Limit Theorems for Random Billiard Models

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Limit Theorems for Random Billiard Models

by

Timothy Chumley

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of Doctor of Philosophy

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Chapter 1

Introduction

This chapter presents an informal introduction to a general framework for creating simple random mechanical model systems which we call random billiards with microstructure. The main results of the thesis pertain to two mathematical models—one of gas particle diffusion through cylindrical channels and the other of a minimalistic heat engine—each of which is centered around the random billiard framework. Section 1.2 presents a rudimentary introduction to deterministic billiard systems needed to motivate random billiard models in general. Section 1.3, which presents a deterministic billiard system—an unfolding of Sinai’s celebrated billiard—and then derives a corresponding random billiard is a first example presented to give a flavor of random billiard models. The rest of the thesis is structured as follows. Chapter 2 introduces the cylindrical channel model and gives an overview of the results of a probabilistic analysis of the model. For the most part precise statements and proofs of the main probabilistic limit theorems are presented in Chapter 3. Chapter 4 presents a random billiard model of a minimalistic heat engine and a preliminary experimental analysis of its operation. One interesting aspect of the model, which is first alluded to at the end of Section 2.5, is its relationship with the channel of Chapters 2 and 3.
1.1 General framework and motivation

By a random billiard we mean a billiard system in which the standard rule of specular reflection is replaced with a Markov transition probabilities operator $P$—often referred to as a collision operator—that gives, at each collision of the billiard particle with the boundary of the billiard domain, the probability distribution of the post-collision velocity for a given pre-collision velocity. A random billiard with microstructure is a random billiard for which $P$ is derived from a choice of geometric or mechanical structure on the boundary of the billiard domain. More specifically, a Markov operator $P$ arising from a random billiard with microstructure is derived by the following general method. We select one or more dynamical variables of a given deterministic mechanical system and turn them into random variables with fixed in time probability distributions. It is natural to choose for the latter the asymptotic probability distribution that those variables attain in the original deterministic system. The result of this construction is a sequence of post-collision velocities that forms a Markov chain whose transition probabilities are governed by $P$ and whose dynamics are not far removed in certain ways from the deterministic system that gave rise to it. For example, in all of the models we present, the velocity factor of the flow-invariant measure in the phase space of the deterministic system becomes a stationary measure for the associated random process, suggesting that the deterministic and random systems have closely related ergodic theories. As physical motivation for such a construction, one might imagine that the measurement scale of the billiard system at the boundary is microscopic in a sense that from a macroscopic observer’s viewpoint, the post-boundary-collision scattering appears random. Figure 1.1 gives a somewhat fanciful example of a billiard system from which a random billiard with microstructure is defined.

From a more broad perspective, there are several sources of motivation for
Figure 1.1: An arbitrary wall system defining a random billiard with microstructure. One may choose to derive the operator $P$ by letting, for instance, the velocity of the spring-attached masses to be a Gaussian random variable with mean zero and variance a function of the spring constant.

random billiards with microstructure, some purely mathematical and others more applied. From the purely mathematical perspective, we have a well-motivated class of Markov chains and more general stochastic processes from which to study issues of general probabilistic interest such as nonstandard limit theorems. The generalized billiard systems of the kind considered may also provide worthwhile examples of random (often hyperbolic) dynamical systems with singularities— that is, random counterparts of the widely studied chaotic billiards for which [12] is a reference. From the more applied perspective, the processes studied may be useful in the study of kinetic theory of gases, as suggested in the model to be presented in Chapters 2 and 3 below. Further, the random billiard framework provides simple Newtonian models for the interaction of a molecule with a heat bath which can be used to study thermostatic action fairly explicitly from a probabilistic perspective. This idea in particular is the subject of Chapter 4.
1.2 Basic facts on deterministic billiards

This section gives a brief overview of some basic properties of deterministic billiards needed for our discussion of random billiards in the next section. Most importantly, is a description of the billiard flow-invariant volume in phase space and the so-called cosine law for billiard reflection.

Billiard systems, broadly conceived, are Hamiltonian systems on manifolds with boundary, the boundary points representing collision configurations. Most commonly, the configuration manifold is a region in the Euclidean plane having piecewise smooth boundary, although higher dimensional systems are widely studied and will be encountered throughout this paper. Higher dimensional billiards typically describe mechanical systems consisting of several rigid constituent masses interacting only through collisions. The configuration manifold is endowed with the Riemannian metric defined by the kinetic energy bilinear form. In particular, the (linear) collision map at boundary points of the configuration manifold is a linear isometry under the assumption of energy conservation. The collision map is often taken to be the standard Euclidean reflection, that is, a map that fixes all the vectors tangent to the boundary while sending a vector perpendicular to the boundary to its negative. In this paper the Riemannian metric on configuration space will always have constant coefficients (associated to masses of the constituent rigid parts of the system) and so will be an Euclidean metric.

Figure 1.2: A version of Sinai’s Billiard on the left, and the Bunimovich stadium on the right. These are two examples of ergodic billiard systems.
Figure 1.2 shows two famous examples of the basic kind of billiard system. In each case, the \textit{billiard table} is a planar region whose boundary consists of piecewise smooth curves; the \textit{billiard particle} undergoes uniform rectilinear motion in the interior of the region, bouncing off specularly after hitting the boundary.

In general, let $M$ denote the billiard’s configuration manifold. This is the planar regions in the 2-dimensional examples of Figure 1.2. The \textit{phase space} is the bundle of tangent vectors $TM$ on which one defines the \textit{flow map} $\varphi_t$. The flow map assigns to each time $t$ and tangent vector $(q, v) \in TM$ the state (i.e., the position and velocity) $\varphi_t(q, v)$ of the billiard trajectory at time $t$ having initial conditions $(q, v)$ at time 0.

It will be assumed here that the billiard particle is not subject to a potential function or any form of interaction other than elastic collision. For a more general perspective see [16]. Thus the speed of billiard trajectories (given in terms of the mechanically determined Riemannian metric) is a constant of motion, usually arbitrarily set to 1, and the flow map $\varphi_t$ is often restricted to the submanifold of unit vectors in $TM$. The precise definition of the billiard flow contains some important fine print, dealing with the issue of singular trajectories; for example, those trajectories that end at corners or graze the boundary of $M$. For the omitted details (in dimension 2) see [12].

A fact of special significance is that the billiard flow map leaves invariant a canonical volume form on phase space. There is also an associated invariant volume form on the space of unit vectors on the boundary of $M$. The existence of these invariant volumes is fundamental for the ergodic theory of billiard systems and for the probability theory we wish to employ later, so we take a moment to describe them in detail. Let $d$ be the dimension of $M$ and $S^+$ the subset of $TM$ consisting of unit vectors at boundary points of $M$ pointing towards the interior.
Figure 1.3: A piece of the boundary of a billiard region, showing the unit hemisphere at a point \( q \). The unit normal vector \( n \) points to the interior of the \( d \)-dimensional manifold \( M \) and \( v \) is a unit tangent vector to \( M \) at \( q \) forming an angle \( \theta \) with \( n \). If \( d\omega \) denotes the \((d-1)\)-dimensional volume on the unit hemisphere at the boundary point \( q \) of \( M \), then \( d\nu = \cos \theta \, d\omega \) is the factor of the invariant volume accounting for velocities at \( q \).

The unit normal vector \( n_q \) is contained in \( S^+_q \); we denote by \( \theta \) the angle between a given \( v \in S^+_q \) and \( n_q \) and by \( d\omega(v) \) the \((d-1)\)-dimensional volume element at \( v \) over \( S^+_q \). Also let \( dV(q) \) denote the volume element at \( q \) on the boundary of \( M \) (associated to the induced Riemannian metric). The billiard flow \( \varphi_t \) induces a map \( T \) on \( S^+ \) as follows: for each \( v \in S^+_q \) write \( (q(t), v(t)) = \varphi_t(q, v) \), where \( t \) is the moment of next collision with the boundary; then \( T(q, v) := (q(t), \overline{v(t)}) \), where \( \overline{v} \) indicates the reflection of \( v \) back into \( S^+ \). We refer to \( T \) as the billiard map. The transformation \( T \) is said to preserve, or leave invariant a measure \( \nu \) on \( S^+ \) if (writing \( u = (q, v) \))

\[
\int_{S^+} f(u) \, d\nu(u) = \int_{S^+} f(T(u)) \, d\nu(u)
\]

for every integrable function \( f \). The next proposition is well-known.

**Proposition 1.1.** \( T \) leaves invariant on \( S^+ \) the measure element

\[
d\nu(q, v) := \cos \theta \, dV(q) \, d\omega(v).
\]  

(1.1)

For a proof (of a more general expression) under much more general conditions
that allow for potentials and non-flat Riemannian metrics see [16].

Figure 1.4: With probability 1, the set of return points to a piece of the boundary of an ergodic billiard satisfies the cosine law: the post-collision angles \( \theta \in [-\pi/2, \pi/2] \) have the distribution \( d\mu(\theta) := \frac{1}{\pi} \cos \theta \, d\theta \). The set of positions, indicated by \( r \) in the figure, are distributed uniformly. Polygonal (and polyhedral) billiard tables, as in the figure, will often appear below, although it is not well understood when such billiards are ergodic. See [22] for further remarks.

The existence of this invariant measure on \( S^+ \) is the starting point of the ergodic theory of billiard systems. We always assume that the measure is finite and typically rescale it so that \( \nu(S^+) = 1 \); in this case it is natural to interpret \( \nu \) as a probability measure. A billiard system is said to be \textit{ergodic} if \( S^+ \) cannot be decomposed as a disjoint union of two measurable subsets, both invariant under \( T \) and having positive measure relative to \( \nu \). Ergodicity can also be expressed in terms of the equality of time and space means:

\[
\lim_{N \to \infty} \frac{1}{N} \sum_{i=0}^{N-1} f(T^i(q,v)) = \int_{S^+} f(q,v) \, d\nu(q,v), \quad (1.2)
\]

where \( f \) is any integrable function on \( S^+ \). (See [25] for a general reference for ergodic theory as a chapter in the mathematical theory of dynamical systems.) The existence of the limit, and the equality in 1.2 under the ergodicity assumption, is the content of the celebrated ergodic theorem of Birkhoff. Below, we refer to the identity itself as the \textit{ergodic theorem}.

Proving that a billiard system is ergodic is generally a technically difficult task. In fact, a significant part of the general theory of dynamical systems, particularly hyperbolic (strongly chaotic) systems, has been developed in pursuit of establish-
ing ergodicity for such statistical mechanical systems as hard spheres models of a
gas. (See, e.g., [4] or [9], chapter 8.)

An immediate consequence of the ergodic theorem is that the long term dis-
tribution of post collision angles of an ergodic billiard in any dimension satisfies
the cosine law, whereas the distribution of collision points on the boundary of
\( M \) is uniform relative to the measure \( dV \). More precisely, let \( v_1, v_2, \ldots \) be the
velocities immediately after collisions registered at each moment that a billiard
trajectory returns to a segment of the boundary of \( M \) having positive measure.
Then for almost all initial conditions the set of angles is distributed according to
\( d\mu(v) = C \langle n, v \rangle d\omega(v) \), where \( C \) is a normalizing constant and the angle brackets
denote inner product and \( \langle n, v \rangle = \cos \theta \), where \( \theta \) is the angle between \( v \) and \( n \).

1.3 An unfolding of Sinai’s billiard

This section presents an example deterministic system and then derives our first
example of a random billiard system. While the example presented will not be
revisited, it gives a flavor for the models to come.

1.3.1 Asymptotic distributions

The billiard table of Figure 1.5 represents a container divided in two chambers
by a porous solid screen composed of small circular scatterers. The scatterers are
separated by small gaps. A billiard particle represents a spherical gas molecule.
One is interested, for example, in how a “gas” consisting of a large number of
billiard particles injected at time \( t = 0 \) into, say, the left chamber, will expand to
fill up the entire container.

This billiard table can be regarded as an “unfolding” of Sinai’s billiard shown
Figure 1.5: A billiard model of a container divided by a solid porous screen consisting of small circular scatterers separated by small gaps.

on the left of Figure 1.2, and from this observation it can be shown that the associated billiard flow is ergodic. Figure 1.5 shows one long segment of trajectory, indicating the initial velocity vector and the image of that vector under the billiard flow at time $t$. This is an example of a (semi-) dispersing billiard, which are well-studied models of chaotic dynamics (see [12]). Trajectories are highly unstable in their dependence on initial conditions due to the presence of the circular scatterers.

Consider Figure 1.6, where we focus on one fundamental cell of the solid screen. We define the reduced phase space of this system as the set

$$ S = \{0, 1\} \times [0, 1] \times [-\pi/2, \pi/2]. $$

A state of the form $(k, r, \theta)$ gives the initial condition of a trajectory that enters into the scattering region from the left ($k = 0$) or the right ($k = 1$) chamber at a position $r$ in the interval $[0, 1]$, with velocity $v = (-1)^k \cos \theta e_1 + \sin \theta e_2$, where $e_1$ and $e_2$ are the standard basis vectors of $\mathbb{R}^2$. The reduced billiard map $T : S \to S$ then gives the end state of a trajectory that begins and is stopped at $S$. The billiard motion on the full table is an appropriate composition of $T$ with a similar return map on a rectangular table.

Given a long trajectory of a billiard particle, we register the values $k_1, k_2, \ldots$ in $\{0, 1\}$, which is the sequence of sides of the container the particle occupies at each moment it enters the scattering region; $r_1, r_2, \ldots$ in $[0, 1]$, the sequence of
Figure 1.6: The core of the dynamics of the divided chambers billiard can is in the motion near a fundamental cell of the scattering screen.

positions along the flat boundary segments of the fundamental cell at which the particle enters the region; and \( \theta_1, \theta_2, \ldots \) in \([-\pi/2, \pi/2]\), the sequence of angles the particle’s velocity makes with the normal vector to those boundary segments.

A remark about the first sequence will be observed shortly; first note that the long term distribution of the \( r_i \) is uniform along the unit interval. This follows from the above observation on the form of the invariant measure and the ergodic theorem, and is observed in the numerical experiment of Figure 1.7.

Figure 1.7: Long term distribution of entry positions into a fundamental cell of the scattering screen. The graph was obtained by numerically simulating the billiard motion over a period of \( 10^7 \) entries into the scattering region.

The distribution of the angles \( \theta_i \) is given, as expected, by the cosine law. This is shown in Figure 1.8. Finally, we remark that the asymptotic fraction of particles on each side of the chamber is \( 1/2 \) but omit numerical evidence.
1.3.2 A random billiard derived from Sinai’s billiard

We are now ready to construct our random billiard. Recall that the general idea is as follows. Starting with the deterministic system—in this case the unfolding of Sinai’s billiard—we take some of its dynamical variables and assume that they are random variables. The resulting system will be expressed as a Markov chain with non-discrete state space. The selection of variables and choice of probability law assumed for them can vary, but we use the following procedure: the probability law for a given random variable is taken to be the asymptotic distribution that the variable assumes in the deterministic system from which the random system is derived.

For our example at hand, we do the following. The screen of circular scatterers is replaced with a vertical line. Upon colliding with this line, the billiard particle changes both direction and chamber as prescribed by transition probabilities with state space \( S' = \{0, 1\} \times [-\pi/2, \pi/2] \), where the first factor indicates as before the side of the divided container (0 for left and 1 for right) and the second factor gives the angle along which the particle impinges on or scatters off the dividing screen. Recall the deterministic map \( T \) defined on the reduced phase space \( \{0, 1\} \times [0, 1] \times [-\pi/2, \pi/2] \) of the fundamental cell shown in Figure 1.6. The velocity and chamber of the billiard particle immediately after collision with the scattering line are then
defined to be random variables obtained from $T$ and the pre-collision side and angle variables by letting the position $r \in [0, 1]$ be random, uniformly distributed over the unit interval.

To obtain the transition probabilities operator, we refer back to the notation set in Figure 1.6. We wish to describe the transition probabilities kernel on $S'$ as a family of probability measures $\mu_{k,\theta}$ indexed by the elements of $S'$. If $f$ is any bounded measurable function on $S'$, then by definition the conditional expectation of $f$ evaluated on the post-collision state, given the pre-collision state $(k_-, \theta_-)$ is

$$(Pf)(k_-, \theta_-) := \int_{S'} f(k_+, \theta_+) \, d\mu_{k_-, \theta_-}(k_+, \theta_+) := \int_0^1 f(T(k_-, r, \theta_-)) \, dr$$

where $T$ is the reduced billiard map of the fundamental cell of Figure 1.6 and $r \in [0, 1]$ is the position coordinate along either of the entry line segments.

![Figure 1.9: A random billiard model for the divided container experiment. The screen of circular scatterers is replaced with a scattering line.](image)

Thus, in this model of random billiard we have replaced the screen of scatterers by a line segment separating the two chambers and a scattering (Markov) operator $P$ that updates the direction of the velocity at every collision with that line segment. It turns out that the operator $P$ has many nice properties. First, the measure $\overline{\mu}$ which assigns probability $1/2$ to $k = 0, 1$ and the cosine distribution to $\theta$ turns out to be the unique stationary distribution for $P$. Second, $P$ can be defined on the Hilbert space of square-integrable functions on $S$ with the measure
$\mu$, where it is a self-adjoint operator of norm 1. We refer to [16, 18, 19] for more information about similar operators and their spectral theory.
Chapter 2

First look at the channel model

This chapter is intended to be an introduction to a random billiard model of gas diffusion in cylindrical channels of the form $\mathbb{R}^k \times \mathbb{B}^{n-k}$ and a first look at corresponding results. The main technical results and their precise statements are left to Chapter 3. The current chapter is organized as follows. Section 2.1 presents an idealized experiment of gas diffusion through a channel with a “microscopically rough” boundary surface and asks how transport properties of the gas are affected by such roughness. Section 2.2 introduces the collision operators of interest and the stationary distributions of the Markov chains they define. Section 2.3 presents two of the main (random) observables of interest—the displacement of the gas along the channel’s major axis between collisions and the flight time between collisions—and how certain moments of these observables are affected by the dimensions of the channel. Section 2.4 gives a preview of the main technical result of the model: one-dimensional projections of the particle’s path converge to a Brownian motion with diffusion constant expressed in terms of the spectrum of the defining collision operator. Section 2.5 concludes the chapter with a series of examples which begin to show how the shape of the surface contour can influence diffusion through the channel.
2.1 An idealized experiment and the main question

Figure 2.1 depicts an ideal experiment in which a small amount of gas composed of point-like, non-interacting masses is injected into a (for simplicity of exposition 2-dimensional) channel and the amount of outflowing gas per unit time is recorded. The graph on the right-hand side shows a typical exit flow curve. Possible gas transport characteristics that can be obtained from such an experiment are the mean value and higher moments of the molecular time of escape.

The central question then is: what can these time characteristics of the gas outflow tell us about the microscopic interaction (i.e., scattering properties) between gas molecules and the surface of the plates?

For a more precise formulation of this question, we begin by describing the classical surface scattering operators that model the microscopic collisions of the point mass. We refer to the boundary of the channel region as the (wall) surface, irrespective of its actual dimension.

Let $\mathbb{H}$ denote the upper-half plane, consisting of vectors $(v_1, v_2)$ with positive second component. Elements of $\mathbb{H}$ represent velocities of a point mass immediately after a collision with the surface. By identifying $(v_1, -v_2)$ and $(v_1, v_2)$, we may regard pre-collision velocities as also being in $\mathbb{H}$. A collision event is then specified by a measurable map $v \in \mathbb{H} \mapsto \eta_v \in \mathcal{P}(\mathbb{H})$, where $\mathcal{P}(\mathbb{H})$ indicates the space of probability measures on the upper-half plane. The measurability condition is understood as follows: For every essentially bounded Borel measurable function $\phi$ on $\mathbb{H}$, the function

$$v \mapsto (P\phi)(v) := \int_{\mathbb{H}} \phi(u) \, d\eta_v(u)$$
is also measurable. We refer to $P$ as the collision operator. This operator specifies the transition probabilities of Markov chains with state space $\mathbb{H}$ giving the sequence of post-collision velocities from which the molecular random flight inside the channel can be obtained. That is, if $P$ acts on an indicator function $\mathbb{1}_A$ for some measurable set $A \subset \mathbb{H}$ then one can think of $P\mathbb{1}_A(v)$ as the probability that velocity of the point mass immediately after collision falls in the set $A$ given that it’s precollision velocity was $v$.

![Figure 2.1](image)

**Figure 2.1:** Idealized experiment in which a small pulse of gas is injected into a 2-dimensional channel and the gas outflow is recorded. The graph on the right represents the rate at which gas escapes. From this function it is possible to derive mean exit time of escape $\tau$. The main problem is to relate easily measured properties of the gas outflow, such as $\tau$, to the microscopic scattering characteristics of the channel surface.

If now $\tau = \tau(L, r, s)$ denotes the expected exit time of the random flight, where $s$ is the molecular root-mean square velocity, then a more restricted form of the general question is to understand how $\tau$ depends on $P$. (This expected exit time is easily measured in actual experiments involving gas diffusion using the rate of gas outflow as represented on the right hand side of Figure 2.1; see, for example, [29] for so-called TAP-experiments in chemical kinetics.)

Although the analysis of $P$ is generally simpler in dimension 2, an interesting complication arises here that is not present in the case of a 3-dimensional cylinder; namely, with respect to the stationary distribution of velocities for natural collision operators (see the next subsection), molecular displacement between collisions
has infinite variance and standard central limit theorems for Markov chains do not apply. The same is true for the random flight in the region $\mathbb{R}^2 \times [-r, r]$ between two parallel plates. In this regard, the random flight in a 3-dimensional cylindrical channel is simpler. (For an early study of two parallel plates case, see in [7].) Infinite variance of the in-between collisions displacements requires a generalization of the central limit theorem of Kipnis and Varadhan in [26] that is proved in this paper.

