Journal of Statistical Physics, Vol. 25, No. 3, 1981

The Kinetic Boundary Layer for the Fokker–Planck Equation with Absorbing Boundary

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Received January 23, 1980; revised June 12, 1980

The Fokker–Planck equation for the distribution of position and velocity of a Brownian particle is a particularly simple linear transport equation. Its normal solutions and an apparently complete set of stationary boundary layer solutions can be determined explicitly. By a numerical algorithm we select linear combinations of them that approximately fulfill the boundary condition for a completely absorbing plane wall, and that approach a linearly increasing position space density far from the wall. Various aspects of these approximate solutions are discussed. In particular we find that the extrapolated asymptotic density reaches zero at a distance x_M beyond the wall. We find $x_M = 1.46$ in units of the velocity persistence length of the Brownian particle. This study was motivated by certain problems in the theory of diffusion-controlled reactions, and the results might be used to test approximate theories employed in that field.

KEY WORDS: Brownian motion; Fokker–Planck equation; boundary layer; Milne problem; half-range expansion; diffusion-controlled reactions.

1. INTRODUCTION

The flow of a reactant in a diffusion-controlled reaction can often be described in terms of Brownian motion of a particle in the presence of absorbing or partially absorbing boundaries.[1,2] The simplest description is obtained through a diffusion or Smoluchowski equation for the probability density of the particle position with either absorbing or "radiative"[1] boundary conditions. In the former case the density is put equal to zero at the boundary, while in the latter the outward normal flux is proportional to the density with a phenomenological proportionality constant. This tradi-

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0022-4715/81/0700-0569$03.00/0

tional theory has often been criticized[(1,2),2]; in particular there seems to be no clear way of relating the proportionality constant in the radiative boundary conditions to a microscopic picture of the reaction kinetics.

The reasons for the inadequacy of the Smoluchowski equation can be exhibited by inspecting its derivation from a more detailed description of Brownian motion due to Klein[(3)] and Kramers,[(4)] in terms of the probability density for the velocity and position of the Brownian particle. The Smoluchowski equation can be recovered[(5)] from this description via a procedure of the Chapman–Enskog type. This derivation breaks down, however, near a wall or at places where the potential varies rapidly; there a so-called kinetic boundary layer occurs.[(6)] This breakdown is caused by the large deviations from the Maxwellian velocity distribution that must occur, e.g., near an absorbing boundary, whereas for validity of the Smoluchowski equation approximate local equilibrium is required.

Exactly solvable problems in which a kinetic boundary layer occurs are extremely rare. Some solvable cases are known[(6,7)] for the BGK model, a drastically simplified linearized Boltzmann equation, and for some modifications of it; a few more for the one-speed neutron transport equation, which is equivalent to the equation of radiative transfer for gray matter.[(8)] Therefore an at least partially solvable Brownian motion problem exhibiting a nontrivial kinetic boundary layer should be of some intrinsic interest, apart from its utility for testing approximate descriptions of diffusion-controlled reactions.

The case studied in the present paper is that of Brownian motion in a half-space bounded by a plane wall. Moreover, we restrict ourselves to the case in which the wall absorbs all particles impinging on it; some cases with selectively absorbing walls will be treated in a subsequent study.[(9)] The problem treated in the present paper was posed long ago by Chang and Uhlenbeck,[(10)] but it has thus far resisted attempts at an exact solution. As a further restriction, we shall consider only stationary solutions with translational invariance parallel to the wall. Thus we are led to the Brownian motion analog of the well-known Milne problem in radiative transfer theory.

The solution of the Milne problem (and of the several solvable problems for the BGK model) proceeds in two steps. First one constructs a special set of stationary solutions that depend, in general, exponentially on the distance to the wall. Secondly one uses a special expansion theorem (half-range completeness) to combine them in such a way that the boundary condition is fulfilled. In our case the special solutions can be constructed explicitly, as was first shown by Pagani.[(11)] His results are reca-

[2]Reference 1 and 2 contain many references to earlier work in this field.

pitulated, to the extent that we need them, in Section 2. However, a half-range completeness theorem does not yet exist. We therefore used a numerical procedure, described in Section 3, to determine linear combinations of the special solutions that come closest, in a sense to be specified, to obeying the requisite boundary condition. As the number of special solutions in the linear combination increases, these approximate solutions appear to exhibit a slow but steady convergence towards a solution with correct behavior at the wall.

