Random billiards with wall temperature and associated Markov chains

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Abstract

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 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*, or RBM for short, is a random billiard for which P is derived from a choice of geometric/mechanical structure on the boundary of the billiard domain, as explained in the text. Such systems provide simple and explicit mechanical models of particle-surface interaction that can incorporate thermal effects and permit a detailed study of thermostatic action from the perspective of the standard theory of Markov chains on general state spaces.

The main focus of the present paper is on the operator P itself and how it relates to the mechanical and geometric features of the microstructure, such as mass ratios, curvatures, and potentials. The main results are as follows: (1) we give a characterization of the stationary probabilities (equilibrium states) of P and show how standard equilibrium distributions studied in classical statistical mechanics such as the *Maxwell-Boltzmann distribution* and the *Knudsen cosine law* arise naturally as generalized invariant billiard measures; (2) we obtain some of the more basic functional theoretic properties of P, in particular that P is under very general conditions a self-adjoint operator of norm 1 on a Hilbert space to be defined below, and show in a simple but somewhat typical example that P is a compact (Hilbert-Schmidt) operator. This leads to the issue of relating the spectrum of eigenvalues of P to the geometric/mechanical features of the billiard microstructure; (3) we explore the latter issue, both analytically and numerically in a few representative examples. Additionally, (4) a general algorithm for simulating the Markov chains is given based on a geometric description of the invariant volumes of classical statistical mechanics. Our description of these volumes may have independent interest.

1 Introduction

This extended introduction contains some definitions and an overview of the main results. Additional results and refinements are discussed throughout the text.

1.1 Physical motivation

Consider the idealized and somewhat fanciful billiard system shown in Figure 1. At a "macroscopic scale" it consists of a point particle, henceforth called the *molecule*, and a billiard table having piecewise smooth boundary (only a small part of which is shown). We often refer to the boundary

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as the *wall*. At a "microscopic scale," both the wall and the molecule may reveal further geometric and mechanical structure that can affect the outcome of a collision. Thus collisions are not necessarily specular; to specify the outcome of a collision it is necessary to consider the interaction between molecule and wall at this finer scale. We suppose that the wall system is kept at a constant statistical state, say, a canonical ensemble distribution with a given temperature, and wish to follow the evolution of the statistical state of the molecule. The outcome of a molecule-wall *collision event* is then shown to be described by a time-independent transition probabilities operator P, to be defined later as an operator on an L^2 space over the set of pure states of the molecule. This operator, which is canonically defined by the mechanical/geometric features of the wall and molecule microstructure and the constant statistical state of the wall, replaces the mirror-reflection map of an ordinary billiard. We call a system of this kind a *random billiard with microstructure*, or RBM.

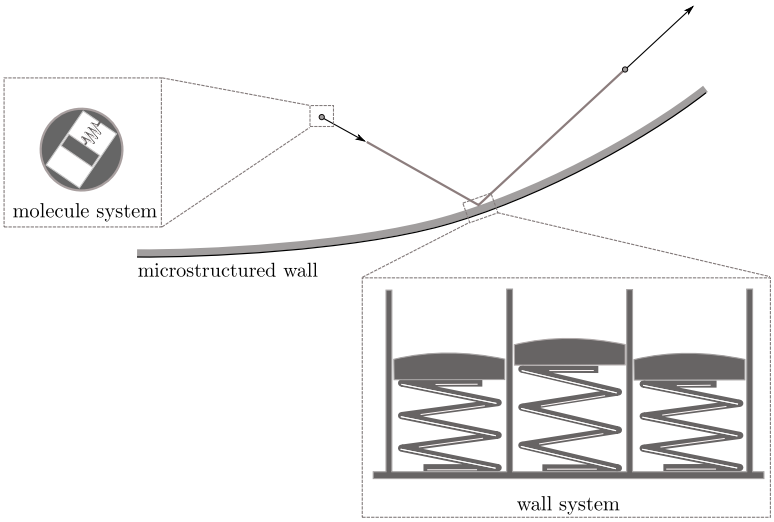

Figure 1: An arbitrary molecule-wall system defining a random billiard with microstructure.

Discrete-time Markov chains associated to P are interpreted as a sequence of random states of the molecule taken immediately after each collision, starting from some initial probability distribution. (This interpretation is valid at least for simple shapes of the billiard domain such as cylinders or balls; see Section 2.4 of [7] and the concept therein of an *attaching frame*, for an elaboration of this comment). Besides determining the equilibrium states of the molecule as the stationary (i.e., P-invariant) probability distributions for the Markov chain, the operator P contains information about rates of decay of correlations and spectral data, which can in principle be used to derive transport coefficients such as the diffusion constant of a gas of non-interacting molecules moving inside a "billiard channel." (See Figure 3.)

This paper develops some of the above ideas in detail, focusing on the billiard-Markov operator P and its relationship with the microstructure. The main results are concerned with defining P for any given Newtonian molecule-wall system, deriving its basic functional analytic properties, describing stationary probability distributions, and illustrating with concrete examples some of the spectral properties of P.

There are several sources of motivation for this work, some purely mathematical and others more applied. On the purely mathematical side, we seek to have well-motivated classes of Markov chains that can be used to investigate issues of general interest in probability theory, such as spectral gap, mixing times, central limit theorems, etc. The statistical mechanics perspective combined with the

choice of very simple mechanical models yields a great variety of new and interesting types of Markov chains. We also believe that generalized billiard systems of the kind we are considering may provide fruitful examples of random (often hyperbolic) dynamical systems with singularities, i.e., random counterparts of the widely studied chaotic billiards, for which [3] is a recommended reference. On the more applied side, the kinds of processes we are studying here may be useful in kinetic theory of gases as suggested, for example, in [8] in the context of Knudsen diffusion studies. In the theory of Boltzmann equations, operators such as our P may serve to specify boundary conditions for gas-wall systems. (See, for example, [2] for some background on this point.) Our random collision operators provide very natural and simple Newtonian models for the interaction of a molecule with a heat bath that can be used to study thermostatic action fairly explicitly and often analytically from the perspective of the general theory of Markov chains. (See [5] for a mathematical model of a heat engine built on the ideas of the present paper.)

1.2 The surface-scattering set-up

Our first step is to introduce the definition of *billiard microstructure.* Before doing so, it will be helpful to make some informal remarks. The reader is urged to look at (the right hand side of) Figures 2, 5, 11, 12, 15 as we introduce the general set-up.

Since this paper is mainly concerned with the interaction between the molecule and the (microstructured) wall rather than the dynamics of the macroscopic system per se, the curvature of the wall will not play a role, and we may regard it as flat. We think of the wall as a horizontal "ground" of dimension k (equal to 0, 1, or greater). Although not strictly necessary for the main conclusions, it is convenient to assume that the wall microstructure is periodic; thus the ubiquitous appearance of a torus factor $\mathbb{T}^k$ throughout the paper. We think of the center of mass of the molecule as moving in $\mathbb{R}\times\mathbb{T}^k$, where the factor $\mathbb{R}$ is the set of vertical positions of the center of mass above the horizontal ground.

The molecule is not necessarily a point particle; its internal structure contributes additional degrees of freedom. The internal configurations of the molecule comprise a manifold $\overline{M}_{\text{mol}}$; thus the full manifold of configurations of the molecule when not interacting with the wall, is the product manifold $M_{\text{mol}} = \overline{M}_{\text{mol}} \times \mathbb{R} \times \mathbb{T}^k$. For example, when the molecule is a rigid body in $\mathbb{R}^3$, one would take for $\overline{M}_{\text{mol}}$ the rotation group $SO(3)$.

Similarly, the wall may have internal moving parts, whose possible configurations comprise a manifold M_{wall}. These are Riemannian manifolds; their metrics are derived from the system's kinetic energy, hence the geometry is defined in terms of the distribution of masses.

If molecule and wall did not interact, the joint system would be described by the product Riemannian manifold $M_{\text{mol}} \times M_{\text{wall}}$. In addition to potential functions, interactions can happen through elastic collisions. Thus the configuration manifold of the total system is taken to be a submanifold with boundary $M \subset M_{\text{mol}} \times M_{\text{wall}}$ (having the same dimension as the latter product manifold), where boundary points correspond to collision configurations.

Implicit in this general picture is the elementary idea that a mechanical system whose component masses may collide elastically can be described in terms of the motion of a single point particle in a (possibly high dimensional) manifold with boundary. We note that this representation of the system essentially eliminates any clear distinction between internal states of the molecule and those of the wall. For example, in the system of Figure 12, the molecule's rotation and shape end up being incorporated in the microstructure of the boundary of the billiard region. Therefore the term "wall microstructure" more properly refers to characteristics of the interaction, rather than just the wall, and may contain information about the internal structure of the molecule as well.

It will be assumed that the part of the manifold M consisting of those configurations in which molecule and wall may be interacting is finite in volume (relative to the canonical volume measures described later in the paper). What we refer to below as a *collision event* is a trajectory of the total

system that starts somewhere in the non-interacting region of M, enters the region of interaction and eventually returns (due to the condition of finite volume) back into the non-interacting region. It is this scattering process that the paper is mainly concerned with; it constitutes one iteration of the Markov chain associated to P (to be defined later).

We now proceed with the definition of billiard microstructure more formally. (Standard notation from manifold theory will be used freely; we recommend [11] as a reference. In particular, TM will refer to the tangent bundle of a manifold M and by *manifold with boundary* we mean *manifold with corners*, as defined in [11].) Let M be a smooth manifold whose points represent the configurations of a mechanical system. The system consists of two interacting subsystems: the *wall* and the *molecule*. Let smooth Riemannian manifolds M_{wall} and M_{mol} be the configuration spaces of the *wall* and the *molecule* subsystems; to capture the idea that there is an axis along which a distance between the (say, center of mass of the) molecule and the plane of the wall can be defined and that the microstructure on the wall is periodic, we assume that M_{mol} factors as a Riemannian product

$$M_{\text{mol}} = \overline{M}_{\text{mol}} \times \mathbb{R} \times \mathbb{T}^k,$$

where $\overline{M}_{\text{mol}}$ is a *reduced* manifold of molecular configurations that does not account for the overall position of the molecule in space.

In the example of Figure 1, M_{wall} is simply an interval $[0, l]$, representing the range of positions of the wall-bound mass attached to the spring. The Riemannian metric on M_{wall} is derived from the kinetic energy of the wall-bound mass. The manifold $\overline{M}_{\text{mol}}$ may be written in that example as $SO(2) \times [0, h]$, specifying the spatial orientation (or angle of rotation) of the hollowed little disc and the position of the vibrating mass in its interior. The Riemannian metric is, again, derived from the kinetic energy of the molecule system, so metric coefficients are given by the values of masses and moments of inertia. The plane of the wall is aligned with the factor $\mathbb{T}^1$ and the axis perpendicular to the wall at the point of collision defines the factor $\mathbb{R}$ in the product. We disregard the possible ("macroscopic") curvature of the billiard table boundary—the interaction is imagined to happen at a length scale in which boundary curvature cannot be discerned.

Back to the general case, the combined *wall-molecule system* has configuration manifold M with a Riemannian metric and a *potential function* $U : M \to \mathbb{R}$ such that (1) the two subsystems are non-interacting when they are sufficiently far apart (more details below) and, (2) for each value $\mathcal{E}$ of the total energy E, where $E(q, v) = \frac{1}{2}\|v\|^2 + U(q)$ for $(q, v) \in TM$, the subset of the level set $E^{-1}(\mathcal{E})$ consisting of states at which the subsystems are a bounded distance from each other has finite volume with respect to the invariant volume form Ω^E, whose definition is recalled later.

To begin to make sense of these assumptions, we introduce a smooth function $d : M \to \mathbb{R}$, which may be thought of as giving the distance from the center of mass of the molecule to a reference plane parallel to and near the wall. For each real number a define $M_{\text{mol}}(a) := \overline{M}_{\text{mol}} \times (a, \infty) \times \mathbb{T}^k$ and $M(a) = M_{\text{mol}}(a) \times M_{\text{wall}}$, and denote by π_{wall} and $\overline{\pi}_{\text{mol}}$ the projection maps to M_{wall} and $\overline{M}_{\text{mol}}$, respectively. Then we suppose that there exists an $a_0 \in \mathbb{R}$, which can be taken with no loss of generality to be less than 0, such that, for all $a \geq a_0$,

i. the set $\{q \in M : d(q) > a\}$ is isometric to, and will be identified with, $M(a)$;

ii. there are smooth functions $U_{\text{mol}} : \overline{M}_{\text{mol}} \to \mathbb{R}$ and $U_{\text{wall}} : M_{\text{wall}} \to \mathbb{R}$ such that

$$U|_{M(a)} = U_{\text{mol}} \circ \overline{\pi}_{\text{mol}} + U_{\text{wall}} \circ \pi_{\text{wall}}$$

iii. for each value $\mathcal{E}$ of the energy function E, the level set $\{v \in T(M \setminus M(a)) : E(v) = \mathcal{E}\}$ has finite volume relative to Ω^E;

iv. the system is *essentially dynamically complete*, in the following sense: Any smooth curve $t \mapsto c(t)$ that satisfies Newton's equation (with acceleration defined in terms of the Levi-Civita

connection)

$$\frac{\nabla c'(t)}{dt} = -\mathrm{grad}_{c(t)} U$$

can be extended indefinitely in the interior of M, until it reaches the boundary; whenever c intersects the boundary transversely at a regular point $q = c(t)$, it can be extended further back into the interior along the unique solution curve with initial state (q, w), where $w = R_q c'(t)$ and $R_q : TM \to TM$ is the standard reflection map.

In the example of Figure 2, $\overline{M}_{\mathrm{mol}}$ is the two-point set $\{-1, 1\}$ labeling the two sheets of M above a certain distance from the handles. The manifold M_{wall} consists of a single point and the potential function U is constant. We give M, say, the Riemannian metric induced from Euclidean 3-space. More representative examples, in which M_{wall} is non-trivial will be shown later.

As already noted, the various manifolds above may have boundary. Boundary points represent collision configurations. It is necessary to accept manifolds whose boundaries may not be smooth. For concreteness, we adopt here the class of *manifolds with corners* (see [11]), which is general enough to provide plenty of meaningful examples. In particular, M contains a set $\partial_{\mathrm{s}} M$, the *singular boundary*, the complement of which is a smooth manifold with boundary in the ordinary sense of being modeled on open subsets of the upper half space. This complement is the union of the interior set M°, and the (regular) boundary $\partial_{\mathrm{r}} M$. Moreover, $\partial_{\mathrm{s}} M$ is contained in the closure of $\partial_{\mathrm{r}} M$, it is nowhere dense in this closure and has measure 0 in ∂M. Since we are mainly interested in probabilistic questions, it is typically safe to ignore the singular boundary set.

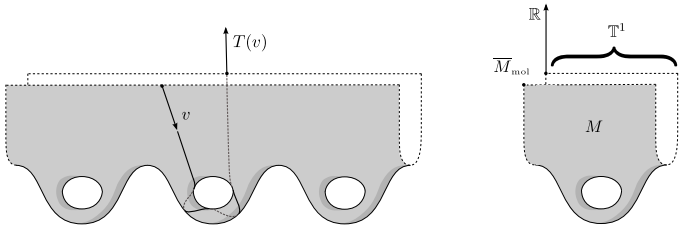

Figure 2: Geodesic motion on a periodic surface representing a molecule-wall scattering process.

If q is a regular boundary point of M and ν is a unit vector perpendicular to the boundary at q, we assume that a motion in M is extended after hitting the boundary at q in such a way that the pre- and post-collision velocities v and v' are related according to the standard linear (reflection) map $v \mapsto v' := v - 2\langle v, \nu\rangle_q \nu$; so "microscopic" collisions are specular. Being an isometry of the kinetic energy metric, this map leaves the energy function E invariant.

Let S be the level set $d = 0$ in M, i.e.,

$$S = \overline{M}_{\mathrm{mol}} \times \{0\} \times \mathbb{T}^k \times M_{\mathrm{wall}}$$

and N_S the restriction of TM to S (more precisely, the pull-back of TM under the inclusion $S \hookrightarrow M$). Informally, crossing S amounts to entering the zone of interaction $M \setminus M(0)$, although S itself lies in the product zone. The vectors in N_S pointing into the zone of interaction form the subset N_S^+. This is the set of *incoming states*. The set of *outgoing states*, N_S^-, is similarly defined as the set of vectors in N_S pointing out of the zone of interaction. Omitting, as we often do, the base point in M when referring to a state in N_S, then $v \mapsto -v$ sends an element of N_S^- to an element of N_S^+. Let $\mathbb{H}$ be the lower half-space in $\mathbb{R}^{k+1}$, the latter space being identified with fibers of $T(\mathbb{R} \times \mathbb{T}^k)$. Then $\mathbb{H} \times \mathbb{R} \times \mathbb{T}^k$ is the submanifold in $T(\mathbb{R} \times \mathbb{T}^k)$ whose vectors point down toward the interaction zone

(so they are projections of vectors in N_S^+). The incoming states now decompose as a product

$$N_S^+ = N_{\text{mol}} \times \mathbb{T}^k \times N_{\text{wall}}$$

where $N_{\text{wall}} := TM_{\text{wall}}$ and $N_{\text{mol}} := T\overline{M}_{\text{mol}} \times \mathbb{H}$.

