SIAM J. APPL. MATH.
Vol. 52, No. 4, pp. 1057–1075, August 1992

011

THE DIFFUSION LIMIT OF FREE MOLECULAR FLOW IN THIN PLANE CHANNELS*

CHRISTOPH BÖRGERS†¶, CLAUDE GREENGARD‡, AND ENRIQUE THOMANN§¶

Abstract. The subject of this paper is free molecular flow in thin channels bounded by parallel plane surfaces on which Maxwell's boundary condition applies. With tools from probability theory, it is proved that in the limit as the domain width h tends to zero, the evolution of the density is described by a diffusion equation, on a timescale of $1/(h \log h^{-1})$, and with a diffusion coefficient of $(2-\alpha)\sqrt{T}/(2\alpha\sqrt{\pi})$ (α is the accommodation coefficient and T is the surface temperature). The logarithmic factor in the timescale is geometry dependent; in thin cylinders of diameter h, the timescale is $1/h$, as Babovsky has proved in [*Journal of Statistical Physics*, 44 (1986), pp. 865–878]. Numerical calculations indicate that the diffusion limit is closely approximated even at fairly large values of h.

Key words. free molecular flow, diffusion limit, rarefied gas lubrication

AMS(MOS) subject classifications. 76P05, 82A40

1. Introduction.

Information is stored and retrieved in magnetic disk storage devices through heads carried on sliders that fly over rotating disks. The sliders are pushed toward the disks by mechanical forces and are pushed away from the disks by increased air pressure in the slider-disk gaps caused by the relative motions of the sliders and the disks. The flow of the air in this gap has traditionally been modeled by the Reynolds lubrication equation [15], which is derived from the compressible Navier–Stokes equations under the assumptions that vertical pressure gradients, temperature variations, and inertia effects are negligible.

However, already in current technology, sliders fly at heights on the order of several molecular mean free paths; future technology will presumably involve even much smaller flying heights. It is doubtful that the Reynolds equation, or even the modified Reynolds equation [7] obtained by incorporation of a slip boundary condition, is a correct model of the physics in such regimes. Consequently, studies have recently been carried out that aim at understanding lubrication in thin regions with a more accurate physical model. Papers [12] and [13] approach the problem of lubrication in thin regions via the linearized BGK model [8, pp. 205ff].

In this paper, we analyze the simplest model of rarefied gas dynamics—free molecular flow—in the region D_h located between two infinite, flat, parallel surfaces, separated by a small distance h,

$$D_h = \{\mathbf{x} = (x, y, z) : (x, y) \in \mathbb{R}^2,\ z \in]0, h[\ \}. \tag{1.1}$$

In the free molecular flow model, gas molecules are assumed to move with constant velocities, as long as they do not collide with a surface, and to be reflected according to Maxwell's boundary condition [8, pp. 118ff.] upon impact with the bounding

* Received by the editors February 11, 1991; accepted for publication (in revised form) July 12, 1991.

† Mathematics Department, University of Michigan, Ann Arbor, Michigan 48109. This author's research was supported in part by National Science Foundation grant DMS-9003965.

‡ IBM Research Division, Thomas J. Watson Research Center, Yorktown Heights, New York 10598.

§ Mathematics Department, Oregon State University, Corvallis, Oregon 97331.

¶ Part of this work was carried out while these authors were visiting the IBM T. J. Watson Research Center, Yorktown Heights, New York 10598.

surfaces. The physical state of the gas is described by a distribution function f_h over the product $D_h \times \mathbb{R}^3$ of position and velocity space, and the equations of free molecular flow describe the evolution of this distribution.

This six-dimensional transport problem admits a greatly simplified description as a two-dimensional (in the (x,y)-plane) diffusion problem in the limit as $h \to 0$. Let ρ_h denote the planar density; i.e., $\rho_h(x,y,t)$ is the number of molecules per unit area (the four-dimensional integral of the molecular distribution function f_h over velocity space and the gap height $]0,h[$) at spatial position (x,y) and time t. We show that when time is appropriately scaled, ρ_h evolves, in the limit as $h \to 0$, as the solution of a diffusion equation.

For free molecular flow in thin tubes of diameter h, the correct timescale for diffusion is $1/h$ [1]. Surprisingly, this timescale is geometry dependent. In fact, we show that for the plane channel, the correct timescale is $1/(h \log h^{-1})$. We prove in this paper that on this timescale, the planar density ρ_h converges to the solution of the diffusion equation

$$\frac{\partial \rho}{\partial t} = \frac{(2-\alpha)\sqrt{T}}{2\alpha\sqrt{\pi}} \left(\frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2} \right), \tag{1.2}$$

where α is the accommodation coefficient and T is the surface temperature.

The diffusion is brought about by the repeated random scatterings of molecules following their collisions with the bounding surfaces. It is noteworthy that a vanishingly small fraction of the collisions accounts for all of the diffusion (see §8).

The tools in our analysis are from probability theory. We represent solutions of the free molecular flow problem by probability distributions of stochastic processes. Our main result, Theorem 6.2, follows from a central limit theorem for a sum of a random number of independent, identically distributed random variables of *infinite variance*. These random variables represent the horizontal displacements—i.e., the displacements in the (x,y)-plane—experienced during molecular trajectories between successive diffuse molecule-surface collisions. The number of these over given time intervals is random—it depends on the trajectory.

The existence of diffusion limits has been demonstrated for other transport problems. Some important examples are the papers [3], [4], and [16]. In the recent paper of Babovsky, Bardos, and Platkowski [2], a diffusion limit is proved for free molecular flow in vanishingly thin regions. Our results, which are based on very different techniques, are an extension of part of the results of [2].

The analysis in [2] yields a diffusion limit under fairly general hypotheses on the boundary condition, with the dependence of the diffusion coefficient on α and on T as in (1.2). However, as Babovsky, Bardos, and Platkowski point out, the reflection kernels in the boundary conditions to which they show their analysis is applicable (for the plane channel case) do not include Maxwell's. Indeed, when time is scaled by h^{-1}, as is assumed in [2], the coefficient of diffusion is infinite for the basic slab geometry (1.1).

The modification of Maxwell's boundary condition to which the analysis of [2] is shown to apply involves a reduction in the rate of reflection of molecules into directions nearly parallel to the boundary. This boundary condition can be handled with the approach presented in this paper. In this case, the horizontal molecular displacements have finite variance, and a more elementary central limit theorem than that needed for the case of Maxwell's boundary condition yields the diffusion result of [2] (with time scaled by $1/h$). The difference in timescales between the two boundary conditions

can be seen to be a consequence of the difference in finiteness of the variances of the displacements.

We conclude this Introduction with an outline of the paper. In §2 we describe free molecular flow with Maxwell's boundary conditions and introduce a stochastic process, whose sample paths are possible molecular trajectories, to represent free molecular flow.

Beginning with §3, we focus on the flow in the plane channels D_h, with h very small. The sample paths of the stochastic process described in §2 consist of a small initial segment, a large number of flight segments that begin and end at diffuse reflections from the boundary, and a small final segment. The horizontal displacements of these flight segments are of infinite variance. In §4 the timescale $t_h = t/(h \log h^{-1})$ is found, and a central limit theorem, Lemma 4.3, is presented. This theorem describes the probability distribution, as $h \to 0$, of the sums of the horizontal displacements between successive diffuse reflections, under the hypothesis that the number of these flight segments is given by the integer part of the ratio of t_h to the expected duration between diffuse reflections.

The number of flight segments of which a molecular trajectory consists is, of course, random, and so to prove that the limit $h \to 0$ leads to diffusion, we need a central limit theorem for a random number of flight segments. An appropriate result, Lemma 5.4, is presented in §5.

The main result of this paper, Theorem 6.2, is given in §6. This theorem states that, for fixed $t > 0$, the planar density at time t_h converges weakly to a solution of the diffusion equation (1.2) at time t. The proof of the theorem relies on Lemma 5.4.

In §7 we present the results of a Monte Carlo simulation of free molecular flow. These results illustrate that the probability distribution at time t_h of a molecule with given initial state is quite close to its limiting normal distribution (given in §6), even for fairly large values of h.