The numerical results are presented and discussed in Section 4. In addition to a three-dimensional picture of the distribution over position and velocity in the boundary layer we present results for the velocity distribution at the wall and for the mean density and the mean-squared velocity as a function of the distance from the wall (the mean velocity follows directly from probability conservation). Far from the wall the density increases linearly with distance, as one expects from the diffusion equation. When this asymptotic solution is extrapolated across the boundary region it reaches zero not at the wall (as the solution of the diffusion equation with absorbing boundary would) but at some distance beyond it. The value we find for this "Milne extrapolation length" is, in the appropriate dimensionless units, approximately twice the value found in the radiative transfer problem. The density in the actual solution is everywhere lower than that of the extrapolated asymptotic solution, but of course it stays finite at the wall. The mean-squared velocity increases as one approaches the wall, but the spread in velocity around the mean, which may be called the "temperature" of the particles absorbed or transmitted at the wall, becomes significantly lower than that in the bulk.

2. STATIONARY SOLUTIONS OF THE FOKKER-PLANCK EQUATION

In this paper we discuss the one-dimensional Fokker-Planck equation

$$\frac{\partial P(u,x,t)}{\partial t}=\left[\gamma\left(\frac{1}{m\beta}\frac{\partial^2}{\partial u^2}+\frac{\partial}{\partial u}u\right)-u\frac{\partial}{\partial x}\right]P(u,x,t) \qquad (2.1)$$

The function $P(u,x,t)$ denotes the probability distribution for the components u and x of the velocity and position of the Brownian particle perpendicular to the plane wall, m is its mass, γ the friction coefficient for its motion through the fluid, and β equals $(k_B T)^{-1}$. Stationary solutions of (2.1) on the range $x>0$ can be made into stationary solutions of the three-dimensional problem in a half-space bounded by a plane wall by means of a multiplication with a Maxwell distribution for the velocity components parallel to the wall (and the constant function with respect to the parallel components of the position). Our discussion of the stationary solutions of (2.1) follows the treatment by Pagani[11] and is similar to a discussion of nonstationary plane-wave solutions by Résibois.[12]

We begin by observing that the operator

$$\mathcal{C} = \frac{1}{m\beta}\frac{\partial^2}{\partial u^2} + \frac{\partial}{\partial u}u \tag{2.2}$$

has eigenvalues $-n$ ($n = 0, 1, 2, \ldots$) and associated eigenfunctions

$$\varphi_n(u) = c_n H_n\left[\left(\tfrac{1}{2}m\beta\right)^{1/2}u\right]\exp\left[-\tfrac{1}{2}m\beta u^2\right] \tag{2.3}$$

where $H_n(x)$ is the nth Hermite polynomial in the convention used by Erdélyi *et al.*[13] and c_n a normalization constant. From the orthogonality property of the Hermite polynomials, and from the form of the first two of them, it follows that in any linear combination

$$f(u, x) = \sum_n a_n(x)\varphi_n(u) \tag{2.4}$$

the coefficient $a_0(x)$ is proportional to the probability density in x space and $a_1(x)$ to the probability current. Normal stationary solutions[5] must be such that $a_0(x)$ is a stationary solution of the diffusion equation

$$\frac{\partial a_0(x,t)}{\partial t} = \frac{1}{m\beta\gamma}\frac{\partial^2}{\partial x^2}a_0(x,t) \tag{2.5}$$

Thus $a_0(x)$ must depend linearly on x. The two independent stationary solutions of (2.1) corresponding to densities 1 and x are

$$\hat{\psi}_0(u, x) = (m\beta/2\pi)^{1/2}\exp\left[-(1/2)m\beta u^2\right] \tag{2.6}$$

and

$$\psi_0'(u, x) = (m\beta/2\pi)^{1/2}(x - \gamma^{-1}u)\exp\left[-(1/2)m\beta u^2\right] \tag{2.7}$$

as one checks easily by substitution.