A *collision event* is defined as an application of the map $T : N_S^+ \to N_S^-$, which gives the return state from an initial state in N_S^+, obtained by integrating the equations of motion. Under our general assumptions this map is defined on almost all initial states by Poincaré recurrence, and for many systems of interest it can be shown that T is smooth on a dense open set of full measure. We make this almost everywhere smoothness a standing assumption. For simplicity, we indicate the domain of T simply by N_S^+, ignoring the fact that it is really defined on an open dense subset of full measure. It is convenient to redefine T by composing it with the reflection map $R : N_S^- \to N_S^+$, so that T becomes a self-map of N_S^+. Thus we add to the above list of assumptions:

v. the return map T is smooth on an open dense subset of N_S^+ of full measure.

1.3 The Markov operator

Let η be any given probability measure on $\mathbb{T}^k \times N_{\text{wall}}$. The physically most natural and interesting choice for η corresponds to taking the product of the uniform distribution on $\mathbb{T}^k$ and the Gibbs canonical distribution on TM_{wall} with parameter $\beta = 1/kT$, whose definition is recalled later. The choice of measure fixes the statistical state of the wall system. The collection of possible states of the molecule system is the space $\mathcal{P}(N_{\text{mol}})$ of Borel probability measures on N_{mol}. We now define the map

$$P : \mathcal{P}(N_{\text{mol}}) \to \mathcal{P}(N_{\text{mol}})$$

that associates to each statistical state $\mu \in \mathcal{P}(N_{\text{mol}})$ the new state $\mu P := (\pi \circ T)_*(\mu \otimes \eta)$. Notations and general explanations are further provided in Section 2. The interpretation is that, to obtain the return statistical state of the molecule, we take its present state μ, form the combined state $\mu \otimes \eta$ of the system, let it evolve under T, thus yielding $T_*(\mu \otimes \eta)$, and finally project the outcome back to N_{mol} under the natural projection $\pi : N_S^+ \to N_{\text{mol}}$. The asterisk indicates the push-forward operation on measures.

Consider again the system of Figure 2 as an example. In that case M_{wall} is trivial (a single point), $N_{\text{wall}} = \mathbb{T}^1$, and N_{mol} is identified with $\{-1, 1\} \times \mathbb{H}$, where $\mathbb{H}$ is the half-plane in $\mathbb{R}^2$. It does not make sense in this case to consider a Gibbs canonical distribution—a natural measure η here is the uniform probability distribution on $\mathbb{T}^1$. Since in this example the speed of the particle does not change, we consider not the full N_{mol} but a level set for the energy (say, only states with unit velocity). So we let $N_{\text{mol}} = \{-1, 1\} \times (-\pi/2, \pi/2)$, which parametrizes the sheet number (± 1) and the angle θ of the incoming trajectory relative to the normal to the wall plane. Ignoring for simplicity the sheet number and focusing on the angular component, we can define P by first indicating how it acts on continuous functions of θ, then defining its action on $\mathcal{P}((-\pi/2, \pi/2))$ by duality, i.e., so that $(\mu P)(f) = \mu(Pf)$, where $\mu(f)$ indicates the integral of f with respect to μ. Thus if f is a function on the angle interval, and $\Psi_\theta(x)$ is the angle of the return state under T for initial state $(\theta, x) \in (-\pi/2, \pi/2) \times \mathbb{T}^1$, then from the general definition we have,

$$(Pf)(\theta) = \int_{\mathbb{T}^1} f(\Psi_\theta(x))\, dx.$$

When the (macroscopic) billiard table is a channel as shown in Figure 3, iterates of P give the post-collision states of a random flight of the molecule (say, in a gas of non-interacting molecules) inside the channel. Diffusion approximation of the random flight and the dependence of the diffusion constant on the spectrum of P are issues of particular interest, which will be investigated in another paper dedicated to central limit theorems for P and related topics.

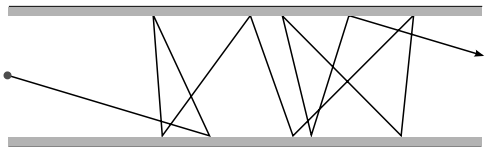

Figure 3: A random flight in a channel. The molecule's state after each collision is specified by P and the pre-collision state. The stationary distribution μ is interpreted as describing the state after the molecule has reached thermal equilibrium with the wall.

1.4 Overview of the main results

The starting point of our analysis is a determination of the stationary probability measures of P. Recall that a probability measure μ is said to be *stationary* for P if $\mu P = \mu$. We consider two possibilities: (1) the space M_{wall} reduces to a point, in which case the wall is regarded as a rigid, unmoving body that does not exchange energy with the billiard particle in a collision. In this case, the measure η that enters in the definition of P is taken to be the normalized Lebesgue measure on $\mathbb{T}^k$; (2) the space M_{wall} has dimension at least one. This means that the wall system has moving parts and energy can be transferred between wall and molecule in a collision. In this case we assume for the purposes of the next theorem that η is the product of the normalized Lebesgue measure on $\mathbb{T}^k$ and the Gibbs canonical measure on the phase space N_{wall} with a fixed parameter β. The latter can be written as follows (a fuller discussion of invariant measures is given in the last section of the paper):

$$d\eta = \frac{e^{-\beta E}}{Z(\beta)} \left| \Omega^E_{\text{wall}} \wedge dE \right|, \tag{1.1}$$

where E is the energy function on N_{wall}, Ω^E_{wall} is the invariant (Liouville) volume form on energy level sets in N_{wall} derived from the symplectic form on this space, and the vertical bars indicate the associated measure. The denominator is a normalization factor.

We consider similar measures on $N_{\text{mol}} := T\overline{M}_{\text{mol}} \times \mathbb{H}$. More precisely, in case (1) we fix a value $\mathcal{E}$ of the energy function of the molecule, which remains constant throughout the process, and consider the microcanonical measure for this value, given by

$$d\mu = \frac{1}{Z(\mathcal{E})} \left| \Omega^{\mathcal{E}}_{\text{mol},S} \right|, \tag{1.2}$$

where S is the hypersurface of separation between the product zone and the zone of interaction, $\Omega^{\mathcal{E}}_{\text{mol},S}$ is the invariant volume form on the part of the level set $E = \mathcal{E}$ above S and the denominator is a normalizing factor. In case (2) we define

$$d\mu = \frac{e^{-\beta E}}{Z(\beta)} \left| \Omega^E_{\text{mol},S} \wedge dE \right|. \tag{1.3}$$

A description of these measures better suited for applications will be given shortly. In the special case when $\overline{M}_{\text{mol}}$ reduces to a point, so that $N_{\text{mol}} := \mathbb{H}$, these measures are as follows: in case (1) we may choose $\mathcal{E}$ so that the molecule state lies in the unit hemisphere in $\mathbb{H}$. Indicating by ω^{sphere} the standard volume form on the unit hemisphere and by ν the unit normal vector to S, say, pointing into the zone of interaction, we have, up to a normalization constant C,

$$d\mu(v) = C\langle v, \nu \rangle \left| \omega^{\text{sphere}} \right|,$$

which we refer to as the *Knudsen* probability distribution; and in case (2)

$$d\mu(v) = C\langle v, \nu\rangle e^{-\beta \frac{m|v|^2}{2}} dV(v),$$

where $\langle v, \nu\rangle$ and $dV(v)$ are, respectively, the standard inner product and volume element in $\mathbb{R}^{k+1}$. This measure is the Maxwell-Boltzmann distribution at boundary points.

Theorem 1. *Let $P : \mathcal{P}(N_{mol}) \to \mathcal{P}(N_{mol})$ be the Markov operator associated to a probability measure η on $\mathbb{T}^k \times N_{wall}$.*

1. *In case (1) above, let η be the normalized Lebesgue measure on $\mathbb{T}^k$. Then the microcanonical distribution 1.2 is a stationary probability for P.*
2. *In case (2) above, let η be the product of the normalized Lebesgue measure on $\mathbb{T}^k$ and the Gibbs canonical distribution on N_{wall} with temperature parameter β. Then the Gibbs canonical distribution on N_{mol} given by 1.3, with the same parameter β, is a stationary probability for P.*

In the particular case when the molecule reduces to a point, the stationary measures are, respectively, the Knudsen distribution in case (1) and the boundary Maxwell-Boltzmann distribution in case (2).

The proof of this theorem is given at the end of Subsection 5.4. The stationary probability is often (but not always) unique and one often obtains convergence of $\mu_0 P^n$ to the stationary state for any initial distribution $\mu_0 \in \mathcal{P}(N_{\mathrm{mol}})$. Thus the dynamic of a Markov chain derived from P describes the process of relaxation of the molecule's state toward thermal equilibrium with the wall. To understand this process in each particular situation it is necessary to study the operator P in more detail; we do this later in the text for a few concrete examples.

The following definition is further elaborated in Section 2. We say that the molecule-wall system is *symmetric* if on the state space N_S^+ are defined two automorphisms $\widetilde{J}$ and $\widetilde{S}$ such that:

i. these maps preserve the natural measure Ω_S^E on $N_S^+(\mathcal{E})$ derived from the symplectic structure;

ii. they respect the product fibration $\pi : N_S^+ = N_{\mathrm{mol}} \times \mathbb{T}^k \times N_{\mathrm{wall}} \to N_{\mathrm{mol}}$ and both induce the same map J on N_{mol}; that is,
$$\pi \circ \widetilde{J} = \pi \circ \widetilde{S} = J \circ \pi;$$

iii. $\widetilde{J}$ is time reversing: $\widetilde{J} \circ T = T^{-1} \circ \widetilde{J}$; and $\widetilde{S}$ commutes with T: $\widetilde{S} \circ T = T \circ \widetilde{S}$.

The existence of the map $\widetilde{J}$ is typically assured by the time reversibility of Newtonian mechanics and the symmetry $\widetilde{S}$ can often be obtained by a simple extension of the original system that does not affect its essential physical properties. (This is akin to defining an orientation double cover of a possibly non-orientable manifold.) The assumption of symmetry is thus a very weak one. These points are further discussed in Section 2 and in some of the specific examples studied later in the paper.

It is natural to consider the associated operator, still denoted P, on the Hilbert space $L^2(N_{\mathrm{mol}}, \mu)$, where μ is one of the stationary probabilities obtained in Theorem 1. We are particularly interested in the spectral theory of P. A first general observation in this direction is the following.

Theorem 2. *Let μ be the stationary measure of P obtained in Theorem 1 and suppose that the system is symmetric. Then P is a self-adjoint operator on $L^2(N_{mol}, \mu)$ of norm 1.*

In particular, P has real spectrum contained in $[-1, 1]$. It is often the case (this will be proved for a simple but representative example later in this paper, and has been shown for special classes of P in previous papers; see [7, 9]) that P is a compact, integral operator (Hilbert-Schmidt). The eigenvalues of P are then invariants of the system, depending in a canonical way on structural parameters like

mass ratios, potential functions, curvatures, etc. The relationship between the spectrum of P and these parameters is one of the central issues in this subject.

Of particular interest is the *spectral gap* of P, defined as 1 minus the spectral radius of the restriction of P to the orthogonal complement to the constant functions. As is well-known (see, for example, [14]) the spectral gap can be used to estimate the exponential rate of convergence of $\mu_0 P^n$ to the stationary distribution in the total variation or the L^2 norm.

A perturbation approach to the spectrum of P, which is valid when the molecule scattering is not far from specular, can be very fruitful. To make sense of this, first define

$$\mathcal{E}_2(v) := E_v\left[\mathrm{dist}(v,V)^2\right],$$

where dist is a distance function on N_{mol}, $v \in N_{\mathrm{mol}}$ is an initial state, V is the random variable representing the scattered state after one collision event, and $E_v[\cdot]$ is conditional expectation given the initial state v. We call $\mathcal{E}_2$ the *second moment of scattering*. Under the identification of N_S^+ and N_S^- (see above), specular reflection corresponds to $V = v$ almost surely and small deviations from specularity correspond to small values of the second moment of scattering. We now define the operator

$$\mathcal{L} := 2(I - P)/\mathcal{E}_2,$$

which we refer to as the *random billiard Laplacian* (or the *Markov Laplacian*) of the system. The billiard Laplacian, for small values of $\mathcal{E}_2$ often approximates a second order differential operator. In the examples studied, this will be seen to be a (densely defined) self-adjoint operator on the same Hilbert space on which P is defined, whose eigenvalue problem amounts to a standard Sturm-Liouville equation.

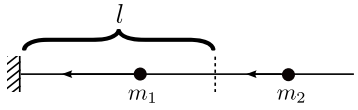

Figure 4: A simple example described in Theorem 3.

In Section 3 we explore these ideas in detail with an example. The example consists of two point masses (see Figure 4) constrained to move along the half-line $[0,\infty)$. Mass m_1, with position coordinate x_1, is restricted to move in the interval $0 \le x_1 \le l$ and m_2, with position coordinate x_2, can move freely on $x_1 \le x_2 < \infty$. The two masses collide elastically with each other, and m_1 collides elastically with walls at 0 and l. The wall at l is regarded as permeable to m_2 but not to m_1. (We imagine m_1 as tethered to the wall on the left by a string of length l that causes m_1 to bounce back when the string is fully stretched, while m_2 is free to move.) The random state η of m_1 is taken to be the product of the uniform distribution over $[0,l]$ and a Gaussian probability with mean 0 and variance σ^2 for its velocity. Mass m_2 is the molecule and mass m_1 is part of the wall system. We refer to this as the *two-masses* system. To simplify notation and for other conveniences we rescale positions and velocities according to $x := \sqrt{m_1/m}\,x_1$ and $y = \sqrt{m_2/m}\,x_2$, where $m = m_1 + m_2$. The main structural parameter of the system is the *mass-ratio* $\gamma := \sqrt{m_2/m_1}$. We let P_γ represent the Markov operator with mass-ratio γ. Further details are explained in Section 3. We summarize in the next theorem some of the main conclusions obtained for the two-masses example. (Further refinements and numerical calculations are described in that section.)

Theorem 3 (Case study)**.** *The following assertions hold for the two-masses system with* $\gamma < 1/\sqrt{3}$*:*

1. *P_γ has a unique stationary distribution μ. Its density relative to Lebesgue measure on $(0,\infty)$ is given by*

$$\rho(v) = \sigma^{-1} v \exp\left(-\frac{v^2}{2\sigma^2}\right).$$

2. *For an arbitrary initial probability distribution μ_0, we have $\|\mu_0 P_\gamma^n - \mu\|_{TV} \to 0$ exponentially fast in the total variation norm.*

3. *P_γ is a Hilbert-Schmidt operator.*

4. *If φ is a function of class C^3 on $(0,\infty)$, then the billiard Laplacian has the form*

$$(\mathcal{L}\varphi)(v) = \lim_{\gamma\to 0} \frac{(P_\gamma\varphi)(v) - \varphi(v)}{2\gamma^2} := \left(\frac{1}{v} - \frac{v}{\sigma^2}\right)\varphi'(v) + \varphi''(v).$$

Equivalently, $\mathcal{L}$ can be written in Sturm-Liouville form as $\mathcal{L}\varphi = \rho^{-1}\frac{d}{dv}\left(\rho\frac{d\varphi}{dv}\right)$, which is a densily defined self-adjoint operator on $L^2((0,\infty),\mu)$.

Based on part 4 of the above theorem and a simple analysis of the corresponding Sturm-Liouville eigenvalue problem (the equation in part 4 is, after the change of coordinate $x = v^2/2$, Laguerre's equation), we can make an educated guess as to the asymptotic value, for small γ, of the spectral gap of P_γ: it is given by $4\gamma^2$. Although we do not prove this claim here, we offer in Section 3 numerical evidence for its validity. This gives the following refinement of item 2 of Theorem 3:

$$\|\mu_0 P_\gamma^n - \mu\|_{TV} \le C(1 - 4\overline{\gamma}^2)^n$$

where C is a positive constant and $\overline{\gamma}/\gamma \to 1$ as the mass-ratio parameter γ approaches 0.

Theorem 3 is proved in Section 3. Section 4 discusses further examples in less detail.

1.5 An algorithm for the Markov chain simulation

The map T generating the deterministic discrete dynamical system involved in the definition of P is essentially a kind of *billiard map* [3] in a very general setting. For applications of Theorem 1, particularly in numerical simulations of the Markov chains, we need a convenient expression for the corresponding invariant *billiard measure* and for the Gibbs distributions. We recall that the standard invariant billiard measure for planar billiards can be described as follows: If states of the billiard system are represented by coordinates (s,θ), where $s \in [0,1]$ is proportional to arclength measured from a reference point on the boundary of the billiard table (assuming that this boundary has finite length) and $\theta \in [-\pi/2, \pi/2]$ measures the angle that a unit velocity vector based at the point represented by s makes with the inward pointing normal vector, then $d\mu(s,\theta) = \frac{1}{2}\cos\theta\, ds\, d\theta$ is the canonical invariant probability measure on the two-dimensional state space of the billiard system. See, for example, [3]. We wish to have a similar description of the invariant billiard measure on boundary components of general Riemannian manifolds in the presence of potential functions. Although this is something rather classical and possibly relatively well-known, we could not find it in the literature in a form that is convenient for our needs. It may thus be of some interest to highlight such an expression here. After doing this, we give at the end of this subsection the outline of an algorithm for generating Markov chains associated to general microstructures.