A curious fact, which shows how sensitively the results depend on the molecule-surface interaction model, is that a vanishingly small portion of the collisions—those that result in reflections into velocities that are nearly parallel to the boundary—accounts for all of the diffusion; most flight segments can be set equal to zero without affecting convergence to the diffusion limit. This is shown in §8 (Proposition 8.1).

In §9 we point out very briefly that our results can be extended to regions of finite length. For the case of vacuum boundary conditions, the density approaches the solution of the diffusion equation (1.2) with homogeneous Dirichlet boundary conditions.

Finally, in §10, we describe very briefly the diffusion limit for free molecular flow in thin tubes. The timescale for diffusion is longer for this case. The difference in timescales is a consequence of the fact that the displacements of molecules between successive collisions with the thin tube surface are of finite variance, contrary to the plane channel case (Babovsky has proved even more than the existence of a diffusion limit for the thin tube problem—he has shown that the axial component of a molecular trajectory converges to a Brownian motion [1]).

2. Stochastic representation of free molecular flow. Let $D \subset \mathbb{R}^3$ be an open spatial region with smooth boundary ∂D, and unit exterior normal vector field $\mathbf{n}$. We denote the spatial coordinates by $\mathbf{x} = (x, y, z)$, the corresponding velocity coordinates by $\mathbf{u} = (u, v, w)$, the time coordinate by t, and the molecular distribution function by f, so that $f(\mathbf{x}, \mathbf{u}, t)$ is the molecular density at time t, spatial position $\mathbf{x} \in D$, and velocity $\mathbf{u} \in \mathbb{R}^3$. As is customary, we denote the sets of incoming and

outgoing states by

$$\Gamma^- = \{(\mathbf{x}, \mathbf{u}) \in \partial D \times \mathbb{R}^3 : \mathbf{u} \cdot \mathbf{n}(\mathbf{x}) < 0\}$$

and

$$\Gamma^+ = \{(\mathbf{x}, \mathbf{u}) \in \partial D \times \mathbb{R}^3 : \mathbf{u} \cdot \mathbf{n}(\mathbf{x}) > 0\},$$

respectively.

The partial differential equation that describes free molecular flow is the linear transport equation in $D \times \mathbb{R}^3$

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{x}} f = 0, \tag{2.1}$$

where $\nabla_{\mathbf{x}}$ denotes the spatial gradient operator $\nabla_{\mathbf{x}} = (\partial/\partial x, \partial/\partial y, \partial/\partial z)$.

The appropriate boundary conditions specify, for each $(\mathbf{x}, \mathbf{u}) \in \Gamma^-$, the rate $-\mathbf{u} \cdot \mathbf{n}(\mathbf{x})\ f(\mathbf{x}, \mathbf{u}, t)$ of molecules that enter the domain at $\mathbf{x} \in \partial D$ and velocity $\mathbf{u}$, per unit boundary area, unit time, and unit velocity space volume, as a function of the rate of molecules that exit the domain at the point $\mathbf{x}$. The boundary condition that describes *specular reflection* is given by the requirement that, for all $(\mathbf{x}, \mathbf{u}) \in \Gamma^-$, $f(\mathbf{x}, \mathbf{u}, t) = f(\mathbf{x}, \mathbf{u}^*, t)$, where $\mathbf{u}^*$ is the specularly reflected velocity $\mathbf{u}^* = \mathbf{u} - 2(\mathbf{u} \cdot \mathbf{n})\mathbf{n}$. The boundary condition of *diffuse reflection* is given by the requirement that, for all $(\mathbf{x}, \mathbf{u}) \in \Gamma^-$,

$$f(\mathbf{x}, \mathbf{u}, t) = \frac{2}{\pi T^2} e^{-\mathbf{u}^2/T} \int_{\tilde{\mathbf{u}} \cdot \mathbf{n}(\mathbf{x}) > 0} f(\mathbf{x}, \tilde{\mathbf{u}}, t)\ \tilde{\mathbf{u}} \cdot \mathbf{n}(\mathbf{x})\ d\tilde{\mathbf{u}},$$

where T is the boundary temperature (the gas constant is normalized to be $\frac{1}{2}$).

Maxwell's boundary condition is the combination

$$f(\mathbf{x}, \mathbf{u}, t) = \alpha \frac{2}{\pi T^2} e^{-\mathbf{u}^2/T} \int_{\tilde{\mathbf{u}} \cdot \mathbf{n}(\mathbf{x}) > 0} f(\mathbf{x}, \tilde{\mathbf{u}}, t)\, \tilde{\mathbf{u}} \cdot \mathbf{n}(\mathbf{x})\, d\tilde{\mathbf{u}} + (1 - \alpha) f(\mathbf{x}, \mathbf{u}^*, t) \tag{2.2}$$

of specular and diffuse reflection, where the accommodation coefficient $\alpha \in [0, 1]$ represents the probability of the reflection being diffuse. We assume in the following that $\alpha > 0$; there is no diffusion limit without this assumption.

The subject of this paper is the analysis of the behavior of mild solutions (defined below) of the problem that consists of the partial differential equation (2.1), with boundary condition (2.2) and an initial condition

$$f(\mathbf{x}, \mathbf{u}, 0) = g(\mathbf{x}, \mathbf{u}). \tag{2.3}$$

Our analysis concerns the limit, as the width of D shrinks to zero, of these mild solutions.

The characteristics of the differential equation (2.1) are the straight paths in $D \times \mathbb{R}^3$ of the form $s \mapsto (\mathbf{x} + s\mathbf{u}, \mathbf{u})$. We build a *mild* solution of the free molecular flow problem from these characteristics. The notation is simplified by the hypothesis, imposed henceforth on the initial condition g, that $g \geq 0$ and $\int_{D \times \mathbb{R}^3} g = 1$, for then g can be viewed as a probability density function. Since the problem under study is linear, the results below extend trivially to all integrable initial conditions.

A stochastic process $(\mathbf{X}, \mathbf{U})(t)$, for $0 \leq t < \infty$, with sample paths in $\overline{D} \times \mathbb{R}^3$ ($\overline{D}$ denotes the closure of D) is constructed in the following way. The sample paths

start at random positions $(\mathbf{X}, \mathbf{U})(0) \in D \times \mathbb{R}^3$, the distribution of which is governed by the probability density function g. The sample paths are piecewise characteristic. The first characteristic segment runs from $(\mathbf{X}, \mathbf{U})(0)$ to either a point $(\mathbf{x}, \mathbf{u}) \in \Gamma^+$, or extends to infinity, or remains at a fixed point (if $\mathbf{U}(0) = 0$). When a characteristic terminates at a point $(\mathbf{x}, \mathbf{u}) \in \Gamma^+$, the sample path is reflected and continues as a characteristic that emanates from $(\mathbf{x}, \tilde{\mathbf{u}}) \in \Gamma^-$ and runs to Γ^+ or extends to infinity. The new velocity $\tilde{\mathbf{u}}$ is chosen, with probability α, to be distributed with density $(2/(\pi T^2))|\tilde{\mathbf{u}} \cdot \mathbf{n}|e^{-\tilde{\mathbf{u}}^2/T}$, and with probability $1 - \alpha$, to have the value $\tilde{\mathbf{u}} = \mathbf{u}^*$.

We denote by $\mu(t)$ the probability distribution of $(\mathbf{X}, \mathbf{U})(t)$ and call $\mu(t)$ the *mild solution* of problem (2.1)–(2.3). The solutions of the free molecular flow problem analyzed in this paper are the mild solutions.

The free molecular flow problem has been analyzed in the framework of semigroups in L^p, where $1 \leq p < \infty$ [10, Chap. 21]. Although we make no use of this here, we state the following facts for completeness (see the forthcoming paper [6] for details).

The mild solution $\mu(t)$ is an absolutely continuous probability measure in $D \times \mathbb{R}^3$ (thus $\mu(t)$ can be viewed as a nonnegative element of $L^1(D \times \mathbb{R}^3)$ of integral one). The family of operators $T(t)$, defined by setting $T(t)g = \mu(t)$, is a strongly continuous semigroup of contractions in $L^1(D \times \mathbb{R}^3)$, with infinitesimal generator $-\mathbf{u} \cdot \nabla_{\mathbf{x}}$.