Now, from an appropriate central limit theorem we obtain for $\tau$ the asymptotic expression

$$
\tau(L, r, s) \sim \frac{L^2}{\mathcal{D}\ln\left(\frac{L}{r}\right)}
$$

for long channels in dimension 2, i.e., for large values of $L/r$, where $\mathcal{D} = \mathcal{D}(r, s)$ is the diffusivity of a limit Brownian motion. Therefore, a more specific formulation of the problem is to understand how properties of the collision operator are reflected on $\mathcal{D}$. A simple dimensional argument given in Subsection 2.4 shows that

$$
\mathcal{D}(r, s) = \frac{4rs}{\pi}\eta,
$$

where $\eta$ only depends on the scattering characteristics at the microscopic scale determined by $P$. The choice of constants will become clear shortly.

The typical, but not the only type of operator we consider here is defined by a choice of microscopic contour of the channel wall surface, as suggested by Figure 2.1. The main problem then amounts to finding the functional dependence of $\eta$ on geometric parameters of the surface microstructure. These parameters are scale invariant and are typically length ratios and angles. The presence of the logarithmic term in $\tau$ is related to some surprising properties of $\mathcal{D}$, as will be noted below, and for this reason we give somewhat greater prominence to the two-dimensional set-up in this paper.
2.2 Natural collision operators and microstructures

Let $dV(v)$ denote the standard volume element on $n$-dimensional half-space $\mathbb{H} := \mathbb{H}^n$ and define the probability measure

$$d\mu(\beta)(v) = 2\pi \left( \frac{\beta M}{2\pi} \right)^{\frac{n+1}{2}} \langle v, e_n \rangle \exp \left( -\frac{\beta M}{2} |v|^2 \right) \, dV(v).$$

on $\mathbb{H}$. We refer to $\mu(\beta)$ as the surface Maxwellian, or surface Maxwell-Boltzmann distribution, with parameter $\beta$ and particle mass $M$. Here, $\langle v, e_n \rangle$ denotes the standard inner product (dot product) of $v \in \mathbb{H}^n$ and the unit normal vector, $e_n$, to the boundary surface at the origin. We often denote this normal vector by $n = e_n$. It will be clear in context whether $n$ refers to dimension or to this normal vector.

In physics textbooks, $\beta = 1/\kappa T$, where $T$ is absolute temperature and $\kappa$ is the Boltzmann constant. A simple integral evaluation shows that the mean squared post-collision speed with respect to $\mu(\beta)$ is

$$s_{ms}^2 := \int_{\mathbb{H}^n} |v|^2 \, d\mu(\beta)(v) = \frac{n+1}{\beta M}.$$

Another distribution of collision velocities that arises naturally is concentrated on an hemisphere $S^+(s) := \{ v \in \mathbb{H} : |v| = s \}$; it is defined by

$$d\mu(v) = \frac{\Gamma \left( \frac{\nu+1}{2} \right)}{s^n \sqrt{\pi}^{\frac{n-1}{2}}} \langle v, n \rangle \, dV_{\text{sph}}(v)$$

where $dV_{\text{sph}}(v)$ is the volume element on the hemisphere of radius $s$ induced from the ambient Euclidean space. In dimension 2, $d\mu(v) = \frac{1}{2\pi} \langle v, n \rangle \, dS(v)$, where $dS$ indicates arclength element on $S^+(s)$. Equivalently, $d\mu(\theta) = \frac{1}{2} \cos \theta d\theta$, where $\theta$ is
the angle between \( v \) and the normal vector \( n \).

Before introducing the next definition, we make a few remarks about the action of collision operators on measures. Although a collision operator \( P \) was first introduced in the last section as acting on functions, it naturally makes sense for it to act on measures as follows. Given \( \nu \in \mathcal{P}(\mathbb{H}) \), we define \( \nu P \) by its action on essentially bounded functions: \((\nu P)(f) = \nu(Pf)\), where the action \( \nu(f) \) simply means integration of \( f \) against \( \nu \). Therefore, to say that a measure \( \nu \) is stationary for a collision operator \( P \) means \( \nu P = \nu \). We also noted in the previous section that \( P \) can be thought of as the transition probabilities operator for a Markov chain with state space \( \mathbb{H} \). To say that \( \nu \) is stationary for \( P \) is of course equivalent to \( \nu \) being stationary for the Markov chain \( P \) defines.

**Definition 2.1** (Natural collision operators). The collision operator \( P \) will be called *natural* if one of the following holds: (a) \( \mu_\beta \) is the unique stationary distribution for \( P \), for some \( \beta \); (b) the process defined by \( P \) does not change the particle speed and \( \mu \) is a stationary probability measure for \( P \) for all \( s \). If case (a) holds we say that the surface with associated operator \( P \) has temperature \( T = 1/\kappa \beta \); in case (b) we say that \( P \) represents a *random reflection*. In addition, we demand in both cases that \( P \) and its stationary probability satisfy the detailed balance condition (see equation (20.5) of [30]). We use \( \nu \) throughout the paper to indicate either \( \mu_\beta \) or \( \mu \).

The natural operators of particular interest to us are those defined by a choice of surface microscopic structure. We briefly describe them here. (See [16], [17], [18], and [19] for more details.) By *surface (micro-)*structure we mean that the channel wall’s surface has a periodic relief composed of *cells*, each consisting of a mechanical system of moving masses or more simply a fixed geometric shape with no moving parts. (Natural collision operators specified by the former cor-
respond to part (a) of the definition, while the latter correspond to part (b.). Moreover, the wall system, mechanical or purely geometric, is assumed to be at a “microscopic” length scale that, by definition, is incommensurate with that of the channel defined, say, by the radius of the ball factor $\mathbb{B}^{n-k}$. At a collision event, the point particle enters a cell of the wall system, undergoes one or more deterministic collisions with it, transferring energy between wall and particle in case (a), and leaves with a seemingly—from the perspective of the channel length scale—random velocity $V$. (See Figure 2.2.) Because of this assumption of incommensurability between the micro and macro scales, the relevant scattering properties specifying $P$ are invariant under homotheties. Thus in dimension 2 we may, when convenient, assume that the width of each cell is 1.

This incommensurability also dictates our assumption that the particle position on the entrance of a cell at the beginning of a collision event is a uniformly distributed random variable. When the wall system has moving parts, the kinetic state of the cell at the moment the particle enters a cell is also drawn from a fixed probability distribution (a canonical Gibbs state at temperature $T$). Under these assumptions, $V$ is an actual random variable and it can be shown (see [16]) that the associated collision operator $P$ is natural according to Definition 2.1. The periodicity condition is not essential—all the basic facts discussed here hold,
for example, for random structures, defined as probabilistic mixtures of periodic micro-structures.

The operator $P$ can be expressed as follows. Let $f$ be, say, a continuous bounded function on $\mathbb{H}$, and let $V_+$ be the random velocity immediately after the collision of a particle with incoming velocity $V_- = v$. Then

$$(Pf)(v) = \mathbb{E}[f(V_+)|V_- = v].$$

For example, in the purely geometric case of random reflections in dimension 2, $P$ is given by

$$(Pf)(\theta) = \int_0^1 f(\Psi_\theta(r)) \, dr$$

where $\Psi_\theta(r)$ is the angle $V$ makes with the normal vector $n$ and $r \in [0, 1]$ is the position at which the particle enters a cell before collision. A similar integral over $\mathbb{T}^k$ defines $P$ in general dimension.

![Diagram](image)

Figure 2.3: An example of a wall system with moving parts. Mass $m_0$ can move freely up and down, bouncing off elastically against the fixed floor and an upper limit that is permeable to $m_1$.

Figure 2.3 illustrates a wall system with micro-structure having moving parts. The periodic relief is assigned a mass $m_0$ and can move vertically and freely over a short range of distances $[0, a]$ from the fixed base, bouncing off elastically at the lower and upper limits. The point particle of mass $m_1$ enters the wall system with velocity $v$ at a uniformly random location along $[0, 1]$. Upon entrance, the velocity of the wall is assumed to be normally distributed with mean 0 and a given
variance $\sigma^2$, where $m_0\sigma^2$ is proportional to the wall temperature; the particle then goes on to interact deterministically with the wall, leaving with random velocity $V$. This is a very special example of wall system for which $P$ is natural. For other examples and details about random billiards with microstructures omitted here see [16]. See also [20] for a detailed analysis of this and other examples in the context of stochastic processes in velocity space $\mathbb{H}$ having stationary measure $\mu_\beta$ or $\mu$.

If we assume that the wall is static and has infinite mass, the system of the figure becomes purely geometric and the particle mass plays no role. In this case the operator $P$ describes a random reflection. We refer to the subclass of natural operators derived from microscopic structures (either static or having moving parts, with arbitrary surface contours) as operators associated to surface microstructures. An interesting question suggested by [1] is whether general natural operators are limits of operators associated to surface microstructures.

**Proposition 2.1.** The operators for the classes of examples of Figures 2.2 and 2.3 are natural.

**Proof.** See [16, 20] for proofs of these basic issues related to stationary measures and more examples. \qed

Occasionally, $\nu$ will stand for either of the two measures $\mu_\beta$ or $\mu$ of Definition 2.1. Because $P$ and $\nu$ are assumed to satisfy the detailed balance condition, $P$ is a self-adjoint operator of norm 1 on $L^2(\mathbb{H}, \nu)$. A further assumption for the main results below is that $P$ be quasi-compact; that is, the spectral radius of $P$ restricted to the orthogonal complement of the constant function in $L^2(\mathbb{H}, \nu)$ is strictly less than 1. Quasi-compactness for natural collision operators for the types of systems illustrated in Figure 2.2 is known to hold in a number of cases. The static version of the system of Figure 2.2 (for the specific shape shown in the figure) has this
property (see [18], [19]), and the operator for the one-dimensional version of the moving wall is known to be compact (see [16]); the case of the two-dimensional moving wall is still open. Further examples of shapes of systems of the static type having quasi-compact $P$ will be provided later in this paper.

Noting the two roles of $P$, as a self-adjoint operator on $L^2(\mathbb{H}, \nu)$ and as a Markov transition probabilities operator, a useful characterization of powers of $P$ is as follows. Let $V_0, V_1, \ldots$ be a stationary Markov chain with transitions $P$ and initial distribution $\nu$ and let $\Psi, \Phi \in L^2(\mathbb{H}, \nu)$. Then it is not difficult to show that

$$\langle \Psi, P^k \Phi \rangle = \mathbb{E}_\nu [\Psi(V_i) \Phi(V_{i+k})]$$

for any $i \geq 0$, where $\mathbb{E}_\nu$ indicates expectation given that $V_0$ is distributed according to $\nu$.

### 2.3 Between-collisions displacements and times

The logarithmic term in Equation 2.1 is a special feature of the random billiard process in regions bounded by parallel plates in arbitrary dimensions (in particular 2-dimensional channels bounded by a pair of parallel lines), and it is not present in the more typical cylindrical channel region $\mathbb{R}^k \times \mathbb{B}^{n-k}$ for $k = 1, \ldots, n - 2$. Ultimately, this is due to the mean square displacements being infinite in the two-plates case and finite in the other cases, as will be seen later. This elementary but key observation is highlighted in the next proposition.

Let $\mathcal{C} := \mathbb{C}^n := \mathbb{R}^k \times \mathbb{B}^{n-k}$ denote the channel region. Of special interest are the low dimensional cases: $n - k = 1$, for $n = 2, 3$ (two-dimensional channels and slabs in dimension 3) and $k = 1, n = 3$ (cylindrical channels in dimension 3). Let $\mathbb{H}_q$ represent the upper-half space consisting of vectors $v \in T_q \mathcal{C}$, $q \in \partial \mathcal{C}$, such
that $\langle n, v \rangle > 0$, where $n$ is the unit vector in $H_q$ perpendicular to $\partial C$ and $\langle \cdot, \cdot \rangle$ is the inner product given by restriction of the standard dot product in $\mathbb{R}^n$. If $q'$ is the next collision point of the trajectory $t \mapsto q + tv$, let $Z(v)$ denote the natural projection to the "horizontal" factor $\mathbb{R}^k$ of the vector $q' - q \in \mathbb{R}^n$. We refer to $Z(v)$ as the (horizontal) displacement vector for the given $v$. See Figure 2.4. The time of free flight between the collisions at $q$ and $q'$ will be indicated by $\tau_b(v)$.

Figure 2.4: The between-collisions displacement vector $Z(v)$, where $v$ is the post-collision velocity at a boundary point of the channel region. The time between two consecutive collisions is denoted in this section $\tau_b(v)$.

**Proposition 2.2.** Let $\nu$ be either of the two probability measures of Definition 2.1 (denoted there $\mu_\beta$ and $\mu$). This is a probability measure on $H \cong T_qC$ (concentrated on a hemisphere in the case of $\mu$), for a given collision point $q \in \partial C$. Let $Z_a$ denote the product of $Z$ and the indicator function of the cone $H(a) := \{v \in H : |Z(v)| \leq ar\}$ for $a > 0$. Also define for any unit vector $u \in \mathbb{R}^k$ the orthogonal projection $Z^u_a := \langle u, Z_a \rangle$. Then, if $n - k \geq 2$,

$$E_\nu [(Z^u)^2] = \lim_{a \to \infty} E_\nu [(Z^u_a)^2] = \frac{4r^2}{(n - k)^2 - 1}.$$ 

If $n - k = 1$, then the asymptotic expression

$$E_\nu [(Z^u_a)^2] \sim 4r^2 \ln a$$

holds. The expected time of free flight $\tau_b$ (here 'b' is for 'between collisions') is
finite for both types of measures and \( n - k \geq 1 \). For the stationary measure \( \mu \) supported on the hemisphere of speed \( s \),

\[
E_\mu [\tau_b] = \frac{2r \sqrt{\pi}}{s(n - k)} \frac{\Gamma \left( \frac{n+1}{2} \right)}{\Gamma \left( \frac{n}{2} \right)}.
\]

For \( \mu_\beta \), the corresponding expression is

\[
E_{\mu_\beta} [\tau_b] = \frac{r}{n - k} \sqrt{2\pi \beta M}
\]

where \( M \) is particle mass.

For a sketch of the proof, see Section 3.3.1.

Before considering random flights in \( \mathcal{C} \), we need to mention a technical point of geometric interest that only arises in dimensions \( n > 3 \), having to do with whether the operator \( P \) actually gives rise to a well-defined process in \( \mathcal{C} \). The issue is that in order for a fixed \( P \) to induce a scattering operator at each \( T_q \mathcal{C} \), \( q \in \partial \mathcal{C} \), we need to be able to identify the positive part (say, inward pointing) of this tangent space with the half-space \( \mathbb{H} = \{ v \in \mathbb{R}^n : \langle v, e_n \rangle > 0 \} \). Such identification amounts to specifying an orthonormal frame on the tangent space at each boundary point, which provides the information of how the model microstructure is “aligned” with the channel wall. Introducing a frame field on \( \partial \mathcal{C} \) has, however, the effect that the scattering operator \( P_q \) at each boundary point \( q \) becomes a conjugate of \( P \) under an orthogonal transformation, rather than \( P \) itself. For all the cases in dimensions 2 and 3, namely \((n = 2, k = 1), (n = 3, k = 1), (n = 3, k = 2)\), there is a natural frame (the parallel transported frame over the boundary of the channel) with respect to which \( P_q = P \) for all \( q \). In the general case, \( T_q \mathcal{C} \) has a canonical orthogonal decomposition into a “horizontal” part, naturally identified with \( \mathbb{R}^k \), and a vertical part that splits orthogonally into the normal direction \( \mathbb{R}^{n_q} \) and
the complement $\mathbb{V}_q$ of dimension $n - k - 1$. We can now understand the issue as follows: Let $v$ be a velocity vector of a particle that emerges from a collision at $q \in \partial C$ and will collide again next at $q'$. In order that the Markov chain in velocity space be given by iterates of the same operator $P$, we need a field of orthonormal frames with respect to which $v$, at $q$, and its mirror reflection at $q'$ have the same representation as vectors in $\mathbb{R}^n$. The components of these two vectors in $\mathbb{V}_q^\perp$ and $\mathbb{V}_{q'}^\perp$, respectively, agree if we choose the canonical (parallel) frame, but on the subspaces $\mathbb{V}_q$ themselves no such frame exists in general. With this in mind, and to avoid complicating the picture by introducing such frame fields as additional structure, we simply assume without further mention that $P$ is $\mathbb{V}$-isotropic, that is, it is invariant under conjugation by orthogonal linear maps that restrict to the identity on $\mathbb{R}^k \oplus \mathbb{R}e_n$. Notice that this assumption is vacuous in dimensions 2 and 3.

### 2.4 Diffusivity, spectrum and mean exit time

Let $\overline{X}_t$, $t \geq 0$, be a piecewise linear path in the channel region $C$ describing a random flight governed by a natural collision operator $P$. Recall that $P$ is a self-adjoint operator on $L^2(\mathbb{H}, \nu)$. We assume throughout that $P$ is quasi-compact. (This is one of the conditions needed for Theorem 3.1, below.)

We wish to consider a diffusion process in $\mathbb{R}^k$ obtained by an appropriate scaling limit of the projection of $\overline{X}_t$ to the $\mathbb{R}^k$ factor of $C$. Let this projection be denoted $X_t$, and assume $X_0 = 0$. The sequence of post-collision velocities of $\overline{X}_t$ is a stationary Markov chain $V_0, V_1, \ldots$, with initial distribution $\nu$. The displacement vectors, previously defined, are random variables $Z_0, Z_1, \ldots$. Thus $X_t$, at collision times, are sums of the $Z_i$. The $a$-scaled random flight is defined
as follows. Let $h(a)$, $a > 0$, be

$$h(a) = \begin{cases} 
a & \text{for } n - k \geq 2 \\
/a \log a & \text{for } n - k = 1. 
\end{cases}$$

Define the *scaled channel system* with scale parameter $a > 0$ to be the channel system with radius $r/a$ and root-mean-square velocity $h(a)s_{ms}$. (If $\nu = \mu$, $s_{ms}$ is the constant speed throughout the process and if $\nu = \mu \beta$, $s_{ms}^2 = (n+1)/\beta M$.) The random flight paths and their projection are defined as the paths for the $a$-system. We denote them by $X_{a,t}$ and $X_{a,t}$, respectively. The $a$-scaled free displacement with post-collision velocity vector $v$ is $a^{-1}Z(v)$, and the displacements associated to the $V_j$ are $a^{-1}Z_j$. For any $\tau > 0$, over a time interval $[0, \tau]$, the number of collisions of $X_t$ with $\partial C$ will written $N_\tau$. For the $a$-scaled system this number is $N_{a,\tau} := N_{ah(a)\tau}$. For the cases in which $n - k = 1$, when $E_{\nu}[|Z|^2]$ is infinite, it will be necessary to also consider the $a$-truncation $Z_a$ of $Z$ introduced above in Proposition 2.2. The $a$-scaled $a$-truncation of $Z$ and $Z_j$ will be written $a^{-1}Z_a$ and $a^{-1}Z_{a,j}$. Finally, we will like to follow the projected random flight along an axis set by a unit vector $u \in \mathbb{R}^k$. Thus we define $Z^u, X^u_t, Z^u_a$, etc., to be the orthogonal projections of $Z, X_t, Z_a$, etc., on $\mathbb{R}u$.

Theorem 2.1 below gives conditions under which $X_{a,t}$ converges to Brownian motion for large $a$. In this subsection, we wish to focus on the variance (or diffusivity) of the limit Brownian motion, and provide an interpretation of this constant in a way that does not make use of the physically somewhat artificial scaling just introduced. The precise conditions for the diffusion limit to exist when $Z$ has infinite variance relative to $\nu$ (i.e., for $n - k = 1$) are not yet fully clear; for Theorem 2.1 we make the following additional assumption that will be verified in the examples discussed later.
**Assumption 1.** Define for $\gamma > 1$ the set $H_\gamma(a) := \{v \in H : |Z^u(v)| \leq ar/\log a\}$ and let $Z^u_{a,\gamma,j}$ be the product of $Z^u_j$ by the indicator function of $H_\gamma(a)$. Then, for any $t > 0$,

$$\lim_{a \to \infty} \mathbb{E}_\nu \left[ \left( \frac{1}{a} \sum_{j=0}^{N_{a,t}} Z^u_{a,\gamma,j} \right)^2 \right]$$

exists for all unit vectors $u \in \mathbb{R}^k$.

This assumption, which will only be needed when $n - k = 1$, will be explained later in the context of Theorems 3.1 and 3.2. It is not needed for $n - k \geq 2$, when $Z$ has finite variance and Theorem 2.1 is for the most part a consequence of well known limit theorems, in particular the central limit theorem for reversible Markov chains as formulated by Kipnis and Varadhan in [26].

**Theorem 2.1** (Diffusion limit). Let $P$ be quasi-compact and, if $n - k = 1$, suppose that Assumption 1 holds. Then the $a$-scaled projected random path $X^u_{a,t}$, for a unit vector $u \in \mathbb{R}^k$, converges weakly as $a \to \infty$ to a Brownian motion in $\mathbb{R}u$ with diffusion constant $D^u$ further specified below. In particular, $X^u_{a,t}$ converges in distribution for each $t > 0$ to a normal random variable in $\mathbb{R}u$ with mean 0 and variance $tD^u$. The following statements concerning $D^u$ also hold:

1. For the purpose of having a baseline value for $D^u$, suppose that $P$ maps probability measures to $\nu$. In other words, let the velocity process on $H$ be i.i.d. with probability measure $\nu$. Let $n - k \geq 2$. Then, denoting the constant $D^u_0$ in this special case,

$$D^u_0 = \frac{4}{\sqrt{2\pi(n+1)}} \frac{n-k}{(n-k)^2 - 1} r^{s_m s_n}$$

when $\nu = \mu_\beta$ and

$$D^u_0 = \frac{2}{\sqrt{\pi}} \frac{\Gamma\left(\frac{n}{2}\right)}{\Gamma\left(\frac{n+1}{2}\right)} \frac{n-k}{(n-k)^2 - 1} r^s$$
when \( \nu = \mu \). Recall that \( s_{ms} \) is the root-mean-square velocity for \( \mu_\beta \), and that \( \mu \) is concentrated on the hemisphere of radius \( s \) in \( \mathbb{H} \). Being independent of \( u \), we denote these values by \( D_0 \).

2. For \( n - k = 1 \), the baseline diffusivities are

\[
D_0 = \frac{4}{\sqrt{2\pi(n + 1)}} r s_{ms}
\]

when \( \nu = \mu_\beta \) and

\[
D_0 = \frac{2}{\sqrt{\pi}} \frac{\Gamma \left( \frac{n}{2} \right)}{\Gamma \left( \frac{n+1}{2} \right)} r s
\]

when \( \nu = \mu \), supported on the hemisphere of radius \( s \).