Since the next theorem is of some independent interest, having to do with a representation of the standard volume measures of classical statistical mechanics, the notation is similar but independent of what was used above. Thus let M be a smooth Riemannian manifold with corners, which could be either M_{wall}, M_{mol}, or the previous M of the combined system, and $U : M \to \mathbb{R}$ any smooth potential function. As always, we let the kinetic energy be defined by the Riemannian metric, $\kappa(v) = \frac{1}{2}\|v\|^2$,

and consider the Hamiltonian flow on $N = TM$ with standard energy function $E := \kappa + U \circ \tau$, where $\tau : N \to M$ is the base-point projection. Let m be the dimension of M and S an $(m-1)$-dimensional submanifold of the boundary of M. Let $N_S^+(\mathcal{E})$ be the intersection of N_S^+, defined just as in the more specialized setting of the molecule-wall systems, with the constant energy submanifold $E = \mathcal{E}$ of N. We assume that the return map $T : N_S^+(\mathcal{E}) \to N_S^+(\mathcal{E})$ is defined (in the a.e. sense described above); let ν be the unit normal vector field on S pointing towards the interior of M; and for any given value $\mathcal{E}$ define $h_\mathcal{E} : M(\mathcal{E}) \to \mathbb{R}$, where $M(\mathcal{E}) := \{q \in M : U(q) \le \mathcal{E}\}$ and

$$h_\mathcal{E}(q) := \sqrt{2(\mathcal{E} - U(q))}. \tag{1.4}$$

Extend $h_\mathcal{E}$ to all of M by setting $h_\mathcal{E} = 0$ on the complement of $M(\mathcal{E})$. Now let W be an open set in $M(\mathcal{E})$ on which is defined an orthonormal frame of vector fields $e_1, \dots, e_m$; let $N_W(\mathcal{E})$ be the part of $N(\mathcal{E})$ above W, and let $F_\mathcal{E} : W \times S^{m-1} \to N_W(\mathcal{E})$ be the map such that

$$F_\mathcal{E}(q, u) = \left(q, h_\mathcal{E}(q) \sum_{i=1}^m u_i e_i(q)\right),$$

where S^{m-1} is the unit sphere in $\mathbb{R}^m$. Then $F_\mathcal{E}$ is a diffeomorphism and $u \mapsto F_\mathcal{E}(q, u)$ maps the unit sphere bijectively onto the fiber of $N(\mathcal{E})$ above q. If W intersects S or more generally ∂M, we assume that at any $q \in W \cap \partial M$ the vector $e_m(q)$ is perpendicular to $T_q(\partial M)$.

The Riemannian volume form on M will be denoted by ω^M and that on S by ω^S. Recall that the relationship between ω^M and ω^S is that $\omega^S = \nu \lrcorner \omega^M$, the interior multiplication of ω^M by the unit normal vector field on S. Let ω^{sphere} be the Euclidean volume form on S^{m-1}, which is obtained from the standard volume form on $\mathbb{R}^m$ by interior multiplication with the unit radial vector field. In Section 5 we define the (microcanonical) invariant forms Ω^E and Ω_S^E on $N(\mathcal{E})$ and $N_S^+(\mathcal{E})$, respectively, in terms of the symplectic form and prove the following.

Theorem 4 (Invariant volumes)**.** *For any choice of orthonormal frame over an open set $W \subset M(\mathcal{E})$, and given the frame map $F_\mathcal{E} : W \times S^{m-1} \to N_W(\mathcal{E})$ defined above, the form Ω^E satisfies*

$$F_\mathcal{E}^* \Omega^E = \pm m h_\mathcal{E}^{m-2} \omega^M \wedge \omega^{sphere}.$$

If W is a neighborhood of a point in S, we similarly have

$$F_\mathcal{E}^* \Omega_S^E = \pm \cos\theta \, h_\mathcal{E}^{m-1} \omega^S \wedge \omega^{sphere},$$

where $\theta(v)$ is the angle that $v \in T_qM$ makes with $\nu(q)$ for $q \in S$. Apart from the unspecified signs, these expressions do not depend on the choice of local orthonormal frame.

The first volume form is invariant under the Hamiltonian flow, and the second is invariant under the return map to S. We refer to the latter as the *billiard volume form* and to the former as the *Liouville volume form*. The Gibbs canonical distribution with temperature parameter β is then the probability measure obtained from the volume form

$$e^{-\beta E} h_\mathcal{E}^{m-2} dE \wedge \omega^M \wedge \omega^{\text{sphere}}$$

on N; similarly the Gibbs volume form is defined on N_S^+ using the billiard volume form just introduced above. These volumes on N and on N_S^+ are also invariant under the Hamiltonian flow and under T, respectively. The probability measure on $N_S^+(\mathcal{E})$ associated to the billiard volume form may also be called the *Gibbs microcanonical distribution*. Note how the probability of states in the microcanonical distribution depends on the potential function (thus on the position in M) due to the term $h_\mathcal{E}^{m-1}$.

Given the representation of the invariant volumes of Theorem 4, we can state the Markov chain algorithm as follows.

MC1. Start with a $\xi_{\text{old}} \in N_{\text{mol}}$, representing the state of the molecule prior to a collision event;

MC2. Choose $\mathcal{E}$ with probability density proportional to $\exp(-\beta\mathcal{E})$, representing the energy of the wall system;

MC3. Choose $q \in M_{\text{wall}}(\mathcal{E}) = \{q \in M_{\text{wall}} : U_{\text{wall}}(q) \leq \mathcal{E}\}$ with probability density proportional to $h_{\mathcal{E}}^{m-2}$ relative to the Riemannian volume (which defines uniform distribution), where m is the dimension of M_{wall};

MC4. Choose a random vector u over the unit sphere in $T_q M_{\text{wall}}$ with the uniform distribution;

MC5. Set the state of the wall prior to the collision event to $(q, h_{\mathcal{E}}(q)u)$;

MC6. Use the combined state $(\xi_{\text{old}}, q, h_{\mathcal{E}}(q)u)$ as the initial condition of the molecule-wall system prior to collision and let it evolve according to the deterministic equations of motion until the molecule leaves the zone of interaction; record the state ξ_{new} of the molecule at this moment.

This procedure is illustrated in Subsection 4.2 with an example that is similar to that of Section 3 but now involving a non-constant potential function. Similarly interpreting Theorem 1, a (typically unique) stationary distribution for a Markov chain with transitions $\xi_{\text{old}} \mapsto \xi_{\text{new}}$ can be sampled from in the following way:

SD1. Choose $\mathcal{E}$ with probability density proportional to $\exp(-\beta\mathcal{E})$;

SD2. Choose q in $\overline{M}_{\text{mol}} \times \mathbb{T}^k$ with probability density proportional to $h_{\mathcal{E}}^{m-1}$, where m is now the dimension of the latter manifold;

SD3. Choose a random vector u over the unit sphere in $T_q M_{\text{mol}}$ with probability density proportional to $\cos\theta$, where θ is the angle between the velocity of the molecule's center of mass and the normal to the submanifold S (which the molecule has to cross to enter the region of interaction);

SD4. Set the sample value of the equilibrium state of the molecule to be $(q, h_{\mathcal{E}}(q)u)$.

Theorem 4 is proved in Subsection 5.5, Proposition 15.

2 Random dynamical systems

In this section we derive a few general facts concerning random dynamical processes with the main goal of proving Theorem 2. The notation employed below is independent of that of the rest of the paper.

2.1 The Markov operator in general

Let $\pi : \mathcal{M} \to X$ denote a *measured fibration*, by which we simply mean a measurable map between Borel spaces together with a family of probability measures $\eta = \{\eta_x : x \in X\}$ on fibers, so that $\eta_x(\pi^{-1}(x)) = 1$ for each x. The family is measurable in the following sense: If $f : M \to [0, \infty]$ is a Borel function then $x \mapsto \eta_x(f)$ is Borel, where $\eta_x(f)$ indicates the integral of f with respect to η_x. We refer to η as the *probability kernel* of the fibration.

A *random system* on X is specified by the data (π, T, η, μ), where π is a measured fibration with probability kernel η, μ is the *initial probability distribution* on X, and $T : \mathcal{M} \to \mathcal{M}$ is a measurable map. We think of the map T as the generator of a deterministic dynamical system on the state space $\mathcal{M}$. A point ξ in $\mathcal{M}$ represents a fully specified state of the system, of which the "observer" can only have partial knowledge represented by $\pi(\xi)$. (It is not assumed that T maps fibers to fibers.)

From this we define a Markov chain with state space X as follows. Let μ be a probability measure on X representing the statistical state of the (observable part of the) system at a given moment. Then the state of the system at the next iteration is given by

$$\mu \mapsto \mu P := (\pi \circ T)_* \mu \circ \eta.$$

The notation should be understood as follows. From μ and η we define a probability measure $\mu \circ \eta$ on M so that for any, say L^∞ function $f : M \to \mathbb{R}$

$$(\mu \circ \eta)(f) = \int_X \eta_x(f)\, d\mu(x).$$

The push-forward operation on measures is defined by $T_*\nu(f) := \nu(f \circ T)$. The result is an operator P taking probability measures to probability measures, which we refer to as the *Markov operator*. When it is helpful to be more explicit we write, say, $P_{\eta,T}$ or P_η, instead of P.

The probability kernel η is the family of *transition probabilities* of the Markov chain. In keeping with standard notation, we let P act on measures (states) on the right, and on functions (observables) in the left. Thus Pf is the function such that $\mu(Pf) = (\mu P)(f)$ for all μ. It follows that

$$(Pf)(x) = \int_{\pi^{-1}(x)} f(\pi \circ T(\xi))\, d\eta_x(\xi).$$

We say that η is the *disintegration* of a probability measure ν on $\mathcal{M}$ relative to a probability μ on X if $\nu = \mu \circ \eta$.

A probability measure ν on $\mathcal{M}$ is *invariant* under T if $T_*\nu = \nu$, and a probability measure μ on X is *stationary* for the random system if $\mu P = \mu$.

Proposition 1. *Let ν be a T-invariant probability measure on the total space $\mathcal{M}$ of the random system (π, T, η, μ) and suppose that η is the disintegration of ν with respect to $\mu := \pi_*\nu$. Then $\pi_*\nu$ is a stationary probability measure on X.*

Proof. This is immediate from the definitions:

$$(\pi_*\nu)P = (\pi \circ T)_*(\pi_*\nu) \circ \eta = \pi_* T_* \nu = \pi_* \nu.$$

We have used that $\pi_*(\mu \circ \eta) = \mu$. □

Let μ be a probability measure on X and define the Hilbert space $L^2(X, \mu)$ with inner product

$$\langle f, g \rangle := \int_X f \overline{g}\, d\mu.$$

Proposition 2. *Let (π, T, η, μ) be a random system, where T is an isomorphism (thus it has a measurable inverse) of the measure space $\mathcal{M}$ and $\nu := \mu \circ \eta$ is T-invariant. Let $P_{\eta,T}$ be the associated Markov operator. Then $P_{\eta,T}$, regarded as an operator on $L^2(X, \mu)$, has norm $\|P_{\eta,T}\| = 1$ and its adjoint is $P^*_{\eta,T} = P_{\eta,T^{-1}}$.*

Proof. Jensen's inequality implies

$$\|P_{\eta,T} f\|^2 = \int_X \left| \int_{\pi^{-1}(x)} f(\pi \circ T(\xi))\, d\eta_x(\xi) \right|^2 d\mu(x) \le \int_X \int_{\pi^{-1}(x)} |f(\pi \circ T(\xi))|^2\, d\eta_x(\xi)\, d\mu(x).$$

The integral on the right equals $\int_{\mathcal{M}} |f|^2 \circ \pi \circ T\, d\nu = \int_{\mathcal{M}} |f|^2 \circ \pi\, d\nu$, by T-invariance of ν. As $f \circ \pi$ is constant on fibers, this last integral is $\|f\|^2$, showing that the norm of the operator is bounded by 1. Taking $f = 1$ shows that the norm actually equals 1. To see that the adjoint equals the operator associated to the inverse map, simply observe the identity

$$\int_{\mathcal{M}} f(\pi(\xi)) \overline{g}(\pi(T(\xi)))\, \nu(\xi) = \int_{\mathcal{M}} f(\pi(T^{-1}(\xi)) \overline{g}(\pi(\xi))\, \nu(\xi),$$

which is due to T-invariance of ν. □

2.2 Time reversibility and symmetry

Let (π, T, η, μ) be a *T-invariant random system*, which means by definition that $\nu = \mu \circ \eta$ is a T-invariant measure so, in particular, μ is stationary. We say that the system is *time reversible* if there is a measurable isomorphism $\tilde{J} : \mathcal{M} \to \mathcal{M}$ respecting π and ν, in the sense that it maps fibers to fibers and $\tilde{J}_* \nu = \nu$, and satisfies

$$T \circ \tilde{J} = \tilde{J} \circ T^{-1}.$$

Since $\tilde{J}$ respects π, it induces a measure preserving isomorphism $J : X \to X$ (for the measure μ) such that $J \circ \pi = \pi \circ \tilde{J}$. We denote also by J the induced composition operator on $L^2(X, \mu)$, so that $Jf := f \circ J$. Notice that such J is a unitary operator on $L^2(X, \mu)$. We call $\tilde{J}$ the *time-reversing map* of the system.

Proposition 3. *Let (π, T, η, μ) be a T-invariant random system with time-reversing map $\tilde{J}$, and J its associated unitary operator on $L^2(X, \mu)$. Then $P^*_{\eta,T} = J^* P_{\eta,T} J$.*

Proof. A straightforward consequence of the definitions is that

$$\left(P_{\eta,T} J f\right)(x) = \int_{\pi^{-1}} (f \circ \pi)\left(T^{-1} \circ \tilde{J}(\xi)\right) d\eta_x(\xi),$$

from which we obtain

$$\langle P_{\eta,T} J f, Jg \rangle = \int_{\mathcal{M}} (f \circ \pi)\left(T^{-1} \circ \tilde{J}(\xi)\right) \overline{g}\left(\pi \circ \tilde{J}(\xi)\right) d\nu(\xi).$$

The last integral is now seen to be equal to $\int_M f(\pi(\xi)) \overline{g}(\pi(T(\xi)))\, d\nu(\xi) = \langle f, P_{\eta,T} g \rangle$ by using the invariance of ν under $\tilde{J}$ and T. □

We say that $\tilde{S} : \mathcal{M} \to \mathcal{M}$ is an *automorphism*, or a *symmetry* of the random system if it is a measurable isomorphism commuting with T that respects π and $\nu = \mu \circ \eta$. Thus $\tilde{S}$ covers a measure preserving isomorphism of X, which we denote by S.

Definition 1. *The T-invariant, time reversible random system (π, T, η, μ) with time reversing map $\tilde{J}$ will be called* symmetric *if there exists an automorphism $\tilde{S}$ whose induced map S on X coincides with the map J induced from $\tilde{J}$.*

Proposition 4. *Let (π, T, η, μ) be a symmetric (hence time-reversible and T-invariant) random system. Then the Markov operator $P_{\eta,T}$ is self-adjoint. In particular, $P_{\eta,T^{-1}} = P_{\eta,T}$.*

Proof. Given Proposition 3, it is enough to verify that $P_{\eta,T}$ commutes with the operator J. Keeping in mind that $J = S$, $T \circ \tilde{S} = \tilde{S} \circ T$, and that ν is $\tilde{S}$-invariant, we obtain

$$\begin{aligned}
\int_{\mathcal{M}} f\left(J \circ \pi \circ T(\xi)\right) \overline{g}\left(\pi(\xi)\right) d\nu(\xi) &= \int_{\mathcal{M}} f\left(\pi \circ \tilde{S} \circ T(\xi)\right) \overline{g}\left(\pi(\xi)\right) d\nu(\xi) \\
&= \int_{\mathcal{M}} f\left(\pi \circ T(\xi)\right) \overline{g}\left(\pi \circ \tilde{S}^{-1}(\xi)\right) d\nu(\xi) \\
&= \int_{\mathcal{M}} f\left(\pi \circ T(\xi)\right) \overline{g}\left(J^{-1} \circ \pi(\xi)\right) d\nu(\xi).
\end{aligned}$$

This means that $\langle P_{\eta,T} J f, g \rangle = \langle P_{\eta,T} f, J^{-1} g \rangle$. The claim follows as J is unitary. □

Corollary 1. *Let (π, T, η, μ) be a T-invariant random system, where T is an involution, i.e., T^2 equals the identity map on $\mathcal{M}$. Then the Markov operator $P_{\eta,T}$ is self-adjoint.*

Proof. Since $T = T^{-1}$, the identity map on I is both a time reversing map and a symmetry of the system. □

The situation indicated in Corollary 1 essentially describes a general stationary Markov chain satisfying *detailed balance.* In that case, X is the state space of the Markov chain, $\mathcal{M} = X \times X$ (or, more generally, a measurable equivalence relation on X), and η_x is a probability measure on X for each $x \in X$. For T we take the (groupoid) inverse map $(x, y) \mapsto (y, x)$. As a special case, we suppose that X is countable and write in more standard notation $p_{xy} := \eta_x(\{y\})$ and $\pi_x := \mu(\{x\})$. Then the random system is symmetric as defined above exactly when the Markov chain on X with transition probabilities (p_{xy}) and stationary distribution (π_x) satisfies the detailed balance condition $\pi_x p_{xy} = \pi_y p_{yx}$ for all $x, y \in X$.

