Abstract: This paper is concerned with stochastic processes that model multiple (or iterated) scattering in classical mechanical systems of billiard type, defined below. From a given (deterministic) system of billiard type, a random process with transition probabilities operator $P$ is introduced by assuming that some of the dynamical variables are random with prescribed probability distributions. Of particular interest are systems with weak scattering, which are associated to parametric families of operators $P_h$, depending on a geometric or mechanical parameter $h$, that approaches the identity as $h$ goes to 0. It is shown that $(P_h - I)/h$ converges for small $h$ to a second order elliptic differential operator $L$ on compactly supported functions and that the Markov chain process associated to $P_h$ converges to a diffusion with infinitesimal generator $L$. Both $P_h$ and $L$ are self-adjoint (densely) defined on the space $L^2(\mathbb{H}, \eta)$ of square-integrable functions over the (lower) half-space $\mathbb{H}$ in $\mathbb{R}^m$, where $\eta$ is a stationary measure. This measure’s density is either (post-collision) Maxwell-Boltzmann distribution or Knudsen cosine law, and the random processes with infinitesimal generator $L$ respectively correspond to what we call MB diffusion and (generalized) Legendre diffusion. Concrete examples of simple mechanical systems are given and illustrated by numerically simulating the random processes.

1. Introduction

The purpose of this section is to explain informally the nature of the results that will be stated in detail and greater generality in the course of the paper.

A type of idealized multi-scattering experiment is depicted in Fig. 1. The figure represents the flight of a molecule between two parallel solid plates. At each collision, the molecule impinges on the surface of a plate with a velocity $v$ and, after interacting with the surface in some way (which will be explicitly described by a mechanical model), it scatters away with a post-collision velocity $V$. The single scattering event $v \mapsto V$, for some specified molecule-surface interaction model, is given by a random map in the
following sense. Let $\mathbb{H}$ denote the half-space of vectors $v = (v_1, v_2, v_3)$ with negative third component. It is convenient to also regard the scattered velocity $V$ as a vector in $\mathbb{H}$ by identifying vectors that differ only by the sign of their third component. A scattering event is then represented by a map from $\mathbb{H}$ into the space of probability measures on $\mathbb{H}$, which we call for now the *scattering map*; the probability measure associated to $v$ is the law of the random variable $V$. Thus the scattering map encodes the “microscopic” mechanism of molecule-surface interaction in the form of a random map, whose iteration provides the information about velocities needed to determine the sample trajectories of the molecule.

The mechanical-geometric interaction models specifying the scattering map will be limited in this paper to what we call a mechanical system of *billiard type*. Essentially, it is a conservative classical mechanical system without “soft” potentials. Interactions between moving masses (comprising the “wall sub-system” and the “molecule sub-system,” using the language of [7]) are billiard-like elastic collisions.

An example of a very simple interaction mechanism (in dimension 2) is shown in Fig. 2. That figure can be thought to represent a choice of wall “microstructure.” In addition to a choice of mechanical system representing the wall microstructure, the specification of a scattering map requires fixing a statistical kinetic state of this microstructure prior to each collision. For the example of Fig. 2, one possible specification may be as follows: (1) the precise position on the horizontal axis (the dashed line of the figure) where the molecule enters the zone of interaction is random, uniformly distributed over the period of the periodic surface contour; (2) at the same time that the molecule crosses the dashed line (which arbitrarily sets the boundary of the interaction zone), the position and velocity of the up-and-down moving wall are chosen randomly from prescribed probability distributions. The most natural are the uniform distribution (over a small interval) for the position, and a one-dimensional normal distribution for the velocity, with mean zero and constant variance. (The variance specifies the wall temperature, as will be seen.) In fact, one general assumption of the main theorems essentially amounts to the constituent masses of the wall sub-system having velocities which are normally distributed and in a state of equilibrium (specifically, energy equipartition is assumed). In this respect, a random-mechanical model of “heat bath” is explicitly given. Once the random pre-collision conditions are set, the mechanical system describing the interaction evolves deterministically to produce $V$. Note that a single collision event may consist of several “billiard collisions” at the “microscopic level.”

Having specified a scattering map (by the choices of a mechanical system and the constant pre-collision statistical state of the wall), a random dynamical system on $\mathbb{H}$ is defined, which can then be studied from the perspective of the theory of Markov chains on general state spaces ([13]).