To obtain nonnormal stationary solutions we try the ansatz

$$\psi(u, x) = \exp\left[-\kappa\gamma x - \lambda u\right]\chi(u) \tag{2.8}$$

Substitution in (2.1) and the stationarity requirement lead to

$$\left[\frac{1}{m\beta}\frac{\partial^2}{\partial u^2} + \frac{\partial}{\partial u}\left(u - \frac{2\lambda}{m\beta}\right) + (\kappa - \lambda)u + \frac{\lambda^2}{m\beta}\right]\chi(u) = 0 \tag{2.9}$$

Comparison with (2.2) shows that with the choice

$$\kappa = \lambda, \qquad \lambda^2 = nm\beta \qquad (n = 0, 1, 2, \ldots) \tag{2.10}$$

one obtains solutions of the form

$$\psi_{\pm n}(u,x) = c_n' H_n\Big\{\big[(1/2)m\beta\big]^{1/2}\big[u \mp 2(n/m\beta)^{1/2}\big]\Big\}$$
$$\exp\Big\{-(1/2)m\beta\big[u \mp (n/m\beta)^{1/2}\big]^2 \mp \gamma x(nm\beta)^{1/2}\Big\} \qquad (2.11)$$

with c_n' a normalization constant. The solution with $n = \pm 0$ is proportional to $\hat{\psi}_0(u,x)$ given by (2.6); we shall find it convenient to choose a slightly different normalization for $\psi_0(u,x)$ later.

It was shown by Pagani[11] that the $\psi_m(u,0)$ obey the orthogonality relations

$$\int_{-\infty}^{+\infty}\psi_m(u,0)\psi_n(u,0)u\exp\big[(1/2)m\beta u^2\big]\,du = 0$$
$$\text{for } m \neq n; \quad m,n = 0, \pm 1, \pm 2, \ldots \qquad (2.12a)$$

and

$$\int_{-\infty}^{+\infty}\psi_m(u,0)\psi_0'(u,0)u\exp\big[(1/2)m\beta u^2\big]\,du = 0 \qquad \text{for } m = \pm 1, \pm 2, \ldots \qquad (2.12b)$$

In particular, (2.12a) with $n = 0$ shows that none of the functions $\psi_n(u,x)$ with $n = \pm 1, \pm 2, \ldots$ carries a probability current. In addition it was shown that the set of functions consisting of the $\psi_n(u,0)$ with $n = 0, \pm 1, \pm 2, \ldots$ and $\psi_0'(u,0)$ constitute a basis in the space of functions $\chi(u)$ for which $u\chi(u)$ is square integrable on the full range $-\infty < u < +\infty$. These orthogonality and completeness relations would enable one to solve boundary value problems of the following type: determine the stationary solution of (2.1) when $P(u,0)$ is prescribed.

Unfortunately, the boundary value problems encountered in practice are mostly of a different type. For an absorbing boundary at $x = 0$ of a medium occupying the region $x > 0$ the boundary condition at the wall affects only the positive velocities:

$$P(u,0) = 0 \qquad \text{for } u > 0 \qquad (2.13)$$

It is supplemented by conditions on $P(u,x)$ far from the wall. The problem that poses itself naturally is: determine a (stationary) solution of (2.1) satisfying (2.13) that approaches a normal solution, i.e., a linear combination of (2.6) and (2.7), at large x. Such a solution must clearly have the form

$$\psi(u,x) = \tilde{c}_0\Big[\psi_0'(u,x) + \sum_{n=0}^{\infty} d_n\psi_{+n}(u,x)\Big] \qquad (2.14)$$

According to the remark following (2.12b), the constant $\tilde{c}_0$ can be fixed by specifying the stationary probability current towards the wall. The remaining problem is to choose the d_n in such a way that (2.13) is satisfied:

$$\psi_0'(u,0) + \sum_{n=0}^{\infty} d_n \psi_{+n}(u,0) = 0 \qquad \text{for } u > 0 \tag{2.15}$$

A sufficient condition for the existence of a unique solution to (2.15) is: the functions $\psi_n(u,0)$ $(n = 0, 1, 2, \ldots)$ are linearly independent and form a basis in a suitable class of functions on the range $0 < u < +\infty$. The solution can be written in closed form if we succeed in finding functions $\tilde{\psi}_n(u)$ such that

$$\int_0^{\infty} \tilde{\psi}_n(u) \psi_m(u,0)\, du = \delta_{nm} \qquad (n, m = 0, 1, 2, \ldots) \tag{2.16a}$$

$$\sum_{n=0}^{\infty} \psi_n(u,0) \tilde{\psi}_n(u') = \delta(u - u')\left[u, u' \in (0, \infty)\right] \tag{2.16b}$$

(half-range orthogonality and completeness theorems). For the BGK model[7] and for the one speed neutron transport equation[8] theorems of this type could be proved (with a continuous index n). For our case such theorems are not yet available. Hence we proceeded to treat the problem (2.15) by numerical means.