2.3 Quotients

A minor technical issue to be mentioned later calls for a consideration of *quotient random systems.* Suppose that G is a group of symmetries of the random system (π, T, η, μ) and that the action of G on $\mathcal{M}$, as well as the induced action on X, are *nice* in the sense that the quotient measurable spaces are countably separated. (See, for example, [15], where such actions are called *smooth.* In the situations of main concern to us, G is a finite group acting by homeomorphisms of a metric space, in which case the condition holds.) Without further mention let the actions of G be nice.

We denote the quotient system by $(\overline{\pi}, \overline{T}, \overline{\eta}, \overline{\mu})$, and the other associated notions, such as $\overline{\mathcal{M}}$ and $\overline{\nu}$, are similarly indicated with an over-bar. The quotient maps $\mathcal{M} \to \overline{\mathcal{M}}$ and $X \to \overline{X}$ will both be indicated by p. These maps and measures are all defined in the most natural way. For example, $\overline{T}$ is the transformation on $\overline{M}$ such that $\overline{T} \circ p = p \circ T$, which exists since G commutes with T, $\overline{\mu} = p_* \mu$, etc. Since G leaves μ invariant, it is represented by unitary transformations of $L^2(X, \mu)$ commuting with $P_{\eta,T}$. So it makes sense to restrict $P_{\eta,T}$ to the closed subspace $L^2_G(X, \mu)$ of G-invariant vectors, which is isomorphic to the Hilbert space $L^2(\overline{X}, \overline{\mu})$ under the map $p^* : L^2(\overline{X}, \overline{\mu}) \to L^2_G(X, \mu)$ that sends f to $f \circ p$. Thus we may identify the quotient Markov operator $P_{\overline{\eta},\overline{T}}$ with the restriction of $P_{\eta,T}$ to the G-invariant subspace.

We use these remarks later in situations where the initial system does not have any symmetries that would allow us to apply Proposition 4, but it can nevertheless be regarded as the quotient of another system having the necessary symmetry.

3 A case study: the two-masses system

In this section we prove Theorem 3 and further refinements, which are concerned with one simple but illustrative molecule-wall system. Other examples are described more briefly in the next section.

3.1 Description of the example

Let x_1, x_2 represent the positions of two point masses that can move on the half-line $[0, \infty)$, with respective masses m_1 and m_2. Mass m_1, called the *bound mass*, is restricted to the interval $[0, l]$, and it reflects elastically upon hitting 0 or l, moving freely between these two values. Mass m_2, called the *free mass*, moves freely on the interval $[x_1, \infty)$, and collides elastically with m_1 when $x_2 = x_1$. There are no forces or interactions of any kind other than collisions. We are interested in the following "scattering experiment": Mass m_2 starts at some place along the half-line with coordinate $x_2 > l$ and speed $s > 0$, moving towards the origin. It eventually collides with m_1, possibly several times, before reversing direction and leaving the interval $[0, l]$. When it finally reaches again a point with coordinate $x_2 > l$, we register its new speed $S > 0$ (now moving away from the origin). It is assumed that we can measure s and S exactly, but that the state of m_1 at the moment the incoming mass crosses the boundary $x_2 = l$ is only known up to a probability distribution.

More specifically, at the moment the incoming mass m_2 crosses the position l into the interval of interaction with m_1, we take x_1 to be a random variable uniformly distributed over $[0, l]$ and that

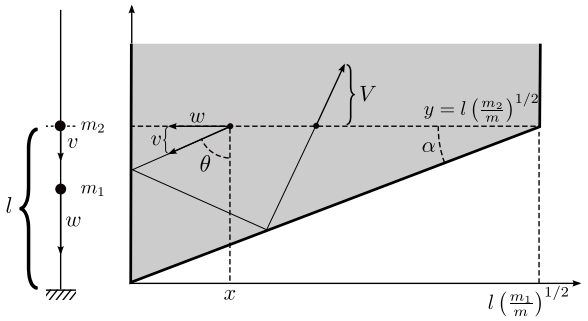

Figure 5: A two-dimensional billiard system corresponding to the one-dimensional scattering example described in the text. For the random system, start with a $v \in (0, \infty)$, then choose a random (uniform) position along the horizontal dashed line and a random value for w according to a given, fixed, probability distribution on $\mathbb{R}$. Then let the billiard particle move, billiard fashion, inside the triangle, with that initial position and initial velocity $we_1 - ve_2$, where e_i are the standard basis of $\mathbb{R}^2$. Eventually, the billiard particle returns to the horizontal dashed line. When it does, let V be the absolute value of the vertical component of the particle's velocity. Then $v \mapsto V$ is the random map for the free particle scattered velocity.

the velocity $v_1 \in \mathbb{R}$ of the bound mass is also random, although we do not yet specify its probability distribution. It is imagined that l is very small ("microscopic") and that the bound mass is part of the wall, whose precise dynamical state is thus only known probabilistically. We wish to investigate the random process $s \mapsto S$, which gives the random speed of the free particle after one collision with the wall system (consisting of possibly many collisions between m_2 and m_1), given the speed of the same particle before the collision.

The state of the system at a moment when $x_2 = l$ is fully described by the triple (x_1, v_1, s). It will be convenient to use coordinates $x := \sqrt{m_1/m}\, x_1$, $y = \sqrt{m_2/m}\, x_2$, $w = \sqrt{m_1/m}\, v_1$ and $v = \sqrt{m_2/m}\, s$, where $m = m_1 + m_2$. A configuration of this two-particle system corresponds to a point (x, y) in the billiard table region depicted in Figure 5. By doing this coordinate change we now have ordinary billiard motion, i.e., uniform rectilinear motion between collisions and specular collisions at the boundary segments. (The coordinate change turns the kinetic energy of the system into the norm, up to uniform scaling, associated to the standard inner product in $\mathbb{R}^2$.)

States of the two-particle system are represented by tangent vectors on the billiard region. Expressing the situation in the language of Section 2, let $\mathcal{M}$ be the set of states for which $y = l\sqrt{m_2/m}$ (see Figure 5); omitting the y-coordinate, we write $\mathcal{M} := \left\{(x, w, v) : x \in \left[0, l\sqrt{m_1/m}\right], v > 0\right\}$. The observable (pure) states are points in $X = (0, \infty)$ and we let $\pi : \mathcal{M} \to X$ be the projection on the third coordinate. The transformation $T : \mathcal{M} \to \mathcal{M}$ is the billiard return map to the horizontal dashed line of Figure 5. We choose the measure η_v on the fiber of $v \in X$ to be the product $\lambda \otimes \zeta$ of the normalized Lebesgue measure on $\left[0, l\sqrt{m_1/m}\right]$ and a fixed probability measure ζ on $\mathbb{R}$.

For each choice of ζ, we obtain a Markov operator P of a random process with state space $(0, \infty)$. Such a process may be interpreted as a sequence of successive collisions of the free mass with the "microstructured wall." It may be imagined that the free particle actually moves in a finite interval of arbitrary length bounded by two such walls having the same probabilistic description, so that the process defined by P describes the evolution of the random velocity of mass m_2 as it collides alternately with the left and right walls.

3.2 Stationary probability distributions

For concreteness, let us choose the measure ζ to be the absolutely continuous probability measure on $\mathbb{R}$ with Gaussian density $\rho_{\text{wall}}(w) = (\sigma\sqrt{2\pi})^{-1}\exp\left(-\frac{1}{2}w^2/\sigma^2\right)$. This amounts to assuming that the state of the bound mass satisfies the Gibbs canonical distribution with temperature proportional to σ^2. One should keep in mind that by the above change of coordinates the kinetic energy of the bound mass is simply $\frac{1}{2}w^2$, so it makes sense to refer to σ^2 as the *temperature* of the wall.

Proposition 5. *Let P be the Markov operator with state space $(0,\infty)$ for the random process of the two-masses system. We assume that the state of the bound mass (or the wall system) has the Gibbs canonical distribution $\lambda\otimes\zeta$ with wall temperature σ^2. Then P has a unique stationary distribution μ, whose density relative to the Lebesgue measure on $(0,\infty)$ is the Maxwell-Boltzmann distribution with the same temperature:*

$$\rho_{\mathit{free}}(v) = \sigma^{-2}v\exp\left(-\frac{v^2}{2\sigma^2}\right).$$

If η is any Borel probability measure on $(0,\infty)$, then ηP^n converges in the weak- topology to the stationary probability measure.*

Proof. We begin by showing that the Maxwell-Boltzmann distribution is indeed stationary for P without invoking the more general Theorem 1. Let μ denote the probability measure with density ρ_{free}. Then the probability measure $\nu = \mu\circ\eta$ on $\mathcal{M}$ is $\mu\otimes\zeta\otimes\lambda$, which has density

$$\rho(x,v,w) = Cv\exp\left(-\frac{v^2+w^2}{2\sigma^2}\right)dx\,dv\,dw,$$

where C is a normalization constant. Let θ be the angle in $[-\pi/2,\pi/2]$ between the initial velocity of the billiard particle in Figure 5 and the normal vector to the horizontal dashed line pointing downward, and r the Euclidean norm of the velocity vector. Then ν can be written, in polar coordinates, as $d\nu(x,\theta,r) = Cr^2\exp\left(-\frac{r^2}{2\sigma^2}\right)\cos\theta\,dx\,d\theta\,dr$ where C is now a different normalization constant. For each value of r, the measure $\cos\theta\,dx\,d\theta$ is invariant under the billiard map restricted to a constant energy surface (see [3]; also compare with our more general Theorem 4). In our case, it is invariant under the return billiard map T restricted to each coordinate r-slice. Therefore, v is itself T-invariant. We can then apply Proposition 1 to conclude that μ is P-stationary. It will be shown shortly that P is an integral operator of the form $(Pf)(v) = \int_0^\infty \kappa(v,u)f(u)\,du$, where $\kappa(v,u) > 0$ for each v and all u. In particular, it is indecomposable and non-periodic, and for each v, $\delta_v P$ is absolutely continuous with respect to the Lebesgue measure on the half-line. By, say, Theorem 7.18 of [1], the stationary measure is unique and the claimed convergence holds. □

Reverting to the non-scaled variables and introducing the parameter β such that $\beta^{-1} = m_1\sigma_1^2$, where σ_1^2 is the variance of the velocity of the bound mass m_1, then the stationary distribution for the speed of the free mass has density

$$\rho_{\text{MB}}(v_2) = \beta m_2 v_2\exp\left(-\beta\frac{m_2v_2^2}{2}\right).$$

We interpret β as the reciprocal of the wall temperature.

3.3 The random map

Proposition 5 gives the equilibrium (stationary) state of the free mass velocity process. This equilibrium state is arrived at by iterating a random map on $(0,\infty)$ with transition probabilities operator

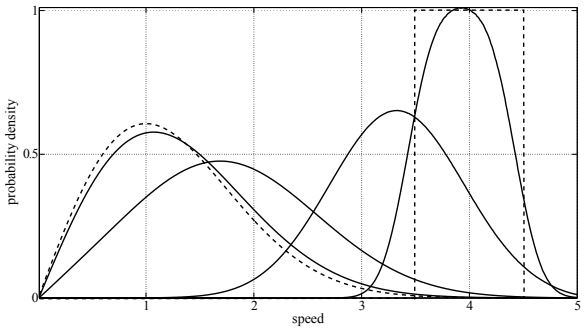

Figure 6: Evolution of an initial probability measure, μ_0, of the free mass velocity, having a step function density. The graphs in dashed line are the initial and the limit density $v\exp(-v^2/2)$, and the other graphs, from right to left, are the densities of $\mu_0 P^n$ at steps $n = 1, 10, 50, 100$, of the Markov chain of Proposition 5. We have used a finite rank approximation of P obtained by numerically simulating the mechanical system with mass ratio $m_1/m_2 = 100$.

P. We wish now to describe this random map more explicitly. In the following analysis, we assume that $m_1 > 3m_2$. (This condition limits the number of branches of the random affine map shown below, which otherwise increases with the ratio m_1/m_2.) First we set some notation: Let $\gamma := \sqrt{m_2/m_1} = \tan\alpha$, where α is the angle of the billiard table triangle indicated on Figure 5. Define

$$a := \frac{1-\gamma^2}{1+\gamma^2}, \quad b := \frac{2\gamma}{1+\gamma^2}, \quad \overline{a} := \frac{1-6\gamma^2+\gamma^4}{(1+\gamma^2)^2}, \quad \overline{b} := \frac{4\gamma(1-\gamma^2)}{(1+\gamma^2)^2}.$$

Also define the functions

$$p_v(w) := \frac{\gamma}{\sqrt{1+\gamma^2}}\frac{|w|}{v}, \quad q_v(w) := \frac{2(1-\gamma^2)}{1+\gamma^2} - \frac{4\gamma}{1+\gamma^2}\frac{|w|}{v},$$

and introduce the partition of $(0,\infty)$ into intervals $I_w^i = |w|I^i$, $i = 1,2,3,4$, where

$$I_1 := (0, \tan\alpha], \quad I_2 := (\tan\alpha, \tan(2\alpha)], \quad I_3 := (\tan(2\alpha), \tan(3\alpha)], \quad I_4 := (\tan(3\alpha), \infty).$$

It is useful to note that $\tan(2\alpha) = 2\gamma/(1-\gamma^2)$ and $\tan(3\alpha) = \gamma(3-\gamma^2)/(1-3\gamma^2)$. The simplifying assumption $m_1 > 3m_2$ is equivalent to $\alpha < \pi/6$. The random map can now be expressed as follows: Choose $w \in \mathbb{R}$ at random with probability ζ (say, the Gaussian probability with temperature σ^2) and define the affine maps

$$F_1^w(v) := av + bw, \quad F_2^w(v) := av - bw, \quad F_3^w(v) := -\overline{a}v + \overline{b}w.$$

These are the deterministic branches of the random map (see Figure 7).

Finally, let $F^w : (0,\infty) \to (0,\infty)$ be the piecewise affine random map defined on each interval I_w^i of the partition as follows. Case I: If $w \geq 0$, then $F^w(v) = F_1^w(v)$. Case II: If $w < 0$, then

$$F^w|_{I_w^1}(v) := F_1^{|w|}(v) \qquad F^w|_{I_w^2}(v) := \begin{cases} F_1^{|w|}(v) & \text{w. prob. } p_v(w) \\ F_3^{|w|}(v) & \text{w. prob. } 1-p_v(w) \end{cases}$$

$$F^w|_{I_w^3}(v) := \begin{cases} F_1^{|w|}(v) & \text{w. prob. } p_v(w) \\ F_2^{|w|}(v) & \text{w. prob. } q_v(w) \\ F_3^{|w|}(v) & \text{w. prob. } 1-q_v(w)-p_v(w) \end{cases} \qquad F^w|_{I_w^4}(v) := \begin{cases} F_1^{|w|}(v) & \text{w. prob. } p_v(w) \\ F_2^{|w|}(v) & \text{w. prob. } 1-p_v(w) \end{cases}$$

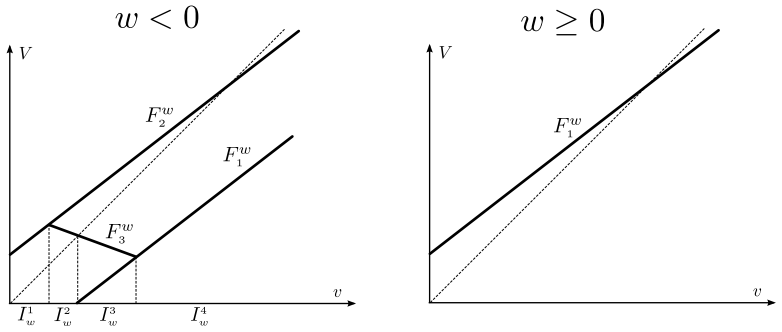

Figure 7: Graph of the random map F. The dashed line is the graph of the identity map.

('w. prob.' = 'with probability.') These expressions are obtained using the standard idea of "unfolding" the polygonal billiard table and some tedious but straightforward work.

3.4 A remark about symmetry

Before continuing with the analysis of the example, let us briefly examine a small modification of it to illustrate a general point concerning symmetries.

The modified example is shown in Figure 8. By Proposition 4, its Markov operator is self-adjoint on $L^2(\mathbb{R}, \mu_{\text{sym}})$, where μ_{sym} is the even measure on the real line whose conditional probability distribution, conditional on the event that the free mass approaches from the right-hand side of the wall, equals the stationary measure asserted in Proposition 5. Denoting this operator by P_{sym}, then $P_{\text{sym}} = (P + P^*)/2$, where P is the Markov operator of the first version of the example.