3. The diffusion constant for a general \( P \) can now be written as \( D^u = \eta(u) D_0 \), where \( \eta(u) \) has the following expression in terms of the spectrum of \( P \). First consider the case \( n - k \geq 2 \) and define a probability measure on the spectrum by

\[
\Pi^u(d\lambda) := \|Z^u\|^{-2} \langle Z^u, \Pi(d\lambda) Z^u \rangle,
\]

where \( \Pi \) is projection-valued spectral measure associated to \( P \) and the inner product and norm are those of \( L^2(\mathbb{H}, \nu) \). Then

\[
\eta(u) = \int_{-1}^{1} \frac{1 + \lambda}{1 - \lambda} \Pi^u(d\lambda).
\] (2.2)

Notice that \( \eta(u) \) is quadratic in \( u \). Now suppose \( n - k = 1 \) and define for each \( a \) the probability measure

\[
\Pi^u_a(d\lambda) := \|Z^u_a\|^{-2} \langle Z^u_a, \Pi(d\lambda) Z^u_a \rangle
\]

on the spectrum and the function \( \eta_a(u) = \int_{-1}^{1} \frac{1 + \lambda}{1 - \lambda} \Pi^u_a(d\lambda) \). Then the limit
\[ \lim_{a \to \infty} \eta_a(u) \text{ exists and defines a quadratic function } \eta(u) \text{ of } u. \]

**Proof.** The limit theorems in probability theory we require are standard in the case \( n - k \geq 2 \) and will be proved later for \( n - k = 1 \) in Theorems 3.1 and 3.2. Here we only indicate how \( D_0 \) and the expression for \( \eta(u) \) in terms of the spectrum of \( P \) are obtained.

Recall that \( N_{a,t} = N_{ah(a)t} \) is the number of collisions of the \( a \)-scaled random flight with the boundary of the (\( a \)-scaled) channel region during time interval \([0, t]\). Let \( \tau_j \) denote the time duration of the step with (non-scaled) displacement \( Z_j \). Then, as
\[
(\tau_0 + \cdots + \tau_{N_T-1})/N_T \leq T/N_T \leq (\tau_0 + \cdots + \tau_{N_T})/N_T
\]
for any \( T > 0 \), we can apply Birkhoff’s ergodic theorem to obtain
\[
E_{\nu}[\tau_b] = \lim_{T \to \infty} T/N_T,
\]
where we have used a previous notation \( \tau_b \) for the random time between consecutive collisions.

Although not necessary in this case, we use here the truncated displacement \( Z_a \), so that the derivation of the spectral formula will also apply to the infinite variance case to be discussed later (under the more stringent conditions needed in that case). It will be shown later in Proposition 3.3 that, for any \( t > 0 \),
\[
D^u = \lim_{a \to \infty} \frac{1}{a^2 t} \mathbb{E}_{\nu} \left[ \left( \sum_{j=0}^{N_{a,t}-1} Z_{a,j}^u \right)^2 \right]. \tag{2.3}
\]
In the i.i.d. case, this gives
\[
D^u = \lim_{a \to \infty} \mathbb{E}_{\nu} \left[ (Z_a^u)^2 \right] \frac{N_{a,t}}{a^2 t} = \lim_{a \to \infty} \frac{h(a)}{a} \mathbb{E}_{\nu} \left[ (Z_a^u)^2 \right] \frac{N_{ah(a)t}}{ah(a)t} = \lim_{a \to \infty} \frac{h(a)}{a} \mathbb{E}_{\nu} \left[ (Z_a^u)^2 \right] \mathbb{E}_{\nu}[\tau_b].
\]
We can now invoke Proposition 2.2 to obtain the values claimed for \( D^u \) in the i.i.d. case.
Next we obtain the spectral formula for $\eta(u)$, beginning from expression 2.3. This expression holds without further assumptions in the finite variance case, and it follows from Assumption 1 when $n - k = 1$ as will be shown later in Proposition 3.3. Because $P$ has positive spectral gap and $Z_a^u$ has zero mean, the measure $\Pi$ has compact support in the interval $(-1, 1)$. In particular, $1 - \lambda$ is bounded away from zero on the support of $\langle Z_a^u, \Pi(d\lambda) Z_a^u \rangle$. Now observe that, for $j \geq i$,

$$
\mathbb{E}_\nu [Z_{a,j}^u Z_{a,i}^u] = \langle Z_a^u, P^{j-i} Z_a^u \rangle = \int_{-1}^1 \lambda^{j-i} \|Z_a^u\|^2 \Pi_a^u(d\lambda).
$$

With this in mind, we obtain for a fixed $N$ after some algebraic manipulation,

$$
\mathbb{E}_\nu \left[ \left( \sum_{j=0}^{N-1} Z_{a,j}^u \right)^2 \right] = \int_{-1}^1 \left( N + 2 \sum_{j=1}^{N-1} \sum_{i=0}^{j-1} \lambda^{j-i} \right) \|Z_a^u\|^2 \Pi_a^u(d\lambda)
$$

$$
= \int_{-1}^1 \frac{1 + \lambda}{1 - \lambda} \left[ N + O(1) \right] \|Z_a^u\|^2 \Pi_a^u(d\lambda).
$$

The expectation on the right-hand side of limit 2.3 can be written as

$$
\frac{1}{a^2 t} \sum_{N=1}^\infty \mathbb{E}_\nu \left[ \left( \sum_{j=0}^{N-1} Z_{a,j}^u \right)^2 \right] \mathbb{P}(N_{a,t} = N)
$$

$$
= \int_{-1}^1 \frac{1 + \lambda}{1 - \lambda} \mathbb{E}_\nu \left[ N_{a,t} + O(1) \right] \frac{h(a)}{a} \|Z_a^u\|^2 \Pi_a^u(d\lambda).
$$

Keeping in mind the relationship between the expectation of $N_{a,t}$ and $\mathbb{E}_\nu[\tau_b]$ observed above in the derivation of the i.i.d. case, we have

$$
\lim_{a \to \infty} \frac{1}{a^2 t} \mathbb{E}_\nu \left[ \left( \sum_{j=0}^{N_{a,t}-1} Z_{a,j}^u \right)^2 \right] = \lim_{a \to \infty} \frac{h(a)}{a} \frac{\mathbb{E}_\nu \left[ (Z_a^u)^2 \right]}{\mathbb{E}_\nu[\tau_b]} \int_{-1}^1 \frac{1 + \lambda}{1 - \lambda} \Pi_a^u(d\lambda)
$$

$$
= D_0 \int_{-1}^1 \frac{1 + \lambda}{1 - \lambda} \Pi^u(d\lambda).
$$
This proves the claimed form of the diffusion constant. The necessary central limit theorem and weak invariance principle required to prove convergence to Brownian motion (in the case $n - k = 1$) will be shown later.

We remark now on a simple interpretation of the diffusivity $\mathcal{D}$ in the context of the idealized experiment described earlier that allows us to obtain $\mathcal{D}$ without recourse to the somewhat physically artificial $a$-scaling. In order to keep the discussion simple, only the case $k = 1$ is considered, although the main idea can be generalized in obvious ways.

Consider a channel $\mathcal{C}(L) = [-L, L] \times \mathbb{B}^{n-1}(r)$ of length $2L$ and recall that $\tau(L, r, s)$ is the mean exit time from $\mathcal{C}(L)$, introduced in Subsection 2.1, where $s$ is root-mean-square speed. The following elementary dimensional properties are easily derived:

(i) $\tau(L, r, s) = \tau(aL, ar, as)$

(ii) $\tau(L, r, s) = a\tau(L, r, as)$

(iii) $\tau(aL, r, s) = ah(a)\tau(L, r/a, h(a)s)$

where the third property is a consequence of the first two. It also follows from (i) and (ii) that the function $F(L/r) := (s/r)\tau(L, r, s)$ is independent of $s$, dimensionless (that is, devoid of physical units), and scale invariant.

We are interested in the asymptotic behavior of $\tau(L, r, s)$ as $L$ grows to infinity. Since the mean exit time from the interval $[-r, r]$ for Brownian motion with diffusivity $\mathcal{D}$ starting at 0 is $r^2/\mathcal{D}$ we expect, given Theorem 2.1 and the above properties of the mean exit time,

$$
\tau(L, r, s) \sim \begin{cases} 
\frac{L^2}{\mathcal{D}} & \text{if } n - k \geq 2 \\
\frac{L^2}{\mathcal{D} \ln(L/r)} & \text{if } n - k = 1.
\end{cases}
$$

(2.4)
Notice, in particular, the expected relation

\[ \mathcal{D} = C(P)rs, \]

where \( C(P) = \lim_{a \to \infty} ah(a)/F(a) \), being independent of \( L, r, s \), is a characteristic number of the scattering process at a microscopic scale. This asymptotic expression is indeed true, and it is a consequence of the following proposition, which will be proved later.

**Proposition 2.3.** Let \( L > 0 \) and \( \mathcal{T} \) be the function on the space of continuous paths \( \gamma : [0, \infty) \to \mathbb{R} \) defined by \( \mathcal{T}(\gamma) := \inf\{t \geq 0 : |\gamma(t)| \geq L\} \), where the infimum of the empty set is taken to be \(-\infty\). Let \( \mathbb{E}_0^a \) denote expectation with respect to the law of the process \( t \mapsto X_{a,t} \), conditioned to start at 0 and \( \mathbb{E}_0^B \), similarly defined, for the Brownian motion with diffusion constant \( \mathcal{D} \). Then

\[ \lim_{a \to \infty} \mathbb{E}_0^a[\mathcal{T}] = \mathbb{E}_0^B[\mathcal{T}] = \mathcal{D}^{-1}L^2 \]

and the asymptotic expression 2.4 holds.

### 2.5 Examples of diffusivity for geometric microstructures

We limit our attention in this subsection to operators associated to static microstructures in dimension 2. Therefore, the main question of interest in how the shape of the surface contour influences the signature parameter \( \eta = \mathcal{D}/\mathcal{D}_0 \) of the particle-surface interaction. For the examples given here, \( \eta \) can be obtained exactly. It will be noticed that the examples are variations on a theme: they are built out of arcs of circle and straight lines and correspond to focusing billiards.
For the focusing semicircle structure of Figure 2.5 it will be shown that

$$\eta = \frac{1 - \frac{1}{4} \log 3}{1 + \frac{1}{4} \log 3}. \quad (2.5)$$

This value is reminiscent of the limit variance seen in central limit theorems for the stadium billiard of deterministic billiard dynamics (see [5]).

A simple modification of the semicircles contour is shown in Figure 2.6. It consists of semicircles as in the first example separated by flat sections. We introduce the parameter $h = l/(l+2r) \in (0, 1)$, which gives the proportion of the top line occupied by the flat part.

The diffusivity for the shapes of Figure 2.6, as a function of $h$, is given by

$$D(h) = D_0 \frac{\eta + h}{1 - h}. \quad (2.6)$$

where $\eta$ is the signature diffusivity parameter of the example of Figure 2.5. Clearly, for the $h = 0$ limiting case, the microscopic cell is simply the semicircle and $D(0) = D$. At the other end, as $h$ approaches 1 the diffusivity increases without
bound. Of course, for a completely flat surface, the transport ceases to be a diffusion at all and becomes (a much faster) deterministic motion.

The next example refers to the surface of Figure 2.7. In this case, the parameter $h$ measures the length of the middle wall relative to the period length of the contour.

For the middle wall of relative height $h < 1/2$ and $h = 1/2$, the values are, respectively,

$$D(h) = D_0 \frac{1 - \frac{1}{4} \log 3}{1 + \frac{1}{4} \log 3}, \quad D(1/2) = D_0 \frac{1 + \frac{1}{4} \log 3}{1 - \frac{1}{4} \log 3}. \quad (2.7)$$

Observe, in particular, that the diffusivity does not change, and has the same $\eta$ as the example of Figure 2.5, until the middle walls reach the top of the cell. At that point the diffusivity changes discontinuously to $D(1/2)$.

A related phenomenon is seen in the next family of examples, shown in Figure 2.8. It is obtained from the first example by adding a flat floor of relative length $h = l/(l + 2r) \in [0, 1)$. It will be shown for this parametric family that

$$D(h) = D_0 \frac{1 + \zeta_h}{1 - \zeta_h}, \quad (2.8)$$

where

$$\zeta_h = -\frac{1 + 3h}{4} \frac{1 - h}{1 + h} \log \frac{3 + h}{1 - h}.$$

At the $h = 0$ limit we naturally have the same $\eta$ as for the first example.
What happens when $h$ approaches 1 is perhaps more surprising. In this case $\mathcal{D}(h)$ approaches the baseline value $D_0$. Recall that this is the diffusivity of the process where at each collision event the particle reflects, independent of the pre-collision angle, according to the stationary measure $\nu$. From the perspective of a single collision event, collisions are nearly mirror-like; on the other hand, from a multiple scattering perspective the collision process reaches equilibrium instantaneously making the surface ideally rough in a sense. This peculiar phenomenon and the discontinuity in $\mathcal{D}$ seen in the previous example are due to the fact that the diffusivity is determined only by collisions which occur at angles nearly parallel to the channel walls, a result made explicit in Proposition 3.3. An allusion to this property is found in [7].

The computation of $\mathcal{D}$ for these examples will be given in Section 3.2.

We conclude the section by pointing out that all of our examples here have been for channels where the microstructure has no moving parts; or in the language of Definition 2.1, represent random reflections. However, Figure 4.13 in Chapter 4 alludes to a channel model similar to the one in the current chapter where the collision operator represents a wall with temperature. While not the same as
the current chapter’s channel models, we wish to point out that the channel in
Chapter 4 arises in a somewhat unexpected manner and presents a novel example
of collision operators for walls with temperature.
Chapter 3

Technical aspects of channel model

3.1 The main limit theorems in the infinite variance case

Let $P$ be a natural collision operator with stationary measure $\nu$. Define for each $v \in \mathbb{H}$ the measure $P(v, A) = (P1_A)(v)$ for $A \subset \mathbb{H}$ measurable. Let $\Omega = \mathbb{H}^N$ and denote by $\mathcal{F}$ the product Borel $\sigma$-algebra. Define a measure $\mathbb{P}$ on cylinder sets as

$$\mathbb{P}(\{\omega \in \Omega : \omega_0 \in A_0, \ldots, \omega_n \in A_n\}) = \int_{A_0} \int_{A_1} \cdots \int_{A_n} P(\omega_{n-1}, d\omega_n) \cdots P(\omega_0, d\omega_1) \mu(d\omega_0),$$

for $A_0, \ldots, A_n \subset \mathbb{H}$ measurable and extend it to $\mathcal{F}$. The coordinate projections $V_i : \Omega \to \mathbb{H}$ given by $V_i(\omega) = \omega_i$, for $i = 0, 1, \ldots$, thought of as random variables on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$, constitute a Markov chain. Because $\nu$ is stationary for $P$, it follows that the Markov chain is stationary.

Being a natural operator, $P$ together with $\nu$ satisfy the detailed balance con-
dition, which implies it is self-adjoint on $L^2(\mathbb{H}, \nu)$. We also assume from now on that $P$ is quasi-compact, and so has a spectral gap. These assumptions imply that the chain is $\rho$-mixing. That is,

$$\sup \{ \text{corr}(X, Y) : X \in L^2(\mathcal{F}_0^k), Y \in L^2(\mathcal{F}_k^\infty), k \geq 1 \} = O(\rho^n),$$

for some $\rho$ such that $0 < \rho < 1$, where the notations are as follows: $\text{corr}(X, Y)$ is the correlation between $X$ and $Y$, $L^2(\mathcal{F}_0^k)$ is the space of square integrable functions measurable with respect to the $\sigma$-algebra $\mathcal{F}_0^k$ generated by $V_0, \ldots, V_k$ and $L^2(\mathcal{F}_k^\infty)$ is the space of square integrable functions for the $\sigma$-algebra generated by $V_j$, for $j \geq k + n$.

Consider the $a$-scaled channel system, as defined earlier, with channel radius scaled down by $a$ and each post-collision velocity scaled up by the previously defined $h(a)$. Let $X_{a,t}$ be the position at time $t$ along the horizontal axis of the particle for the $a$-scaled random flight starting at $X_{a,0} = 0$; let $N_{a,t}$ be the number of collisions with the walls for the scaled system during the time interval $[0, t]$. Notice that $N_{a,t} = N_{ah(a)t}$, where $N_s$ is, by definition, the number of collisions during $[0, s]$ for the non-scaled system.

In what follows, $h(a) = a/\log a$ and $Z$ will be any real measurable function on $\mathbb{H}$ slowly varying at infinity, in the sense that $\mathbb{E}_\nu [Z^2 1_{|Z| \leq a}] \sim C \log a$ as $a \to \infty$, where $C > 0$ is a constant and $a_n/b_n$ means $a_n/b_n \to 1$ as $n \to \infty$. The various notations used before for the inter-collision displacement function will be used for this general $Z$. Thus, for example, $Z_j = Z(V_j)$. However, the $a$-truncation $Z_a$ of $Z$ will be understood more generally as follows: If $I(a)$ is an interval whose endpoints are functions of the scaling parameter, we write $Z^{I(a)} := Z 1_{\{Z \in I(a)\}}$, and if there is no ambiguity about which interval is being assumed we write $Z_a := Z^{I(a)}$. Combining notations, $Z_{a,j} = Z_a(V_j)$, for the non-scaled observable $Z$, while the corresponding
a-scaled quantity (for the a-scaled system with radius $r/a$ and root-mean-square speed $h(a)s$) is $a^{-1}Z_{a,j}$. Unless explicitly stated otherwise, $Z_a$ is associated to the interval $I(a) = [-a, a]$. The probability measure $\Pi_a(d\lambda)$ on the spectrum on $P$ is defined as before for a general $Z$: $\Pi_a(d\lambda) := \|Z_a\|^{-2} \langle Z_a, \Pi(d\lambda)Z_a \rangle$. While we make no claims on the existence of a weak limit of the measures $\Pi_a$ we note that there exists a subsequence of $\Pi_a$ that converges weakly to a probability measure which we will call $\Pi_0$.

If a sequence of random variables converges in distribution to a normal random variable with mean 0 and variance $\sigma^2$, we say for short that the sequence converges to $\mathcal{N}(0, \sigma^2)$.

**Theorem 3.1** (Central limit theorem). Suppose $P$ is a quasi-compact natural operator and that Assumption 1 holds. Then, for any $t > 0$, the sum $\sum_{j=0}^{N_a,t-1} a^{-1}Z_j$ converges to $\mathcal{N}(0, tD)$ as $a \to \infty$, where

$$D = \lim_{a \to \infty} \frac{1}{a^2t} \mathbb{E}_\nu \left[ \left( \sum_{j=0}^{N_a,t-1} Z_{a,j} \right)^2 \right].$$

**Theorem 3.2** (Weak invariance principle). Under the same assumptions as in Theorem 2.1, let $X_{a,t} \in \mathbb{R}^k$ be the particle at time $t$ in the a-scaled system with radius $r/a$ and root-mean-square velocity $h(a)s$. Then $X_{a,t}$ converges weakly to $B_t$, a Brownian motion with diffusivity given by the quadratic form $D^\nu$.

We note that it is still possible, without Assumption 1, to prove a central limit theorem and weak invariance principle for the inter-collision displacements—only slight modifications of the statements and proofs are needed. However, Assumption 1 allows us to express the variance of the limit distribution in the central limit theorem in terms of the observable $Z$ and the operator $P$. So while more general statements can be made and proven, we choose when possible to
emphasize the connection between macroscopic data—the limit variance in the central limit theorem—and microscopic data encoded in the operator $P$ and its spectrum.

We also note that Assumption 1 may be reduced to a statement about covariances. Observe that

$$E \left[ \left( \sum_{j=0}^{N_{a,t}-1} a^{-1} Z_{a,j} \right)^2 \right] = E \left[ a^{-2} \sum_{j=0}^{N_{a,t}-1} Z_{a,j}^2 \right] + E \left[ a^{-2} \sum_{0 <|i-j|<N_{a,t}} Z_{a,i} Z_{a,j} \right].$$

As already seen in the proof of Theorem 2.1 the limit of the first summand exists in general. Thus the assumption may be restated as requiring the existence of the limit of the second summand of covariances. In the case of strictly stationary $\rho$-mixing sequences with finite variance and a relatively light (less than exponential) condition on the rate of mixing, the scaled limit of variances is known to always exist (see for example [8]). As far as we are aware, the corresponding result in our setting—whether such a limit always exists for exponentially fast $\rho$-mixing stationary sequences with infinite variance—has not been addressed.

The remainder of the paper is organized as follows. Section 3.1.1 outlines the proof of the central limit theorem as a sequence of technical lemmas, leaving the proofs of the lemmas for Section 3.3.2. In Section 3.1.2 we prove the weak invariance principle and Proposition 2.3 on convergence of mean exit times. The computation of diffusivity for the examples of Section 2.5 is given in Section 3.2. The first subsection there outlines a general technique for such computations, while the last two subsections are devoted to the computation of diffusivity for a periodic focusing semicircle micro-geometry and related parametric families.
3.1.1 Outline of proof of the central limit theorem

In this section we explain the skeleton of the proof of Theorem 3.1 as a sequence of lemmas, leaving the proofs of the lemmas for Section 3.3.2. Now $Z$ represents more generally an integrable scalar (rather than vector) random variable so that $\mathbb{E}[|Z|] < \infty$, having mean 0 and slowly varying at infinity; that is, $\mathbb{E}[(Z_a)^2] = O(\ln a)$. Although $Z$ is more general than before, we find it convenient to continue to refer to $Z$ as the displacement. The typical random variable we wish to apply the below theorems to are the projections of the displacement vector $Z^u$ considered before. For a channel in $\mathbb{R}^2$ bounded by parallel lines, we are mainly interested in $Z(v) = rv_1/v_2$, where $v = (v_1, v_2)$, with vector $(0, 1)$ being perpendicular to the boundary lines.