3. THE NUMERICAL SOLUTION PROCEDURE

To find an approximate numerical solution of the problem (2.15) one may determine for various values of N the quantities d_n^N that minimize

$$\int_0^{\infty} |\psi_N(u)|^2 \rho(u)\, du \equiv D_N^2 \tag{3.1}$$

with

$$\psi_N(u) = \psi_0'(u,0) + \sum_{n=0}^{N-1} d_n^N \psi_n(u,0) \tag{3.2}$$

and $\rho(u)$ a suitably chosen positive weight function. Variation of (3.1) leads to

$$I_n + \sum_{m=0}^{N-1} G_{nm} d_m^N = 0 \qquad (n = 0, 1, 2, \ldots) \tag{3.3}$$

with

$$I_n = \int_0^{\infty} \psi_0'(u,0) \psi_n(u,0) \rho(u)\, du \tag{3.4a}$$

and

$$G_{nm} = \int_0^{\infty} \psi_n(u,0) \psi_m(u,0) \rho(u)\, du \tag{3.4b}$$

If the $\psi_n(u,0)$ have the half-range orthogonality and completeness properties stated in the preceding section, the D_N^2 formed with the aid of the solutions of (3.3) should approach zero, and the d_n^N themselves should approach well-defined limits for $N \to \infty$. Moreover, the functions

$$\tilde{\psi}_n^N(u) \equiv \sum_{m=0}^{N-1} \left(G_N^{-1}\right)_{nm} \psi_m(u,0)\rho(u) \tag{3.5}$$

then approach the $\tilde{\psi}_n(u)$ of (2.16). One expects that the required completeness properties hold for a broad class of weight functions $\rho(u)$, if at all. In view of the speed of convergence of our procedure and the manageability of round-off errors an appropriate choice appears to be

$$\rho(u) = u \exp\left[(1/2)m\beta u^2\right] \tag{3.6}$$

For this choice explicit, albeit complicated, expressions for I_m and G_{nm} can be found, as is discussed further in the Appendix.

4. RESULTS

The coefficients d_n^N were determined from (3.3) for all $N \leqslant 140$ and all $n \leqslant N$, with the choice (3.6) for the weight function. We shall first present a few aspects of the resulting approximate solution of type (2.14) in graphical form, then a table with more precise numerical values, and finally we shall discuss the possibility of extrapolating some of the results towards $N = \infty$. More detailed results are given elsewhere.[14] The calculations were carried out on the CYBER-175 of the RWTH Computing Center.

In Fig. 1 we show the approximation $P_{140}(u,x)$ to the solution (2.14) with boundary condition (2.15), using 140 boundary solutions with coefficients determined from (3.3). As our unit of velocity we chose the thermal velocity $(m\beta)^{-1/2}$ and as our unit of length the distance traveled by a particle of unit velocity during a velocity decay time γ^{-1}. This "velocity persistence length" plays a role similar to that of the mean free path in kinetic theory.[5] The solution is shown for $|u| \lesssim 3$ and $0 < x < 3$. The units for $P(u,x)$ are arbitrary, and the constant $\tilde{c}_0$ in (2.14) is hence irrelevant. For $x = 3$ the solution is already close to a Maxwell distribution. At $x = 0$ the deviations from the correct boundary condition (2.15) are still noticeable; the probability distribution $P_{140}(u,0)$ even assumes negative values in the "forbidden region" $u > 0$.

To show the convergence of $P_N(u,0)$ with increasing N in more detail we present in Fig. 2 this function for $N = 35$, 70, and 140. For large $|u|$ the curves are indistinguishable, and the region in which appreciably negative probabilities and violation of (2.15) occur shrinks roughly equally with each doubling of N. Eventual convergence towards a function satisfying (2.15) is