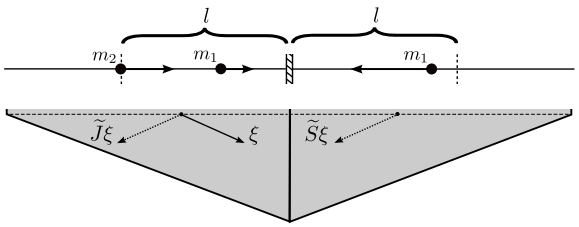

Figure 8: A symmetric version of the example of Figure 5 (top of figure). The free particle may approach the wall from the left or from the right, with equal probabilities. The states of the bound masses on the right and left are equally distributed and independent. The map $\widetilde{J}$ is the time reversing map, and $\widetilde{S}$ is a symmetry compatible with $\widetilde{J}$, in the sense that Proposition 4 applies.

Although this remark illustrates a useful general point made in Subsection 2.3, it turns out that P is already self-adjoint in the present case. In fact, the map J on X introduced in the definition of time reversibility is in this case the identity so the symmetry $\widetilde{S}$ can be taken to be the identity map and Proposition 4 applies to the original system.

3.5 The integral kernel and compactness

We now wish to show that the operator P on $L^2((0,\infty), \mu)$ is Hilbert-Schmidt. This is the content of the below Proposition 6.

It is not difficult to show that P is an integral operator, $(Pf)(v) =: \int_0^\infty \kappa(v,u) f(u)\,du$, whose integral kernel κ has the following description. Write $\rho_\sigma(w) := \rho_{\text{wall}}(w)$ to emphasize the parameter σ of the Gaussian distribution. Then,

$$\kappa(v,u) = \rho_{b\sigma}(u-av)\sum_{i=1}^{5} Q_i\left(v, \frac{u-av}{b}\right)\mathbb{1}_{J_i(v)}(u) + \rho_{\overline{b}\sigma}(u+\overline{a}v)\sum_{i=1}^{2}\overline{Q}_i\left(v, \frac{u+\overline{a}v}{\overline{b}}\right)\mathbb{1}_{\bar{J}_i}(u)$$

where $\mathbb{1}_A$ is the indicator function of a set A, the Q_i are

$$Q_1(v,w) = Q_2(v,w) = 1, \quad Q_3(v,w) = p_v(w), \quad Q_4(v,w) = q_v(w), \quad Q_5(v,w) = 1 - p_v(w),$$

the $\overline{Q}_i$ are

$$\overline{Q}_1(v,w) = 1 - p_v(w), \quad \overline{Q}_2(v,w) = 1 - p_v(w) - q_v(w),$$

the intervals J_i and $\bar{J}_i$ are

$$J_1 = (av,\infty), J_2 = (\overline{c}v,\infty), J_3 = (av,\overline{c}v), J_4 = (0, v/\overline{c}), J_5 = (v/\overline{c}, av), \bar{J}_1 = (v,\overline{c}v), \bar{J}_2 = (\underline{c}v, v)$$

and, finally,

$$\underline{c} = \frac{\gamma^2(3+3\gamma^2+\gamma^4)}{(1+\gamma^2)(3-\gamma^2)}, \quad \overline{c} = \frac{3-\gamma^2}{1+\gamma^2}.$$

Let μ be the measure on $(0,\infty)$ having density $\rho_{\text{free}}(v) = \sigma^{-2} v \exp\left(-v^2/2\sigma^2\right)$ and $K(v,u)$ the integral kernel of P relative to μ. Thus $(Pf)(v) = \int_0^\infty K(v,u) f(u)\,d\mu(u)$. Then there exists a constant C such that

$$K_0(v,u) := \rho_{b\sigma}(u-av)/\rho_{\text{free}}(u) = \frac{C}{u}\exp\left\{-\frac{1}{2\sigma^2}\left(\frac{u-av}{b}\right)^2 + \frac{u^2}{2\sigma^2}\right\}. \tag{3.1}$$

Define $\overline{K}_0(v,u)$ similarly, by substituting $\overline{a}$ and $\overline{b}$ for a and b.

Proposition 6. *Let $\widetilde{K}(v,u)$ be one of the following kernels:*

$$K_0(v,u)\mathbb{1}_{(cv,\infty)}(u), \quad \overline{K}_0(v,u)\mathbb{1}_{(cv,\infty)}(u), \quad \text{or} \quad K_0(v,u)\,q_v\left(\frac{u-av}{b}\right)\mathbb{1}_{(0,v/\overline{c})}(u)$$

where c is a positive constant. Then $\widetilde{K}$ has finite Hilbert-Schmidt norm with respect to the measure μ on $(0,\infty)$. It follows that P is a Hilbert-Schmidt self-adjoint operator.

Proof. This amounts to showing that $\int_0^\infty \int_0^\infty K(v,u)^2\,d\mu(v)\,d\mu(u) < \infty$. Expressing the integrand in terms of the Lebesgue measure $dv\,du$, omitting multiplicative constants, and setting $\sigma = 1$ for simplicity, we have to show, for the first of the three kernels, that

$$I := \int_0^\infty \int_0^\infty \exp\left\{-\left(\frac{u-av}{b}\right)^2 + u^2 - \frac{u^2+v^2}{2}\right\}\frac{v}{u}\mathbb{1}_{(cv,\infty)}(u)\,dv\,du < \infty.$$

Making the substitution $s = v/u$, we obtain

$$I = \int_0^\infty u \int_0^{1/c} \exp\left\{-u^2\left(\left(\frac{1-as}{b}\right)^2 + \frac{s^2-1}{2}\right)\right\} s\,ds\,du,$$

which clearly is finite. The second kernel is treated in the same manner. To deal with the third kernel, first observe that

$$f(s) := \left(\frac{1-as}{b}\right)^2 + \frac{s^2-1}{2} \geq \epsilon := \frac{1}{2}(1-a^4)/(1+a^2)^2 > 0$$

for all s. We have used $a^2 + b^2 = 1$ and $a = (1-\gamma^2)/(1+\gamma^2) < 1$. The same change of variables, $s = v/u$, now yields

$$I = 2\int_0^\infty u \exp\left(-\epsilon u^2\right) \int_{\overline{c}}^\infty \exp\left\{-u^2\left(\left(\frac{1-as}{b}\right)^2 + \frac{s^2-1}{2} - \epsilon\right)\right\} ds\, du$$

where the identity $q_v((u-av)/b) = 2/s$ for $u < v/\overline{c}$ was used. The value of the integral in s decreases in u as $O(1/u)$, so I converges. The actual kernel of P is a sum of kernels of the three types considered, so it also has finite Hilbert-Schmidt norm. It is interesting to note that the norm worsens as γ approaches 0. □

It is clear from the description of the integral kernel of P (and by using the general results and definitions from, say [12]) that Markov chains associated to P are Lebesgue-irreducible, strongly aperiodic, recurrent, and admit a unique stationary probability.

3.6 A perturbation approach to the spectrum of P

For convenience, we make the velocity variables dimensionless by dividing them by σ, which is the standard deviation of the velocity of the wall-bound mass. In this way, the stationary probability distribution for the free mass becomes $\rho(z) = z\exp(-z^2/2)$, where $z = v/\sigma$. The specific form of the (dimensionless) velocity distribution of the wall mass will be unimportant, but we assume that it has mean zero and variance 1. Having fixed the temperature, the main parameter of interest is $\gamma = \sqrt{m_2/m_1}$. We denote by P_γ the Markov operator acting on $L^2((0,\infty),\mu)$, where $d\mu(z) = \rho(z)\, dz$. Then the main remark of this subsection is the following proposition.

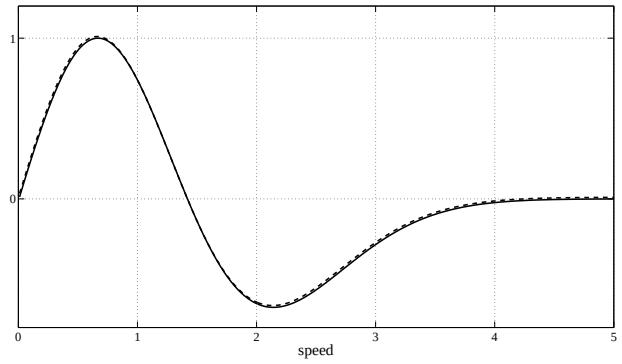

Figure 9: Comparison of the second eigendensity of P, obtained by numerical approximation, and the second eigendensity of the billiard Laplacian $\mathcal{L}$, which is $(1-z^2/2)\rho(z)$, both normalized so as to have maximum value 1. The graph of the latter (dashed line) has been intentionally offset upwards by a small amount to better distinguish the two. We have used $\gamma = 0.1$; the numerical value for the second eigenvalue of P (after $\lambda = 1$) was found to be 0.9606, to be compared with $1 + 2\gamma^2(-2) = 0.9600$, which uses the eigenvalue -2 of $\mathcal{L}$.

Proposition 7. *If ϕ is a function of class C^3 on $(0,\infty)$ vanishing at 0 and ∞, then*

$$\lim_{\gamma\to 0} \frac{(P_\gamma\varphi)(z) - \varphi(z)}{2\gamma^2} = (\mathcal{L}\varphi)(z)$$

holds for all $z > 0$ where $\mathcal{L}$, the billiard Laplacian *of the system of Example 5, is defined by*

$$(\mathcal{L}\phi)(z) := \left(\frac{1}{z} - z\right)\varphi'(z) + \varphi''(z).$$

Equivalently, $\mathcal{L}$ can be written in Sturm-Liouville form as $\mathcal{L}\varphi = \rho^{-1}\frac{d}{dz}\left(\rho\frac{d\varphi}{dz}\right)$. This is a densely defined, self-adjoint operator on $L^2((0,\infty),\mu)$.

Proof. For the sake of brevity, we give the basic idea of the proof in the special when the velocity distribution of the wall-bound mass is Bernoulli, taking values ±1 with equal probabilities 1/2. We make the additional simplification of ignoring the branch F_3^w of the random map (see Figure 7). Notice that the intervals I_w^1, I_w^2, I_w^3 (same figure) lie in $[0, 3\gamma + O(\gamma^2)]$, so only F_1^w and F_2^w are expected to be important. Thus we consider the simpler random system define as follows. Let $F_1(z) := az + b$ and $F_2(z) := az - b$, where we approximate $a = 1 - 2\gamma^2$ and $b = 2\gamma$. Let $p := \gamma/z$. Then the approximate random dynamics corresponds to applying F_1 with probability $(1+p)/2$ and F_2 with probability $(1-p)/2$. Define the k-th moment of scattering as

$$\mathcal{E}_k(z) := E_z\left[(Z-z)^k\right] = \frac{1+\gamma/2}{2}\left(F_1(z)-z\right)^k + \frac{1-\gamma/2}{2}\left(F_2(z)-z\right)^k,$$

where Z is the random speed after collision, z is the speed before collision, and $E_z[\cdot]$ indicates expectation given z. From this general expression we derive

$$\mathcal{E}_1(z) = 2\gamma^2\left(\frac{1}{z} - z\right), \quad \mathcal{E}_2(z) = 4\gamma^2 + O(\gamma^4), \quad \mathcal{E}_k(z) = O(\gamma^k).$$

Now, we expand $(P_\gamma\varphi - \varphi)(z)/2\gamma^2 = E_z\left[(\varphi(Z) - \varphi(z))/2\gamma^2\right]$ in Taylor polynomial approximation up to degree 2 and obtain

$$\frac{(P_\gamma\varphi - \varphi)(z)}{2\gamma^2} = \frac{1}{2\gamma^2}\left(\varphi'(z)E_z[Z-z] + \frac{1}{2}\varphi''(z)E_z\left[(Z-z)^2\right] + E_z\left[O\left(|Z-z|^3\right)\right]\right) = (\mathcal{L}\varphi)(z) + O(\gamma),$$

proving the main claim in this very simplified case. The general case, although much longer and tedious to check, can still be obtained in a similar straightforward manner. □

An *eigenmeasure* of P is defined as a signed measure ν such that $\nu P = \lambda\nu$. The density of an eigenmeasure relative to Lebesgue measure on the half-line will be referred to as an *eigendensity* of P. They have the form $\phi\rho$, where ρ is the stationary probability density and ϕ is an eigenfunction, $P\phi = \lambda\phi$. Based on the proposition, the first few eigenvalues and eigendensities of P for sufficiently small values of γ are expected to be approximated by those of the operator $I + 2\gamma^2\mathcal{L}$. We do not study this spectral approximation problem here (this is part of a more general study that will be presented elsewhere), but only point out the numerical agreement for the second eigenvalue and eigendensity shown in Figure 9.

The spectral theory for $\mathcal{L}$ corresponds to a standard Sturm-Liouville problem. In fact, under the change of coordinates $x = z^2/2$, $\mathcal{L}$ is (up to a constant multiple −2) the differential operator of Laguerre's equation

$$2\left(xe^{-x}\phi_x\right)_x = \lambda e^{-x}\phi.$$

Polynomial solutions exist for $\lambda = -2n$, where n is a non-negative integer, and the corresponding eigenfunctions are easily obtained by textbook methods. The second polynomial eigenfunction (the first being the constant function) is given by $\phi(z) = 1 - z^2/2$, associated to eigenvalue $\lambda = -2$. Thus it is natural to expect that the spectral gap of P is approximately $4\gamma^2$ for small values of γ. This is confirmed numerically by the graph of Figure 10.

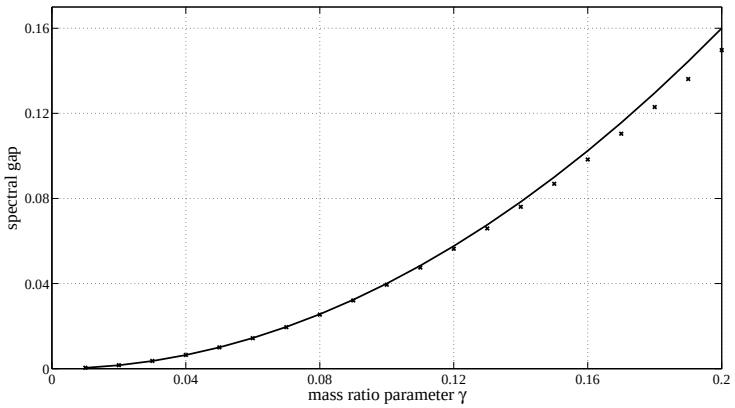

Figure 10: Asymptotics of the spectral gap of P for small values of the mass-ratio parameter γ. The discrete points are the values of the gap obtained numerically. The solid curve is the graph of $f(\gamma) = 4\gamma^2$, suggested by approximating P by a second order differential equation.

4 Other examples

We give a few further examples of simple systems to illustrate the content of the main theorems.

4.1 Wall systems without moving parts

In this subsection we very briefly consider examples having a trivial wall system, for which the Gibbs canonical distribution does not make sense. These are nevertheless interesting, and we have studied them in some detail in previous papers. (See [7, 9, 10].) Our only concern here is to see how they fit into the present more general set-up.

By assumption, M_{wall} reduces to a single point. If we further assume that the molecule is a point particle, then the only dynamical variable of interest is the velocity before and after the collision event, $v, V \in \mathbb{H}$, where $\mathbb{H}$ is a half-space in $\mathbb{R}^{k+1}$. By conservation of energy, $\|v\| = \|V\|$, so it suffices to take the hemisphere S^+ of unit vectors in $\mathbb{H}$ as the state space for the Markov chains. The only random variable is the point in $\mathbb{T}^k$, assumed to be uniformly distributed. Given a continuous function f on S^+, the Markov operator applied to f takes the form

$$(Pf)(v) = \int_{\mathbb{T}^k} f(\Psi_v(x))\, dx, \tag{4.1}$$

where $\Psi_v(x)$ is the post-collision velocity with initial conditions (x, v). A first example was suggested by Figure 2. Planar billiards, as in Figure 11, provide a large and interesting general class of examples of a purely geometric nature, for which the operator P is canonically determined by the billiard shape.

In the next proposition, let $J : S^+ \to S^+$ be the linear involution that sends the north pole to itself and points on the equator to their antipodes. We use the same symbol to denote the induced composition operator on functions on S^+. A unit of the periodic contour which, for the example of Figure 11, is shown on the right-hand side of the figure, will be called a *billiard cell*. A billiard cell is *symmetric* if it is invariant under $u \mapsto -u$ in $\mathbb{T}^k$ (which induces the map J on velocities)

Proposition 8. *For the systems without internal moving parts as described by the operator P in*

4.1, the probability measure μ on S^+ defined by

$$d\mu(v) := \frac{\Gamma(k/2+1)}{\pi^{k/2}} \langle v, n \rangle \, dA(v),$$

is stationary, where dA is the Euclidean k-dimensional volume form on S^+, n is the unit vector perpendicular to the boundary of $\mathbb{H}$, pointing towards the billiard surface, and the inner product is the standard dot product. On the Hilbert space $L^2(S^+, \mu)$, the operator P is bounded of norm 1 and satisfies $P^* = JPJ$. If the billiard cell is symmetric, then P is self-adjoint.