3. Molecular flights between surfaces. We now restrict our attention to the domains D_h, defined in (1.1). For each h, we denote by $(\mathbf{X}, \mathbf{U})_h(t)$ the stochastic process defined above, for the domain D_h, with initial probability density function g_h.

Denote by $(X, Y)_h(t)$ the first two components of $(\mathbf{X}, \mathbf{U})_h(t)$. For each $t \geq 0$, denote by $\nu_h(t)$ the probability distribution of $(X, Y)_h(t)$. Thus, for every Borel set $S \subset \mathbb{R}^2$,

$$\nu_h(t)(S) = \mu_h(t)(S \times [0, h] \times \mathbb{R}^3).$$

By definition, $\nu_h(0)$ is absolutely continuous, and its Radon–Nikodym derivative is the initial planar density, given by

$$(x, y) \mapsto \int_0^h \int_{\mathbb{R}^3} g_h(x, y, z, \mathbf{u}) d\mathbf{u} dz.$$

We will show that ν_h converges to the solution of a diffusion equation in $\mathbb{R}^2$.

In the following, for expository clarity, we use physical terminology for certain mathematical objects and relations. The precise mathematical statements should be clear from the context. For example, we call sample paths of the process $(\mathbf{X}, \mathbf{U})_h(t)$ *flights*, and one or more characteristic pieces of these sample paths *flight segments*. We refer, even more informally, to the flights of a *molecule*, and write that the molecule is reflected specularly or diffusely.

Consider the diffuse reflection of a molecule from the lower or upper surface at $(x, y) = (0, 0)$. Its velocity is distributed in the half-space $\mathbb{R}^2 \times \mathbb{R}^+$, at the lower surface, or $\mathbb{R}^2 \times \mathbb{R}^-$, at the upper surface, according to the probability density function

$$\frac{2}{\pi T^2} |w| \, e^{-\mathbf{u}^2/T} \tag{3.1}$$

(observe that $|w| = |\mathbf{u} \cdot \mathbf{n}|$). The horizontal coordinates of the point of impact with the opposite surface are given by $h\tilde{\xi}$, where $\tilde{\xi}$ is a radially symmetric $\mathbb{R}^2$-valued random

variable of length $\sqrt{u^2+v^2}/|w|$. The distribution function of $\tilde{\xi}$ is given, at each $r>0$, by

$$P(|\tilde{\xi}|<r)=\frac{2}{\pi T^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{\sqrt{u^2+v^2}/r}^{\infty} we^{-\mathbf{u}^2/T}dwdudv=\frac{r^2}{1+r^2}. \tag{3.2}$$

Differentiating (3.2) with respect to r, we find that the probability density function of $|\tilde{\xi}|$, which we denote by $\tilde{G}$, is given by

$$\tilde{G}(r)=\frac{2r}{(1+r^2)^2}. \tag{3.3}$$

The components $\tilde{X},\tilde{Y}$ of $\tilde{\xi}$ are uncorrelated random variables—$E(\tilde{X}\tilde{Y})=0$—as is clear from the symmetry of $\tilde{\xi}$. However, they are not independent.

A molecule that leaves a surface with velocity distributed according to (3.1) collides with the opposite surface at time $h\tilde{\tau}$, where $\tilde{\tau}=1/|w|$. The expected flight time is given by $hE(\tilde{\tau})$, where

$$E(\tilde{\tau})=\frac{2}{\pi T^2}\int_0^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\tilde{\tau}(\mathbf{u})\,|w|\,e^{-\mathbf{u}^2/T}d\mathbf{u}=\frac{2}{T}\int_0^{\infty}\frac{1}{|w|}|w|\,e^{-w^2/T}dw=\sqrt{\frac{\pi}{T}}.$$

The flight segments that follow successive collisions are independent when all collisions are diffuse (this is the case when $\alpha=1$). In general, however, the segments are not independent; for example, the flight lengths and times prior to and following specular reflections are identical. Since the basis of our analysis is the application of a central limit theorem to the sums of the horizontal displacements between molecule-surface collisions, it is inconvenient to deal with dependent flight segments. Fortunately, this apparent difficulty is easily overcome by the following observation. The flights between successive diffuse reflections are independent and the displacement and flight duration between consecutive diffuse reflections are random variables whose distributions can be explicitly calculated (they depend on the accommodation coefficient α).

Let us denote by n the random number of specular reflections experienced by a molecule between successive diffuse reflections. The integer-valued random variable n has the following distribution. For each integer $k\geq 0$,

$$P(n=k)=\alpha(1-\alpha)^k, \tag{3.4}$$

and so n has expected value

$$E(n)=\sum_{k=0}^{\infty}k\alpha(1-\alpha)^k=\frac{1-\alpha}{\alpha},$$

and second moment

$$E(n^2)=\sum_{k=0}^{\infty}k^2\alpha(1-\alpha)^k=\frac{(1-\alpha)(2-\alpha)}{\alpha^2}.$$

We define the random variable ξ by setting $\xi=(1+n)\tilde{\xi}$, so that $h\xi$ is the horizontal displacement of a molecule between two successive diffuse reflections. Since n and $\tilde{\xi}$

are independent, we find, for each $r > 0$, that

$$\begin{aligned} P(|\xi| \le r) &= P\left((1+n)|\tilde{\xi}| \le r\right) \\ &= \sum_{k=1}^{\infty} P\left((1+n) = k \text{ and } k|\tilde{\xi}| \le r\right) \\ &= \sum_{k=1}^{\infty} P((1+n) = k) \int_0^{r/k} \tilde{G}(s)ds, \end{aligned}$$

and the probability density function G of $|\xi|$ is given by

$$G(r) = \sum_{k=1}^{\infty} \alpha(1-\alpha)^{k-1} k^{-1} \tilde{G}(k^{-1}r).$$

The durations of the flight segments immediately before and after specular reflections are the same. Thus, defining the random variable $\tau = (1+n)\tilde{\tau}$, we have that the length of time between successive diffuse reflections is given by $h\tau$. The expected duration is $hE(\tau)$, where $E(\tau) = E((1+n)\tilde{\tau}) = E(1+n)E(\tilde{\tau}) = \sqrt{\pi}/(\alpha\sqrt{T})$.

4. A central limit theorem for a deterministic number of flight segments. Having described the probability distributions of the horizontal displacements between successive diffuse reflections and of the durations of these flights, we continue by studying the distributions of sums of these random variables. For each positive integer k, we denote by S_k the sum $S_k = \sum_{i=1}^{k} \xi_i$, where the ξ_i denote independent realizations of the variable ξ. A molecule that begins its flight at the origin in $\mathbb{R}^2$ on one of the two bounding surfaces has reached the horizontal position hS_k as it experiences its kth diffuse reflection.

If the second moments of ξ were finite (it can easily be checked that $E(|\xi|^2) = \infty$), then the central limit theorem for random variables of finite variance would imply that hS_k converges, in distribution, to a normal distribution when $k = O(h^{-2})$. To find an appropriate k such that hS_k converges to a (nondegenerate) normal distribution, and to demonstrate this convergence, we proceed by finding an expansion arund the origin for the characteristic function of ξ. In contrast to the finite variance case, where the second-order Taylor expansion is used, we use an expansion with a logarithmic factor.

We first investigate $\tilde{\phi}$, the characteristic function of $\tilde{\xi}$, defined for $\lambda \epsilon \mathbb{R}^2$ by setting

$$\tilde{\phi}(\lambda) = E\left(e^{i\lambda\cdot\tilde{\xi}}\right).$$

LEMMA 4.1. *The characteristic function $\tilde{\phi}$ admits the asymptotic expansion*

$$\tilde{\phi}(\lambda) = 1 + \frac{|\lambda|^2}{2}\log|\lambda| + O(|\lambda|^2),$$

as $\lambda \to 0$.