Lemma 3.1. Let $\tau_b$ be the random inter-collision time. Then $(ah(a)t)^{-1}N_{a,t}$ converges to $1/\mathbb{E}_\nu[\tau_b]$ almost surely for each $t > 0$ as $a \to \infty$. In particular, let

$$n_{a,t} := \left\lfloor \frac{ah(a)t}{\mathbb{E}_\nu[\tau_b]} \right\rfloor,$$

where $[x]$ denotes the integer part of $x$. Then $N_{a,t}/n_{a,t} \to 1$ almost surely.

The proof of Lemma 3.1 has already been given in the proof of Theorem 2.1 in Section 2.4.

Lemma 3.2. Let $n_{a,t}$ be defined as in Lemma 3.1. If $\sum_{j=0}^{n_{a,t}-1} a^{-1} Z_j$ converges in distribution to $N(0, t\mathcal{D})$ then so does $\sum_{j=0}^{n_{a,t}-1} a^{-1} Z_j$.

The next lemma shows that one can work with the $a$-truncated random variables $Z_{a,j}$ instead of the $Z_j$.

Lemma 3.3. The quantity $\sum_{j=0}^{n_{a,t}-1} a^{-1} (Z_j - Z_{a,j})$ converges to 0 in probability as $a \to \infty$. 

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To address the issue of statistical dependence among the displacements, we employ Bernstein’s big-small block technique. That is, we break the sum of truncated displacements into alternating big and small blocks in such a way that the small blocks are negligible and the big blocks are in a sense independent. Let \( \alpha = 0.01, \beta = 0.6 \) and define \( b_{a,t} = \left\lfloor n_{a,t}^{\beta} \right\rfloor \) and \( s_{a,t} = \left\lceil n_{a,t}^{\alpha} \right\rceil \). These are the lengths of the big blocks and small blocks, respectively. Define the big blocks as

\[
U_{a,t} = \sum_{j=1}^{b_{a,t}} a^{-1} Z_{a,(i-1)(b_{a,t}+s_{a,t})+j},
\]

for \( 1 \leq i \leq k_{a,t} \), where \( k_{a,t} \) is the largest integer \( i \) for which \((i-1)(b_{a,t}+s_{a,t})+b_{a,t} < n_{a,t} - 1\). Note that \( k_{a,t} \sim n_{a,t}^{1-\beta} \). Next define the small blocks \( V_{a,i} \) as the sums that remain between the big blocks. That is,

\[
V_{a,i} = \sum_{j=1}^{s_{a,t}} a^{-1} Z_{a,(i-1)(b_{a,t}+s_{a,t})+b_{a,t}+j},
\]

for \( 1 \leq i < k_{a,t} \), and \( V_{a,k_{a,t}} = a^{-1} \left( Z_{a,(k_{a,t}-1)(b_{a,t}+s_{a,t})+b_{a,t}+1} + \cdots + Z_{a,n_{a,t}-1} \right) \), so that

\[
\sum_{j=0}^{n_{a,t}-1} a^{-1} Z_{a,j} = \sum_{i=1}^{k_{a,t}} (U_{a,i} + V_{a,i}).
\]

The next lemma shows that it will suffice to consider only the big blocks as the sum of the small blocks is negligible in probability.

**Lemma 3.4.** The sum \( \sum_{i=1}^{k_{a,t}} V_{a,i} \) converges to 0 in probability as \( a \to \infty \).

The proof of Theorem 3.1 has by now been reduced to showing that \( \sum_{i=1}^{k_{a,t}} U_{a,i} \to N(0,tD) \) as \( a \to \infty \). Therefore, the theorem will be proved if we show that the characteristic function of this sum converges to the characteristic function of the normal random variable. By the next lemma, the big blocks are asymptotically independent in the sense that the characteristic function of their sum can be
estimated by the product of their characteristic functions.

**Lemma 3.5.** Convergence \[ \left| \mathbb{E}\left[ \exp\left( i\mu \sum_{i=1}^{a,t} U_{a,i} \right) \right] - \prod_{i=1}^{k_{a,t}} \mathbb{E}\left[ \exp\left( i\mu U_{a,i} \right) \right] \right| \rightarrow 0 \] holds for all \( \mu \) in \( \mathbb{R} \) as \( a \rightarrow \infty \).

Combining the above with the following lemma then gives the proof of Theorem 3.1.

**Lemma 3.6.** The convergence \[ \prod_{i=1}^{k_{a,t}} \mathbb{E}\left[ \exp\left( is U_{a,i} \right) \right] \rightarrow \exp\left( -\frac{s^2}{2} tD \right) \] holds for all \( s \in \mathbb{R} \) as \( a \rightarrow \infty \).

### 3.1.2 Proof of the weak invariance principle

We give now a proof of Theorem 3.2 and of Proposition 2.3. To show weak convergence in the space \( C[0,\infty) := C([0,\infty),\mathbb{R}^k) \) of continuous paths in \( \mathbb{R}^k \) it suffices to show that the finite dimensional distributions of the projection of \( X_a \) along each coordinate axis of \( \mathbb{R}^k \) converge weakly to those of Brownian motion \( B \) and the collection \( X_a \) in \( C[0,\infty) \) is tight (see, for example, [6]). In fact, with regard to the second condition it suffices to show tightness of the collection restricted to \( C[0,t] \) for all \( t > 0 \) (see, for example, [37]). Thus the following two propositions are sufficient to prove the theorem. We assume without loss of generality that dimension \( k = 1 \).

**Proposition 3.1.** Under the conditions of Theorem 3.2, the random vectors \( (X_{a,t_1}, \ldots, X_{a,t_l}) \) converge weakly to \( (B_{t_1}, \ldots, B_{t_l}) \) as \( a \rightarrow \infty \) for all \( l \) and all \( t_1 < \cdots < t_l \in [0,\infty) \).

**Proof.** The proof is by induction on \( k \). For the case \( k = 1 \) we begin by writing

\[ X_{a,t_1} = \left( \sum_{j=0}^{a,t_1-1} a^{-1} Z_j \right) + R_{a,t_1}, \]
where $R_{a,t_1}$ is the signed distance traveled in the time between collision $N_{a,t_1}$ and $t_1$. We claim that $R_{a,t_1} \to 0$ in probability as $a \to \infty$. Indeed note that $|R_{a,t_1}| \leq |a^{-1}Z_{N_{a,t_1}}|$ so, for any $\epsilon > 0$

$$\mathbb{P}(|R_{a,t_1}| > \epsilon) \leq \mathbb{P}(|a^{-1}Z_{N_{a,t_1}}| > \epsilon) \leq \frac{\mathbb{E}[|Z|]}{\epsilon a},$$

which goes to 0 as $a \to \infty$. It follows that $X_{a,t_1}$ converges in distribution to $B_{t_1}$ by Theorem 3.1.

Next we consider the case $l > 1$. It suffices to show that $\sum_{i=1}^l \xi_i X_{a,t_i}$ converges in distribution to $\sum_{i=1}^l \xi_i B_{t_i}$ as $a \to \infty$ for any $(\xi_1, \ldots, \xi_l) \in \mathbb{R}^l$. We first write

$$\sum_{i=1}^l \xi_i X_{a,t_i} = \xi_1 X_{a,t_1} + \cdots + \xi_{l-2} X_{a,t_{l-2}} + (\xi_{l-1} + \xi_l) X_{a,t_{l-1}} + \xi_l (X_{a,t_l} - X_{a,t_{l-1}})$$

Arguing as in the previous case and using the techniques of truncation and Bernstein’s method as in the proof of the central limit theorem we conclude that the first $l - 1$ summands above are asymptotically independent from the last so that, by the induction hypothesis, the sum

$$\xi_1 X_{a,t_1} + \cdots + \xi_{l-2} X_{a,t_{l-2}} + (\xi_{l-1} + \xi_l) X_{a,t_{l-1}} + \xi_l (X_{a,t_l} - X_{a,t_{l-1}})$$

converges in distribution as $a \to \infty$ to

$$\xi_1 B_{t_1} + \cdots + \xi_{l-2} B_{t_{l-2}} + (\xi_{l-1} + \xi_l) B_{t_{l-1}} + \xi_l B_{t_l - t_{l-1}} = \sum_{i=1}^l \xi_i B_{t_i}.$$ 

This concludes the proof of the proposition. \qed

**Proposition 3.2.** Let $t > 0$ and define

$$u(a, \delta) := \sup \{|X_{a,u} - X_{a,v}| : |u - v| < \delta \text{ and } u, v \in [0, t]\}.$$
Then \( \lim_{\delta \to 0} \lim_{a \to \infty} \mathbb{P}(u(a, \delta) > \epsilon) = 0 \) for all \( \epsilon > 0 \).

**Proof.** Let \( \epsilon > 0 \) and \( \delta < t \). For simplicity we assume \( \delta \) divides \( t \) and let \( n = t/\delta \). The argument holds in general with only minor modification. Let \( 0 = t_0 < \cdots < t_n = t \) be the equidistant partition of \([0, t]\). Observe that

\[
\mathbb{P}(u(a, \delta) > \epsilon) \leq \mathbb{P}
\left(
\max_{0 \leq j \leq n-1} \sup_{s \in [t_j, t_{j+1}]} |X_{a,s} - X_{a,t_j}| > \epsilon/3
\right)
\leq \sum_{j=0}^{n-1} \mathbb{P}
\left(
\sup_{s \in [t_j, t_{j+1}]} |X_{a,s} - X_{a,t_j}| > \epsilon/3
\right).
\]

Introducing the notation \( D^t_k := \sum_{j=k}^{k-1} Z_{a,j} - \sum_{j=k}^{N_{a,t}-1} Z_{a,t} \), then for any \( 0 \leq j \leq n - 1 \), the event

\[
\sup \{|X_{a,s} - X_{a,t_j}| : s \in [t_j, t_{j+1}]\} > \epsilon/3
\]

implies that

\[
\max_{N_{a,t_j} \leq k \leq N_{a,t_j+1}} |D^t_k| > a \epsilon/6.
\]

Next let \( n_\delta = \left\lceil \frac{ah(a)t}{v/r\pi} \right\rceil \) and let \( A(j, \delta) \) denote the event \( N_{a,t_{j+1}} - N_{a,t_j} + 1 \leq n_\delta \). Then the probability \( \mathbb{P}\left(\sup_{s \in [t_j, t_{j+1}]} |X_{a,s} - X_{a,t_j}| > \epsilon/3, A(j, \delta)\right) \) is bounded above by

\[
\mathbb{P}\left(\max_{N_{a,t_j} \leq k \leq N_{a,t_j+1}} |D^t_k| > a \epsilon/6, A(j, \delta)\right) \leq \mathbb{P}\left(\max_{N_{a,t_j} \leq k \leq N_{a,t_j+n_\delta}} |D^t_k| > a \epsilon/6\right)
\leq 2 \mathbb{P}\left(\max_{1 \leq k \leq n_\delta} \sum_{i=0}^{k-1} Z_i > a \epsilon/6\right)
\leq 4 \mathbb{P}\left(\sum_{i=0}^{n_\delta-1} Z_i > a \epsilon/6\right),
\]

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where the last two inequalities follow as in the proof of Lemma 3.2. Therefore,

\[
\mathbb{P}(u(a, \delta) > \epsilon) \leq \sum_{j=0}^{n-1} \mathbb{P} \left( \sup_{s \in [t_j, t_{j+1}]} |X_{a,s} - X_{a,t_j}| > \epsilon/3 \right) \\
\leq \sum_{j=0}^{n-1} \left( 4\mathbb{P} \left( \sum_{i=0}^{n-1} Z_i > a\epsilon/6 \right) + \mathbb{P}(A(j, \delta)^c) \right) \\
= n \left( 4\mathbb{P} \left( \sum_{i=0}^{n-1} Z_i > a\epsilon/6 \right) + \mathbb{P}(A(j, \delta)^c) \right) \\
= \frac{t}{\delta} \left( 4\mathbb{P} \left( \sum_{i=0}^{n-1} Z_i > a\epsilon/6 \right) + \mathbb{P}(A(j, \delta)^c) \right).
\]

Notice that the number of collisions in the interval \([t_j, t_{j+1}]\) is precisely \(N_{a,t_j} - N_{a,t_j} + 1\) and so by Lemma 3.1, \(\frac{1}{n_\delta} (N_{a,t_j+1} - N_{a,t_j} + 1) \to 1\) almost surely as \(a \to \infty\). From this it follows that \(\mathbb{P}(A(j, \delta)^c) \to 0\) almost surely as \(a \to \infty\), independent of \(j\) and \(\delta\). From Theorem 3.1

\[
\frac{1}{\delta} \mathbb{P} \left( \sum_{i=0}^{n-1} a^{-1} Z_i > \epsilon/6 \right) \to \frac{2}{\delta^{3/2} \sqrt{2\pi D}} \int_{\epsilon/6}^\infty e^{-x^2/2\delta D} dx
\]

as \(a \to \infty\). Letting \(\delta \to 0\) on the right-hand side above then gives the result. \(\square\)

**Proof of Proposition 2.3.** The equality in the statement of the proposition is a standard fact on the mean exit time of Brownian motion from an interval. We prove here only the convergence of mean exit times. Note that by the continuous mapping theorem \(\tau(X_a)\) converges in distribution to \(\tau(B)\). (Of course \(\tau\) is not continuous on all of \(C[0, \infty)\) but it’s not difficult to show that it is \(\mathbb{P}_0^B\)-a.s. continuous.) Therefore, to show the convergence of mean exit times it suffices to show that the collection of \(\tau(X_a)\) is uniformly integrable. That is, it suffices to show that for any \(\epsilon > 0\) there exists \(M > 0\) such that \(\mathbb{E}_0^a [\tau \mathbb{1}_{\{\tau > M\}}] < \epsilon\) for all \(a\).

Note that for all \(\epsilon > 0\) there exists \(\delta \in (0, 1)\) such that \(\mathbb{P}_x^B(\tau < \epsilon) > \delta\) for all \(x \in (-L, L)\). Since \(\tau(X_a)\) converges to \(\tau(B)\) in distribution it follows, similarly,
that for any \( \epsilon > 0 \) there exists some \( \delta \in (0, 1) \) and \( a_0 \) such that \( \mathbb{P}_x^a(\tau < \epsilon) > \delta \) for all \( a \geq a_0 \) and for all \( x \in (-L, L) \). If we let \( \epsilon = 1 \) and let \( \delta \) be the corresponding value in \((0, 1)\) then it follows by induction and the strong Markov property that \( \mathbb{P}_0^a(\tau > k) \leq (1 - \delta)^k \) for every positive integer \( k \) and \( a \geq a_0 \). Therefore, if we choose \( M' \) large enough so that \( \sum_{k=M'}^{\infty} (k+1)(1-\delta)^k < \epsilon \), then for \( a \geq a_0 \)

\[
\mathbb{E}_0^a \left[ \tau \mathbb{1}_{\{\tau > M'\}} \right] \leq \sum_{k=M'}^{\infty} (k+1)\mathbb{P}_0^a(\tau > k) \leq \sum_{k=M'}^{\infty} (k+1)(1-\delta)^k < \epsilon.
\]

It is also straightforward to see that there exists \( M'' > 0 \) such that \( \mathbb{E}_0^a \left[ \tau \mathbb{1}_{\{\tau > M''\}} \right] < \epsilon \) for \( a < a_0 \). Letting \( M = \max\{M', M''\} \) then gives the uniform integrability. \( \square \)

### 3.2 Examples

This section is devoted to showing how the diffusivity \( \mathcal{D} \) encodes surface microscopic structure when our operator \( P \) represents a random reflection. The structure of the section is as follows. The first subsection gives a general outline for computing \( \mathcal{D} \) independent of any given surface microscopic structure. The second subsection computes \( \mathcal{D} \) in the case that the surface of the walls is given by a periodic arrangement of focusing semicircles. The last subsection gives \( \mathcal{D} \) for certain parametric families of surfaces derived from the semicircle example of the previous subsection.

#### 3.2.1 General Technique

While in general, under Assumption 1, the diffusivity is given by

\[
t\mathcal{D} = \lim_{a \to \infty} \mathbb{E} \left[ \left( a^{-1} \sum_{j=0}^{N_{a,t}} Z_j^{I(a)} \right)^2 \right],
\]
where $I(a)$ is the interval given in Theorem 3.1, it is possible to consider a significantly reduced truncation without altering the value of $D$.

Let $\eta \in (0, 1)$ and define $J(a) := \{x : \exp(\log^\eta a) < |x| < a/\log^\eta a\}$. The following proposition shows that we may use the truncated displacements $Z^J(a)$ in computing $D$ so that in fact a vanishingly small cone of trajectories determine the diffusivity.

**Proposition 3.3.** Under the assumptions of Theorem 3.1,

$$tD = \lim_{a \to \infty} E \left[ \left( a^{-1} \sum_{j=0}^{N_{a,t}-1} Z^J_J(a) \right)^2 \right].$$

**Proof.** As in the proof of Theorem 2.1, the second moment on the right above may be expressed as the spectral integral

$$E \left[ \left( a^{-1} \sum_{j=0}^{N_{a,t}-1} Z^J_J(a) \right)^2 \right] = \int_{-1}^{1} \frac{1 + \lambda}{1 - \lambda} \frac{h(a)}{ah(a)} \left( \frac{h(a)}{a} \|Z^J_J(a)\|^2 \right) \Pi_{Z^J_J}(d\lambda).$$

where $\Pi_{Z^J_J}(d\lambda) = \|Z^J_J\|^{-2} \left\langle Z^J_J, \Pi(d\lambda)Z^J_J \right\rangle$ is a probability measure on the spectrum of $P$. Now observe that if $W := Z^I-I(a)$, then

$$\left\langle Z^J_J, \Pi(d\lambda)Z^J_J \right\rangle = \left\langle Z^I-I - W, \Pi(d\lambda) \left( Z^I-I - W \right) \right\rangle$$

$$= \left\langle Z^I-I, \Pi(d\lambda)Z^I-I \right\rangle - 2 \left\langle W, \Pi(d\lambda)Z^I-I \right\rangle + \left\langle W, \Pi(d\lambda)W \right\rangle$$

and $\|W\|_2^2 = O(\ln^\eta a)$. Therefore,

$$\|Z^I-I\|^2 - Z^I-I \leq 2\|W\|_2 \|Z^I-I\|_2 + \|W\|_2^2 = O(\ln^{\eta'} a)$$

for some $\eta' \in (0, 1)$. Multiplying both sides of the inequality by $h(a)/a = 1/\ln a$ and taking the limit as $a \to \infty$ implies that $Z^J_J$ and $Z^I-I$ grow at the same rate,
and that in the limit formula for $D$ we can use $Z^{J(a)}$ rather than $Z^{I(a)}$. □

With the previous proposition in mind we use the shorthand notation $Z_a := Z^{J(a)}$ through the rest of the subsection without the risk of ambiguity.

If we expand

$$E \left[ \left( a^{-1} \sum_{j=0}^{N_{a,t}-1} Z_{a,j} \right)^2 \right] = E \left[ a^{-2} \sum_{j=0}^{N_{a,t}-1} Z_{a,j}^2 \right] + E \left[ 2a^{-2} \sum_{1 \leq i < j \leq N_{a,t}-1} Z_{a,i} Z_{a,j} \right],$$

the limit of the first term has been shown in the proof of Theorem 2.1 to be $D_0$, which is independent of the microstructure. Let $C(a)$ be a function that increases slower than $ah(a)$ but is otherwise to be determined by a specific microstructure.

For the second term we break the sum into two pieces as follows

$$a^{-2}E \left[ 2 \sum_{1 \leq i < j \leq N_{a,t}-1} Z_{a,i} Z_{a,j} \right] = a^{-2}E \left[ \sum_{0 < |i-j| \leq C(a)} Z_{a,i} Z_{a,j} \right] + a^{-2}E \left[ \sum_{C(a) \leq |i-j| \leq N_{a,t}-1} Z_{a,i} Z_{a,j} \right].$$

The first term on the right above will be determined by the microstructure, but the second term actually vanishes.

**Lemma 3.7.** We have $\lim_{a \to \infty} a^{-2} E \left[ \sum_{C(a) \leq |i-j| \leq N_{a,t}-1} Z_{a,i} Z_{a,j} \right] = 0.$
Proof. Observe that

\[ a^{-2} \sum_{C(a) \leq |i-j| \leq N_{a,t} - 1} |\mathbb{E}[Z_{a,i}Z_{a,j}]| = a^{-2} \sum_{i=1}^{N_{a,t}-C(a)} \sum_{j=i}^{N_{a,t}-C(a)} |\mathbb{E}[Z_{a,i}Z_{a,j+C(a)}]| \]

\[ = 2a^{-2} \mathbb{E}[Z_{a,0}^2] \sum_{i=1}^{N_{a,t}-C(a)} \sum_{j=i}^{N_{a,t}-C(a)} |\text{corr}(Z_{a,i}, Z_{a,j+C(a)})| \]

\[ \leq 2a^{-2} \mathbb{E}[Z_{a,0}^2] \sum_{i=1}^{N_{a,t}-C(a)} \sum_{j=i}^{N_{a,t}-C(a)} |\rho(C(a) + j - i)| \]

\[ \leq \frac{M}{ah(a)} \sum_{i=1}^{N_{a,t}-C(a)} \sum_{j=i}^{N_{a,t}-C(a)} \rho^{C(a)+j-i}, \]

where \( M > 0 \) is a constant and \( 0 < \rho < 1 \) is the essential spectral radius. Further,

\[ \sum_{i=1}^{N_{a,t}-C(a)} \sum_{j=i}^{N_{a,t}-C(a)} \rho^{C(a)+j-i} = \rho^{C(a)} \left( \frac{1}{1-\rho} \left( N_{a,t} - C(a) - \frac{1 - \rho^{N_{a,t}-C(a)+1}}{1-\rho} \right) + 1 \right). \]

Taking expectation and letting \( a \to \infty \) then gives the result. \( \square \)

3.2.2 Semicircle Microstructure

This section is devoted to computing the diffusivity of the channel system whose walls consist of a periodic focusing semicircle microscopic structure. The first subsection is devoted to a thorough analysis of the operator \( P \) for this geometry. We show that \( P \) is quasicompact and give an explicit formula for \( P \) for a certain range of pre-collision angles. The second subsection is devoted to the computation of \( D \) using the method outlined in the above section.