Proof. This follows from the general description of invariant measures of Theorem 4 and the fact that the conditions of Proposition 4 are satisfied. See also [9]. □

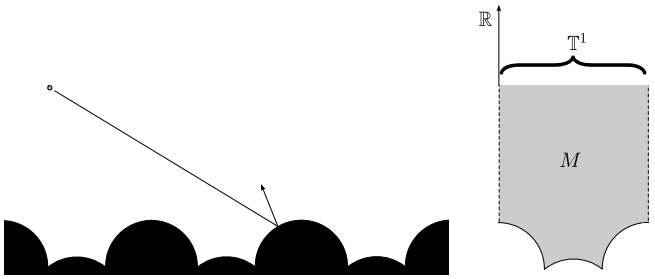

Figure 11: Billiard collisions between a point particle and wall with periodic contour. A point particle reflects off of a hard surface with periodic relief in ordinary billiard fashion. Here $\overline{M}_{\text{mol}}$ and M_{wall} consist of a single point each, and M is the subset of $\mathbb{R} \times \mathbb{T}^1$ indicated on the right-hand side of the figure. It is given the induced flat metric and the potential function is constant.

The operator P is often (and, for the specific contour of Figure 11, this is a consequence of results in [7] or [9]) a Hilbert-Schmidt operator. A problem of particular interest is the relationship between its spectrum of eigenvalues and the geometric features of the billiard cell. We refer to [9] and [10] for more information.

Another example to which Proposition 8 applies is shown in Figure 12. In this case, the wall is featureless but the molecule is not: M_{wall} consists of a single point and $\overline{M}_{\text{mol}}$ can be identified with the circle S^1. We assume constant potentials. Since the wall is translation invariant, the length scale for $\mathbb{T}^1$ is not specified (and not needed). Let l be the fixed length of the arm connecting the two masses and $m = m_1 + m_2$ the total mass. Let (x, y) represent the coordinates of the center of mass of the dumbbell molecule. Then the configuration manifold is given by

$$M = \left\{ ([\theta], x, y) : \min \left\{ y - \frac{m_2}{m} l \sin\theta, y + \frac{m_1}{m} l \sin\theta \right\} \geq 0 \right\}.$$

Here $[\theta]$ is element in $S^1 = \mathbb{R}/2\pi\mathbb{Z}$. A (θ, y)-cross section of M is shown in Figure 13. By introducing the scaled angle coordinate

$$z := \frac{\sqrt{m_1 m_2}}{m} l\theta$$

the kinetic energy, as a function of the coordinates $(x, y, z, \dot{x}, \dot{y}, \dot{z})$ on the tangent bundle of M, takes the form

$$E(x, y, z, \dot{x}, \dot{y}, \dot{z}) = \frac{1}{2} m \left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2 \right),$$

which corresponds to the standard Euclidean metric in regions of $\mathbb{R}^3$. In terms of these new coordinates, collisions are described by ordinary specular reflection on the boundary of M. (We are assuming here that the surface is perfectly smooth in the physical sense, i.e., there is no tangential transfer of momentum between the particles and the surface.)

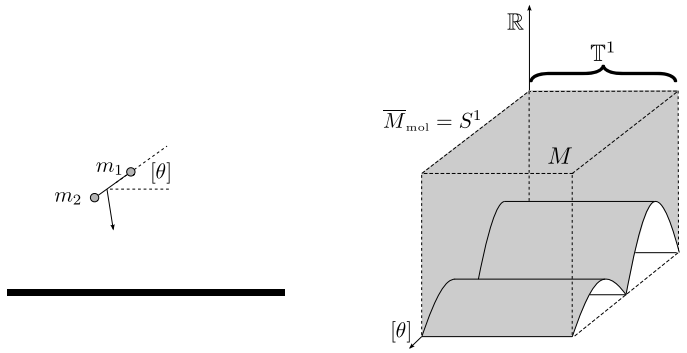

Figure 12: Collision of a rotating dumbbell with a flat surface.

By restricting attention to a cross section (x = constant) this 3-dimensional system can be reduced to a 2-dimensional system (see Figure 13) that is very similar to the one of Figure 11, with z taking the role of the length coordinate on $\mathbb{T}^1$ in the first example. If we assume that z is random, uniformly distributed, then we have a system that is of essentially of the same kind as that of the previous example.

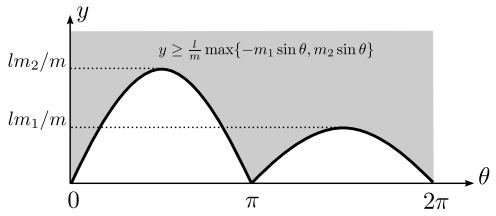

Figure 13: A cross section of the manifold with boundary depicted in Figure 12.

Letting the normalized speed $u = v/v_{\max}$ of the center of mass of the dumbbell molecule be the variable of interest (assuming, for simplicity, that the constant horizontal momentum is zero), then P is regarded as a Markov operator with state space $[0,1]$, where $v_{\max} = \sqrt{2\mathcal{E}/m}$ is the maximal speed that can be attained for a given, fixed, energy value. Writing $u = \sin\theta$ for $\theta \in [0,\pi]$, the stationary distribution μ given by Proposition 8 has the form

$$d\mu(\theta) = \frac{1}{2}\sin\theta\, d\theta.$$

It is easily shown that, for any initial probability distribution for θ, the corresponding Markov chain is (Lebesgue measure)-irreducible and aperiodic, and μ is the unique stationary probability measure.

Notice that P does not depend on the length l separating the two masses since changing l only produces a homothety change of the rescaled region of Figure 13 (i.e., after the change of variables from θ to z). So P only depends on the mass-ratio. Let $\gamma := \sqrt{m_1/m_2}$. It is convenient to set

$l = (\gamma^{-1} + \gamma)/2\pi$. With this choice, the billiard cell contour in the y, z coordinate plane is bounded below by the graph of the function

$$y = \frac{1}{2\pi} \max\left\{-\gamma \sin(2\pi z), \gamma^{-1} \sin(2\pi z)\right\}$$

for $z \in [0, 1]$.

Based on the results and arguments from [7] and [9] one should expect P to be an integral operator (Hilbert-Schmidt, or at least quasi-compact). We do not attempt to show this here, but only offer the numerical observation about the dependence of the spectral gap of P on the mass-ratio parameter γ shown in Figure 14. The graph exhibits a great deal of structure which, at this moment, we do not know how to interpret.

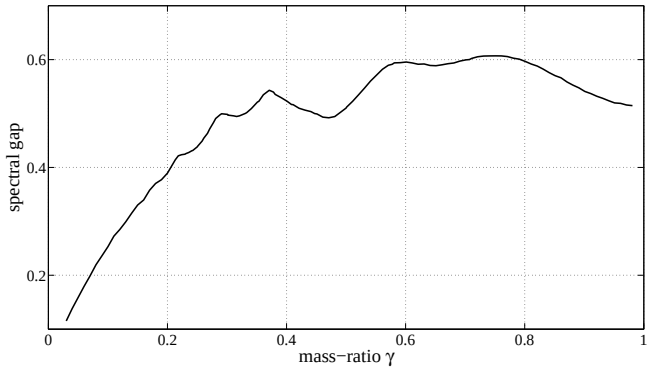

Figure 14: The spectral gap of P as function of the parameter $\gamma = \sqrt{m_1/m_2}$, where $m_2 > m_1$.

4.2 Adding potentials

For an example with a non-constant potential function, consider the system on the left-hand side of Figure 15. This is similar to the two-masses system of Section 3 except that we add a linear spring potential acting on mass m_1. Thus we consider a spring-mass with (essentially point) mass m_1, which comprises the wall subsystem, and a point mass m_2 corresponding to the molecule subsystem. Suppose for simplicity that the free mass m_2 can only move vertically, so the whole set-up should be regarded as one-dimensional. It is assumed that there are no potentials involved other than the elastic potential of the spring. (In particular, no gravity.) Then M_{wall} is an interval, $\overline{M}_{\text{mol}}$ is a single point, the torus component has dimension 0, and M is the subset of $\mathbb{R} \times M_{\text{wall}}$ indicated on the right-hand side of the figure.

The region of interaction is the interval $[0, l]$, where l is a positive number. Let x_1, x_2 indicate the positions of the masses m_1 and m_2 in physical space (on the left-hand side of the figure). Using the scaled coordinates

$$x = \sqrt{\frac{m_1}{m}}\left(x_1 - \frac{l}{2}\right), \quad y = \sqrt{\frac{m_2}{m}}\, x_2$$

for the respective positions of m_1 and m_2, the energy function for the system with linear spring potential is given by

$$E(x, y, \dot{x}, \dot{y}) = \frac{m}{2}\left(\dot{x}^2 + \dot{y}^2 + \frac{k}{m_1} x^2\right).$$

The motion in M between two collisions (of the two masses or of m_1 with the bottom wall or the semi-permeable wall at l) is given by the functions of t:

$$x(t) = x_0 \cos\left(\sqrt{\frac{k}{m_1}}\, t\right) + \dot{x}_0 \sqrt{\frac{m_1}{k}} \sin\left(\sqrt{\frac{k}{m_1}}\, t\right), \quad y(t) = \dot{y}_0 t + y_0. \tag{4.2}$$

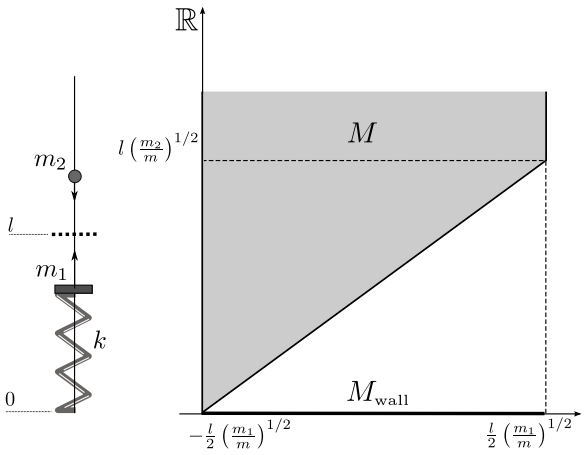

Figure 15: Collision of a point mass with a spring-mass system.

The state variable of the Markov chain in this case is taken to be the speed $v = |\dot{y}| \in (0, \infty)$ of m_2. It is assumed that the statistical state of m_1 is a Gibbs distribution with parameter β. For concreteness, we describe chain transitions $v_{\text{old}} \mapsto v_{\text{new}}$ in algorithmic fashion:

1. Choose independent, uniform random numbers U_1, U_2 in $[0,1]$, and a sign $s \in \{-,+\}$ with equal probabilities;
2. Let $\mathcal{E} = -\frac{1}{\beta} \ln U_1$; thus $\mathcal{E} \in (0,\infty)$ has probability density $\beta \exp(-\beta \mathcal{E})$;
3. Let $L(\mathcal{E}) := \min\left\{1, \frac{l}{2}\left(\frac{k}{2\mathcal{E}}\right)^{1/2}\right\}$ and $x = \left(\frac{2\mathcal{E}m_1}{mk}\right)^{1/2} \sin\left((2U_2 - 1)\arcsin(L(\mathcal{E}))\right)$; thus x has probability density proportional to $h_{\mathcal{E}}^{-1}$ over the interval $-L(\mathcal{E})\sqrt{2\mathcal{E}m_1/mk} \le x \le L(\mathcal{E})\sqrt{2\mathcal{E}m_1/mk}$, where $h_{\mathcal{E}}(x) := \sqrt{2(\mathcal{E} - U(x))}$ and $U(x) = kmx^2/m_1$ is the spring potential in the scaled coordinate;
4. Set $(x, sh_{\mathcal{E}}(x))$ to be the state of the mass m_1 when m_2 enters the region of interaction, and $(l\sqrt{m_2/m}, v_{\text{old}})$ the state of m_2. Let the system evolve, deterministically with this initial condition until m_2 is back at position $l\sqrt{m_2/m}$. Along the way, assume that collisions with the boundary of the two dimensional region on the right side of Figure 15 are specular and in between collisions the trajectory satisfies equations 4.2. When m_2 reemerges at $l\sqrt{m_2/m}$ set v_{new} equal to its new speed.

By Theorems 1 and 4, this Markov process has stationary probability given by the Maxwell-Boltzmann distribution (after reverting to the variables prior to scaling, with speed $u = \sqrt{m/m_2}v$)

$$d\mu(u) = \beta m_2 u \exp\left(-\beta \frac{m_2 u^2}{2}\right) du. \tag{4.3}$$

See Figure 16 for a numerical verification of the stationary distribution.

In comparing theses distributions with the corresponding textbook expressions, the reader should keep in mind the distinction between the Maxwell-Boltzmann distribution in the interior of gas container (with the velocity sampled at random times) and the similar distribution on the wall of the container. The latter has density proportional to

$$\beta m\, v \cdot n \|v\|^{d-1} \exp\left(-\beta \frac{m\|v\|^2}{2}\right)$$

in dimension d, where n is the unit normal to the wall surface.

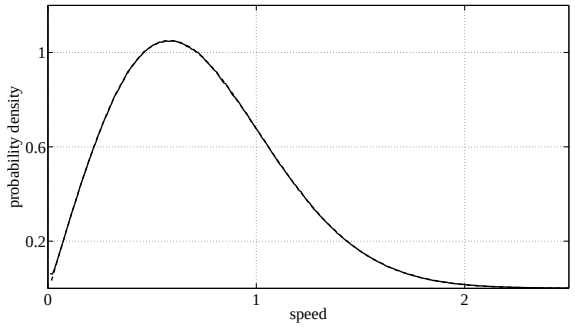

Figure 16: The figure superposes the graph of the stationary distribution 4.3 and the same distribution obtained by numerically simulating the Markov chain according to the algorithm described above.

5 Invariant volume forms

The main purpose of this section is to prove Theorems 1 and 4.

5.1 Definitions

Recall the function $d : M \to \mathbb{R}$ introduced in Subsection 1.2. The set $S \coloneqq \overline{M}_{\text{mol}} \times \{0\} \times \mathbb{T}^k \times M_{\text{wall}}$ is the level set $d = 0$. It will be convenient in this section to disregard the part of M given by $d > 0$ and consider S as a submanifold of the boundary of M. Observe that S lies in the interior of the product region, where the molecule and wall subsystems are non-interacting. Thus it makes sense to define over a neighborhood of S in M the unit vector field ν along the $\mathbb{R}$-factor of M_{mol}. We choose the direction of ν so that it points towards the region of interaction. The restriction of ν to S is then a unit vector field perpendicular to TS, pointing into M. Let $N \coloneqq TM$ and $N_S \coloneqq \iota^* TM$, the pull-back of TM to S under the inclusion map $\iota : S \to M$. Also define the subset N_S^+ of N_S consisting of v such that $\langle v, \nu \rangle > 0$, $N_S^- \coloneqq -N_S^+$, and $N_S^0 \coloneqq TS$. These are all bundles over S. We often denote fibers of a bundle using subscripts, as in $N_q = T_q M$. When this is inconvenient, we use function form, so that $N_S(q)$, for example, is the fiber of N_S above $q \in S$. Projection maps for these bundles will be denoted by the same symbol τ. Projection maps for other fibrations will typically be denoted by π.

Clearly, the reflection map R maps $N_S^\pm$ to $N_S^\mp$ and N_S^0 to itself. More generally, we can define N_∂ as the restriction (pull-back) of N to ∂M, and $N_\partial^\pm$ as we did in the case of N_S. The notation $N^{\partial\pm}$ may also be used when convenient. On regular points of the boundary, the reflection map is defined

on N_∂. If we wish to emphasize that something is taking place over regular points of the boundary (or regular points of the function E), we may indicate this by adding a subscript such as in $N_{\mathrm{reg}}^{\partial+}$.

Let $\langle\cdot,\cdot\rangle$ be a Riemannian metric on M and $U : M \to \mathbb{R}$ the potential function. Unless explicitly stated otherwise, functions and tensor fields are assumed to be smooth on interior and regular boundary points. The Riemannian metric defines the *kinetic energy* function $\kappa : TM \to \mathbb{R}$ given by

$$\kappa(q,v) := \frac{1}{2}\|v\|_q^2 := \frac{1}{2}\langle v, v\rangle_q.$$

The (total) *energy* function of the Newtonian system on M with potential U is $E : TM \to \mathbb{R}$ such that

$$E(q,v) := \kappa(q,v) + U(q).$$

We write $N(\mathcal{E}) := \{(q,v) \in N : E(q,v) = \mathcal{E}\}$. Clearly, the base point projection $\tau : N \to M$ maps $N(\mathcal{E}) \smallsetminus$ zero section into $M^{\mathcal{E}} := \{q \in M : U(q) < \mathcal{E}\}$. The intersection of $N(\mathcal{E})$ with N_S is denoted $N_S(\mathcal{E})$. Similar notations are used for the various related sets defined earlier. Whenever convenient, we specify points in N simply by v instead of (q,v). For example, we typically write $q = \tau(v)$, T_vN, $d\tau_v$, etc., for $v \in N$.

Let ∇ be the Levi-Civita covariant derivative operator. If $X(s)$ is a vector field along a differentiable curve $s \mapsto c(s)$ such that $v = c'(0)$, the covariant derivative of X along c at $s = 0$ will be written $\frac{\nabla X}{ds}\big|_{s=0}$ or, when appropriate, $\nabla_v X$. The *horizontal bundle* H over N is the subbundle of TN defined as the kernel of the *connection map* $K_v : T_vN \to T_{\tau(v)}M$, which is derived from ∇ as follows. Let $v'(0) \in T_vN$, where $s \mapsto v(s)$ is a differentiable curve in N such that $v(0) = v$; then

$$K_v v'(0) = \frac{\nabla}{dt}\Big|_{t=0} v(t).$$

Write $\xi := v'(0)$ and $w := d\pi_v \xi$. Let Y be a smooth section of π over a neighborhood of $q = \pi(v)$ such that $Y(q) = v$ and $dY_q w = \xi$. Then $K_v\xi = \nabla_w Y$.

