensional stationary case and in the absence of external forces, its solution has the form

$$f(x, \mathbf{v}) = f(x_0, \mathbf{v}) \exp\left\{-\frac{1}{v_x}\int_{x_0}^{x} J_2(x', \mathbf{v}) dx'\right\} + \frac{1}{v_x}\int_{x_0}^{x} J_1(x', \mathbf{v}) \exp\left\{-\frac{1}{v_x}\int_{x'}^{x} J_2(x'', \mathbf{v})\, dx''\right\} dx' \tag{2.2}$$

Here the initial cross section x_0 for $v_x < 0$ is taken to the left of x, while for $v_x < 0$ it is taken to the right. The above expression describes the obvious fact that the number of particles in a given velocity band v, dv at x is equal to the number of particles on the trajectory through x_0 (taking into account their decrease

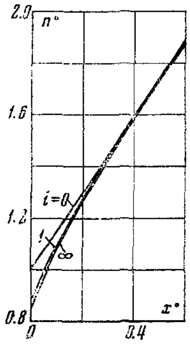

Fig. 1

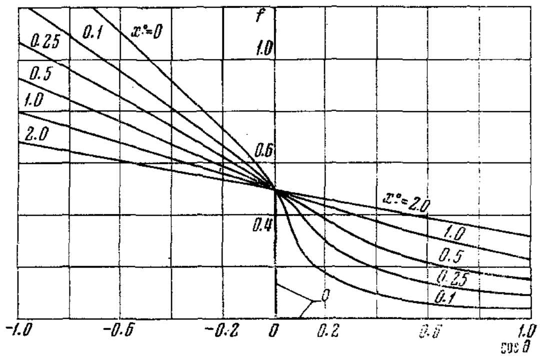

Fig. 2

due to collisions) plus those particles which entered it along the path and reached x without collision. If we take the cross section x_0 far from x, the first term in (2.2) drops out. Hence, in this case the form of the initial distribution function $f(x_0, v)$ is not significant because of the strong damping along the length.

For the sequel we actualize the form of the collision integral. Since by the foregoing the scattering centers are assumed to be fixed, the collision integral can be significantly simplified:

$$J_{st} = n_0 \int_o [f(\mathbf{v}') - f(\mathbf{v})] \, v\sigma(v, \vartheta) \, do \tag{2.3}$$

where n_0 is the density of the scattering centers.

The integral J_2 in (2.3) is found at once

$$J_2 = n_0 v \sigma_0 (v) = 1/\tau (v) \tag{2.4}$$

where $\sigma_0(v)$ is the complete scattering cross section.

Then the solution of (2.2) takes the form

$$f(x, \mathbf{v}) = \frac{1}{v_x} \int_{x_0}^{x} J_1(x', \mathbf{v}) \exp\left(-\frac{x - x'}{v_x \tau}\right) dx' \tag{2.5}$$

If we now multiply both sides of (2.5) by v_x and integrate with respect to v, we find the flux crossing the cross section x

$$j(x) = \int_{\mathbf{v}} \int_{x}^{x} J_1(x', \mathbf{v}) \exp\left(-\frac{x - x'}{v_x \tau}\right) dx' d\mathbf{v} \tag{2.6}$$

It is easy to see that (2.6) coincides with the expression obtained on the basis of the mean free path method [1], where

$$J_1(x', \mathbf{v}) = \frac{\chi(x', \mathbf{v})}{\tau}$$

In the general case the distribution function for the scattered particles $\chi(x', v)$ depends on their distribution before collision $f(x', v)$ and the actual form of the scattering cross section $\sigma(\vartheta)$. But for a cross section of elastic spheres, when the particles are scattered uniformly over the sphere $|v| = \text{const}$, the function $\chi(x', v)$ becomes isotropic and is determined by the average number of particles over the sphere. Hence,

$$J_1(x', \mathbf{v}) = \frac{1}{4\pi\tau} \int_o f(x', \mathbf{v}) \, do \tag{2.7}$$

Assuming further that the distribution of v is monoenergetic and integrating (2.5) with respect to v, we obtain an integral equation for the particle density of this group

$$n(x) = \frac{1}{4\pi} \int_{x_0}^{x} \int_{\Omega} n(x') \exp\left(-\frac{x-x'}{\lambda \cos\theta}\right) \frac{dx' d\Omega}{\lambda \cos\theta} \tag{2.8}$$

where θ is the angle between the velocity v and the X axis.

Having determined n(x), we can then find the angular distribution function

$$f(\Omega) = \frac{1}{n} \frac{dn}{d\Omega}$$

If λ is independent of v, Eq. (2.8) is also satisfied by the total particle density.