A closer look at \( P \)

To show that \( P \) is quasicompact we employ the technique of conditioning (see [18] and [19] for more details). The general idea of conditioning in this setting
is to obtain a compact operator by considering \( P \) conditional on the event that trajectories satisfy a given property. As we will see, the compactness of this conditional operator will imply \( P \) is quasicompact.

Let \( Q \) denote the the microscopic cell bounded by the semicircle and its diameter such that \( \partial Q = \Gamma_0 \cup \Gamma_1 \) where we renormalize so that the diameter \( \Gamma_0 \) is identified with \([0, 1]\) and \( \Gamma_1 \) is the semicircle with radius \(1/2\). Let \( \Psi_\theta(r) \in [0, \pi] \) denote the angle between the outgoing vector \( V \) and \( \Gamma_0 \) given that the trajectory enters \( Q \) with angle \( \theta \) at position \( r \).

We define a measurable partition of \( M = I \times V = [0, 1] \times [0, \pi] \) as follows: let \( M_1 \subset M \) be the subset of initial conditions whose billiard trajectories undergo exactly one or two collisions with \( \partial Q \) before returning to \( \Gamma_0 \). Define \( P_1 \) as \( P \) conditional on the event \( M_1 \), and similarly define \( P_2 \) from \( M_2 = M \setminus M_1 \). More precisely, if we let \( M_j(\theta) = \{ r \in I : (r, \theta) \in M_j \} \) and define \( \alpha_j(\theta) = \lambda(M_j(\theta)) \) for each \( j = 1, 2 \) and \( \theta \in V \), then for each \( f \in L^\infty(V, \mu) \), define

\[
(P_j f)(\theta) = \begin{cases} 
\frac{1}{\alpha_j(\theta)} \int_{M_j(\theta)} f(\Psi_\theta(r)) dr, & \alpha_j(\theta) \neq 0 \\
0, & \alpha_j(\theta) = 0.
\end{cases}
\]

We call \( P_j \) the conditional operators associated to the partition \( M_j \). Note that it makes sense to write \( Pf = \alpha_1 P_1 f + \alpha_2 P_2 f \). Let \( \mu_j \) be the measure on \( V \) defined such that \( d\mu_j = \frac{\alpha_j}{(\lambda \times \mu)(M_j)} d\mu \). It follows that \( P_j \) is self adjoint on \( L^2(V, \mu_j) \).

Next note that \( P_1 \) has an integral kernel. Let \( W_\theta^i = \{ r \in I : (r, \theta) \in M_i \} \). Then \( W_\theta^1 \) is the countable (or finite) union of open intervals \( W_{\theta,j} \) for which the restriction \( \Psi_{\theta,j} = \Psi_{\theta}|_{W_{\theta,j}} \) is a diffeomorphism from \( W_{\theta,j} \) onto its image \( V_{\theta,j} \). Define \( \Gamma_\theta(\varphi) = \sum_j \chi_{V_{\theta,j}}(\varphi) \Lambda_{\theta,j}(\varphi)^{-1} \), where \( \Lambda_{\theta,j}(\varphi) = \frac{1}{2} |\Psi_\theta'(\Psi_{\theta,j}^{-1}(\varphi))| \sin \varphi \). Let

\[
\omega_1(\theta, \varphi) = \frac{(\lambda \times \mu)(M_1) \Gamma_\theta(\varphi)}{\alpha_1(\theta) \alpha_1(\varphi)}.
\]
It follows by way of change of variables that the operator $P_1$ on $L^2(V, \mu_1)$ is given by

$$(P_1 f)(\theta) = \int_V f(\varphi) \omega_1(\theta, \varphi) d\mu_1(\varphi).$$

To show $P_1$ is compact, it will suffice to show $\omega_1$ is square integrable on $V \times V$. To this end, we first look at the function $\Psi_\theta(r)$. By the symmetry of the semicircle $\Psi_\theta(r)$ satisfies

$$\Psi_\theta(r) = \pi - \Psi_{\pi-\theta}(1-r).$$

It follows that it suffices to consider only $\theta \in (0, \pi/2)$.

**Proposition 3.4.** The function $\Psi_\theta(r)$ has the following properties:

1. Let $\theta \in (0, \pi/2)$ and let $n \geq 1$ be the number of collisions a trajectory with initial data $(r, \theta)$ makes with the semicircle. Then

$$\Psi_\theta(r) = \begin{cases} 
2n \sin^{-1}((2r - 1) \sin \theta) + n\pi - \theta, & r \in [0, 1/2] \\
2n \sin^{-1}((2r - 1) \sin \theta) - (n - 2)\pi - \theta, & r \in (1/2, 1]. 
\end{cases}$$

2. Let $\theta \in (\pi/4, \pi/2)$. Then $\Psi_\theta(r)$ has the following points of discontinuity in $[0, 1]$:

$$r_0^{(n)} = \frac{1}{2} \sin\left[\frac{(n\pi - \theta)/(2n + 1)}{2 \sin \theta}\right], \quad r_1^{(n)} = \frac{1}{2} + \frac{\sin\left[\frac{(n - 1)\pi + \theta}/(2n + 1)\right]}{2 \sin \theta},$$

$n \geq 1$.

3. Let $\theta \in (0, \pi/4)$. Then $\Psi_\theta(r)$ has only one point of discontinuity given by

$$r' = \frac{1}{2} + \frac{\sin \theta/3}{2 \sin \theta}.$$
are possible and hence the formula in 1. is only valid for $n = 1, 2$. Further, we make more precise what is meant by the points of discontinuity given in 2. and 3. If $r \in \left(r_0^{(1)}, r_1^{(1)}\right)$, then the initial conditions $(r, \theta)$ give a billiard trajectory which makes only one intermediary collision. And for $n \geq 2$, if $r \in \left(r_0^{(n)}, r_0^{(n-1)}\right) \cup \left(r_1^{(n-1)}, r_1^{(n)}\right)$, then the initial conditions $(r, \theta)$ give a billiard trajectory which makes $n$ intermediary collisions. For $0 < \theta < \pi/4$, the situation is simpler. The initial conditions $(r, \theta)$ for $r \in (0, r')$, give one intermediary collision, and for $r$ in the complementary subinterval of $I$, there are two intermediary collisions. The proof of the proposition is by elementary trigonometry.

![Figure 3.1: Definition of $\bar{r}$](image)

**Proposition 3.5.** The operator $P_1$ on $L^2(V, \mu_1)$ is compact.

**Proof.** As $P_1$ is given as an integral operator $(P_1f)(\theta) = \int_V f(\varphi)\omega_1(\theta, \varphi)d\mu_1(\varphi)$ it suffices to show that $\omega_1 \in L^2(V \times V, \mu_1 \times \mu_1)$. By symmetry, we have the identity $\omega_1(\theta, \varphi) = \omega_1(\pi - \theta, \pi - \varphi)$ and the square of the $L^2$-norm of $\omega_1$ is

$$2 \int_0^{\pi/2} \int_V \omega_1^2(\theta, \varphi)d\mu_1(\varphi)d\mu_1(\theta).$$

Thus we show that the following two integrals are finite:

$$\int_0^{\pi/4} \int_V \omega_1^2(\theta, \varphi)d\mu_1(\varphi)d\mu_1(\theta), \quad \int_\pi^{\pi/2} \int_V \omega_1^2(\theta, \varphi)d\mu_1(\varphi)d\mu_1(\theta). \quad (3.1)$$
First consider the second integral. Let $\pi/4 < \theta < \pi/2$. Using the notation established in the previous proposition and further above, $W^1_{\theta} = (r_0^{(1)}, r_1^{(1)})$. Correspondingly, $V_{\theta, 1} = (\pi/3 - \theta/3, \pi - \theta/3)$.

Moreover, $\Psi_{\theta, 1}(r) = \pi - \theta + 2 \sin^{-1}((2r - 1) \sin \theta)$. It follows that

$$|\Psi'(\Psi^{-1}_{\theta, 1}(\varphi))| = \frac{4 \sin \theta}{\sin \left(\frac{\varphi + \theta}{2}\right)}$$

Now observe that

$$\int_{\pi/4}^{\pi/2} \int_{V} \omega^2_1(\theta, \varphi) d\mu_1(\varphi) d\mu_1(\theta) = \int_{\pi/4}^{\pi/2} \int_{V} \frac{\Gamma_0(\varphi)^2}{\alpha_1(\theta) \alpha_1(\varphi)} d\mu(\varphi) d\mu(\theta)$$

$$= \int_{\pi/4}^{\pi/2} \int_{V_{\theta, 1}} \sin \theta \frac{1}{\alpha_1(\theta) \alpha_1(\varphi)} |\Psi'(\Psi^{-1}_{\theta, 1}(\varphi))|^2 \sin \varphi d\varphi d\theta.$$

Now because $\theta, \phi$ are bounded away from zero in the above integrals and because $\alpha_1(\theta) > 0$ for all $\theta$, it follows that the above integral is finite.

We show that the first integral in (3.1) is finite. Let $0 < \theta < \pi/4$. Here $W^1_{\theta}$ is given by the single interval $W_{\theta, 1} = (0, r')$ and $V_{\theta, 1} = (\pi - 3\theta, \pi - \theta/3)$. Moreover, $\Psi_{\theta, 1}(r) = \pi - \theta + 2 \sin^{-1}((2r - 1) \sin \theta)$ as in the previous case. Hence $|\Psi'(\Psi^{-1}_{\theta, 1}(\varphi))|$ is also as above. It follows that it suffices to show the following integral is finite:

$$\int_{\pi/4}^{\pi/4} \int_{\pi/4}^{\pi/4} \sin^2 \left(\frac{\varphi + \theta}{2}\right) \sin \theta \sin \varphi d\varphi d\theta.$$

Note that for $\pi - 3\theta < \varphi < \pi - \theta/3$, we have $\varphi \geq \theta$, which implies $\sin \left(\frac{\varphi + \theta}{2}\right) \leq \frac{\varphi + \theta}{2}$.
\[ \int_0^{\pi/4} \int_{\pi - 3\theta}^{\pi - \theta/3} \sin^2 \left( \frac{\varphi + \theta}{2} \right) \, d\varphi \, d\theta \leq \int_0^{\pi/4} \int_{\pi - 3\theta}^{\pi - \theta/3} \frac{\sin \varphi}{\sin \theta} \, d\varphi \, d\theta \]
\[ = \int_0^{\pi/4} \int_{\theta/3}^{3\theta} \frac{\sin \varphi}{\sin \theta} \, d\varphi \, d\theta \]
\[ \leq \int_0^{\pi/4} \frac{1}{\sin \theta} \left( \frac{(3\theta)^2 - (\theta/3)^2}{2} \right) d\theta, \]

which is finite. \( \Box \)

Having shown that \( P_1 \) is compact we are now ready to show that \( P \) is quasi-compact. This this a consequence of the following general fact. (See Theorem 9.9 in [36].)

**Proposition 3.6.** Let \( K \) and \( T \) be bounded self adjoint operators on a Hilbert space and suppose that \( K \) is compact. Then the essential spectrum of \( T + K \) is contained in the essential spectrum of \( T \). In particular, if \( \| T + K \| = 1 \) and \( \| T \| < 1 \), then the spectral gap \( \gamma(T + K) \) of \( T + K \) satisfies

\[ \gamma(T + K) \geq \min \{ 1 - \| T \|, \gamma(K) \}. \]

The quasicompactness of \( P \) then follows from letting \( K = \alpha_1 P_1 \) and \( T = \alpha_2 P_2 \) and noting that \( 1 - \| T \| \geq \inf \alpha_1 > 0. \)

**Computation of \( D \)**

In this subsection we use the shorthand \( Z_a := Z^{J(a)} \) and \( Z_{a,j} := Z^{J(a)}(\Theta_j) \) where \( J(a) \) is as given at the start of Section 3.2.1.

We show, for the example of Figure 2.5, that \( D = \frac{4w}{\pi^2} \frac{1 + \zeta}{1 - \zeta} \) where \( \zeta = -\frac{1}{4} \log 3. \)
Following the discussion in Section 3.2.1 we aim to compute

$$\lim_{a \to \infty} a^{-2} \sum_{0 < |i-j| < C(a)} \mathbb{E}[Z_a,iZ_{a,j}]$$

where we choose $C(a) = \log_3 \log a$. By stationarity, we are interested in computing $\mathbb{E}[Z_{a,0}Z_{a,j}]$ for $j < C(a)$. That is, we are interested in the first $C(a)$ collisions of trajectories with a shallow initial angle. Now although we’ve chosen these truncations of the between collision displacements because, as seen in the previous section, the transition probability kernel has a straightforward explicit formula for such pre-collision angles, they are not without their own complications. It’s clear that to keep track of the trajectories whose $j$th displacement falls out of the truncation range, making $Z_{a,0}Z_{a,j}$ vanish, quickly becomes intractable. For this reason, we introduce the following so-called widened truncation, which, as we will show, will not change the diffusivity.

Consider a trajectory for which $Z_0 \in J(a)$. I follows that, for large enough $a$,

$$|Z(3^j\Theta_0)| \leq |Z_j| \leq |Z(3^{-j}\Theta_0)|,$$

for all $j < C(a)$. A straightforward estimate then shows that

$$3^{-j} \exp(\log^\gamma a) - C_1 < |Z_j| < 3^j a/ \log^\gamma a + C_1$$

where $C_1 > 0$.

Define $K(a) := \{ x : 3^{-C(a)} \exp(\log^\gamma a) < |x| < 3^{C(a)}a/ \log^\gamma a+C_1 \}$. For the rest of the subsection we will consider the new truncated displacement $Z^{K(a)}$ as well as $Z^{J(a)}$, which we will continue to denote $Z_a$. Note that each $Z^{K(a)}_j = Z^{K(a)}(\Theta_j)$ is nonzero. Moreover, the following lemma shows that it suffices to compute
Lemma 3.8. The following equality of limits holds:

$$\lim_{a \to \infty} \sum_{0 < |i-j| < C(a)} a^{-2} \mathbb{E} Z_{a,i} Z_{a,j} = \lim_{a \to \infty} a^{-2} \sum_{0 < |i-j| < C(a)} \mathbb{E} Z_{a,i} Z_{a,j} K(a)$$

Proof. Define $I_1 := \{ x : 3^{-C(a)} \exp(\log^\eta a) < |x| < \exp(\log^\eta a) \}$ and $I_2 := \{ x : a/\log^\gamma a < |x| < 3C(a) a/\log^\gamma a + C_1 \}$. Note that $K(a) = I_1(a) \cup I_2(a)$. Hence it suffices to show

$$\lim_{a \to \infty} a^{-2} \sum_{0 < |i-j| < C(a)} \mathbb{E} \left[ Z_{a,i} \left( Z_{j,1}^{I_1(a)} + Z_{j,2}^{I_2(a)} \right) \right] = 0.$$ 

Observe that

$$a^{-2} \mathbb{E} \left[ Z_{a,i} \left( Z_{j,1}^{I_1(a)} + Z_{j,2}^{I_2(a)} \right) \right] \leq a^{-2} \mathbb{E}^{1/2} \left[ Z_{a,i}^2 \left( \mathbb{E}^{1/2} \left[ \left( Z_{j,1}^{I_1(a)} \right)^2 \right] + \mathbb{E}^{1/2} \left[ \left( Z_{j,2}^{I_2(a)} \right)^2 \right] \right) \right]$$

$$= O \left( a^{-2} \log^{1/2} a (\log \log a)^{1/2} \right),$$

where the last step is due to $\mathbb{E} \left[ Z_{a,i}^2 \right] = O(\log a)$ and $\mathbb{E} \left[ \left( Z_{j,1}^{I_1(a)} \right)^2 \right] = O(\log \log a)$. Since the sum contains roughly $O(N_{a,i} C(a)) = O \left( a^2 \frac{\log \log a}{\log a} \right)$ such terms, the result follows. \qed

Let $q_i = Z_i/Z_{i-1}$ for $i \geq 1$. The next lemma is a key technical tool in the computation.

Lemma 3.9. Let $1 \leq j < O(\log \theta)$. Then $\mathbb{E} [q_1 \cdots q_j \mid \Theta_0 = \theta] = \zeta^j + AB^{j-1} \theta^2 + O(\theta^4)$ for constants $A, B$ independent of $\theta$.

Proof. Observe that for $\theta$ sufficiently small, using the integral kernel for $P$ derived
in the previous subsection

\[ \mathbb{E}[q_1 \mid \Theta_0 = \theta] = \frac{1}{\cot \theta} \left( \int_{3\theta/4}^{\pi/2} \cot \varphi \frac{\cos \left( \frac{\varphi + \theta - \pi}{2} \right)}{4 \sin \theta} \, d\varphi + \int_{\theta/3}^{3\theta/4} \cot \varphi \frac{\cos \left( \frac{\varphi + \theta}{4} \right)}{8 \sin \theta} \, d\varphi \right) \]

\[ = \frac{1}{\cos \theta} \left( -\frac{1}{4} \int_{\theta/3}^{3\theta/4} \cot \varphi \cos \left( \frac{\varphi - \theta}{2} \right) \, d\varphi + \frac{1}{8} \int_{\theta/3}^{3\theta/4} \cot \varphi \cos \left( \frac{\varphi + \theta}{4} \right) \, d\varphi \right). \]

One may check that

\[ \frac{1}{\cos \theta} \int_{\theta/3}^{3\theta/4} \cot \varphi \cos \left( \frac{\varphi - \theta}{2} \right) \, d\varphi = 2 \log 3 + D_1 \theta^2 + O(\theta^4), \]

where \( D_1 \) is a constant, and likewise for the second integral above, albeit with a constant different from \( D_1 \). The case \( j = 1 \) then follows.

Let \( V_\theta = (\theta/3, 3\theta) \cup (\pi - 3\theta, \pi - \theta/3) \). Observe that

\[ \mathbb{E}[q_1 q_2 \mid \Theta_0 = \theta] = \mathbb{E}[\mathbb{E}[q_1 q_2 \mid \Theta_0 = \theta, \Theta_1 = \varphi] \mid \Theta_0 = \theta] \]

\[ = \int_{V_\theta} \mathbb{E}[q_1 q_2 \mid \Theta_0 = \theta, \Theta_1 = \varphi] \, P(\theta, d\varphi) \]

\[ = \int_{V_\theta} \frac{z(\varphi)}{z(\theta)} \mathbb{E}[q_2 \mid \Theta_0 = \theta, \Theta_1 = \varphi] \, P(\theta, d\varphi) \]

\[ = \int_{V_\theta} \frac{z(\varphi)}{z(\theta)} (\zeta + A\varphi^2 + O(\varphi^4)) \, P(\theta, d\varphi) \]

\[ = \zeta \mathbb{E}[q_1 \mid \Theta_0 = \theta] + \int_{V_\theta} \frac{z(\varphi)}{z(\theta)} (A\varphi^2 + O(\varphi^4)) \, P(\theta, d\varphi) \]

\[ = \zeta^2 + A\theta^2 + O(\theta^4) + \int_{V_\theta} \frac{z(\varphi)}{z(\theta)} (A\varphi^2 + O(\varphi^4)) \, P(\theta, d\varphi). \]

Next, one may check that

\[ \int_{V_\theta} \frac{z(\varphi)}{z(\theta)} (A\varphi^2 + O(\varphi^4)) \, P(\theta, d\varphi) = \frac{1}{\cos \theta} \left( -\frac{1}{4} \int_{\theta/3}^{3\theta/4} \cot \varphi (A\varphi^2 + O(\varphi^4)) \cos \left( \frac{\varphi - \theta}{2} \right) \, d\varphi \right. \]

\[ + \frac{1}{8} \int_{\theta/3}^{3\theta/4} \cot \varphi (A\varphi^2 + O(\varphi^4)) \cos \left( \frac{\varphi + \theta}{4} \right) \, d\varphi \right) \]

\[ = AB\theta^2 + O(\theta^4) \]
The case \( j = 2 \) follows. The rest of the argument follows by a similar induction argument.

With the above lemma in place we are ready to compute the correlations.

**Lemma 3.10.** For \( 1 \leq j < C(a) \), \( \mathbb{E} \left[ Z_{a,0}Z_{j}^{K(a)} \right] = 4r^2\zeta^j \Lambda(a) + AB^{j-1}\Gamma(a) \), where \( \Lambda(a) \sim \log a \), \( \Gamma(a) = O(\exp(-2\log^a a)) \), and \( A, B \) are the constants given in Lemma 3.9.

**Proof.** Recall the interval \( J(a) = \{ x : \exp(\log^a a) < |x| < a/\log a \} \). Observe that

\[
\mathbb{E} \left[ Z_{a,0}Z_{j}^{K(a)} \right] = \int_0^\pi Z_a(\theta)^2 \mathbb{E} \left( q_1 \cdots q_j \mid \Theta_0 = \theta \right) \mu(d\theta) = 2 \int_0^\pi Z(\theta)^2 \mathbb{E} \left( q_1 \cdots q_j \mid \Theta_0 = \theta \right) \mathbb{I}_{J(a)} \mu(d\theta) = 2 \int_0^\pi Z(\theta)^2 (\zeta^j + AB^{j-1}\theta^2 + O(\theta^4)) \mathbb{I}_{J(a)} \mu(d\theta).
\]

We remark that because we are only considering here \( \theta \) such that \( \exp(\log^a a) < Z(\theta) < a/\log^a a \), and hence \( |\log \theta| < C \log a \) for some constant \( C \), it follows that \( j < C(a) \) is sufficiently small so that we may apply Lemma 3.9.

It is straightforward to compute \( \int_0^\pi Z(\theta)^2 \mathbb{I}_{J(a)} \mu(d\theta) \sim 2r^2 \log a \). And moreover

\[
\int_0^\pi Z(\theta)^2 O(\theta^2) \mu(d\theta) = \int_0^\pi O(\theta) \mathbb{I}_{J(a)} d\theta = O \left( (\exp(\log^a a))^{-2} \right).
\]

The result now follows. \( \square \)

The summation of correlations is the final piece to our computation.