Let V denote the *vertical bundle*, which is the vector bundle over N whose fiber above a $v \in N$ is the tangent space to $N_{\pi(v)}$ at v. Thus V_v is the kernel of $d\pi_v$, the projection $d\pi_v : H_v \to T_qM$ is a linear isomorphism, and the direct sum decomposition $TN = H \oplus V$ holds. If X is a smooth vector field on M, then the horizontal lift of X is the smooth section of H given by

$$v \mapsto X^H(v) := (d\tau_v|_{H_v})^{-1} X(\tau(v)).$$

For each $v \in N$ with $q = \tau(v)$, define the linear isomorphism $l_v : T_qM \to V_v$, called the *vertical lift* map, by

$$l_v(w) := \frac{d}{ds}\Big|_{s=0} (v + sw).$$

The alternative notation $w^V(v)$ or w_v^V will also be used later instead of $l_v(w)$. If X is a smooth vector field on M, then the vertical lift of X is the smooth section of V given by

$$v \mapsto X^V(v) := (X(\tau(v)))_v^V.$$

5.2 Contact, symplectic, and volume forms

The manifold N is equipped with the canonical contact form θ defined by $\theta_v(\xi) := \langle v, d\tau_v\xi\rangle_q$, for $v \in N(q)$. It is well-known that $d\theta$ is non-degenerate, hence a symplectic form on N. In terms of the Riemannian metric,

$$d\theta_v(\xi_1,\xi_2) = \langle K_v\xi_1, d\tau_v\xi_2\rangle - \langle K_v\xi_2, d\tau_v\xi_1\rangle \tag{5.1}$$

from which it easily follows that $d\theta$ is indeed non-degenerate and that V and H are Lagrangian subbundles.

The *Hamiltonian vector field* (associated to the energy function E) is the vector field X^E on N such that

$$X^E \lrcorner d\theta = -dE. \tag{5.2}$$

One easily shows that E and $d\theta$ are invariant under X^E. Thus $X^E E = 0$ and $\mathcal{L}_{X^E} d\theta = 0$, where $\mathcal{L}_X$ indicates the Lie derivative along X. The contact form θ, however, is not in general invariant but satisfies $\mathcal{L}_X \theta = dL$, where L is the Lagrangian function $L(q,v) := \kappa(q,v) - U(q)$. The Hamiltonian vector field can be written as

$$X^E = Z - (\operatorname{grad} U)^V \tag{5.3}$$

where the *geodesic spray* Z is the vector field on N defined, at each v, as the horizontal lift of v to H_v. In particular, $d\pi_v Z(v) = v$ and $d\pi_v X^E = v$. Observe that (q,v) is a critical point of E exactly when $X^E(v) = 0$, which can only happen when $v = 0$ and q is critical for U.

The *Hamiltonian flow* is the (local) flow of X^E, which we denote by $t \mapsto \Phi_t := \Phi_t^{X^E}$. The flow lines project under π to curves $c(t)$ on M that satisfy Newton's equation, and any solution of Newton's equation lifts to a flow line in N. It will be convenient to let $t \mapsto \Phi_t(v)$ represent a trajectory of the system through its entire history, which may include collisions and reflections with the boundary of M. The Hamiltonian vector field is essentially complete, in the sense defined in Section 1.2 (part (iv) of list of assumptions).

Proposition 9. *Let $v \in N(\mathcal{E})$ be a regular point for E and let $q = \tau(v)$ be either an interior point of M or in the regular boundary $\partial_r M$. Then $T_v N(\mathcal{E})$ consists of $\xi \in T_v N$ such that*

$$d(U \circ \tau)_v \xi + \langle v, K_v \xi \rangle_q = 0. \tag{5.4}$$

The projection $d\tau_v : T_v N(\mathcal{E}) \to T_q M$ is surjective. In fact, for each $w \in T_q M$,

$$w^\wedge(v) := w^H(v) - \|v\|^{-2} dU_q(w) W(v) \in T_v N(\mathcal{E})$$

satisfies $d\tau_v w^\wedge(v) = w$. The space $T_v N^{\partial+}(\mathcal{E})$ consists of all $\xi \in T_v N$ such that 5.4 holds and $d\tau_v \xi$ is tangent to ∂M.

Proof. These claims are easily derived by observing that Equation 5.1, the definition of X^E in 5.2, and Equation 5.3, imply

$$dE_v(\xi) = d\theta_v(\xi, X^E) = \left\langle K_v \xi, d\tau_v X^E \right\rangle - \left\langle K_v X^E, d\tau_v \xi \right\rangle = \langle v, K_v \xi \rangle + \langle \operatorname{grad} U, d\tau_v \xi \rangle.$$

Of course, ξ lies in $T_v N(\mathcal{E})$ iff $dE_v(\xi) = 0$ on regular points of E. □

Proposition 10. *Let $N^\partial_{reg}(\mathcal{E})$ be the subset of $N^\partial(\mathcal{E})$ consisting of those v for which $\tau(v)$ is a point in the regular boundary of M and let $\iota : N^\partial_{reg}(\mathcal{E}) \to N$ be the inclusion map. Then $\iota^* d\theta$ is a symplectic form on $N^\partial_{reg}(\mathcal{E}) \setminus T(\partial_{reg} M)$. Furthermore, the reflection map $R : N^\partial_{reg}(\mathcal{E}) \to N^\partial_{reg}(\mathcal{E})$ leaves $\iota^*\theta$ and $\iota^* d\theta$ invariant.*

Proof. Here and in what follows, we assume that all points under consideration are regular for E and, if on the boundary, that they are regular boundary points. If $v \neq 0$, then v is necessarily regular for E. With this in mind, we omit references to 'regular' in the notation from now on.

The main issue is to check that $\omega := \iota^* d\theta$ is non-degenerate. Let $\xi \in T_v N^\partial(\mathcal{E})$ and assume that $\omega_v(\xi, \eta) = 0$ for all $\eta \in T_v N^\partial(\mathcal{E})$, where v is not tangent to the boundary of M. First choose $\eta \in V_v$

such that $K_v\eta$ is orthogonal to v. Then $0 = \omega_v(\xi,\eta) = -\langle K_v\eta, d\tau_v\xi\rangle$, so $d\tau_v\xi$ is orthogonal to all w such that $w \perp v$. That is, $d\tau_v\xi$ is a scalar multiple of v. By Proposition 9 this vector is tangent to the boundary, thus zero by assumption, and ξ must be a vertical vector. Let now η be an arbitrary tangent vector to $N^\partial(\mathcal{E})$ at v. Then as $0 = \omega_v(\xi,\eta) = \langle K_v\xi, d\tau_v\eta\rangle$ and $d\tau_v\eta$ is tangent to ∂M we conclude that $K_v\xi$ is a scalar multiple of the normal vector n at $\tau(v)$, that is, $\xi = \lambda n^V(v)$ for some $\lambda \in \mathbb{R}$. From Proposition 9 it follows that $0 = d(U\circ\tau)_v\xi + \langle v, K_v\xi\rangle_{\pi(v)} = \lambda\langle v, n\rangle_{\tau(v)}$, which implies that $\lambda = 0$. Therefore, $\xi = 0$. □

It is useful to introduce the *Sasaki metric* on N, which is the Riemannian metric defined by

$$\langle \xi,\eta\rangle_v := \langle d\tau_v\xi, d\tau_v\eta\rangle_q + \langle K_v\xi, K_v\eta\rangle_q$$

for all $\xi,\eta \in T_vN$ and $q = \tau(v)$. In terms of this metric the vertical and horizontal subbundles are mutually orthogonal and H_v, V_v are isometric to T_qM under $d\tau_v$ and K_v, respectively.

Define the vector field

$$\eta := (\text{grad } E)/\|\text{grad } E\|^2,$$

the gradient and norm being associated to the Sasaki metric. Observe that $dE(\eta) = 1$, so that $E\circ\Phi_s^\eta = E + s$, where Φ_s^η denotes the local flow of η. It is not difficulty to obtain the expressions

$$\text{grad } E = W + (\text{grad U})^H, \quad \|\text{grad } E\|_v^2 = \|v\|_q^2 + \|\text{grad } U\|_q^2$$

where W is the *canonical vertical vector field*, defined by $W_v := v_v^V$ for each $v \in N$.

Let $\Omega := (d\theta)^m$, where $m = \dim M$. Then Ω is a volume form (i.e., a non-vanishing form of top degree) on N. It is also invariant under the Hamiltonian flow since $\mathcal{L}_X d\theta = 0$.

Proposition 11. *Let X^E be the Hamiltonian vector field for the energy function E, and η the vector field introduced in the previous paragraph. Define $\Omega^E := \eta \lrcorner \Omega$. Then*

1. $\Omega = dE \wedge \Omega^E$;
2. $X^E \lrcorner \Omega^E = m(d\theta)^{m-1} + m(m-1)(\eta\wedge d\theta)\wedge dE\wedge(d\theta)^{m-1}$;
3. $\mathcal{L}_{X^E}\Omega^E = dE \wedge (\eta \lrcorner \mathcal{L}_{X^E}\Omega^E)$.

It follows that the restriction of Ω^E to each level set $N(\mathcal{E})$ is non-vanishing (a volume form) and invariant under the Hamiltonian flow, and that the restriction of $X^E \lrcorner \Omega^E$ to the same level sets equals $m(d\theta)^{m-1}$.

Proof. For part 1, write $dE\wedge\Omega^E = f\Omega$ and take the interior multiplication on both side with η to conclude that $f\Omega^E = \Omega^E$. As Ω^E does not vanish, we have $f = 1$. For part 2, observe that

$$X^E \lrcorner (\eta\lrcorner\Omega) = X^E \lrcorner \left(m\,(\eta\lrcorner d\theta)\wedge(d\theta)^{m-1}\right) = m\,d\theta\left(\eta, X^E\right)(d\theta)^{m-1} - m(\eta\lrcorner d\theta)\wedge\left(X^E\lrcorner(d\theta)^{m-1}\right).$$

But $d\theta(\eta, X^E) = dE(\eta) = 1$ by the definition of X^E and η. Also $X^E \lrcorner (d\theta)^{m-1} = -(m-1)dE\wedge(d\theta)^{m-2}$. For part 3, obtain from $\mathcal{L}_{X^E}(dE\wedge\Omega) = 0$ that $dE\wedge\mathcal{L}_{X^E}\Omega^E = 0$ and take the interior multiplication on both sides of this equation with η. □

5.3 Billiard maps

We fix an energy value $\mathcal{E}$ and assume that $N(\mathcal{E})$ has finite volume relative to Ω^E. Here we will let S denote more generally than before (the regular part of) a submanifold of the boundary of M. For any given $v \in N_S^+(\mathcal{E})$, define

$$\mathcal{T}(v) := \inf\{t > 0 : \Phi_t(v) \in N_S^+(\mathcal{E})\},$$

which is ∞ if the flow line never returns to $N_S^+(\mathcal{E})$. By Poincaré's recurrence applied to the Hamiltonian flow, $\mathcal{T}$ is finite with probability 1 with respect to the flow-invariant probability measure derived from Ω^E. Now define the return map $N_S^+(\mathcal{E})$ by $T := R \circ \Phi$, where $\Phi(v) := \Phi_{\mathcal{T}(v)}(v)$, R being the reflection map. Then T is almost everywhere defined, and by one of our standing assumptions it is almost surely smooth. (Section 1.2, assumption (v); see [3] for how this point concerning smoothness is argued in the simpler case of plane billiards.) We denote by $\Omega^{E,S}$ the pull-back of $X^E \lrcorner \Omega^E$ to $N_S^+(\mathcal{E})$ under the inclusion map. By Proposition 11 this form agrees with the pull-back of $m(d\theta)^{m-1}$.

Proposition 12. *The return map $T : N_S^+(\mathcal{E}) \to N_S^+(\mathcal{E})$ preserves $\Omega^{E,S}$ almost everywhere.*

Proof. This involves a standard argument, which we briefly recall. Let $v \in N_S^+(\mathcal{E})$ admit a neighborhood $\mathcal{U}$ where T is smooth. Let $c : [0, \mathcal{T}(v)] \to N(\mathcal{E})$ be the orbit segment connecting v to $\Phi_{\mathcal{T}(v)}(v)$, and γ_1 a closed curve contained in $\mathcal{U}$. Let D be a smooth embedded disc contained in $\mathcal{U}$ that is bounded by γ_1, and denote by γ_2 the image of γ_1 under Φ. Then γ_1 sweeps out a surface Σ under the Hamiltonian flow such that the boundary of Σ is the union of γ_1 and $-\gamma_2$, where the negative sign indicates orientation. Notice that the restriction of $d\theta$ to Σ is 0 as E is constant on this surface and the interior multiplication of $d\theta$ by the Hamiltonian vector field is $-dE$. So

$$0 = \int_\Sigma d\theta = \int_{\gamma_1} \theta - \int_{\gamma_2} \theta = \int_{\gamma_1} [\theta - \Phi^*\theta] = \int_D d[\theta - \Phi^*\theta].$$

As γ_1 and D can be made arbitrarily small, we conclude that $\Phi^* d\theta = d\theta$. Since R also preserves $d\theta$ according to Proposition 10, the same holds for T. Therefore, T leaves $\Omega^{E,S}$ invariant as claimed. □

5.4 Product systems

We next specialize some of the above facts to product systems. The notation here is independent of that of the rest of the paper. Let $M = M_1 \times M_2$. Let $\tau_i : N_i := TM_i \to M_i$ and $\tau : N := TM \to M$ be the tangent bundle maps and let π_i be the projection $M \to M_i$. The induced projection $N \to N_i$ will also be written π_i, so it makes sense to write $\pi_i \circ \tau = \tau_i \circ \pi_i$. If there is some possibility of confusion we may write, for example, $(q_i, v_i) = (q_i, (d\pi_i)_q v)$ instead of $v_i = \pi_i(v)$ for a given v in N. Either way, the product Riemannian metric reads

$$\langle v, w \rangle_q = \langle v_1, w_1 \rangle_{q_1} + \langle v_2, w_2 \rangle_{q_2}.$$

Vertical and horizontal lifts, and the corresponding subbundles of TN decompose as expected in terms of the respective notions on N_i. In particular, the Sasaki metric is similarly decomposed as $\langle \cdot, \cdot \rangle = \pi_1^* \langle \cdot, \cdot \rangle_1 + \pi_2^* \langle \cdot, \cdot \rangle_2$. The canonical contact form θ on $N = N_1 \times N_2$ becomes $\theta = \pi_1^* \theta_1 + \pi_2^* \theta_2$, where θ_i is the contact form on N_i, and the invariant volume form $\Omega = \pi_1^* \Omega_1 \wedge \pi_2^* \Omega_2$. Whenever convenient, we omit explicit reference to the projection maps and write, for example, $\Omega = \Omega_1 \wedge \Omega_2$ or $\theta = \theta_1 + \theta_2$.

Assuming that the potential function U on M has the form $U = U_1 \circ \pi_1 + U_2 \circ \pi_2$, where U_i is a smooth function on M_i, the energy function becomes $E = E_1 \circ \pi_1 + E_2 \circ \pi_2$ and the Hamiltonian vector field on N is written as $X^E = X_1 + X_2$, where X_i is characterized by being π_i-related to the Hamiltonian vector field on N_i associated to E_i and π_j-related to 0 for $j \neq i$. The (Sasaki) gradient of E will be written, with slight abuse of notation, as grad E = grad E_1 + grad E_1 and the vector field $\eta := (\text{grad } E)/\|\text{grad } E\|^2$ becomes

$$\eta = \frac{\|\text{grad } E_1\|^2}{\|\text{grad } E_1\|^2 + \|\text{grad } E_2\|^2} \eta_1 + \frac{\|\text{grad } E_2\|^2}{\|\text{grad } E_1\|^2 + \|\text{grad } E_2\|^2} \eta_2.$$

Proposition 13. *Let $\Omega^E := \eta \lrcorner \Omega$ be the invariant volume form on the energy level $N(\mathcal{E})$ and similarly define $\Omega_i^{E_i} := \eta_i \lrcorner \Omega_i$ on level sets $N_i(\mathcal{E}_i)$. Then the level sets $N(\mathcal{E})$ can be measurably partitioned as a disjoint union of product manifolds*

$$N(\mathcal{E}) = \bigsqcup N_1(\mathcal{E}_1) \times N_2(\mathcal{E} - \mathcal{E}_1)$$

where the elements of the partition are the level sets of $E_1 : N(\mathcal{E}) \to \mathbb{R}$, and the invariant volume Ω^E has the decomposition

$$\Omega^E = dE_1 \wedge \Omega_1^{E_1} \wedge \Omega_2^{E_2}$$

adapted to this partition.