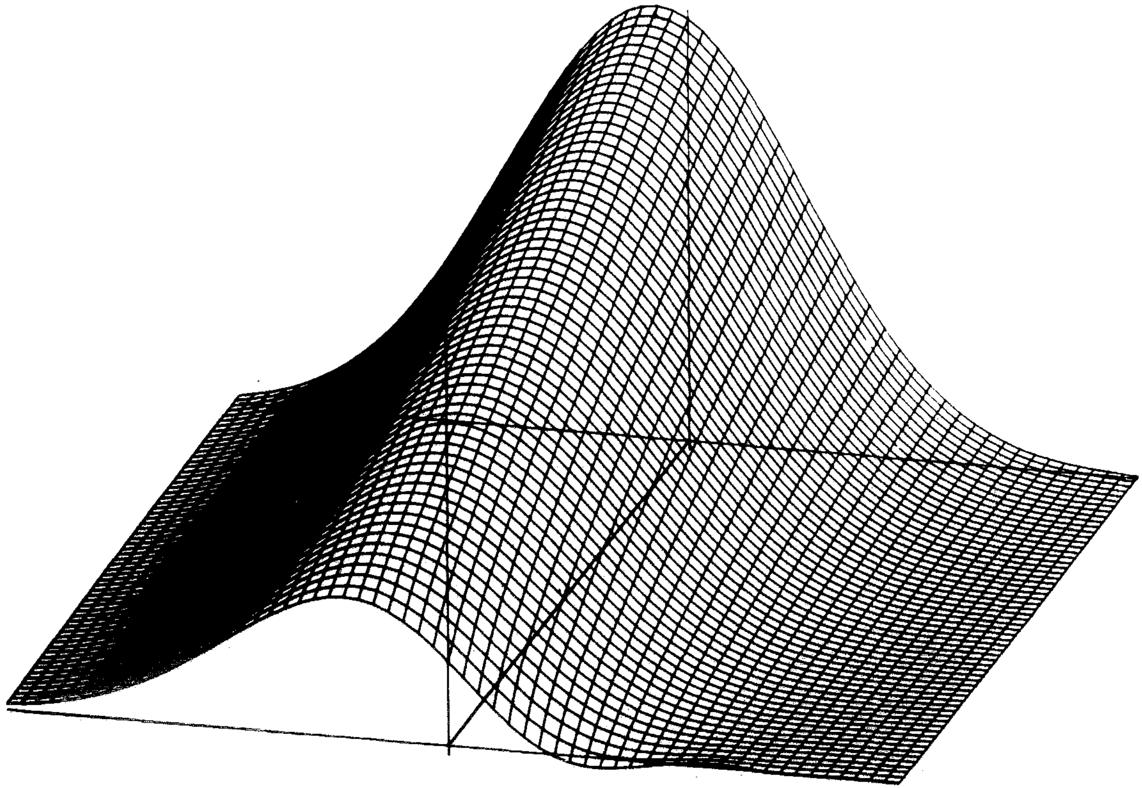

Fig. 1. The approximate stationary solution of the Fokker–Planck equation with absorbing boundary, constructed with 140 boundary layer solutions. The velocity coordinate (horizontal) runs from -3 to $+3$, the position coordinate (towards the rear) from 0 to 3 in units specified at the beginning of Section 4.

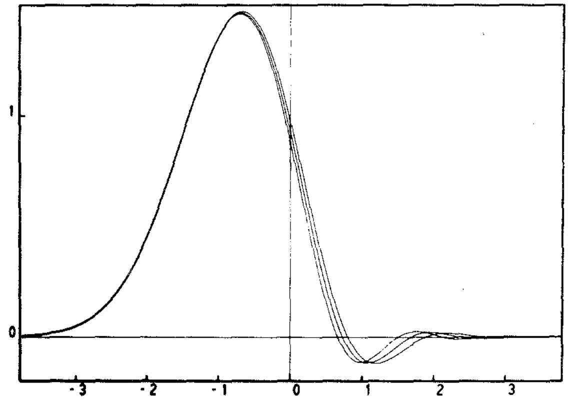

Fig. 2. The velocity distribution at the wall for the approximate solutions with 140, 70, and 35 boundary layer solutions (the leftmost curve corresponds to $N = 140$).

indicated, but it is equally clear that an unrealistically high N would be needed to exhibit it on the scale of this figure.

In Fig. 3 we show the integral $n_{140}(x)$ of $P_{140}(u,x)$ over velocities, i.e., the probability density in position space, for a value of $\tilde{c}_0$ that is unity in our system of units, in which $m\beta = \gamma = 1$. For large x this function should approach

$$n_{140}^{\text{as}}(x) = x + d_0^{140}(2\pi)^{1/2} \equiv x + x_M^{140} \tag{4.1}$$

since all $\psi_n(u,x)$ with $n > 0$ decay exponentially with x. The factor $(2\pi)^{1/2}$ is caused by our normalization $G_{00} = 1$. The function (4.1) is