Proof. Since $\tilde{\xi}$ has a radially symmetric distribution, the characteristic function $\tilde{\phi}$ is radially symmetric as well, and is given by the Bessel transform

$$\tilde{\phi}(\lambda) = \frac{1}{2\pi}\int_0^{\infty} \tilde{G}(r) \int_0^{2\pi} e^{i|\lambda|r\cos\theta} d\theta dr = \frac{1}{\pi}\int_0^{\infty} \frac{r}{(1+r^2)^2} \int_0^{2\pi} e^{i|\lambda|r\cos\theta} d\theta dr.$$

Making use of the change of variables $R = r|\lambda|$, we find that

$$\begin{aligned}
\tilde{\phi}(\lambda) - 1 &= \frac{1}{\pi}\int_0^\infty \int_0^{2\pi} \frac{r}{(1+r^2)^2}(e^{i|\lambda| r\cos\theta} - 1)d\theta dr \\
&= \frac{|\lambda|^2}{\pi}\int_0^\infty \int_0^{2\pi} \frac{R}{(|\lambda|^2+R^2)^2}(e^{iR\cos\theta} - 1)d\theta dR \\
&= \frac{|\lambda|^2}{\pi}\int_0^1 \int_0^{2\pi} \frac{R}{(|\lambda|^2+R^2)^2}(e^{iR\cos\theta} - 1)d\theta dR + O(|\lambda|^2) \\
&= \frac{|\lambda|^2}{\pi}\int_0^1 \int_0^{2\pi} \frac{R}{(|\lambda|^2+R^2)^2}\left(iR\cos\theta - \frac{1}{2}R^2\cos^2\theta + O(R^3)\right)d\theta dR + O(|\lambda|^2) \\
&= -\frac{|\lambda|^2}{2}\int_0^1 \frac{R^3}{(|\lambda|^2+R^2)^2}dR + O(|\lambda|^2) \\
&= -\frac{|\lambda|^2}{4}\left(\frac{-1}{1+|\lambda|^2} + \log(|\lambda|^2+1) - 2\log|\lambda|\right) + O(|\lambda|^2) \\
&= \frac{|\lambda|^2}{2}\log|\lambda| + O(|\lambda|^2).
\end{aligned}$$

□

We next find an appropriate expansion for the characteristic function ϕ of ξ, defined by

$$\phi(\lambda) = E\left(e^{i\lambda\cdot\xi}\right) = E\left(e^{i\lambda\cdot(1+n)\tilde{\xi}}\right).$$

LEMMA 4.2. *As* $\lambda \to 0$,

$$\phi(\lambda) = 1 + \frac{2-\alpha}{2\alpha^2}|\lambda|^2\log|\lambda| + O(|\lambda|^2).$$

Proof. We have that

$$\begin{aligned}
\phi(\lambda) &= \frac{1}{2\pi}\int_0^\infty \int_0^{2\pi} G(r)e^{i|\lambda| r\cos\theta}d\theta dr \\
&= \frac{1}{2\pi}\int_0^\infty \int_0^{2\pi} \sum_{k=1}^\infty \alpha(1-\alpha)^{k-1}k^{-1}\tilde{G}(k^{-1}r)e^{i|\lambda| r\cos\theta}d\theta dr \\
&= \sum_{k=1}^\infty \alpha(1-\alpha)^{k-1}\tilde{\phi}(k\lambda) \\
&= 1 + \frac{1}{2}\sum_{k=1}^\infty \alpha(1-\alpha)^{k-1}k^2|\lambda|^2\log|\lambda| + O(|\lambda|^2) \\
&= 1 + \frac{2-\alpha}{2\alpha^2}|\lambda|^2\log|\lambda| + O(|\lambda|^2).
\end{aligned}$$

□

An expansion for the characteristic function of hS_k now follows easily. From the independence of the ξ_i, we have that

$$E(e^{i\lambda\cdot hS_k}) = (E(e^{ih\lambda\cdot\xi}))^k = (\phi(h\lambda))^k = \left(1 + \frac{2-\alpha}{2\alpha^2}|\lambda|^2h^2\log h + O(h^2)\right)^k. \tag{4.1}$$

We can conclude from (4.1) that k should be $O(1/(h^2 \log h^{-1}))$ in order for the hS_k to converge to a normal distribution. A timescale can now be deduced such that the number of flight segments over the appropriately scaled time interval is of this order in h.

For real $t > 0$, define

$$m_h(t) = \left[\frac{t}{hE(\tau)}\right] = \left[\frac{\alpha\sqrt{T}\, t}{\sqrt{\pi} h}\right], \tag{4.2}$$

where $[a]$ denotes the largest integer less than or equal to a. Now fix a time $t > 0$ and define

$$t_h = t/h \log h^{-1}.$$

It follows from (4.1) that, as $h \to 0$,

$$(\phi(h\lambda))^{m_h(t_h)} \to e^{-t\sigma^2|\lambda|^2/2}, \tag{4.3}$$

where $\sigma^2 = (2-\alpha)\sqrt{T}/\alpha\sqrt{\pi}$. The limit in (4.3) is the characteristic function of a two-dimensional, normally distributed, random variable with covariance matrix $t\sigma^2$ times the identity matrix, whose probability density function $K_{t\sigma^2}$ is given by

$$K_{t\sigma^2}(x,y) = \frac{1}{2\pi t\sigma^2} e^{-(x^2+y^2)/2t\sigma^2}.$$

We denote the corresponding distribution by $\Phi_{t\sigma^2}$. An immediate consequence is that the probability distribution of $hS_{m_h(t_h)}$ converges weakly (i.e., in the dual space of the continuous and bounded functions on $\mathbb{R}^2$) to $\Phi_{t\sigma^2}$.

LEMMA 4.3. *As* $h \to 0$, $hS_{m_h(t_h)} \Rightarrow \Phi_{t\sigma^2}$.

(The symbol $\Rightarrow$ denotes convergence, in distribution, of the distribution of the random variables on the left-hand side to the distribution on the right-hand side.) This result can also be verified by use of Theorem 2 in [14, p. 128].

5. A central limit theorem for a random number of flight segments. We have proved that a molecule that is emitted at $(x,y) = (0,0)$ from one of the surfaces diffusely at time zero has an approximately normally distributed horizontal position after $m_h(t_h)$ diffuse reflections, where $m_h(t_h)$ is the integer part of the ratio of t_h to the expected duration between successive diffuse reflections. The actual number of collisions a molecule experiences is random. We see in this section that, nevertheless, the distribution of the horizontal position of the molecule at the time of the last collision experienced before time t_h converges to $\Phi_{t\sigma^2}$.

Denote by $N_h(t)$ the random variable whose value is the number of collisions experienced by the molecule before time t. That is,

$$h\sum_{i=1}^{N_h(t)} \tau_i \le t, \qquad h\sum_{i=1}^{N_h(t)+1} \tau_i > t$$

(the τ_i denote independent realizations of the variable τ).

Our goal in this section is to prove that $hS_{N_h(t_h)} \Rightarrow \Phi_{t\sigma^2}$. Observe that $N_h(t_h)$ is not independent of the ξ_i, since larger $|\xi_i|$ are more likely to require longer flight durations and hence are more likely to lead to smaller values of $N_h(t_h)$. Nevertheless,

it is sufficient, for the desired convergence theorem to hold, that $N_h(t_h)/m_h(t_h) \to 1$ in probability as $h \to 0$. In fact, stronger convergence holds.