**Proposition 3.7.** Let \( U(a) = \sum_{0 < |i-j| < C(a)} \mathbb{E} \left[ Z_{a,i}Z_{j}^{K(a)} \right] \). Then

\[
\lim_{a \to \infty} a^{-2}U(a) = \frac{8trv}{\pi} \frac{\zeta}{1-\zeta}.
\]
Proof. Observe that

\[
U(a) = 2 \left[ (N_{a,t} - C(a) + 1) \sum_{i=1}^{C(a)-1} \mathbb{E} \left[ Z_{a,0} Z_i^{K(a)} \right] + \sum_{i=1}^{C(a)-2} \sum_{j=1}^{C(a)-i-1} \mathbb{E} \left[ Z_{a,0} Z_j^{K(a)} \right] \right]
\]

\[
= 2 \left[ (N_{a,t} - C(a) + 1) \sum_{i=1}^{C(a)-1} \left( 4r^2 \zeta^j \Lambda(a) + AB^{j-1} \Gamma(a) \right) + \sum_{i=1}^{C(a)-2} \sum_{j=1}^{C(a)-i-1} \left( 4r^2 \zeta^j \Lambda(a) + AB^{j-1} \Gamma(a) \right) \right]
\]

\[
= 2 \left[ A \Gamma(a) \left( (N_{a,t} - C(a) + 1) \frac{B^C(a) - B}{B(B - 1)} + \frac{B^C(a) + B(C(a) - 2) - B^2(C(a) - 1)}{B(B - 1)^2} \right) + 4r^2 \Lambda(a) \left( (N_{a,t} - C(a) + 1) \frac{\zeta^C(a) - \zeta}{\zeta - 1} + \frac{\zeta^C(a) + \zeta(C(a) - 2) - \zeta^2(C(a) - 1)}{(\zeta - 1)^2} \right) \right].
\]

Dividing by \(a^2\) and letting \(a \to \infty\) gives the result. \(\square\)

The value of \(D\) then follows from adding the value from the proposition above to \(4trv/\pi\) as discussed in Section 3.2.1.

### 3.2.3 Parametric Families

In this section we consider three different parametric families which are derived from the semicircle. Of primary interest will be how the diffusivity of the limiting process for each family changes as a function of the parameter.

We begin with the family formed by adding a middle wall of height \(h\) to the semicircle as shown in the figure above. Suppose \(h < 1/2\); that is, the wall does not extend to the center of the semicircle. It is apparent by inspection that trajectories with a sufficiently small pre-collision angle will never, so to speak, notice the middle wall. And moreover, those trajectories with initial data \((r, \theta)\) that do notice the wall will behave like trajectories in the semicircle with no wall with initial data \((1 - r, \pi - \theta)\) by symmetry. That is, if \(\Psi^h_\theta(r)\) denotes the post-
collision angle of a trajectory with initial data \((r, \theta)\) in the middle wall geometry and similarly \(\Psi_\theta(r) = \Psi_\theta^0(r)\), then \(\Psi_\theta^0(r) = \Psi_{\pi-\theta}(1-r)\) for initial conditions \((r, \theta)\) for which the trajectory hits the middle wall. It follows that the operator \(P_h\) for the middle wall geometry is quasicompact. Moreover, as pointed out earlier, the diffusivity \(D_h\) for \(P_h\) depends only on trajectories with arbitrarily shallow angles by the formula in Proposition 3.3. It follows that the diffusivity \(D(h)\) is constant and equal to the diffusivity for the semicircle with no wall for all \(h < 1/2\).

Further, using the symmetry \(\Psi_\theta^h(r) = \Psi_{\pi-\theta}(1-r)\) and following the proof given for the semicircle, the diffusivity \(D(1/2)\) for the geometry with a middle that extends exactly to the center of the semicircle is given by \(D(1/2) = \frac{4rv}{\pi} \frac{1-\zeta}{1+\zeta}\) where \(\zeta = -\frac{1}{4} \log 3\) as in the semicircle. We summarize these facts as follows.

**Proposition 3.8.** For the middle wall modification of the semicircle with middle wall height \(h\), \(D(h) = D\), for \(h < 1/2\), where \(D\) is the diffusivity for the semicircle with no wall, and for \(h = 1/2\) the diffusivity is given by

\[
D(1/2) = \frac{4rv}{\pi} \frac{1-\zeta}{1+\zeta},
\]

where \(\zeta = -1/4 \log 3\).

It is interesting to note that the diffusivity is not a continuous function of the parameter. We also remark that the case \(h > 1/2\) when the middle wall extends outside the semicircle requires a different analysis altogether, which we leave for a future paper.

Next we look to the geometry formed by splitting the semicircle and adding a flat bottom of length \(h \in (0, 1)\) as shown above. We renormalize the size of the semicircles so that they have radius \((1-h)/2\). We also establish the notation \(a = (1+h)/2, b = (1-h)/2\). While qualitatively similar to the semicircle, the angle function \(\Psi_\theta^h(r)\) requires a new detailed analysis, which we sketch here.
We begin by noting that by symmetry it again suffices to consider only pre-collision angles $\theta \in (0, \pi/2)$. And moreover, for sufficiently small pre-collision angles $\theta$ at most two intermediary collisions are possible within the cell. In the discussion that follows we consider only such $\theta$. Let $r' \in (0, 1)$ be the point of entry for which $\Psi^h_\theta(r)$ is discontinuous. That is, $r'$ is chosen such that trajectories with initial data $(r, \theta)$ for $r \in (0, r')$ experience one intermediary collision, and for those with $r \in (r', 1)$, there are two intermediary collisions. It follows that $\Psi^h_\theta(r) = \pi - \theta - 2\beta_1(r)$ for $r \in (0, r')$ where $\beta_1 = \beta_1(r)$ satisfies $b \sin \beta_1 = (a - r) \sin \theta$. We may also characterize $r'$ as the value of $r$ that satisfies $a \sin(\theta - 2\beta_1) = b \sin \beta_1$. From these observations it follows that

$$
\Psi^h_\theta(0) = \pi - \frac{3 + h}{1 - h} \theta + O(\theta^3), \quad \lim_{r \to (r')-} \Psi^h_\theta(r) = \pi - \frac{1 - h}{3 + h} \theta + O(\theta^3).
$$

Following the notation established in the discussion on the semicircle,

$$V_{\theta,1} = \left[ \pi - \frac{3 + h}{1 - h} \theta + O(\theta^3), \pi - \frac{1 - h}{3 + h} \theta + O(\theta^3) \right].$$

Moreover, if we let $\Theta = \Psi_\theta(r)$ it follows from implicit differentiation that

$$\Theta'(r) = \frac{1}{1 - h} \frac{4 \sin \theta}{\cos \left( \Theta + \theta - \pi \right)}$$

which is the corresponding value in the semicircle case except for the factor of $(1 - h)^{-1}$.

For $r \in (r', 1)$, we have $\Psi^h_\theta(r) = 2\beta_1(r) + 2\beta_2(r) - \theta$, where $\beta_1(r)$ is as above and $\beta_2 = \beta_2(r)$ satisfies $b \sin \beta_2 = h \sin(2\beta_1 - \theta) + \sin \beta_1$. It follows by symmetry that

$$V_{\theta,2} = \left[ \frac{1 - h}{3 + h} \theta + O(\theta^3), \frac{3 + h}{1 - h} \theta + O(\theta^3) \right].$$
Further, by implicit differentiation again

$$\Theta'(r) = \frac{1 + h}{(1 - h)^2} \frac{8 \sin \theta}{\cos (\Theta + \frac{\theta}{4})},$$

which again resembles the semicircle case but for the factor of \((1 + h)(1 - h)^{-2}\).

As in the computation of the diffusivity for the semicircle we find the following.

**Proposition 3.9.** For the flat bottom of length \(h \in (0, 1)\) modification of the semicircle, we have the following value of diffusivity as a function of \(h\):

$$D(h) = \frac{4rv}{\pi} \frac{1 + \zeta_h}{1 - \zeta_h},$$

where

$$\zeta_h = -\frac{1 + 3h}{4} \frac{1 - h}{1 + h} \log \frac{3 + h}{1 - h}.$$

Notice that the limiting case \(h = 0\) gives the diffusivity of the semicircle while \(h = 1\) gives \(\zeta_h = 0\) which gives the diffusivity in the case that at each post-collision angle is chosen independently according to the distribution \(\mu\).

The final family of interest is formed by adding a flat side of length \(h \in (0, 1)\) between semicircles as shown above. The key observation here is that the operator \(P_h\) corresponding to such a geometry can be thought of as a sum of conditional operators given by \(P_h = (1 - h)P + hI\) where \(P\) is the operator corresponding
to the semicircle geometry and $I$ is the identity operator. Such an operator is a
generalized Maxwell-Smoluchowski model as discussed in the introduction. Next
notice that since $P$ and $I$ commute the spectra of $P_h$ and $P$ are the same, and in
fact every spectral value of $P_h$ is given by $(1 - h)\lambda + h$ for some unique spectral
value $\lambda$ of $P$. It follows that

$$
\int_{-1}^{1} \frac{1 + \lambda}{1 - \lambda} \Pi_a^h(d\lambda) = \int_{-1}^{1} \frac{1 + (1 - h)\lambda + h}{1 - (1 - h)\lambda - h} \Pi_a(d\lambda)
= \int_{-1}^{1} \left( \frac{1}{1 - h} \frac{1 + \lambda}{1 - \lambda} + \frac{h}{1 - h} \right) \Pi_a(d\lambda),
$$

where $\Pi_a$ is the spectral measure as given in the statement of Theorem 3.1, and
similary $\Pi_a^h$ is derived from the projection valued measure $\Pi^h$ associated to $P_h$
given by the spectral theorem. The following proposition then follows from the
discussion above and the spectral formulation of the diffusivity.

**Proposition 3.10.** For the flat top of length $h \in (0, 1)$ modification of the semi-
circle, we have the following value of diffusivity as a function of $h$:

$$
\mathcal{D}(h) = \frac{1}{1 - h} \mathcal{D} + \frac{h}{1 - h} \frac{4rv}{\pi} = \frac{4rv}{\pi(1 - h)} \left( h + \frac{1 + \zeta}{1 - \zeta} \right),
$$

where $\mathcal{D}$ is the diffusivity for the unmodified semicircle and $\zeta = -1/4 \log 3$.

### 3.3 Additional proofs

We collect here proofs of some of the more technical propositions and lemmas
from earlier parts of the chapter.
3.3.1 Sketch of proof of Proposition 2.2

The proposition results from tedious but elementary and straightforward integra-
tions. We show a few steps to convey the flavor.

By identifying the tangent space to \( C \) at \( q \in \partial C \) with \( \mathbb{R}^k \oplus \mathbb{R}^{n-k} \), the unit normal vector \( n \) is identified with \( e_n = (0, \ldots, 0, 1) \) and \( \mathbb{H}_q \) is identified with the half-space consisting of vectors \( v = (v_1, v_2) \in \mathbb{R}^k \oplus \mathbb{R}^{n-k} \) such that \( \langle v, e_n \rangle > 0 \).

For such a post-collision velocity \( v \), the point of next collision with the channel boundary is \( q + \tau v \), where \( \tau = \frac{2r \langle v, e_n \rangle}{|v|^2} \) is the time interval between the two collisions and \( Z(v) = 2r \langle v, e_n \rangle v_1/|v_2|^2 \) is the between-collisions displacement vector in “horizontal” factor \( \mathbb{R}^k \) as represented in Figure 2.4. We assume that \( \nu \) has the following general form:

\[
d\nu(v) = C\langle v, n \rangle f \left( |v|^2 \right) dV(v),
\]

in which \( f(x) \) is a nonnegative function on \([0, \infty)\) such that \( \int_0^{\infty} x^n f(x^2) \, dx < \infty \).

We allow \( f \) to be distributional (a delta-measure concentrated on a fixed value of \(|v|\)) so as to include the case where \( \nu \) is supported on an hemisphere. Let \( S_+ := S_n^{-1} \) be the unit hemisphere in \( \mathbb{H} \). Then \( \mathbb{H} \) is diffeomorphic to \( S_+ \times (0, \infty) \) under polar coordinates \( v \mapsto (w, \rho) \), where \( w = v/|v| \) and \( \rho = |v| \), and \( dV(v) = \rho^{n-1} dV_{\text{sph}}(w) \, d\rho \). Also define the notations \( S_+a := S_+ \cap \mathbb{H}(a) \) and \( E(a) := E_\nu[|Z|^2, \mathbb{H}(a)] \).

Then

\[
E(a) = C \int_0^\infty \int_{S_+a} \rho^n f \left( \rho^2 \right) |Z(w)|^2 \langle w, n \rangle \, dV_{\text{sph}}(w) \, d\rho
= C' \int_{S_+a} |Z(w)|^2 \langle w, n \rangle \, dV_{\text{sph}}(w),
\]

where we have used that \( Z(v) = Z(w) \). Here and below, \( C, C', C'' \) are positive constants that can be obtained explicitly.
The image of $S_{+a}$ under the projection map $\pi: w \in S_+ \mapsto \overline{w} \in \mathbb{B}_{a}^{n-1}$ contains the ball $\mathbb{B}_{a}^{n-1}$ of radius $(1 + (2/a)^2)^{-1/2}$, and it is equal to $\mathbb{B}_{a}^{n-1}$ when $n - k = 1$.

The volume elements $dV_{sph}$ on the hemisphere and $dV_{n-1}$ on the ball are related under $\pi$ by $\langle w, n \rangle dV_{sph}(w) = dV_{n-1}(\overline{w})$. Also let $x_1 = \pi_1(x)$ be the natural projection from the unit ball in $\mathbb{R}^{n-1}$ to the unit ball $\mathbb{B}^k$ in the horizontal factor $\mathbb{R}^k$, and $x_2 = \pi_2(x)$ the projection to the complementary factor $\mathbb{R}^{n-k-1}$ in $\mathbb{R}^{n-1}$. Then the limit as $a \to \infty$ of $\int_{S_{+a}} \langle Z(w), w \rangle^2 dV_{sph}(w)$ is, up to multiplicative positive constant, the same as the limit of

$$\int_{\mathbb{B}_a^{n-1}} \frac{(1 - |x_1|^2 - |x_2|^2) |x_1|^2}{(1 - |x_1|^2)^2} dV_{n-1}(x)$$

$$= \int_{\mathbb{B}_k^k} \int_{\mathbb{B}_{n-1}^{n-k-1}} \frac{|x_1|^2}{(1 - |x_1|^2)^2} (1 - |x_1|^2 - |x_2|^2) dV_{n-k-1}(x_2) dV_k(z_1)$$

$$= 2 \text{Vol}(\mathbb{B}^{n-k-1}) \frac{2}{n - k + 1} \int_{\mathbb{B}_k^k} |x_1|^2 (1 - |x_1|^2)^{\frac{n-k-3}{2}} dV_k(x_1)$$

$$= \frac{k}{n - k + 1} \text{Vol}(\mathbb{B}^{n-k-1}) \text{ Vol}(\mathbb{B}^k) \int_0^\infty s^{\frac{n^2}{2}} \frac{s^{\frac{k}{2}}}{s^{\frac{n-k-3}{2}}} ds$$

where the iterated integrals were carried out in polar coordinates, in which volume elements are related by $dV_n(v) = |v|^{n-1} dV_{sph}(v/|v|) d|v|$. The limit of the remaining integral, as $a$ goes to $\infty$, is a Beta-function of the exponents of $s$ in the integrand; it, and the volumes of unit balls, can be written in terms of Gamma-functions and further simplified.

The expected values of $\tau_b(v) = 2r \langle v, n \rangle / |v_2|^2$ are shown by similar computations to take the form

$$E_\mu [\tau_b] = \frac{2r}{s} \frac{\Gamma \left( \frac{n+1}{2} \right)}{\pi^{\frac{n-1}{2}}} I(n, k), \quad E_{\mu_\beta} [\tau_b] = r \left( 2\beta M \right)^{\frac{1}{2}} \frac{\Gamma \left( \frac{n}{2} \right)}{\pi^{\frac{n-1}{2}}} I(n, k),$$

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where $s$ is the speed (or radius) of the hemisphere on which $\mu$ is supported and

$$I(n, k) := \int_{S_+} \frac{(x, n)^2}{|x|^2} dV_{\text{sph}}(x) = \frac{\pi \frac{n}{2}}{(n - k) \Gamma \left( \frac{n}{2} \right)} ,$$

$S_+$ being the hemisphere of radius 1 in $\mathbb{H}$.

Finally, observed that $\mathbb{E}_\nu [ (Z^u_a)^2 ] = \mathbb{E}_\nu [ |Z_a|^2 ] / k$ since $\nu$ is rotationally symmetric in the $\mathbb{R}^k$ subspace. The proposition is now a consequence of these observations.

### 3.3.2 Proofs of CLT lemmas

**Proof of Lemma 3.2.** We again employ the notation

$$D_l := \sum_{j=k}^{l-1} Z_{a,j} - \sum_{j=k}^{n_{a,t}-1} Z_{a,t} .$$

Since $\sum_{j=0}^{N_{a,t}-1} Z_{a,j} = \sum_{j=0}^{n_{a,t}-1} Z_{a,j} + D_{0}^{N_{a,t}}$ it suffices to show $D_{0}^{N_{a,t}} \to 0$ in probability. Before getting to this directly, we begin with a few technical remarks to be used in what follows.

Let $\nu > 1$ and define

$$n_1 = \left[ \left( 1 - \frac{\epsilon^2}{2} \right) n_{a,t} \right] + 1, \quad n_2 = \left[ \left( 1 + \frac{\epsilon^2}{2} \right) n_{a,t} \right] - 1 .$$

Then $\mathbb{P}(n_1 \leq N_{a,t} \leq n_2) \geq 1 - \epsilon$ for a large enough. Let $a^* = \epsilon^\nu a$, $n_{a,t}^* = n_{a,t}^*$. Observe that

$$\epsilon^{2\nu} n_{a,t} \leq \epsilon^{2\nu} a h(a) t \leq \mathbb{E}_{[T_b]} \leq \mathbb{E}_{[T_b]} \leq n_{a,t}^* + 1 .$$

Therefore, $n_2 - n_1 \leq \epsilon^{2\nu} n_{a,t} - 1 \leq n_{a,t}^*$. We are now ready to address the convergence
in probability. Observe that

\[
\mathbb{P}\left(\left|D_{1,N_{a,t}}^{}\right| > a\epsilon\right) = \sum_{j=1}^{\infty} \mathbb{P}\left(N_{a,t} = j, \left|D_{1,N_{a,t}}^{}\right| > a\epsilon\right)
\]

\[
= \sum_{j=n_1}^{n_2} \mathbb{P}\left(N_{a,t} = j, \left|D_{1,N_{a,t}}^{}\right| > a\epsilon\right)
\]

\[
+ \sum_{j \notin [n_1,n_2]} \mathbb{P}\left(N_{a,t} = j, \left|D_{1,N_{a,t}}^{}\right| > a\epsilon\right).
\]

Notice for the second term above that

\[
\sum_{j \notin [n_1,n_2]} \mathbb{P}\left(N_{a,t} = j, \left|D_{1,N_{a,t}}^{}\right| > a\epsilon\right) \leq \sum_{j \notin [n_1,n_2]} \mathbb{P}\left(N_{a,t} = j\right)
\]

\[
= 1 - \mathbb{P}(n_1 \leq N_{a,t} \leq n_2)
\]

\[
\leq \epsilon.
\]

For the first term observe that

\[
\sum_{j=n_1}^{n_2} \mathbb{P}\left(N_{a,t} = j, \left|D_{1,N_{a,t}}^{}\right| > a\epsilon\right) \leq \sum_{j=n_1}^{n_2} \mathbb{P}\left(N_{a,t} = j, \max_{n_1 \leq k \leq n_2} \left|D_k^{}\right| > a\epsilon\right)
\]

\[
\leq \mathbb{P}\left(\max_{n_1 \leq k \leq n_2} \left|D_k^{}\right| > a\epsilon\right).
\]

And notice that

\[
\mathbb{P}\left(\max_{n_a,t<k\leq n_2} \left|D_k^{}\right| > a\epsilon\right) = \mathbb{P}\left(\max_{n_a,t<k\leq n_2} \left|\sum_{i=n_a,t+1}^{k} Z_{a,i}\right| > a\epsilon\right)
\]

\[
= \mathbb{P}\left(\max_{1\leq k\leq n_2-n_a,t} \left|\sum_{i=1}^{k} Z_{a,i}\right| > a\epsilon\right)
\]

\[
\leq \mathbb{P}\left(\max_{1\leq k\leq n_2-n_1} \left|\sum_{i=1}^{k} Z_{a,i}\right| > a\epsilon\right).
\]
Similarly,

\[
P\left( \max_{n_1 \leq k < n_{a,t}} |D_k^{1}| > a\epsilon \right) \leq P\left( \max_{1 \leq k \leq n_2 - n_1} \left| \sum_{i=1}^{k} Z_{a,i} \right| > a\epsilon \right).
\]

It then follows that

\[
P\left( \max_{n_1 \leq k \leq n_2} |D_k^{1}| > a\epsilon \right) \leq 2P\left( \max_{1 \leq k \leq n_2 - n_1} \left| \sum_{i=1}^{k} Z_{a,i} \right| > a\epsilon \right)
\leq 2P\left( \max_{1 \leq k \leq n_{a,t}^{*}} \left| \sum_{i=1}^{k} Z_{a,i} \right| > a\epsilon \right).
\]

Next observe that by the symmetry of \( Z_{a,i} \),

\[
P\left( \left| \sum_{i=1}^{n_{a,t}^{*}} Z_{a,i} \right| > a\epsilon, \max_{1 \leq k \leq n_{a,t}^{*}} \left| \sum_{i=1}^{k} Z_{a,i} \right| > a\epsilon \right)
\leq P\left( \sum_{i=1}^{n_{a,t}^{*}} Z_{a,i} > a\epsilon, \max_{1 \leq k \leq n_{a,t}^{*}} \left| \sum_{i=1}^{k} Z_{a,i} \right| > a\epsilon \right)
\geq \frac{1}{2},
\]

which implies

\[
P\left( \max_{1 \leq k \leq n_{a,t}^{*}} \left| \sum_{i=1}^{k} Z_{a,i} \right| > a\epsilon \right) \leq 2P\left( \sum_{i=1}^{n_{a,t}^{*}} Z_{a,i} > a\epsilon, \max_{1 \leq k \leq n_{a,t}^{*}} \left| \sum_{i=1}^{k} Z_{a,i} \right| > a\epsilon \right)
\leq 2P\left( \sum_{i=1}^{n_{a,t}^{*}} Z_{a,i} > a\epsilon \right).
\]
We summarize and observe that by assumption
\[
\sum_{j=n_1}^{n_2} \mathbb{P}(N_{a,t} = j, D_1^{N_{a,t}} > a\epsilon) \leq 4\mathbb{P}\left(\left|\sum_{i=1}^{n_{a,t}^*} Z_{a,i}\right| > a\epsilon\right)
= 4\mathbb{P}\left(\sum_{i=1}^{n_{a,t}^*} Z_{a,i} > a^*1^{-\nu}\right)
\rightarrow \frac{8}{\sqrt{2\pi tD}} \int_{e^{1^{-\nu}}}^\infty e^{-x^2/2tD} dx,
\]
as \(a \to \infty\). In letting \(\epsilon \to 0\) the last line above vanishes. \(\square\)

**Proof of Lemma 3.3.** Let \(I_1(a) := \{x : a/\log^\gamma(a) < |x| < a \log \log a\}\) and \(I_2 := \{x : |x| > a \log \log a\}\). It will suffice to show that each of the sums \(\sum_{j=0}^{N_{a,t}-1} a^{-1}Z_j\) for \(i = 1, 2\) converges to zero in probability.