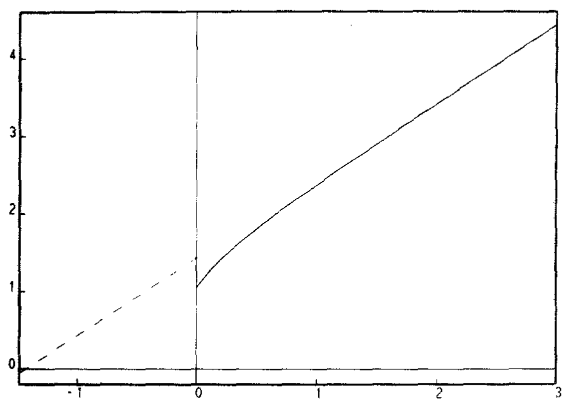

Fig. 3. The density as a function of the distance from the wall for the approximate solution with $N = 140$ (drawn curve) and its asymptote (broken line). The intersection of the asymptote with the horizontal axis is the approximate Milne extrapolation length x_M^{140}.

indicated in Fig. 3 by a broken line. The quantity

$$x_M = \lim_{N\to\infty} x_M^N \tag{4.2}$$

is the analog of the Milne extrapolation length for our problem. On the scale of Fig. 3 the curves $n_{35}(x)$ and $n_{70}(x)$ would be displaced slightly in the vertical direction with respect to $n_{140}(x)$, but the curves $n_N(x) - n_N^{\text{as}}(x)$ would be indistinguishable on this scale for $x \gtrsim 0.1$.

In view of the orthogonality relations (2.12) one finds for the first two moments of $P_N(u,x)$

$$n_N(x)\langle u\rangle_N(x) \equiv \int_{-\infty}^{+\infty} uP_N(u,x)\,du = -1 \tag{4.3}$$

which expresses conservation of probability in the interior, and

$$\begin{aligned} n_N(x)\langle u^2\rangle_N(x) &\equiv \int_{-\infty}^{+\infty} u^2 P_N(u,x)\,du \\ &= x + (2\pi)^{1/2} d_0^N = n_N^{\text{as}}(x) \end{aligned} \tag{4.4}$$

Therefore the average squared velocity of a particle at x in units of $(m\beta)^{-1}$ is given by $n_N^{\text{as}}(x)/n_N(x)$, a function shown in Fig. 4 for $N = 35$, 70, and 140. Since $n_N(x)$ becomes progressively smaller compared to $n_N^{\text{as}}(x)$ as one

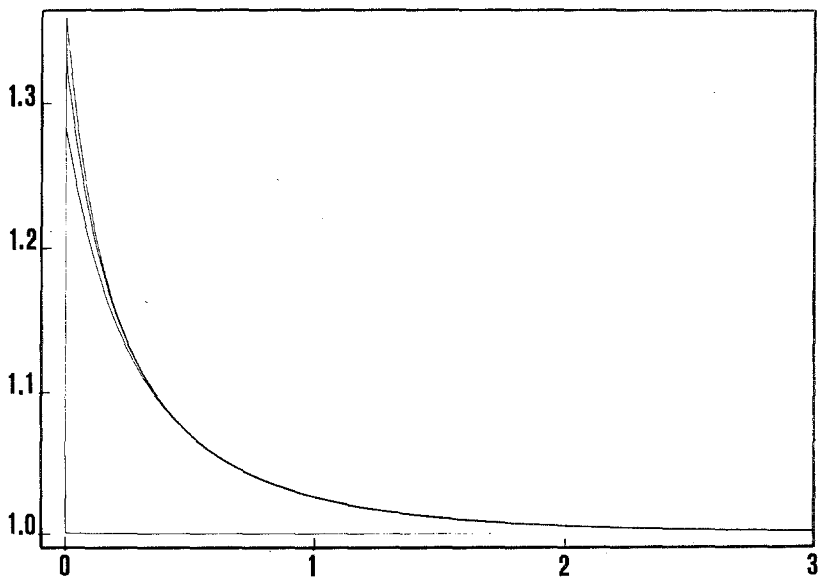

Fig. 4. The mean-squared velocity as a function of the distance from the wall for the approximate solutions with $N = 140$ (upper curve), $N = 70$, and $N = 35$ in units of the squared thermal velocity.

approaches the wall, as is evident from Fig. 3, the mean-squared velocity becomes correspondingly larger. In Fig. 5, we give the spread in velocity

$$[\langle u^2\rangle - \langle u\rangle^2]_N(x) = n_N^{as}(x)/n_N(x) - [n_N(x)]^{-2} \tag{4.5}$$

which decreases strongly as one approaches the wall. If one assumes that particles that reach the wall emerge on the vacuum side without altering their velocity, then the value of (4.5) at the wall might be interpreted as a "temperature" for the velocity component perpendicular to the wall in the emerging beam of Brownian particles. For $N = 140$ its value is 0.464 times the value in the bulk.