LEMMA 5.1. *Let $t > 0$ be fixed. As $h \to 0$,*

$$\frac{N_h(t_h)}{m_h(t_h)} \to 1 \quad \textit{almost surely.}$$

Proof. From the definition of m_h, we have that

$$\frac{N_h(t_h)}{m_h(t_h)} = \frac{N_h(t_h)hE(\tau)}{t_h} \frac{t_h/hE(\tau)}{[t_h/hE(\tau)]}.$$

The second factor on the right-hand side obviously tends to 1 as h tends to zero. We must only show that the first factor tends to 1 almost surely. Observe that $N_h(t_h) = N_1(t_h/h)$. (This equation asserts the equality of two random variables and therefore, strictly speaking, depends on the way in which the underlying probability space Ω is chosen and the random variables are defined as functions on Ω. We assume that these choices are made so that Ω is independent of h and so that, for a given $\omega \in \Omega$, the molecular trajectory for gap height h is obtained from that for gap height 1 by scaling space and time: $(\mathbf{X}, \mathbf{U})_h(t)(\omega) = (h\mathbf{X}, \mathbf{U})_1(t/h)(\omega)$ for all $h > 0$, $t \geq 0$, $\omega \in \Omega$.) Thus

$$\lim_{h\to 0} \frac{N_h(t_h)hE(\tau)}{t_h} = \lim_{h\to 0} \frac{N_1(t_h/h)E(\tau)}{t_h/h} = \lim_{\tilde{t}\to\infty} \frac{N_1(\tilde{t})E(\tau)}{\tilde{t}} = 1$$

almost surely. The last equality is the statement from renewal theory that as the length of a time period tends to infinity, the number of renewals during the period, divided by the length of the period, tends (almost surely) to the inverse of the expected renewal time [9, Thm. 5.5.2]. □

In the finite variance case, a central limit theorem with a random number of terms is proved by Chung [9, Thm. 7.3.2.]. We prove an analogous theorem, using an adaptation of this proof, which avoids the Kolmogorov inequality. We need the following two lemmas.

LEMMA 5.2. *For all positive integers n and positive real B,*

$$P(\max_{k\leq n} |S_k| \geq B) \leq 2P(|S_n| \geq B).$$

Proof. It is clear from the symmetry of the ξ_i that the conditional probability

$$\frac{P(|S_n| \geq B \text{ and } \max_{k\leq n} |S_k| \geq B)}{P(\max_{k\leq n} |S_k| \geq B)} \geq \frac{1}{2},$$

and the lemma follows. □

LEMMA 5.3. *Let $t > 0$, $1 \geq \epsilon > 0$, and $\gamma > 0$ be given, and define $h_* = h/\sqrt{\epsilon^\gamma}$. Then*

$$\epsilon^\gamma m_h(t_h) \leq m_{h_*}(t_{h_*}) + 1.$$

Proof. We have that

$$\epsilon^\gamma m_h(t_h) \leq \epsilon^\gamma \frac{\alpha\sqrt{T}}{\sqrt{\pi}} \frac{t}{h^2 \log h^{-1}} \leq \frac{\alpha\sqrt{T}}{\sqrt{\pi}} \frac{t}{h_*^2 \log h_*^{-1}} \leq m_{h_*}(t_{h_*}) + 1,$$

as claimed. □

LEMMA 5.4. *Fix $t > 0$ and let k_h be a family of random integers such that as $h \to 0$,*

$$\frac{k_h}{m_h(t_h)} \to 1 \quad \textit{in probability.} \tag{5.1}$$

Then

$$hS_{k_h} \Rightarrow \Phi_{t\sigma^2}.$$

Proof. To make the notation less cumbersome, we set $M_h = m_h(t_h)$, for all h (t is fixed). Since $hS_{k_h} = hS_{M_h} + h(S_{k_h} - S_{M_h})$ and $hS_{M_h} \Rightarrow \Phi_{t\sigma^2}$, it suffices [5, Thm. 4.1] to prove that

$$h\,|S_{k_h} - S_{M_h}| \to 0 \quad \text{in probability.}$$

Let $1 \geq \epsilon > 0$ be fixed. We must estimate

$$P\left(h\,|S_{k_h} - S_{M_h}| \geq \epsilon\right) = \sum_{i=1}^{\infty} P\left(k_h = i \text{ and } |S_{k_h} - S_{M_h}| \geq \epsilon h^{-1}\right).$$

We estimate the right-hand side by separately considering k_h near M_h, and k_h away from M_h, showing that S_{k_h} is close to S_{M_h} in the former case, and that the latter case is unlikely.

For this purpose, an appropriate interval about M_h consists of the integers k such that $a_h \leq k \leq b_h$, where $a_h = [(1 - \epsilon^3/2)M_h] + 1$ and $b_h = [(1 + \epsilon^3/2)M_h] - 1$ (the square brackets again denote the greatest integer less than or equal to the real number enclosed by the brackets). Set $h_* = h/\sqrt{\epsilon^3}$. Then, for h sufficiently small,

$$b_h - a_h \leq \epsilon^3 M_h - 1 \leq M_{h_*}, \tag{5.2}$$

by Lemma 5.3.

By hypothesis (5.1) on k_h, $P(a_h \leq k_h \leq b_h) \geq 1 - \epsilon$ for all sufficiently small h. The total contribution from these values of k_h is estimated by

$$\begin{aligned}
&\sum_{i=a_h}^{b_h} P\left(k_h = i \text{ and } |S_{k_h} - S_{M_h}| \geq \epsilon h^{-1}\right) \\
&\leq \sum_{i=a_h}^{b_h} P\left(k_h = i \text{ and } \max_{a_h \leq j \leq b_h} |S_j - S_{M_h}| \geq \epsilon h^{-1}\right) \\
&\leq P\left(\max_{a_h \leq j \leq b_h} |S_j - S_{M_h}| \geq \epsilon h^{-1}\right) \\
&\leq 2P\left(\max_{1 \leq j \leq b_h - a_h} |S_j| \geq \epsilon h^{-1}\right) \\
&\leq 4P\left(|S_{M_{h_*}}| \geq \epsilon h^{-1}\right);
\end{aligned}$$

the last inequality follows from Lemma 5.2 and (5.2). Thus

$$P(h|S_{k_h} - S_{M_h}| \geq \epsilon) \leq P(k_h < a_h \text{ or } k_h > b_h)$$

$$
\begin{aligned}
&+ \sum_{i=a_h}^{b_h} P\left(k_h = i \text{ and } |S_{k_h} - S_{M_h}| \geq \epsilon h^{-1}\right) \\
&\leq \epsilon + 4P\left(|S_{M_{h_*}}| \geq \epsilon h^{-1}\right) \\
&= \epsilon + 4\,P\left(h_* |S_{M_{h_*}}(t)| \geq \frac{1}{\sqrt{\epsilon}}\right) \\
&\to \epsilon + \frac{4}{t\sigma^2} \int_{1/\sqrt{\epsilon}}^{\infty} e^{-r^2/2t\sigma^2} r dr, \qquad (5.3)
\end{aligned}
$$

as $h \to 0$. Since expression (5.3) tends to zero as $\epsilon \to 0$, the proposition is proved. □

As an immediate consequence of Lemmas 5.1 and 5.4, we obtain the following proposition.

PROPOSITION 5.5. *As* $h \to 0$, $hS_{N_h(t_h)} \Rightarrow \Phi_{t\sigma^2}$.

6. The diffusion limit. In §5 we studied the horizontal position, at the time of its last diffuse reflection prior to or at time t_h, of a molecule that is emitted diffusely from a surface at time $t = 0$, and found the limit as $h \to 0$ of the probability distribution of this position. We now investigate the distribution, at the exact time t_h, of the horizontal coordinates of a molecule that, at time zero, is located at an arbitrary state in $D_h \times \mathbb{R}^3$. Our main result, convergence to the solution of a diffusion equation, follows from integration of these distributions over all initial molecular states.

For $(\mathbf{x}, \mathbf{u}) \in D_h \times \mathbb{R}^3$, let $((X,Y)|(\mathbf{x},\mathbf{u}))_h(t)$ denote the horizontal position at time t of a molecule whose initial state is $(\mathbf{x}, \mathbf{u})$.