We first consider the truncation by \(I_2\). As there is no ambiguity, we use the shorthand \(Z_a := Z_{I_2}\) and \(Z_{a,j} = Z_{I_2}(\Theta_j)\). Let \(\epsilon > 0\) and observe that
\[
\mathbb{P}\left(\left|\sum_{j=0}^{N_{a,t}-1} Z_{a,j}\right| > a\epsilon\right) \leq \mathbb{P}\left(\sum_{j=0}^{N_{a,t}-1} |Z_{a,j}| > a\epsilon\right)
= \sum_{N=1}^\infty \mathbb{P}\left(\sum_{j=0}^{N} |Z_{a,j}| > a\epsilon\right) \mathbb{P}(N_{a,t} = N)
\leq \sum_{N=1}^\infty \mathbb{P}(Z_j \in I_2 \text{ for some } j, 0 \leq j \leq N - 1) \mathbb{P}(N_{a,t} = N)
\leq \sum_{N=1}^\infty \sum_{j=0}^{N-1} \mathbb{P}(Z_j \in I_2) \mathbb{P}(N_{a,t} = N)
= \mathbb{E}[N_{a,t}] \mathbb{P}(Z_0 \in I_2).
\]

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Next note that
\[
\mathbb{P}(Z_0 \in I_2) = \int_{0}^{\cot^{-1}(a \log \log a/(2r))} \sin \theta \, d\theta \\
= 1 - \cos \left( \cot^{-1}(a \log \log a/(2r)) \right) = O \left( (a \log \log a)^{-2} \right).
\]

Moreover, a straightforward application of Lemma 3.1 and the dominated convergence theorem shows that \( \mathbb{E} \left[ N_{a,t} \right] = O(ah(a)) \). It follows that
\[
\mathbb{P} \left( \left| \sum_{j=0}^{N_{a,t}-1} Z_{a,j} \right| > a\epsilon \right) \leq O \left( \frac{1}{\log a \cdot (\log \log a)^2} \right) \to 0
\]
as \( a \to \infty \).

Next we consider the truncation by \( I_1 \). As before we use the shorthand \( Z_a := Z_{I_1} \). To show that the sum \( \sum_{j=0}^{N_{a,t}-1} a^{-1} Z_{a,j} \) converges to zero in probability, we use Chebyshev’s inequality. To this end, observe that as in the proof of Theorem 2.1
\[
\mathbb{E} \left[ \left( \sum_{j=0}^{N_{a,t}-1} a^{-1} Z_{a,j} \right)^2 \right] = \int_{-1}^{1} \frac{1}{1 - \lambda} \mathbb{E} \left[ N_{a,t} + O(1) \right] \frac{h(a)}{ah(a)} \| Z_a \|^2 \Pi_{a}(d\lambda),
\]
where we recall \( \Pi_{a} = \| Z_a \|^{-2} \langle Z_a, \Pi(d\lambda) Z_a \rangle \) is the spectral measure associated to \( Z_a \). Note \( \| Z_a \|^2 = O(\log \log a) \) and \( h(a)/a = 1/\log a \), while all other factors in the integrand are bounded as \( a \to \infty \). The result follows.

\textbf{Proof of Lemma 3.4.} Because of the slight difference in definitions, we show separately that \( \sum_{i=1}^{k_{a,t}-1} V_{a,i} \to 0 \) and \( V_{a,k_{a,t}} \to 0 \). To prove each of these, note that by Chebyshev’s inequality, it suffices to show
\[
\mathbb{E} \left[ \left( \sum_{i=1}^{k_{a,t}-1} V_{a,i} \right)^2 \right] \to 0, \quad \mathbb{E} \left[ V_{a,k_{a,t}}^2 \right] \to 0,
\]

respectively. We start with the first. Observe that

\[
\mathbb{E} \left[ \left( \sum_{i=1}^{k_{a,t} - 1} V_{a,i} \right)^2 \right] = k_{a,t} \mathbb{E} \left[ V_{a,1}^2 \right] + 2 \sum_{1 \leq i < j \leq k_{a,t} - 1} \mathbb{E} [V_{a,i}V_{a,j}]
\]

and

\[
\mathbb{E} \left[ V_{a,1}^2 \right] = \mathbb{E} \left[ \left( \sum_{j=0}^{s_{a,t} - 1} a^{-1} Z_{a,j} \right)^2 \right] = \int_{\sigma} \frac{1 + \lambda s_{a,t} + O(1) h(a)}{1 - \lambda ah(a) a} \|Z_a\|^2 \Pi_a(d\lambda) = O \left( (ah(a)^{a-1}) \right).
\]

Therefore, \( k_{a,t} \mathbb{E} \left[ V_{a,1}^2 \right] = O \left( (ah(a)^{a-\beta}) \rightarrow 0 \right. \). The number of terms in the sum \( \sum_{1 \leq i < j \leq k_{a,t} - 1} V_{a,i}V_{a,j} \) is \((k_{a,t} - 1)(k_{a,t} - 2)\) and each term \( V_{a,i}V_{a,j} \) itself contains \( s_{a,t}^2 \) terms of the form \( a^{-2} Z_{a,m}Z_{a,n} \). It follows that

\[
2 \sum_{1 \leq i < j \leq k_{a,t} - 1} \mathbb{E} [V_{a,i}V_{a,j}] = O((ah(a))^{2(1-\beta)+2\alpha-1}) \rightarrow 0.
\]

Finally, the sum in \( V_{a,k_{a,t}} \) contains by definition less than \( b_{a,t} + s_{a,t} \) terms. Just as above, it follows that \( \mathbb{E} \left[ V_{a,k_{a,t}}^2 \right] \leq O((ah(a))^{\beta-1}) \rightarrow 0. \)

**Proof of Lemma 3.5.** Let \( w_i = \exp(i\mu U_{a,i}) \) for \( 1 \leq i \leq k_{a,t} \). Also let \( \sigma_{w_i}^2 = \mathbb{E} \left[ w_i^2 \right] - \mathbb{E}^2 \left[ w_i \right] \). Define \( \mathcal{E}(w_1, w_2) := \mathbb{E} \left[ w_1 w_2 \right] - \mathbb{E} \left[ w_1 \right] \mathbb{E} \left[ w_2 \right] \). Because of the small block gap of size \( s_{a,t} \) between big blocks, \( \|\mathcal{E}(w_1, w_2)\| = |\sigma_{w_1}||\sigma_{w_2}| \text{corr}(w_1, w_2) \leq \)
\[ 4 |\text{corr}(w_1, w_2)| \leq 4 |\rho(s_{a,t})|. \] Moreover,

\[
|\mathbb{E}[w_1 w_2 w_3] - \mathbb{E}[w_1] \mathbb{E}[w_2] \mathbb{E}[w_3]| \leq |\mathcal{E}(w_1, w_2 w_3)| + |\mathbb{E}[w_1] \mathcal{E}(w_2, w_3)| \\
= |\sigma_{w_1}| |\sigma_{w_2 w_3}| \text{corr}(w_1, w_2 w_3) \\
+ |\mathbb{E}[w_1] \mathcal{E}(w_2, w_3)| \\
\leq 4 |\rho(s_{a,t})| + 4 |\rho(s_{a,t})|.
\]

It then follows by induction that

\[
|\mathbb{E} \left[ \exp \left( i \mu \sum_{i=1}^{k_{a,t}} U_{a,i} \right) \right] - \prod_{i=1}^{k_{a,t}} \mathbb{E} \left[ \exp \left( i \mu U_{a,i} \right) \right]| \leq 4 k_{a,t} |\rho(s_{a,t})| \to 0
\]
as \( a \to \infty \).

**Proof of Lemma 3.6.** A simple induction argument shows that if \( z_1, \ldots, z_m, w_1, \ldots, w_m \in \mathbb{C} \) are of modulus at most 1, then

\[
\left| \prod_{i=1}^{m} z_i - \prod_{i=1}^{m} w_i \right| \leq \sum_{i=1}^{m} |z_i - w_i|.
\]

Applying the remark to \( |\mathbb{E} \left[ \exp \left( i \mu U_{a,i} \right) \right]| \) and, for large enough \( a, \left| 1 - \frac{\mu^2}{2 k_{a,t} D} \right| \),
we see
\[
\prod_{i=1}^{k_{a,t}} \mathbb{E} [\exp (i \mu U_{a,i})] - \left(1 - \frac{\mu^2}{2k_{a,t}} t \mathcal{D} \right)^{k_{a,t}} \leq \sum_{i=1}^{k_{a,t}} \left| \mathbb{E} [\exp (i \mu U_{a,i})] - \left(1 - \frac{\mu^2}{2k_{a,t}} t \mathcal{D} \right) \right|
\]
\[
= k_{a,t} \left| \mathbb{E} [\exp (i \mu U_{a,1})] - \left(1 - \frac{\mu^2}{2k_{a,t}} t \mathcal{D} \right) \right|
\]
\[
= \frac{\mu^2}{2} k_{a,t} \mathbb{E} [U_{a,1}^2] - O \left( \mathbb{E} [U_{a,1}^3] \right)
\]
\[
\leq \frac{\mu^2}{2} k_{a,t} \mathbb{E} [U_{a,1}^2] - t \mathcal{D} \]
\[
+ \left| k_{a,t} \mathcal{O} \left( \mathbb{E} [U_{a,1}^3] \right) \right|.
\]

Now, it follows from the spectral representation of \( \mathcal{D} \) that \( |k_{a,t}\mathbb{E} [U_{a,1}^2] - t \mathcal{D}| \to 0 \).

Expanding \( U_{a,1}^3 \) results in \( b_{a,t}^3 \) terms of the form \( a^{-3} Z_{a,i}Z_{a,j}Z_{a,k} \). Suppose \( i \leq j \leq k \) and let \( D_1 = j - i \) and \( D_2 = k - j \). Let \( C(a) = C \log a \), where \( C > 4\beta \).

We separate the terms in the expansion of \( U_{a,1}^3 \) into one group containing those terms whose indices satisfy \( D_1 \leq C(a) \) and \( D_2 \leq C(a) \); and another group with those terms for which \( D_1 > C(a) \) or \( D_2 > C(a) \). Suppose \( Z_{a,i}Z_{a,j}Z_{a,k} \) is in the first group. Then

\[
\mathbb{E} [Z_{a,i}Z_{a,j}Z_{a,k}] \leq \mathbb{E}^{1/3} [ |Z_{a,i}|^3 ] \mathbb{E}^{1/3} [ |Z_{a,j}|^3 ] \mathbb{E}^{1/3} [ |Z_{a,k}|^3 ]
\]
\[
= \mathbb{E} [ |Z_{a,i}|^3 ]
\]
\[
= O (a/ \log^\gamma a).
\]

Moreover, of the \( b_{a,t}^3 \) total terms, \( O (b_{a,t}C(a)^2) \) of them fall into this first group. Thus the contribution of these terms to \( |k_{a,t} \mathbb{E} [U_{a,1}^3]| \) is at most of the order \( O (\log^{1-\gamma} a) \) which is negligible as \( a \to \infty \).

Suppose next that \( Z_{a,i}Z_{a,j}Z_{a,k} \) is in the second group and assume without loss
of generality that \( D_1 > C(a) \). Observe that

\[
\mathbb{E} [Z_{a,i}Z_{a,j}Z_{a,k}] = \text{corr}(Z_{a,i}, Z_{a,j}Z_{a,k}) \mathbb{E}^{1/2} [Z_{a,i}^2] \left( \mathbb{E} \left[ (Z_{a,j}Z_{a,k})^2 \right] - \mathbb{E}^2 [Z_{a,j}Z_{a,k}] \right)^{1/2}.
\]

Recall that \( \mathbb{E} [Z_{a,i}^2] = O(\log a) \). Moreover, by the Cauchy-Schwarz inequality, stationarity, and further direct computation of moments

\[
\mathbb{E} \left[ (Z_{a,j}Z_{a,k})^2 \right] \leq \mathbb{E} [Z_{a,i}^4] = O \left( a^2 / \log^2 a \right)
\]

and

\[
\mathbb{E}^2 [Z_{a,j}Z_{a,k}] \leq \mathbb{E}^2 [Z_{a,j}^2] = O \left( \log^2 a \right).
\]

Finally, using the mixing properties of the process \( \text{corr} (Z_{a,i}, Z_{a,j}Z_{a,k}) \leq \rho (C(a)) = O \left( a^{-C} \right) \). Putting these three estimates together, we see that

\[
a^{-3} \mathbb{E} [Z_{a,i}Z_{a,j}Z_{a,k}] \leq O \left( a^{-(C+2)} \log^{1/2-\gamma} a \right)
\]

Since, \( O \left( b_{a,t}^3 - b_{a,t} C(a)^2 \right) = O \left( b_{a,t}^3 \right) = O \left( a^{6\beta} \log^{-3\beta} a \right) \) terms are in this second group, their contribution to \( \left| k_{a,t} O \left( \mathbb{E} [U_{a,1}^3] \right) \right| \) will be of order at most

\[
O \left( a^{4\beta-C} \log^{1/2-2\beta-\gamma} a \right),
\]

which is indeed negligible with our choice of \( C \). The lemma now follows. \( \square \)
This chapter introduces a random billiard model for a minimalistic heat engine. The heat engine is constructed through a series of steps, each of which is the focus of sections 4.2, 4.3, and 4.4 below. A distinguishing feature of the model is an explicit random billiard model of a heat bath-thermostat which is very closely related to the deterministic system from which it is derived. Section 4.1 introduces this deterministic model. The section serves to motivate the random billiard model but is not strictly necessary for defining the random billiard heat engine. The reader can safely skip past this section on the first read. Section 4.2 begins the construction in earnest, introducing the random billiard heat bath-thermostat—a one dimensional random billiard along a line segment, where collisions of the billiard particle with one distinguished endpoint produce a random post-collision velocity so as to mimic heating or cooling of the particle. Section 4.3 modifies this model slightly so that collisions with both endpoints produce random post-collision velocities, mimicking heat flow when the distributions of post-collision velocities are chosen appropriately. Section 4.4 introduces the heat engine itself and highlights a connection with the channel model of Chapters 2 and 3 first mentioned at the end of Chapter 2. Section 4.5 gives a preliminary analysis of the
The single particle billiard system is a geometric representation of a mechanical system that may consist of many constituent rigid particles interacting with each other through elastic collisions. This simple remark is immediately understood by considering the two-particle, one-dimensional billiard system shown at the top of Figure 4.1.

To be fully specified, the billiard table must be given a Riemannian metric relative to which reflections are specular. The triangular region of Figure 4.1 with the standard Euclidean inner product does not in general define a billiard system since if $m_1 \neq m_2$, the single particle in the triangle, whose $x$ and $y$ coordinates give the positions of the two masses along the interval $[0, L]$, will not reflect specularly when colliding with the diagonal side of the triangle. A simple way to make the collision specular is to absorb the mass values into the position coordinates. Thus we define coordinates $x_{\text{new}} = \sqrt{\frac{m_1}{m}} x$, $y_{\text{new}} = \sqrt{\frac{m_2}{m}} y$ where $m = m_1 + m_2$, and note that the kinetic energy of the system, expressed in the new coordinates, is a constant multiple of the ordinary Euclidean norm. Therefore, a linear transformation that conserves energy becomes an orthogonal map. Conservation of linear momentum means that the component of the pre-collision velocity vector in the direction of the slanted side of the triangle in the new metric equals the same component for the post-collision velocity. Therefore, the normal component of the pre- and post-collision velocities can only be either equal or the negative of each other. Obviously, the latter must the case as there would be no collision
otherwise.

Figure 4.1: The billiard table of the two-particle system.

These new, mass-rescaled coordinates yield a bona fide billiard system on the plane. We call the single particle system in the triangular region with the new metric the billiard representation of the one-dimensional two-particle system. The idea is obviously very general and works in any dimension, for any number of masses. In higher dimensions, say, for the collision of two solid bodies in 3-dimensional space, the basic conservation laws of energy, linear and angular momentum, as well as the imposition of time-reversibility and linearity, do not fully specify the collision map. Further assumptions about the nature of contact, such as being slippery or rubbery, are needed.

4.1.2 Knudsen implies Maxwell-Boltzmann

One has not entered thermodynamics until temperature is somehow brought into the picture, and for our needs this may be done via the Maxwell-Boltzmann distribution of velocities. In the present section we illustrate with a simple example the geometric explanation of how this fundamental distribution arises in the context of billiard dynamics.

The example is shown in Figure 4.2. It consists of point masses $m_1, \ldots, m_k, m$
that can slide without friction on a line. Masses \( m_i \) are restricted to lie in the interval \([0, l]\) and they move independently of each other. Their position coordinates are indicated by \( z_i \); \( m \) can move in the bigger interval \([0, L]\), with position coordinate \( z \). At the endpoints of \([0, l]\) the \( m_i \) bounce off elastically. Mass \( m \) moves freely past \( l \) (dashed line in Figure 4.2), and it collides elastically with the \( m_i \) and with the wall at \( z = L \). We imagine the \( m_i \) as tethered to the left wall by inelastic and massless, but fully flexible strings of length \( l \); when the strings are stretched to the limit of their length, the masses bounce back as if hitting a solid wall at \( l \).

![Figure 4.2: A billiard model that helps explain the origin of the Maxwell-Boltzmann distribution of scattered velocities.](image)

To make the system more symmetric without changing it in any essential way, we regard the wall on the left as a mirror and we keep track of both \( z_i \) and its image \(-z_i\); thus \( z_i \in [-l, l] \) can be negative. (The thickness of the masses is considered negligible in this model.) In this symmetric form, the billiard representation of the system is as shown in Figure 4.3.

Let \( M = m + m_1 + \cdots + m_k \). Changing coordinates to

\[
x_i = \sqrt{m_i/M} \, z_i \quad \text{for} \quad i = 1, \ldots, k, \quad \text{and} \quad x_0 = \sqrt{m/M} \, z,
\]

the kinetic energy form becomes

\[
K(x, \dot{x}) = \left( M/2 \right) \left( \dot{x}_0^2 + \cdots + \dot{x}_k^2 \right).
\]
We may equivalently assume that \((x_1, \ldots, x_k)\) defines a point on the hypercube with coordinates \(x_i\) in \(I_i := [-a_i/2, a_i/2]\), where \(a_i = 2\sqrt{m_i/M}\), having in mind the above comment about mirror image. Mass \(m\) is then constrained to move on the interval \(F(x_1, \ldots, x_k) \leq x_0 \leq \sqrt{m/ML}\) where

\[
F(x_1, \ldots, x_k) := \max\left\{\sqrt{m/m_1}|x_1|, \ldots, \sqrt{m/m_k}|x_k|\right\}.
\]

Figure 4.3: Part of the billiard representation of the system of Figure 4.2 for \(k = 2\) describing the interaction between \(m\) and the masses \(m_1\) and \(m_2\).

Thus the configuration manifold is

\[
M = \left\{(x_0, x) \in I_1 \times \cdots \times I_k \times \mathbb{R} : F(x) \leq x_0 \leq \sqrt{m/ML}\right\},
\]

and collision is represented (due to energy and momentum conservation and time-reversibility), by specular reflection at the boundary of \(M\). We now wish to follow the motion of mass \(m\); geometrically, this amounts to following the image of billiard orbits under the orthogonal projection \(\pi\), as indicated in Figure 4.4. In particular, what can be said about the distribution of values of the projection \(\bar{v}(t) := \pi(v(t))\) of the velocity of typical billiard trajectories over long time spans? The following elementary proposition points to an answer.