Of course our results are reliable only if the $\psi_n(u, 0)$ with $n = 0, 1, 2, \ldots$ are linearly independent and complete on the positive half-line with weight function $\rho(u)$. As a test of the independence we checked whether $\det \mathsf{G}_N$ might approach zero with increasing N. This is clearly not the case; the values stabilize at a value of roughly 0.9. Lack of completeness might manifest itself in the form of a nonzero limit of the distance D_N^2 defined in (3.1). In Table I we give this quantity for the values $N = 20$, 60, 100, and 140. Further we give the approximate extrapolation length x_M^N and the values for the density and the mean-squared velocity at the wall. All are smooth functions of N for intermediate values of N. The four functions

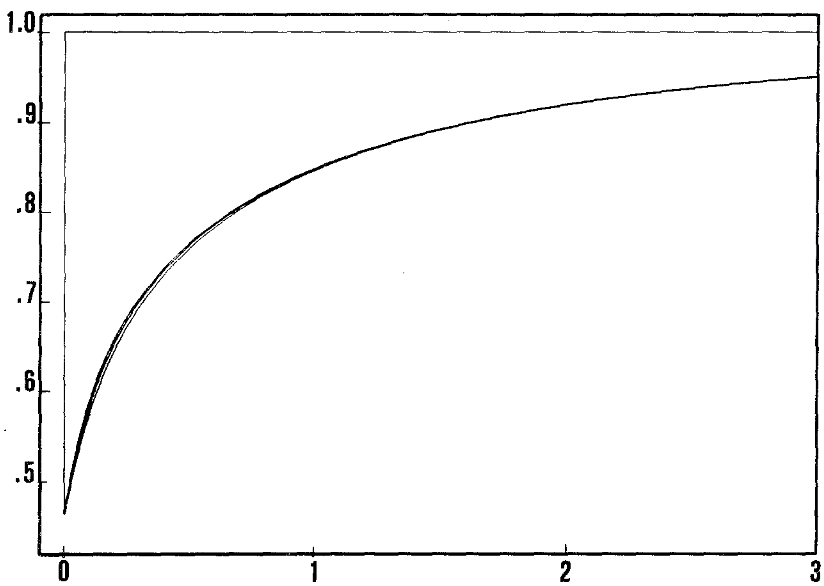

Fig. 5. The spread in velocity as a function of the distance from the wall for the approximate solutions with $N = 140$ (lower curve), $N = 70$, and $N = 35$ in units of the squared thermal velocity (curves only partially resolved).

Table I. The Violation of the Boundary Condition, D_N^2 [Eq. (3.1)], the Approximate Milne Extrapolation Length x_M^N, and the Approximate Density $n_N(0)$ and Mean Square Velocity $\langle u^2\rangle_N(0)$ at the Wall in an Approximate Solution of the Boundary Layer Problem with N Boundary Layer Solutions for Some Values of N

N	D_N^2	x_M^N	$n_N(0)$	$\langle u^2\rangle_N(0)$
20	0.04680	1.4078	1.1138	1.2639
60	0.02743	1.4279	1.0774	1.3253
100	0.02136	1.4344	1.0627	1.3499
140	0.01811	1.4380	1.0537	1.3648

could be fitted well with a three-parameter extrapolation formula of the type

$$q_N = q_\infty + \alpha N^{-\delta} \tag{4.6}$$

In Table II we give the values for q_∞ for the four quantities of Table I. To convey an idea of the reliability of the extrapolation we made separate fits employing the values of the four quantities in the three intervals $20 < N \leqslant 60$, $60 < N \leqslant 100$, and $100 < N \leqslant 140$. The last line gives the value of δ for the third interval. The extrapolation results for D_N^2 are quite compatible with $\lim_{N\to\infty} D_N^2 = 0$, and they do not vary too much when the interval is changed. Similarly the extrapolated values for the Milne extrapolation length are practically the same for the three intervals. Other three-parameter fits[14] for x_M^N also yield $x_M = 1.46$, but their quality is somewhat less than that of (4.5).