Proof. The main point is to verify the stated form of Ω^E. Define α_i by $\eta = \alpha_1\eta_1 + \alpha_2\eta_2$. Now, Ω^E can be written as

$$(\alpha_1\eta_1 + \alpha_2\eta_2) \lrcorner (\Omega_1 \wedge \Omega_2) = \alpha_1\Omega_1^{E_1} \wedge \Omega_2 + \alpha_2\Omega_1 \wedge \Omega_2^{E_2} = \alpha_1\Omega_1^{E_1} \wedge dE_2 \wedge \Omega_2^{E_2} + \alpha_2 dE_1 \wedge \Omega_1^{E_1} \wedge \Omega_2^{E_2}.$$

Since $dE_2 = -dE_1$ on $N(\mathcal{E})$, $\Omega_1^{E_1}$ is an odd-degree form, and $\alpha_1 + \alpha_2 = 1$,

$$\Omega^E = (-\alpha_1 dE_2 + \alpha_2 dE_1) \wedge \Omega_1^{E_1} \wedge \Omega_2^{E_2} = dE_1 \wedge \Omega_1^{E_1} \wedge \Omega_2^{E_2}$$

as claimed. □

The Gibbs canonical distribution on N_i with temperature parameter β_i is the probability measure on N_i defined by the form

$$\zeta_i := \frac{e^{-\beta_i E_i}}{Z_i(\beta_i)} \Omega_i^{E_i} \wedge dE_i,$$

where $Z_i(\beta_i)$ is a normalization constant. The following trivial but key observation must be noted.

Corollary 2. *If the states of the two subsystems are distributed according to the Gibbs canonical distribution with same parameter β, then the state of the product system is also distributed according to the Gibbs canonical distribution with parameter β.*

Proof. Let $E = E_1 + E_2$ and define $Z(\beta) = Z_1(\beta)Z_2(\beta)$. Note that $dE_1 \wedge dE_2 = dE_1 \wedge dE$. Due to Proposition 13,

$$\zeta_1 \wedge \zeta_2 = \pm \frac{e^{-(E_1+E_2)}}{Z_1(\beta)Z_2(\beta)} \Omega_1^{E_1} \wedge \Omega_2^{E_2} \wedge dE_1 \wedge dE_2 = \pm \frac{e^{-\beta E}}{Z(\beta)} \Omega^E \wedge dE.$$

The measure obtained from $\zeta_1 \wedge \zeta_2$ is already normalized, so $Z(\beta)$ is the correct denominator. □

Theorem 1 can now be seen to follow from Corollary 2 and Proposition 1. If the state of the wall system has the Gibbs distribution with parameter β and the state of the molecule system is given, prior to entering the interaction zone, the Gibbs distribution with the same parameter, then the state of the joint (product) system has a probability distribution which is invariant under the deterministic return map to the non-interaction zone. Thus the molecule factor of the state distribution of the total system upon return to the non-interaction zone remains the same.

5.5 Frame description of the volume forms

Let m be the dimension of M and $U \subset M$ an open subset on which is defined a smooth orthonormal frame of vector fields $\{e_1, \ldots, e_m\}$. Let N_U be the subset of elements in N with base point in U. Define

$$\mathcal{N}_U := \{(q, u, \mathcal{E}) \in U \times \mathbb{R}^m \times \mathbb{R} : \|u\| = 1 \text{ and } U(q) < \mathcal{E}\}.$$

Thus $\mathcal{N}_U$ is an open submanifold of $U \times S^{m-1} \times \mathbb{R}$. Let $\mathcal{N}_U(\mathcal{E})$ denote the submanifold mapping to $\mathcal{E}$ under $\pi_3 : \mathcal{N}_U \to \mathbb{R}$. Let $\{c_1, \ldots, c_m\}$ represent the standard basis of $\mathbb{R}^m$ and $u \cdot v$ the ordinary inner product. Observe that

$$c_i^\curlyvee(u) := \left.\frac{d}{ds}\right|_{s=0} \frac{u + sc_i}{\|u + sc_i\|} = c_i - u \cdot c_i \, u$$

is tangent to S^{m-1} at a unit vector u, and $\{c_1^\curlyvee, \ldots, c_{m-1}^\curlyvee\}$ is a basis of $T_u S^{m-1}$ for all u not perpendicular to c_m. For these u, let $\{\varphi_1, \ldots, \varphi_{m-1}\}$ be the dual basis associated to $\{c_1^\curlyvee, \ldots, c_{m-1}^\curlyvee\}$. In terms of this dual basis, the (standard) Riemannian volume form on S^{m-1} is

$$\omega_u^{\text{sphere}} = (-1)^{m-1} u \cdot c_m \, \varphi_1^\curlyvee \wedge \ldots \varphi_{m-1}^\curlyvee. \tag{5.5}$$

This is obtained from $\omega_u^{\text{sphere}} = u \lrcorner (c_1^* \wedge \cdots \wedge c_m^*)$, where the c_i^* constitute the dual standard basis, by evaluating this form on the vectors $c_i^\curlyvee(u)$. The Riemannian volume form on M (up to sign) is

$$\omega^M := e_1^* \wedge \cdots \wedge e_m^*,$$

where the e_i^* form the dual frame on T^*M. By identifying e_i with $(e_i, 0, 0)$ and $c_i^\curlyvee$ with $(0, c_i^\curlyvee, 0)$, we may think of e_i and $c_i^\curlyvee$ as tangent to $\mathcal{N}_U(\mathcal{E})$, and $\{e_1^*, \ldots, e_m^*, \varphi_1^\curlyvee, \ldots, \varphi_{m-1}^\curlyvee\}$ as a frame of 1-forms on $\mathcal{N}_U(\mathcal{E})$.

We now introduce a diffeomorphism $F : \mathcal{N}_U \to N_U$ by

$$F(q, u, \mathcal{E}) = \left(q, h_{\mathcal{E}}(q) \sum_i u_i e_i(q)\right), \tag{5.6}$$

where $h_{\mathcal{E}}(q) := \sqrt{2(\mathcal{E} - U(q))}$. The inverse map is $F^{-1}(q, v) = (q, u, \mathcal{E})$, where $u_i = \|v\|_q^{-1} \langle v, e_i(q)\rangle_q$ and $\mathcal{E} = \frac{1}{2}\|v\|_q^2 + U(q)$.

Proposition 14. *For any given $v, w \in N_q$, define vectors $w_v^\curlyvee$ and $w_v^\wedge$ in $T_v N$ by*

$$w_v^\curlyvee := w_v^V - \|v\|^{-2} \langle v, w\rangle_q W_v \text{ and } w_v^\wedge := w_v^H - \|v\|^{-2} dU(w) W_v.$$

If $\{w_1, \ldots, w_m\}$ is a basis of $T_q M$ and $v \in N(\mathcal{E})$ for some $\mathcal{E} \in \mathbb{R}$, then $\{w_1^\wedge, \ldots, w_m^\wedge, w_1^\curlyvee, \ldots, w_{m-1}^\curlyvee\}$ is a basis for $T_v N(\mathcal{E})$, providing decompositions

$$TN(\mathcal{E}) = T^\curlyvee N \oplus T^\wedge N \text{ and } TN = T^\curlyvee N \oplus T^\wedge N \oplus \mathbb{R}\eta,$$

where $T^\curlyvee N$ and $T^\wedge N$ are spanned by vectors of the form $w^\curlyvee$ and $w^\wedge$, respectively. Define the forms $\omega_{ij}(w) := \langle \nabla_w e_j, e_i\rangle$. Letting $(q, v) = F(q, u, \mathcal{E})$, then

$$dF_{(q,u,\mathcal{E})} c_i^\curlyvee = h_{\mathcal{E}}(q) e_i^\curlyvee(v) \text{ and } dF_{(q,u,\mathcal{E})} e_i = e_i^\wedge(v) + \sum_{r,s=1}^m \omega_{sr}(e_i) u_r e_s^\curlyvee(v).$$

The vector field η transforms under F according to

$$dF_v^{-1} \eta = \left(\frac{grad_q U}{\|v\|^2 + \|dU\|_q^2}, \left(\frac{\|v\|_q^{-1} \sum_j \langle v, e_j\rangle_q \omega_{ji}(grad_q U)}{\|v\|^2 + \|dU\|_q^2}\right)_i, 1\right).$$

Proof. We only obtain $dF_v^{-1}w^V$ and $dF_v^{-1}w^H$ to illustrate the method of calculation. First, $dF_v^{-1}w^V$ equals

$$\frac{d}{ds}\Big|_{s=0} F^{-1}(v+sw) = \frac{d}{ds}\Big|_{s=0}\left(q, \left(\frac{\langle v+sw, e_i\rangle_q}{\|v+sw\|_q}\right), \frac{1}{2}\|v+sw\|_q^2 + U(q)\right) = (0, (\xi_i), \langle v, w\rangle_q),$$

where $\xi_i = \|v\|^{-1}\langle w - \langle v, w\rangle v/\|v\|^2, e_i\rangle = \|v\|^{-1}\langle K_v w^\curlyvee, e_i\rangle$. Before calculating $dF_v^{-1}w^H$, first note that

$$w_v^H = \frac{d}{ds}\Big|_{s=0} \mathcal{P}_{\gamma(s)}v,$$

where $\gamma(s)$ is a differentiable curve such that $\gamma(0) = q$ and $\gamma'(0) = w$, and $\mathcal{P}_{\gamma(s)}v$ indicates the parallel translation of v along γ. Keeping in mind that $\|\mathcal{P}_{\gamma(s)}v\| = \|v\|$ and that $\frac{d}{ds}\big|_{s=0}\langle \mathcal{P}_{\gamma(s)}v, e_i\rangle = \langle v, \nabla_w e_i\rangle$, we obtain

$$\begin{aligned}\frac{d}{ds}\Big|_{s=0} F^{-1}(\mathcal{P}_{\gamma(s)}v) &= \frac{d}{ds}\Big|_{s=0}\left(\gamma(s), \left(\frac{\langle \mathcal{P}_{\gamma(s)}v, e_i\rangle}{\|\mathcal{P}_{\gamma s}v\|}\right), \frac{1}{2}\|\mathcal{P}_{\gamma(s)}v\|^2 + U(\gamma(s))\right)\\ &= \left(w, \left(\|v\|^{-1}\sum_j \langle v, e_j\rangle \omega_{ji}(w)\right), dU(w)\right).\end{aligned}$$

The claimed identities are easily obtained from these. □

We have so far made no special assumptions about the local orthonormal frame $\{e_1, \dots, e_m\}$. Since we may want to consider the invariant volume form Ω^E near boundary points of M, it makes sense to introduce the following concept: The orthonormal frame is said to be *adapted* to a codimension-1 foliation $\mathcal{S}$ of $U \subset M$ if $\{e_1, \dots, e_{m-1}\}$ spans the tangent space to each leaf S of $\mathcal{S}$ at any given point $q \in U$. Recall that the set of elements in N (respectively, in $N(\mathcal{E})$) with base point in S is denoted by N_S (respectively, $N_S(\mathcal{E})$). The set $\{e_1^\wedge, \dots, e_{m-1}^\wedge, e_1^\curlyvee, \dots, e_{m-1}^\curlyvee\}$ is easily seen to be a frame on $N_S(\mathcal{E})$. It was noted before that $\{e_1^\wedge, \dots, e_m^\wedge, e_1^\curlyvee, \dots, e_{m-1}^\curlyvee\}$ is a local, not necessarily orthonormal, frame on $N(\mathcal{E})$, and it can be shown exactly as in Proposition 9 that for a tangent vector to $N(\mathcal{E})$ to actually be tangent to $N_S(\mathcal{E})$ it is necessary and sufficient that its projection be tangent to S. In particular, if $\{e_1, \dots, e_m\}$ is an adapted frame, the distribution in $TN(\mathcal{E})$ spanned by $\{e_1^\wedge, \dots, e_{m-1}^\wedge, e_1^\curlyvee, \dots, e_{m-1}^\curlyvee\}$ is involutive.

Proposition 15. *Define on $N_U \smallsetminus \{$zero section$\}$ the functions*

$$\psi_i(v) := \langle v, e_i\rangle_q \text{ and } \psi_0(v) := \left(\|v\|^2 + \|\text{grad } U\|^2\right)^{-1} dU_q(v),$$

where $\{e_1, \dots, e_m\}$ is an orthonormal frame on U. The Hamiltonian vector field X^E has the form

$$X^E = \sum_{i=1}^m \psi_i e_i^\wedge - \sum_{i=1}^m dU(e_i)e_i^\curlyvee = \sum_{i=1}^m \psi_i e_i^\wedge - \sum_{i=1}^{m-1}\left(dU(e_i) - \frac{dU(e_m)}{\psi_m}\psi_i\right)e_i^\curlyvee. \tag{5.7}$$

The contact form θ restricted to N_U can be written as

$$\theta_v = \psi_0(v)\eta^* + \sum_{i=1}^m \psi_i(v)\epsilon_i^\wedge, \tag{5.8}$$

where $\{\eta^*, \epsilon_1^\wedge, \dots, \epsilon_m^\wedge, \epsilon_1^\curlyvee, \dots, \epsilon_{m-1}^\curlyvee\}$ is the dual basis of $\{\eta, e_1^\wedge, \dots, e_m^\wedge, e_1^\curlyvee, \dots, e_{m-1}^\curlyvee\}$. The volume form Ω^E on each $N(\mathcal{E})$ over the set $U \cap M^{\mathcal{E}}$ can be written as

$$\Omega^E = \psi_m^{-1}\epsilon_m^\wedge \wedge \left(X^E \lrcorner \Omega^E\right) = m\psi_m^{-1}\epsilon_m^\wedge \wedge (d\theta)^{m-1}. \tag{5.9}$$

Now suppose that $\{e_1, \dots, e_m\}$ is adapted to a local codimension-1 foliation $\mathcal{S}$ and let

$$\iota_{\mathcal{S}}^* \theta = \psi_1 \epsilon_1^\wedge + \cdots + \psi_{m-1} \epsilon_{m-1}^\wedge \tag{5.10}$$

be the restriction of θ to the leaves $N_S(\mathcal{E})$. Then $\iota_{\mathcal{S}}^* d\theta$ is a symplectic form on each $N_S(\mathcal{E})$, and it can be written as

$$\iota_{\mathcal{S}}^* d\theta = -\sum_{i,j=1}^{m-1} \left(\delta_{ij} - \frac{\psi_i \psi_j}{h_{\mathcal{E}}^2} \right) \epsilon_i^\wedge \wedge \epsilon_j^\curlyvee + \sum_{i,j=1}^{m-1} \frac{dU(e_j)\psi_i - dU(e_i)\psi_j}{h_{\mathcal{E}}^2} \epsilon_i^\wedge \wedge \epsilon_j^\wedge \tag{5.11}$$

It follows that

$$\iota_{\mathcal{S}}^* (d\theta)^{m-1} = \pm \frac{\psi_m^2}{h_{\mathcal{E}}^2} \epsilon_1^\wedge \wedge \cdots \wedge \epsilon_{m-1}^\wedge \wedge \epsilon_1^\curlyvee \wedge \cdots \wedge \epsilon_{m-1}^\curlyvee, \ \Omega^E = \pm m \frac{\psi_m}{h_{\mathcal{E}}^2} \epsilon_1^\wedge \wedge \cdots \wedge \epsilon_m^\wedge \wedge \epsilon_1^\curlyvee \wedge \cdots \wedge \epsilon_{m-1}^\curlyvee. \tag{5.12}$$

The volume form Ω^E transforms under the diffeomorphism $F : \mathcal{N}_U(\mathcal{E}) \to N_U(\mathcal{E})$ defined by 5.6 according to

$$F^* \Omega^E = \pm m h_{\mathcal{E}}^{m-2} \pi_1^* \omega^M \wedge \pi_2^* \omega^{sphere}$$

The symplectic form on a hypersurface S in U is expressed under F according to

$$F^* (d\theta)^{m-1} = \pm \left(\frac{\psi_m \circ F}{h_{\mathcal{E}}} \right) h_{\mathcal{E}}^{m-1} \pi_1^* \omega^S \wedge \pi_2^* \omega^{sphere}$$

Proof. All of this follows straightforwardly from the definitions and basic facts. We only make a few comments. Identity 5.9 results by noting that $\epsilon_m^\wedge \wedge \left(X^E \lrcorner \Omega^E \right)$ is a $(2m-1)$-form on $N(\mathcal{E})$, thus it can be written as $f\Omega^E$, where the function f is found by applying the interior multiplication with X^E and using that ψ_m is the coefficient of X^E for the basis element $e_m^\wedge$. Item 2 of Proposition 11 is also needed. Identity 5.11 can be derived with little effort by using the identity 5.1, which expresses the symplectic form $d\theta$ in terms of the Sasaki metric. Identity 5.12 is a consequence of 5.11 and the identity $\det(I + ab^t) = 1 + b^t a$, where I is the identity matrix, a, b are column vectors, and b^t is the row vector associated to b after transpose. It should be kept in mind that the $e_i^\curlyvee$ span an $(m-1)$-dimensional subspace at each point, so they are linearly dependent. In fact, they satisfy the equation $\sum_{i=1}^m \psi_i e_i^\curlyvee = 0$. □

Theorem 4 is a corollary of the proposition.

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