**Proposition 4.1.** Let \(S := S^k_{\sigma \sqrt{k} + 1}\) denote the hemisphere of dimension \(k\)
and radius $\sigma\sqrt{k+1}$, consisting of vectors $v = (v_0, \ldots, v_k) \in \mathbb{R}^{k+1}$ such that $v_0 > 0$ and $v_0^2 + \cdots + v_k^2 = (k+1)\sigma^2$. Let $\mu_k$ be the Knudsen cosine probability measure on $S$; thus $d\mu_k(v) = C_kv_0\,dV(v)$, where $V$ is the Euclidean volume measure on $S$ and $C_k$ is a normalizing constant. Let $\nu_k$ be the image of $\mu_k$ under the projection map $\pi(v) = v_0$. Thus the $\nu_k$-measure of an interval $A \subset \mathbb{R}$ is, by definition, 

$$
\nu_k(A) := \mu_k\left(\{v : \pi(v) \in A\}\right).
$$

Then, as $k$ goes to infinity, the sequence of $\nu_k$ converges (in the vague topology of probability measures) to $\nu$ on $(0, \infty)$ such that

$$
d\nu(v_0) = \frac{v_0}{\sigma} \exp\left( -\frac{1}{2} \frac{v_0^2}{\sigma^2} \right) \,dv_0.
$$

We refer to $\nu$ as the post-collision Maxwell-Boltzmann probability measure in dimension 1, with parameter $\sigma^2$. Similarly, let $\nu_{i,k}$ be the probability distribution of $v_i$, $i \neq 0$, given that $v$ is distributed according to $\mu_k$. Then in the limit as $k$ approaches infinity $\nu_{i,k}$ converges to the Gaussian

$$
d\nu_i(v_i) = \frac{\exp\left( -\frac{1}{2} \frac{v_i^2}{\sigma^2} \right) }{\sigma \sqrt{2\pi}} \,dv_i.
$$

**Proof.** For convenience set $R := \sigma\sqrt{k+1}$ and let $S^{k-1}$ be the unit $(k-1)$-sphere in
$\mathbb{R}^k$ centered at the origin. Let $\phi : [0, R] \times S^{k-1} \to S^k_+ (R)$ be the polar coordinates map on the hemisphere, which is defined by

$$
\phi (v_0, v) = \left( v_0, \sqrt{R^2 - v_0^2} v \right).
$$

Let $dV_{S^k_+ (R)}$ denote the volume form on the $k$-dimensional hemisphere of radius $R$ and $dV_{S^{k-1}}$ the volume form on the unit sphere of dimension $k - 1$. A geometric exercise yields the expression of $dV_{S^k_+ (R)}$ in the just defined coordinates as

$$
dV_{S^k_+ (R)} = R \left( R^2 - v_0^2 \right)^{\frac{k-2}{2}} dv_0 dV_{S^{k-1}}.
$$

Given now any bounded function $f(v_0)$ on the interval $[0, R]$, we obtain by a change of variables in integration that

$$
\int_0^R f(v_0) d\nu_k (v_0) = \int_{S^k_+ (R)} f(\pi (v)) d\mu_n (v)
$$

$$
= C_n \int_0^R \int_{S^{k-1}} f(v_0) v_0 R \left( R^2 - v_0^2 \right)^{\frac{k-2}{2}} dv_0 dV_{S^{k-1}}.
$$

Integrating over the unit $(k-1)$-sphere in the last integral gives, for a new constant $D_k$,

$$
\int_0^R f(v_0) d\nu_k (v_0)) = D_k \int_0^R f(v_0) v_0 R \left( R^2 - v_0^2 \right)^{\frac{k-2}{2}} dv_0.
$$

Reverting back to $R = \sigma \sqrt{k + 1}$ and using that $(1 + a/m)^m$ converges to $e^a$ as $m$ tends to infinity, finally gives (for yet another constant $C$ independent of $f$)

$$
\lim_{n \to \infty} \int_0^{\sigma \sqrt{k+1}} f(v_0) d\nu_n (v_0) = C \int_0^{\infty} f(v_0) v_0 \exp \left( -\frac{1}{2} \frac{v_0^2}{\sigma^2} \right) dv_0.
$$
As \( f \) is arbitrary we conclude that

\[
d\nu(v_0) = C v_0 \exp\left(-\frac{1}{2} \frac{v_0^2}{\sigma^2}\right) dv_0.
\]

The constant \( C \) is easily found to be \( 1/\sigma \) by normalization. The claim for the other components of \( v \) is similarly demonstrated.

Proposition 4.1 is a manifestation of the well-known connection between probability theory (and statistical physics) and geometry in high dimensions. An especially intriguing exposition of this connection under the heading of concentration of measures may be found in [21], chapter 3 1/2.

The appearance of the Maxwell-Boltzmann (MB) distribution in our billiard model can now be explained as follows. Observing the velocity of the mass \( m \) amounts to taking the projection \( \pi \) of the velocity of the billiard trajectory as in Figure 4.4; if the billiard system is ergodic (this depends on the ratios of masses, although as far as we know there is no general criterion of ergodicity for polyhedral billiard tables, even in dimension 2), then as indicated earlier the long term distribution of velocities \( v_1, v_2, \ldots \) at the moments \( t_1, t_2, \ldots \) when the billiard particle emerges from the interaction zone on the left-hand side of the polyhedral table follows a cosine distribution. The proposition now implies that the projections \( \pi(v_1), \pi(v_2), \ldots \) should then follow the approximate MB distribution for finite \( n \). The approximation becomes better as the number of masses near the wall of the system of Figure 4.2 increases and the total energy increases proportionally.

Reverting to the initial velocity variables (i.e., before we absorbed the masses to form the above \( v_i \)) and indicating by \( v \) the velocity of \( m \), the post-collision MB
distribution can be written as

$$\rho_{MB}(v) = \beta mv \exp\left(-\beta \frac{mv^2}{2}\right)$$  \hspace{1cm} (4.3)

where $\beta$ is a parameter with units of energy. Later on, after we introduce our random billiard model for a thermostat, we will remark on how equality of $\beta$ for two parts of a system is a necessary condition for stationarity, so we recover the idea of thermal equilibrium. In statistical physics one writes $\beta = 1/kT$, where $k$ is the so-called Boltzmann constant and $T$ is absolute temperature.

Notice the difference between what we have called above the “post-collision” MB distribution and the MB distribution for the particle’s velocity sampled at random times, in which case the velocity can be both positive and negative. If $\rho_{MB}(v_0)$ is the post-collision density shown in $4.3$, then at a random time each velocity $v_0$ should be weighted by the time the particle, having this velocity, takes to go from one end of the interval to the other, which is proportional to $1/v_0$. This term cancels out the factor $v_0$ in $\rho_{MB}(v_0)$, yielding the standard one-dimensional MB-distribution $4.2$.

We point out for later use the model of Figure 4.5 of thermal interaction between gas molecule and wall. The $k$ masses on the far left have a very short range of motion, limited by the first dashed line, compared to $m_1$, which is limited by the second dashed line on the right. The gas molecule, $m_2$, can move across
those lines. As discussed above, when the number of masses constituting the finite “heat bath” grows, the asymptotic distribution of positions of $m_1$ (under the assumption of ergodicity) becomes uniform and the distribution of velocities of $m_1$ becomes Gaussian. The random billiard thermostat to be introduced in the next section will be abstracted from this deterministic model by eliminating the masses on the left (the “heat bath”) and setting the statistical state of $m_1$ equal to the asymptotic distribution (of position and velocity) this mass would have in the deterministic system in the limit of very large $k$.

### 4.2 The random billiard heat bath-thermostat

Figure 4.6: Mass $m_2$ moves freely over the interval until colliding with the wall-bound masses $m_1$. We imagine the latter as tethered to the wall by a string of length $l$. The position of $m_1$ is assumed to be random uniformly over $[0, l]$, and the velocity is random normally distributed with mean 0 and variance $\sigma^2$. At the moment $m_2$ crosses the dashed line and thus enters the zone where it can collide with $m_1$, we choose the state of the latter (its position and velocity) from fixed probability distributions described in the text below. From that point on we follow the deterministic motion of the two masses until $m_2$ leaves $[0, l]$. Prior to every future collision the statistical state of $m_1$ is reset.

We first introduce a random billiard model that will serve as our all-purpose thermostat at a fixed temperature. The model is derived from a deterministic billiard system consisting of two billiard particles which are allowed to travel on a finite length line segment. The details are explained in Figure 4.6. The two particle system can also be represented as a single particle billiard system by the technique of Subsection 4.1.1. This so-called billiard representation of the system is described in Figure 4.7.
As in the channel example of the previous chapters, a collision event—where mass $m_2$ enters the zone of interaction to the left of the dashed line in Figure 4.6 and emerges with a random velocity after colliding with mass $m_1$—is governed by an operator $P$. The operator $P$ generates a Markov chain with state space now $(0, \infty)$ of possible values of the velocity of $m_2$ as it emerges from the interaction zone after each collision event. To write $P$ explicitly first define $\gamma = \sqrt{m_2/m_1}$ and write $P = P_\gamma$ to keep in mind the dependence of the process on this key parameter. Note that $P_\gamma$ depends on the choice of a Gaussian distribution with mean zero and a $\sigma^2$, representing the distribution of velocities of $m_1$. Then $P_\gamma$ acts on, say, bounded continuous functions on the interval $(0, \infty)$ or, dually, on probability measures on that interval according to

$$(P_\gamma f)(v) = \frac{1}{l_1} \int_0^{l_1} \int_{-\infty}^{\infty} f(\varphi_\tau(r, (w, v))) \frac{\exp \left( -\frac{1}{2} \frac{w^2}{\sigma^2} \right)}{\sigma \sqrt{2\pi}} dw \, dr$$

where the following notation is being used: $\tau = \tau(r, w, v)$ is the return time to the entry (dashed-line) side of the triangle of Figure 4.7 given that the (deterministic) billiard trajectory begins at $r \in [0, l_1]$, where $l_1 = l (m_2/m_1)^{1/2}$, $m = m_1 + m_2$, $\varphi_\tau$ is the billiard flow stopped at time $\tau$, and $(w, v)$ is the initial velocity of the billiard particle in dimension 2.

This amounts to giving the post-collision velocity $V$ of $m_2$ by the following procedure. (See Figure 4.7.) When $m_2$ crosses the line into the zone of free motion of $m_1$, the horizontal component $w$ of the billiard particle is chosen according to a Gaussian distribution with mean 0 and variance $\sigma^2$ given above, and the position along the upper side of the triangle indicated by a dashed line is chosen to be random uniform. The trajectory afterwards is ordinary, deterministic billiard motion. The outgoing velocity of $m_2$ is then the vertical component of the velocity of the billiard particle as it emerges out of the triangle.
The basic facts of the billiard-thermostat just defined are given in [16]. We note in particular that $P_\gamma$ as defined has a unique stationary distribution $\mu$ with density $\rho(v) = \sigma^{-1}v \exp(-v^2/(2\sigma^2))$. Moreover, $P_\gamma$ is self adjoint as an operator on $L^2((0, \infty), \mu)$ with norm 1 and is quasi-compact with spectral gap dependent on $\gamma$. Thus $P_\gamma$ is essentially a one-dimensional version of the natural collision operators with surface temperature of Definition 2.1 (a). Any reference to a value of temperature of a wall should be understood as a fixed value $T = m_1\sigma_1^2$.

4.3 Heat flow

Consider the experiment described in Figure 4.8. As the wall-bound mass $m_1$ will be fixed, we may identify the wall temperature with the variance parameter $\sigma_2^2$ of the velocity distribution of $m_1$. The middle particle, of mass $m_2$, will be referred to as the gas molecule.

We first wish to understand what happens to the stationary velocity distribu-
tion of the gas molecule. Figure 4.9 shows the main effect. The key observation is that the mean velocity going away from the warmer wall is greater than the mean velocity moving toward it. This means that energy is being transferred from the warmer wall to the colder one through the back and forth motion of the free mass. The statistical states of the walls being constant, this creates a stationary heat flow between the walls mediated by the free particle.

Figure 4.9: The figure contains 6 graphs, only 4 of which are distinguishable. One pair (the tallest curve) gives the probability distributions of the forward and backward velocities when the two temperatures are equal and relatively small: \( T_1 = T_2 = T_\text{cold} \). Similarly, the shortest pair of graphs corresponds to equal but relatively high temperature: \( T_1 = T_2 = T_\text{hot} \). The two graphs in between show the same distributions when \( T_1 = T_\text{hot} \) and \( T_2 = T_\text{cold} \). Parameters used: \( m_1 = 10, m_2 = 1 \), the number of iterations (collisions with either side) was \( 5 \times 10^7 \) and the hot and cold temperatures are given by the variances \( \sigma^2_\text{hot} = 20 \) and \( \sigma^2_\text{cold} = 1 \).

Let \( Q^{\text{hot}}_i \) and \( Q^{\text{cold}}_i \), for \( i = 1, 2, \ldots \), be the change in energy of the gas molecule before and after each collision, alternately with the hot (say, left) and cold (right) walls, indexed by the collision number \( i \). Unsurprisingly, it is observed numerically that the expected value of the \( Q^{\text{cold}}_i \) over a large number of collisions is the negative of the expected value of the \( Q^{\text{hot}}_i \). Furthermore, this expected value, denoted \( \bar{Q}^{\text{hot}} \),
depends linearly on the difference of temperatures:

\[ \overline{Q}^{\text{hot}} = c(\gamma) (T_{\text{hot}} - T_{\text{cold}}) \]

where \( c(\gamma) \) is a constant which, experimentally, appears to depend only on the main parameter \( \gamma \) of the wall-gas molecule system.

Figure 4.10 gives some evidence for this linear relation. Each line shows the mean energy transferred from the hot wall to the gas molecule for a given value of \( \gamma \). We have set in each case \( \sigma^2_{\text{cold}} = 1 \) whereas \( \sigma^2_{\text{cold}} \) varied from 1 to 11. The graphs were virtually the same after shifting both temperatures by an equal value.

Figure 4.10: From top to bottom, \( m_2 = 1 \), \( m_1 = 3.001, \ldots, 7.001 \). The mean energy transferred for each pair of temperatures (expressed by the values of \( m_1 \sigma^2 \)) and each value of \( \gamma \) was obtained by averaging over \( 3 \times 10^5 \) collisions.

### 4.4 The heat engine

With the numerical evidence of heat flow established in the previous subsection, the natural idea is to take some of the difference in momentum between the forward and backward motion of the gas molecule and impart it on another mass to produce coherent motion.
We describe here (and in Figure 4.11) our heat engine. It consists of two parallel rail tracks, one a short distance above the other. The upper track contains a sliding mass $m_2$ (the gas molecule) and a wall, one side of which is kept at temperature $T_1$ and the other at temperature $T_2$. These walls can only exchange energy indirectly through collisions with the sliding mass.

The gas molecule moves freely at uniform speeds when it is away from the wall; when a collision with the wall occurs we use our model thermostat to obtain the post-collision velocity. The lower rail, of mass $m_1$, will be called the Brownian particle. (When running the engine later on, we typically assume the Brownian mass to be several times bigger than $m_2$.) It can rotate freely, and attached to it is a protruding pin that can move up and down in billiard fashion; that is, it moves freely within a short vertical interval, bouncing off elastically against the limits of the interval.

The maximum height of the pin does not exceed the lowest point of the wall, so it never collides with the wall, but it may collide with the gas molecule depending on how far extended it is. Therefore, the Brownian particle can at any time be at
two possible states: either “open” to the passage of the gas molecule or “closed” to it. The times $\tau_1, \tau_2$ during which it is closed or open, respectively, alternate periodically as the vertical motion of the pin is assumed not to be affected by the horizontal motion of the system. These times only depend on the speed of vertical motion and the lengths $s_1$ and $s_2$ (Figure 4.11.)

We shall refer to this whole apparatus as the Brownian engine, or occasionally the billiard-Markov engine. The billiard representation of the Brownian engine is shown in Figure 4.12.

![Figure 4.12: The 3-dimensional billiard channel associated to the Brownian engine of Figure 4.11. The bottom and top walls reflect at temperatures $T_1$ and $T_2$. This means that the two components of the velocity tangent to those walls are kept the same, while the normal component is prescribed by the thermostat’s random map. All the other walls reflect specularly (after appropriate rescaling of coordinates). We are interested in the projection of the motion along the axis labeled “lower rail.”](image)

The whole system contains 5 moving parts: the gas molecule, the Brownian particle, the moving tip of the obstacle, and one particle bound to each side of the wall. Thus 5 dimensions are required for a full description of the random billiard system, but by not showing the billiard structure of the thermostats we can present it in dimension 3. The variable of special interest is the long axis labeled as “lower rail” giving the rotation of the Brownian particle. When later testing the engine we will want to add a constant force $F$ tangential to the rail so as to investigate the engine’s ability to do work (i.e., rotate) against this force.

Figure 4.13 shows a short segment of trajectory. It is apparent that collisions
with the top and bottom sides are not specular and may not preserve the particle’s speed. Collisions with the diagonal sides, when they occur, are specular.

Figure 4.13: Two-dimensional projection of a small segment of trajectory of the Brownian motor with a force load, obtained by numerical simulation. The circle indicates the beginning. It is apparent from the curvature of trajectory segments that the force is acting towards the right-hand side. Distances are rescaled by the masses, so reflections with the diagonal walls are specular (when such reflections occur).

4.5 Preliminary analysis of heat engine operation

The typical behavior of the engine, first with 0 load, is shown in Figure 4.14.

These graphs suggest that the mass $m_1$ undergoes a noisy rotation, with speed of rotation that depends on the difference in temperature between the walls. When the temperatures are switched, the direction of rotation is reversed.

When the two temperatures are equal, the Brownian particle appears to move according to mathematical Brownian motion. See the right hand side of Figure 4.14, which shows another sample path obtained under the same conditions as the middle graph on the left hand side of the same figure. Viewed at this scale, the Brownian character of the motion is more apparent.

The effect of adding a constant force is shown in Figure 4.15, giving the mean velocity of rotation for a constant load while the temperature of one of the walls is changed. For relatively small temperature differences, the Brownian particle rotates with constant mean velocity in the same direction of the force, so the
Figure 4.14: Left: position of the Brownian particle (with zero load), as a function of time. Parameters: the mass $m_0$ of the thermostat wall system is 10; the Brownian particle mass is $m_1 = 100$ and the gas molecule mass is $m_2 = 1$. The length of the circular rail track is $l = 10^{-4}$ (the vertical axis measures the positive or negative translation along the track) and the number of events (an event being defined as a collision between the two particles, a collision between the gas molecule and one of the walls, or simply the passage of the two particles through a common position along the tracks without collision due to the obstacle’s pin being down) is $N = 10^6$. The temperature parameters are, from the middle graph to the top: $\sigma_1^2 = 1$ and $\sigma_2^2 = 1, 2, 4, 8$. For the lower graphs the two parameters are reversed. A steady translation away from the hot wall and toward the cold wall is apparent. On the right: another sample path obtained under the same conditions as the middle graph on the left. In particular, the two walls have the same temperature and there is no apparent rotation drift.
work is done on the system. When the temperature difference is sufficiently large
the engine rotates against the force, so that work is done by the system.

The efficiency of a heat engine is traditionally defined, since Sadi Carnot’s
pioneering work, as the (negative of the) ratio of the amount of mechanical work
done by the system over the heat taken from the heat source. The analysis of
efficiency is based on a simple energy accounting. At any given time \( t > 0 \), let
\( Q_h(t) \) be the total amount of heat transferred to the system (gas-molecule plus
Brownian particle) since time \( t = 0 \) due to collisions between the gas molecule and
the hot wall. Let \( Q_c(t) \) be the heat similarly transferred to the system from the
cold wall. These heats are obtained by adding up the changes in kinetic energy
of the gas molecule before and after each collision.

![Figure 4.15: The working engine with a force load. The graphs show the mean velocity
of the Brownian particle as a function of time. Common parameters for all graphs: The
values of the masses \( m_0, m_1, m_2 \) are as in Figure 4.14; the force load is \( F = 1 \); the number
of events (as explained in Figure 4.14) is \( N = 10^6 \); the length of the track is \( l = 10^{-4} \);
the temperature parameters, from top to bottom, are: \( \sigma_1^2 = 1 \) and \( \sigma_2^2 = 1, 2, 4, 8 \).

The (internal) energy of the system at time \( t \) is \( E_g(t) + E_b(t) \), where \( E_g(t) \) is the
kinetic energy of the gas molecule and \( E_b(t) \) is the kinetic energy of the Brownian
particle. The work done by a force \( F \) as in Figure 4.11 on the system up to time
\( t \) is denoted by \( W(t) \). When \( W(t) \) is negative, we say that work is done by the
system. Recall that the \( W(t) = (x_b(t) - x_b(0))F \) for a constant \( F \), where \( x_b(t) \)
is the position of the Brownian particle at time \( t \). Over a time interval without
collisions, the change in \( W \) equals the change in kinetic energy of the Brownian particle. Then the following identity holds:

\[
Q_h(t) + Q_c(t) + W(t) = E_g(t) - E_g(0) + E_b(t) - E_b(0).
\]

Now formally define the (mean, at time \( t \)) efficiency over one sample history of the engine, when work \( W \) is negative hence done by the system, as

\[
\epsilon(t) = -\frac{W(t)}{Q_h(t)},
\]

which measures the fraction of heat transferred to the system from the hot wall that is converted to mechanical work over the course of one history of the engine and is, therefore, a random variable.

Experimentally, we observe by running our Brownian engine that the quotient \((E_g(t) - E_g(0) + E_b(t) - E_b(0))/Q_h(t)\) goes to zero relatively quickly when the two temperatures are different. This is illustrated in Figure 4.16.

![Figure 4.16: Comparison of the definition of mean efficiency 4.5 (dashed line) and the alternative form 4.6 (solid line). We have applied a force \( F = 1 \), the same masses as in Figure 4.14, and temperature parameters \( \sigma^2_1 = 1 \), \( \sigma^2_2 = 8 \). The graph shows a short run of 1000 events. On the right, zooming in on part of the graph on the left shows that the efficiency is small but not zero.](image)

The efficiency measured at a steady operation regime may be expected to equal
(almost surely for large $t$) the alternative expression

$$\bar{\epsilon}_t(T_h, T_c) = 1 + \frac{Q_c(t)}{Q_h(t)}$$

(4.6)

where the two heats have opposite signs.

Figure 4.17: The efficiency axis is in percentage units, so maximum efficiency is a little below 0.4%. The vertical bars indicate 99% confidence intervals. The parameters here are: $m_0 = 10, m_1 = 100, m_2 = 1, \sigma_1^2 = 1, \sigma_2^2 = 8$. For each value of the force we have evaluated the efficiency over 40000 runs of the engine, each run of length 2000 elementary events. (The dashed line connecting the mean values is there as a visual aid and has no significance.)

Compared to the classical upper limit of efficiency $1 - T_c/T_h$ derived from the second law of thermodynamics (for non-stochastic systems), our engine has very low efficiency. (See Figure 4.17.) The engine can operate in the reverse direction: for a range of values of the force $F$ and the temperatures $T_c$ and $T_h$, work is positive (done to the system), with the effect of transferring heat from the cold to the hot wall. In this regime, the engine operates as a heat pump.

We offer these informal numerical observations simply as evidence that the engine functions as expected. A model of how a detailed analysis of its operation may be done centered on the idea of entropy production is the stochastic thermodynamic framework of [32]. The stochastic dynamic of our engine is given by a Markov chain, so the first step in the analysis should be to describe the process
in terms of Langevin equations by an appropriate scaling limit, or pursue more
directly the type of analysis of [24].
Bibliography