Fix $(\mathbf{x}_0, \mathbf{u}_0) \in D_1 \times \mathbb{R}^3$, with $w_0 \neq 0$. Let τ_0 denote the time of the first diffuse reflection of a molecule whose initial state is $(\mathbf{x}_0, \mathbf{u}_0)$ (note that τ_0 is random if $\alpha < 1$). Consider the family of initial states $(\mathbf{x}_0, \mathbf{u}_0)_h \in D_h \times \mathbb{R}^3$, defined by setting

$$(\mathbf{x}_0, \mathbf{u}_0)_h = (x_0, y_0, hz_0, \mathbf{u}_0).$$

The duration of the flight segment until the first diffuse reflection, of the molecule initially at state $(\mathbf{x}_0, \mathbf{u}_0)_h$, is given by $h\tau_0$. Similar to earlier notation, we denote by $N_h(t_1, t_2)$ the number of diffuse reflections experienced after time t_1 and before or at time t_2. Now set $k_h = N_h(h\tau_0, t_h) + 1$. Then the horizontal displacement of the molecule through time t_h is given by

$$((X,Y)|(\mathbf{x}_0,\mathbf{u}_0)_h)_h(t_h) - (x_0, y_0) = h\left(\chi + \sum_{i=1}^{k_h-1} \xi_i + \frac{(t_h - t_h^-)}{h\tau_{k_h}} \xi_{k_h}\right), \qquad (6.1)$$

where

$$t_h^- = \min\left\{h \sum_{i=0}^{k_h-1} \tau_i\,,\ t_h\right\}$$

is the time of the last diffuse reflection before or at time t_h (or the time t_h if $h\tau_0 > t_h$), and

$$\chi = (u_0, v_0) \min\left\{\tau_0\,,\ \frac{t_h}{h}\right\}.$$

Let $\Phi_{t\sigma^2}(x_0, y_0)$ denote the normal distribution introduced earlier, but now centered at (x_0, y_0).

LEMMA 6.1. *As* $h \to 0$, $((X,Y)|(\mathbf{x}_0,\mathbf{u}_0)_h)_h(t_h) \Rightarrow \Phi_{t\sigma^2}(x_0,y_0)$.

Proof. It is clear that $h\chi \to 0$ almost surely and, since $(t_h - t_h^-)/\tau_{k_h} < h$, that $\xi_{k_h}(t_h - t_h^-)/\tau_{k_h} \to 0$ almost surely as well. There remains to investigate the middle term of the right-hand side of (6.1).

We have that

$$\frac{k_h - 1}{m_h(t_h)} = \frac{N_h(h\tau_0, t_h)}{m_h(t_h)} = \frac{N_1(\tau_0, t_h/h)E(\tau)}{t_h/h - \tau_0} \frac{t_h/h - \tau_0}{E(\tau)m_h(t_h)}.$$

The second factor on the right-hand side clearly tends to 1 almost surely. As we saw in the proof of Lemma 5.1, the first factor also tends to 1 almost surely. Thus $(k_h - 1)/m_h(t_h) \to 1$ in probability, and, by the central limit theorem, Lemma 5.4,

$$h \sum_{i=1}^{k_h - 1} \xi_i \Rightarrow \Phi_{t\sigma^2}$$

□

Now let us consider the full stochastic process $(\mathbf{X}, \mathbf{U})_t$, i.e., the flight of a molecule with a random initial state. The following theorem can be shown to hold for a wider class of initial data, but for brevity we assume as initial data the functions g_h, defined by the scaling

$$g_h(\mathbf{x}, \mathbf{u}) = \frac{1}{h} g\left(x, y, \frac{z}{h}, \mathbf{u}\right),$$

for all $(\mathbf{x}, \mathbf{u}) = (x, y, z, \mathbf{u}) \in D_h \times \mathbb{R}^3$, where $g \geq 0$ and $\int_{D_1 \times \mathbb{R}^3} g = 1$. In particular, the initial planar density

$$\rho_0(x,y) = \int_{\mathbb{R}^3} \int_0^h g_h(x,y,z,\mathbf{u}) dz d\mathbf{u}$$

does not depend on h.

THEOREM 6.2. *Let* ρ *be the solution of the diffusion equation*

$$\frac{\partial \rho}{\partial t} = \frac{(2-\alpha)\sqrt{T}}{2\alpha\sqrt{\pi}} \left(\frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2} \right),$$

with initial condition

$$\rho(x,y,0) = \rho_0(x,y).$$

Denote by $\rho(t)$ *the function* $\rho(t)(x,y) = \rho(x,y,t)$ *and by* $\nu(t)$ *the probability measure with probability density function* $\rho(t)$. *Fix* $t > 0$. *Then as* $h \to 0$,

$$\nu_h(t_h) \rightharpoonup \nu(t),$$

where the symbol $\rightharpoonup$ *denotes weak convergence of the measures.*

Proof. Let $S \subset \mathbb{R}^2$ be a Borel set. Then

$$\begin{aligned}
\nu_h(t_h)(S) &= P((X,Y)_h(t_h) \in S) \\
&= \int_{D_h \times \mathbb{R}^3} P(((X,Y)|(\mathbf{x}_0,\mathbf{u}_0))_h(t_h) \in S)\ g_h(\mathbf{x}_0,\mathbf{u}_0) d\mathbf{x}_0 d\mathbf{u}_0 \\
&= \int_{D_1 \times \mathbb{R}^3} P(((X,Y)|(\mathbf{x}_0,\mathbf{u}_0)_h)_h(t_h) \in S)\ g(\mathbf{x}_0,\mathbf{u}_0) d\mathbf{x}_0 d\mathbf{u}_0,
\end{aligned}$$

by Fubini's theorem.

From Lemma 6.1, we have that, for all $(\mathbf{x}_0, \mathbf{u}_0) \in D_1 \times \mathbb{R}^3$,

$$P(((X,Y)|(\mathbf{x}_0,\mathbf{u}_0)_h)_h(t_h) \in S) \;\to\; \frac{1}{2\pi t\sigma^2}\int_S e^{-((x-x_0)^2+(y-y_0)^2)/2t\sigma^2}\,dxdy$$

as $h \to 0$. Consequently, by the Lebesgue dominated convergence theorem and Fubini's theorem,

$$\begin{aligned}
\nu_h(t_h)(S) &\to \int_{D_1\times\mathbf{R}^3}\left[\frac{1}{2\pi t\sigma^2}\int_S e^{-((x-x_0)^2+(y-y_0)^2)/2t\sigma^2}\,dxdy\right] g(\mathbf{x}_0,\mathbf{u}_0)dx_0dy_0dz_0d\mathbf{u}_0\\
&= \int_S\left[\frac{1}{2\pi t\sigma^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\rho_0(x_0,y_0)e^{-((x-x_0)^2+(y-y_0)^2)/2t\sigma^2}\,dx_0dy_0\right]dxdy\\
&= \int_S \rho(x,y,t)\,dx\,dy\\
&= \nu(t)(S)
\end{aligned}$$

as $h \to 0$. □

7. Monte Carlo simulation. To illustrate the closeness of the approximation by diffusion for even fairly large values of h, we present the results of a Monte Carlo simulation of molecular trajectories in the slab domain. Consider the trajectory of a molecule that, at time zero, is located on one of the two surfaces, at $(x, y) = (0, 0)$, with velocity distributed according to the probability density function (3.1).

According to Lemma 6.1, the probability distribution of the x-coordinate at time t_h converges weakly to the normal distribution with variance $(2-\alpha)\sqrt{T}t/(\alpha\sqrt{\pi})$. In Fig. 7.1, we have plotted histograms computed from 5,000,000 molecular sample paths for two values of h, together with a graph of the limit normal distribution.

8. Most collisions do not contribute to diffusion. If we modify the stochastic process we have studied so far by prohibiting reflections into arbitrarily small sectors adjacent to the surface (i.e., the set of $\mathbf{u} \in \Gamma^-$ such that $w/|\mathbf{u}| < a$, for some real $a > 0$), the horizontal displacement between successive diffuse collisions is a variable of finite variance, and, consequently, there is no diffusion on a $1/(h \log h^{-1})$ timescale. Conversely, if we fix a sector adjacent to the surface and replace by zero the horizontal displacements that follow reflections outside of this sector, then the diffusion limit is unchanged. In fact, we can even let the sector vanish in the $h\to 0$ limit without affecting this result. Thus a vanishingly small fraction of the flight segments accounts for all of the diffusion. For simplicity, we assume in this section that $\alpha = 1$ and that there are exactly $m_h(t_h)$ collisions (the extension to the general problem studied above is straightforward).