The density and the mean-squared velocity at the wall, which depend more sensitively on the higher boundary solutions, converge much more slowly, as is evident from the tables, and have not settled down yet at $N = 140$. As a check we can use the relation $\langle u^2\rangle = n_{as}/n$, which is exact and obeyed by the entries in Table I, but incompatible with an N depen-

Table II. Extrapolated Values for the Quantities of Table I Using the Fit (4.6) for the Three Intervals Indicated in the First Column. The Last Row Gives the Exponent in (4.6) for the Third Interval.

Interval	D_∞^2	x_M^∞	$n_\infty(0)$	$\langle u^2\rangle_\infty(0)$
21–60	– 0.00044	1.4611	0.8940	1.6013
61–100	– 0.00036	1.4610	0.9078	1.5948
101–140	– 0.00028	1.4609	0.9136	1.5901
Exponent	– 0.48	–0.43	– 0.18	– 0.19

dence of type (4.5) for all three quantities. The discrepancy decreases, however, from 2.1% for the first interval to 0.56% for the last one. The spread in velocity at the wall does not reach its asymptotic N dependence in the range of N values calculated by us; it shows a flat maximum near $N = 100$ at a value around 0.46 (see Fig. 5). Substitution of extrapolated values in (4.4) indicates a limiting value of around 0.40, but the slow convergence does not inspire much confidence in this extrapolation.

In conclusion, our procedure yields a good qualitative picture of the boundary layer and a value for the extrapolation length that should be reliable up to the third significant digit. The slow convergence near $x = 0$, $u = 0$ precludes a precise determination of the velocity distribution at the wall and of its moments. An attempt to determine $\tilde{\psi}_n(u)$ of (2.16) by extrapolation of the expressions (3.5) did not yield reliabile results due to slow convergence.

APPENDIX

In this Appendix we outline the computation of the matrix elements G_{mn} of (3.4b) that involve the $\psi_n(u,0)$ of (2.11). By the transformation $u(\frac{1}{2}m\beta)^{1/2} = t$ and absorption of some constant factors into the normalization constants c_n' to form c_n'' we obtain

$$G_{nm} = c_n'' c_m'' \int_0^\infty tH_n\left[t - (2n)^{1/2}\right] H_m\left[t - (2m)^{1/2}\right]$$
$$\exp\left[t - (n/2)^{1/2} - (m/2)^{1/2}\right]^{-2} dt \qquad \text{(A.1)}$$

The factor t can be eliminated by using[13]

$$tH_n(t-s) = sH_n(t-s) + nH_{n-1}(t-s) + \tfrac{1}{2}H_{n+1}(t-s) \qquad \text{(A.2)}$$

Then by application of

$$H_n(t-s) = \sum_{m=0}^{n} \binom{n}{m} (-2s)^m H_{n-m}(t) \qquad \text{(A.3)}$$

which follows immediately from[13]

$$H_n(t) = (-1)^n \exp(t^2)(d^n/dt^n)\exp(-t^2) \qquad \text{(A.4)}$$

the integrals resulting from (A.1) by substitution of (A.2) can be expressed in terms of integrals of the type

$$K_{nm}(a) = \int_{-a}^{\infty} H_n(t) H_m(t) \exp(-t^2)\, dt \qquad \text{(A.5)}$$

Integration by parts and application of (A.5) and $H_n'(t) = 2nH_{n-1}(t)$ yields the recursion relation (for $m > 0$)

$$K_{nm}(a) = H_n(-a)H_{m-1}(-a)\exp[-a^2] + 2nK_{n-1,m-1}(a) \quad \text{(A.6)}$$

From this recursion relation and $K_{nm}(a) = K_{mn}(a)$ follow closed expressions for K_{nm} with $n \neq m$. The expression for K_{nn} involves also $K_{00}(a)$, which is related simply to the error function. In this way G_{nm} is first expressed in $3(n+1)(m+1)$ different $K_{pq}(a)$, each of which is in turn expressed in $\min(p,q) + \delta_{pq}$ easily calculated terms. The c_n'' are chosen such that $G_{nn} = 1$. The computation of the I_n given by (3.4a) was carried out in a completely analogous fashion.

ACKNOWLEDGMENTS

We thank Dipl.-Math. N. Gwosdzik of the RWTH Computing Center for help and advice, and Mr. A. Weidmüller for assistance in preparing the illustrations. We also thank Dr. Henk van Beijeren for several useful comments. U.M.T. wishes to thank Professor Carlo Cercignani for a helpful discussion during an early stage of this investigation.

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