Then, integrating (2.8) with respect to Ω and transforming to dimensionless coordinates $x^c = x/\lambda$ and $z = |x-x'|/\lambda$, we reduce the equation to the form

$$n(x^\circ) = \frac{1}{2}\left[\int_0^{x^\circ} n(x^\circ - z) E_1(z)\, dz + \int_0^{\infty} n(x^\circ + z) E_1(z)\, dz\right] \tag{2.9}$$

where the kernel $E_1(z)$ is the exponential integral [4, 10].

In the same way, taking (2.8) and (2.9) into account, we have for the angular part of the distribution function

$$f(x^\circ, \theta) = \frac{1}{2n(x^\circ)} \int_0^{(x^\circ \sec\theta,\ \infty)} n(x^\circ - t\cos\theta) e^{-t}\, dt \tag{2.10}$$

in which $t = z|\sec\theta|$. Here the first upper limit is taken for $0 \leq \theta < {}^1\!/_2\pi$ and the second for ${}^1\!/_2\pi \leq \theta < \pi$.

3. Numerical Solutions of the Above Equations and Discussion of Results. It follows from the form of (2.9) that the solution of that equation may differ by a constant factor proportional to the flux I at the wall. At large distances from the wall $x^\circ \gg 1$, the solution must become linear, the true gradient being established very slowly for $x^\circ \gg 1$ because the factor $E_1(z)$ decreases rapidly. Hence the correct choice of the zero-order approximation is very important when (2.9) is solved by iteration.

As a very exact initial approximation for $x^\circ \gg 1$ we can take the diffusion distribution (1.5)

$$n^\circ = 1 + 3/2\ x^\circ \tag{3.1}$$

It is interesting to note that for linear flight, when we obtain an equation of the type (2.9) with kernel e^{-z}, the zero-order approximation (1.5) in the form $n^\circ = 1 + x^\circ$ is the exact solution, as we easily see by direct substitution.

The numerical solution of (2.9) converges rapidly by iteration from the approximation (3.1) (Fig. 1). Thus, by the second iteration the density at the origin $n_2^\circ(0)$ is greater than the exact value $n_\infty^\circ(0) = 0.855$ by not more than 0.65%, and the sixth iteration yields an accuracy at the origin of not worse than $\varepsilon = 10^{-4}$, and perturbation of the solution with respect to x° for a given accuracy extends to not more than 4 or 5 digits.

When $x^\circ \gtrsim 0.5$ the solution is slightly larger than the approximation (3.1).

Judging from Fig. 1, the discrepancy between the diffusion distribution and the exact distribution is not more than 15% even at $x = 0$. This approximation is virtually exact outside the λ-layer when the boundary condition (1.4) holds at its boundary. But the solution for linear particle flight is also exact inside the λ-layer.

With the aid of (2.10) we can then compute the angular distribution function (Fig. 2) from the solution $n^\circ(x)$. We compare it with the distribution in the diffusion approximation. Assuming both limits in (2.10) to be infinite and transforming to dimensional variables, we obtain the diffusion approximation

$$f(x, \theta) = \frac{1}{2}\left(1 - \frac{\lambda}{n}\frac{dn}{dx}\cos\theta\right) \quad (3.2)$$

The last term in (3.2) is a measure of the deviation of the distribution from the equilibrium value. Comparing (3.2) with the exact solution, we note that for particles moving towards the wall ($\cos\theta < 0$), they differ insignificantly in the λ-layer, while for $\cos\theta > 0$ the distorting effect of the wall is small, particularly from a small distance from the wall ($x^{\circ}\sec\theta \leqslant 1$). But even for $x^{\circ} = 1$ this difference is insignificant, while for $x^{\circ} = 2$ both distributions coincide virtually completely.

That the appropriateness of the diffusion approximation is good in this case, which is far from equilibrium, can be explained by two reasons. The first is that the form of the function $\chi(x' v)$ plays a significant role here, remaining spherically symmetric for the chosen scattering law and any anisotropy of the distribution function. If the scattering law departs from the model of elastic spheres, the accuracy of the approximation decreases in the λ-layer.

The second reason is as follows. By (1.3) and (1.4) the density must formally vanish at a distance λ_D beyond the wall. Positioning the wall at $x = 0$ so as to be opaque to particles from the left and absorb particles from the right results in the destruction of the mechanism for forming the fluxes $j_{\pm}$ near it. But the perturbation, as simple estimates show, cannot exceed 15-20% because of the smallness of the density on the left, which is confirmed by the numerical results.

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