Let R_h be a family of positive reals. The probability that a flight segment leads to a displacement greater than $h\,R_h$ is given by

$$P(|\xi| > R_h) = \int_{R_h}^{\infty}\frac{2r}{(1+r^2)^2}dr = \frac{1}{1+R_h^2},$$

which tends to zero as $h\to 0$ if $R_h\to\infty$. Nevertheless, if all of the flight segments with $|\xi| \le R_h$ are replaced by flights of zero length, the diffusion limit is unchanged as long as R_h grows sufficiently more slowly than $1/h$.

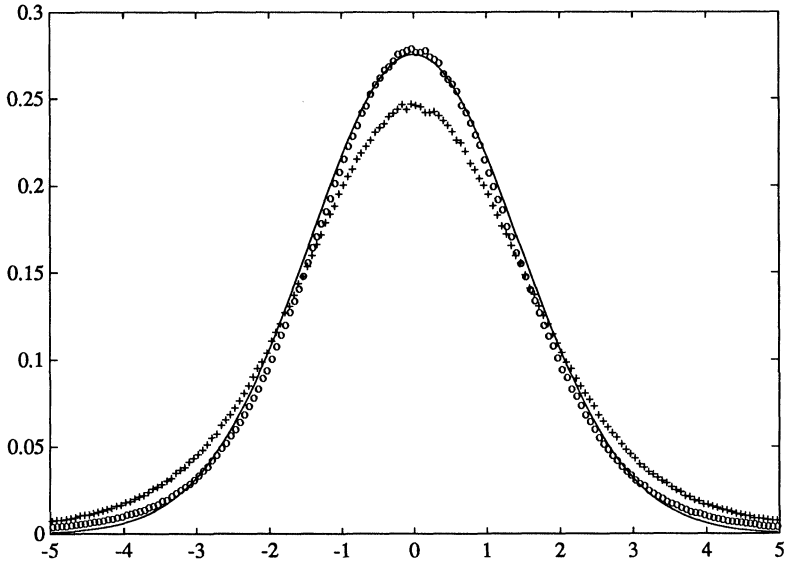

FIG. 7.1. *Distributions of the x-coordinate at time t_h. Histograms for $h = 0.25$ ("+") and $h = 0.025$ ("o"), and the graph of the limit density (solid line). The parameters $\alpha = 0.7$, $T = 1$, and $t = 2$ were used.*

PROPOSITION 8.1. *Assume that $\log R_h / \log h^{-1} \to 0$ as $h \to 0$, and denote by Θ_h the characteristic function of the interval $]R_h, \infty[$. Then*

$$h \sum_{i=1}^{m_h(t_h)} \Theta_h(|\xi_i|)\xi_i \;\Rightarrow\; \Phi_{t\sigma^2}$$

as $h \to 0$.

Proof. By Lemma 4.3,

$$h \sum_{i=1}^{m_h(t_h)} (1 - \Theta_h(|\xi_i|))\xi_i \;+\; h \sum_{i=1}^{m_h(t_h)} \Theta_h(|\xi_i|)\xi_i = h \sum_{i=1}^{m_h(t_h)} \xi_i \;\Rightarrow\; \Phi_{t\sigma^2}.$$

Thus it suffices to prove that $h\sum_{i=1}^{m_h(t_h)}(1 - \Theta_h(|\xi_i|))\xi_i \to 0$ in probability.

By symmetry, the random variable $(1 - \Theta_h(|\xi|))\xi$ has zero expectation. Since we have assumed that $\alpha = 1$, the probability density function of $|\xi|$ is the function $\tilde{G}$ defined in (3.3), and the covariance matrix of $(1 - \Theta_h(|\xi|))\xi$ is the identity matrix multiplied by γ_h^2, where

$$\begin{aligned}\gamma_h^2 &= \frac{1}{2} E\left((1 - \Theta_h(|\xi|))|\xi|^2\right) \\ &= \int_0^{R_h} \frac{r^3}{(1+r^2)^2} dr \\ &= \frac{1}{2}\left(\log(1 + R_h^2) - \frac{R_h^2}{1 + R_h^2}\right).\end{aligned}$$

By the central limit theorem for double arrays [9, Thm. 7.1.2], the series

$$\frac{\sum_{i=1}^{m_h(t_h)}(1-\Theta_h(|\xi_i|))\xi_i}{\sqrt{m_h(t_h)}\sqrt{\gamma_h^2}}$$

converges in distribution, as $h\to 0$, to a normal distribution.

By the definition of m_h and the hypothesis on R_h,

$$h\sqrt{m_h(t_h)}\sqrt{\gamma_h^2} \;\to\; 0,$$

as $h\to 0$. Consequently,

$$h\sum_{i=1}^{m_h(t_h)}(1-\Theta_h(|\xi_i|))\xi_i = \frac{\sum_{i=1}^{m_h(t_h)}(1-\Theta_h(|\xi_i|))\xi_i}{\sqrt{m_h(t_h)}\sqrt{\gamma_h^2}}\; h\sqrt{m_h(t_h)}\sqrt{\gamma_h^2}$$
$$\to 0 \quad \text{in probability.}$$

□

9. Regions of finite length. The above results for infinitely long domains can be extended to the case of semi-infinite and finite length domains. For example, consider the region located between two semi-infinite flat plates separated by a distance h, $\{(x,y,z) : x\in\mathbb{R}^+, y\in\mathbb{R}, z\in\,]0,h[\}$. Let Maxwell's boundary condition apply on the surfaces $\mathbb{R}^+\times\mathbb{R}\times\{0,h\}$, and let the vacuum boundary condition be given on $\{0\}\times\mathbb{R}\times\,]0,h[$: $f(0,y,z,\mathbf{u},t)=0$ if $u>0$.

A mild solution can be defined from the obvious generalization of the stochastic process defined in §2. The only necessary change is that sample paths be absorbed when they reach the open boundary $x=0$. Of course, contrary to the case of §3, the integral of the distribution function f now decreases with time.

A diffusion limit can be deduced from the analysis above and a reflection principle which is well known in similar contexts [11]. We sketch the ideas very briefly. Let the family of initial conditions

$$f(x,y,z,\mathbf{u},0)=\frac{1}{h}g\left(x,y,\frac{z}{h},\mathbf{u}\right)$$

be given. At time t, the density of molecules at location (x,y) is given by the integral, over (x',y'), of the probability that molecules get from (x',y') to (x,y) without leaving the domain by crossing the plane $x=0$. This probability is the total probability of traveling between the two regions minus the probability that the molecule exits the domain before time t and then gets to (x,y). The latter probability approaches, as $h\to 0$, the probability that a molecule travels from $(-x',y')$ to (x,y). Consequently, the density as $h\to 0$ is given by the solution to the problem in $\mathbb{R}\times\mathbb{R}\times\,]0,h[$ studied in §3, with oddly reflected initial data

$$\tilde{g}(x,y,z,\mathbf{u})=\begin{cases} g(x,y,z,\mathbf{u}) & \text{if } x>0,\\ -g(-x,y,z,\mathbf{u}) & \text{if } x<0.\end{cases}$$

This density is the solution of the following diffusion problem in $\{(x,y) : x\in\mathbb{R}^+, y\in\mathbb{R}\}$:

$$\begin{aligned}\rho_t &= \frac{(2-\alpha)\sqrt{T}}{2\alpha\sqrt{\pi}}(\rho_{xx}+\rho_{yy}),\\ \rho(x,y,0) &= \rho_0(x,y),\\ \rho(0,y,t) &= 0.\end{aligned}$$

Similarly, consider the domain $]0,1[\times \mathbb{R} \times]0,h[$, with boundary conditions

$$f(0,y,z,\mathbf{u},t) = 0 \quad \text{for } u > 0,$$
$$f(1,y,z,\mathbf{u},t) = 0 \quad \text{for } u < 0.$$

One can use the above reflection argument, but iterated infinitely often. The result is that, as $h \to 0$, we get the solution of the following diffusion problem in $\{(x,y) : x \in]0,1[, y \in \mathbb{R}\}$:

$$\begin{aligned} \rho_t &= \frac{(2-\alpha)\sqrt{T}}{2\alpha\sqrt{\pi}}(\rho_{xx} + \rho_{yy}), \\ \rho(x,y,0) &= \rho_0(x,y), \\ \rho(0,y,t) &= 0, \\ \rho(1,y,t) &= 0. \end{aligned}$$

10. On the diffusion limit in thin tubes. In this section, we compare the diffusion limit established in §6 for free molecular flow in plane channels to the diffusion limit of free molecular flow in the tubes, $D_h = \{(x,y,z) : x \in \mathbb{R},\ y^2 + z^2 \le h^2\}$. Refer to [1] for a fuller treatment of this problem, including a proof that the molecular trajectories converge to a Brownian motion.

Consider a molecule that is scattered from the boundary at the point $(x,y,z) = (0,0,-h)$, with velocity (u,v,w) distributed (over the space of velocities such that $w > 0$) according to the probability density function

$$\frac{2}{\pi T^2} w e^{-(u^2+v^2+w^2)/T}.$$

The next collision with the boundary occurs at the point

$$\begin{pmatrix} 0 \\ 0 \\ -h \end{pmatrix} + \frac{2hw}{v^2+w^2}\begin{pmatrix} u \\ v \\ w \end{pmatrix}.$$

We use much of the same notation as we did for the plane channel case, to denote the analogous random variables, and we denote the x-component of the difference between the two collision locations by $h\tilde{\xi}$, where $\tilde{\xi} = 2uw/(v^2+w^2)$.

The expectation of $\tilde{\xi}$ is zero and the variance of $\tilde{\xi}$ is

$$\begin{aligned} E(\tilde{\xi}^2) &= \frac{2}{\pi T^2}\int_0^\infty\int_{-\infty}^\infty\int_{-\infty}^\infty \frac{4u^2w^3}{(v^2+w^2)^2} e^{-(u^2+v^2+w^2)/T} du\,dv\,dw \\ &= \frac{4}{\sqrt{\pi T}}\int_0^\infty\int_{-\infty}^\infty \frac{w^3}{(v^2+w^2)^2} e^{-(v^2+w^2)/T} dv\,dw = \frac{8}{3}. \end{aligned}$$

The x-component of the difference between the locations of successive diffuse reflections is given by $\xi = (1+n)\tilde{\xi}$, where n has the distribution (3.4). Since n and $\tilde{\xi}$ are independent, the first and second moments of ξ are

$$E(\xi) = E(1+n)E(\tilde{\xi}) = 0$$

and

$$E(\xi^2) = E\left((1+n)^2\right) E\left(\tilde{\xi}^2\right) = \frac{8}{3}\left(E(1) + 2E(n) + E\left(n^2\right)\right) = \frac{8(2-\alpha)}{3\alpha^2}.$$

The duration of the flight segment immediately following a diffuse reflection is given by $h\tilde{\tau}$, where $\tilde{\tau} = 2w/(v^2+w^2)$, with expectation

$$hE(\tilde{\tau}) = \frac{2}{\pi T^2}\int_0^\infty\int_{-\infty}^\infty\int_{-\infty}^\infty \frac{2hw^2}{v^2+w^2}e^{-(u^2+v^2+w^2)/T}dudvdw$$
$$= \frac{4h}{\sqrt{\pi T^3}}\int_0^\infty\int_{-\infty}^\infty \frac{w^2}{v^2+w^2}e^{-(v^2+w^2)/T}dvdw = \frac{h\sqrt{\pi}}{\sqrt{T}},$$

as in the case of the slab domain. Set $\tau = (1+n)\tilde{\tau}$. The duration of the flight segment between successive diffuse reflections has expectation

$$hE(\tau) = hE(1+n)E(\tilde{\tau}) = h\sqrt{\pi}/(\alpha\sqrt{T}).$$

Let m_h be defined as in (4.2) and let $S_k = \sum_{i=1}^k \xi_i$, as before. However, contrary to plane channel timescale, it is appropriate here to set $t_h = t/h$. Observe that $h\,S_{m_h(t_h)}$ has expectation zero and variance

$$h^2 m_h(t_h)E(\xi^2) \approx \frac{8(2-\alpha)\sqrt{T}}{3\sqrt{\pi}\alpha}t$$

(equality does not generally hold because $m_h(t_h)$ is the integer part of $t_h/(hE(\tau))$).

By the central limit theorem, we have that as $h\to 0$,

$$hS_{m_h(t_h)} \Rightarrow \Phi_{t\sigma^2},$$

where $\Phi_{t\sigma^2}$ is the one-dimensional normal distribution of mean zero and variance $t\sigma^2$, and

$$\sigma^2 = \frac{8\sqrt{T}(2-\alpha)}{3\sqrt{\pi}\alpha}.$$

Observe that $m_h(t_h)$ is the integer part of the ratio of t_h to the expected duration between consecutive diffuse reflections. The actual number of collisions is random, but the techniques used for the plane channel problem can easily be applied to the present case (which is much easier because of the finiteness of the variance of ξ). The conclusion is that free molecular flow in thin tubes of diameter h leads to diffusion of the axial density (the number of molecules per unit length) on a timescale of $1/h$ and with a diffusion coefficient of $\sigma^2/2$.

Acknowledgments. This paper was inspired by our discussions with Claude Bardos about his work with Professors Babovsky and Platkowski on this subject. We also thank Ed Larsen and Mina Ossiander for their discussions with us about this work.

REFERENCES

[1] H. BABOVSKY, *On Knudsen flows within thin tubes*, J. Statist. Phys., 44 (1986), pp. 865–878.

[2] H. BABOVSKY, C. BARDOS, AND T. PLATKOWSKI, *Diffusion approximation for a Knudsen gas in a thin domain with accommodation on the boundary*, Asymptotic Anal., 3 (1991), pp. 265–289.

[3] C. BARDOS, F. GOLSE, B. PERTHAME, AND R. SENTIS, *The nonaccretive radiative transfer equations: Existence of solutions and Rosseland approximation*, J. Funct. Anal., 77 (1988), pp. 434–460.

[4] A. BENSOUSSAN, J.-L. LIONS, AND G. PAPANICOLAOU, *Boundary layers and homogenization of transport processes*, J. Pub. RIMS Kyoto Univ., 15 (1979), pp. 53–115.
[5] P. BILLINGSLEY, *Convergence of Probability Measures*, John Wiley, New York, 1986.
[6] C. BÖRGERS, C. GREENGARD, AND E. THOMANN, *The free molecular flow semigroup: A stochastic construction*, in preparation.
[7] A. BURGDORFER, *The influence of the molecular mean free path on the performance of hydrodynamic gas lubricated bearings*, ASME J. Basic Engrg., 81 (1959), pp. 94–100.
[8] C. CERCIGNANI, *The Boltzmann Equation and Its Applications*, Springer-Verlag, New York, 1988.
[9] K. L. CHUNG, *A Course in Probability,* 2nd ed., Academic Press, Orlando, FL, 1974.
[10] R. DAUTRAY AND J.-L. LIONS, *Analyse Mathematique et Calcul Numerique Pour les Sciences et les Techniques,* Tome 3, Masson, Paris, 1985.
[11] W. FELLER, *An Introduction to Probability Theory and its Applications,* Vol. 2, 2nd ed., John Wiley, New York, 1971.
[12] S. FUKUI AND R. KANEKO, *Analysis of ultra-thin gas film lubrication based on linearized Boltzmann equation: First report—derivation of a generalized lubrication equation including thermal creep flow*, ASME J. Tribology, 110 (1988), pp. 253–262.
[13] R. GANS, *Lubrication theory at arbitrary Knudsen number*, ASME J. Tribology, 107 (1985), pp. 431–433.
[14] B. GNEDENKO AND A. KOLMOGOROV, *Limit Distributions for Sums of Independent Random Variables*, Addison–Wesley, Reading, MA, 1954.
[15] W. GROSS, L. MATSCH, V. CASTELLI, A. ESHEL, J. VOHR, AND M. WILDMAN, *Fluid Film Lubrication*, John Wiley, New York, 1980.
[16] E. LARSEN AND J. KELLER, *Asymptotic solution of neutron transport problems for small mean free paths*, J. Math. Phys., 15 (1974), pp. 75–81.