A two-stage approach to relaxation in billiard systems of locally confined hard spheres

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We consider the three-dimensional dynamics of systems of many interacting hard spheres, each individually confined to a dispersive environment, and show that the macroscopic limit of such systems is characterized by a coefficient of heat conduction whose value reduces to a dimensional formula in the limit of vanishingly small rate of interaction. It is argued that this limit arises from an effective loss of memory. Similarities with the diffusion of a tagged particle in binary mixtures are emphasized.

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The derivation of the macroscopic transport equations of hydrodynamics and the computation of the associated coefficients for systems described at the microscopic level by Hamilton’s equations of classical mechanics is a central problem of non-equilibrium statistical physics. The periodic Lorentz gas provides an example where this program can be achieved and Fick’s law of diffusion established.

Furthermore, by tweaking the system’s geometry so that tracer particles hop from cell to cell at nearly vanishing rates, memory effects disappear and the dynamics of tracers is well approximated by a continuous time random walk. In this regime, the diffusion coefficient takes on a simple limiting value, given by a dimensional formula, by which we mean that its expression reduces to the square of the length scale of the cell separation multiplied by the hopping rate. Similarly, it was found that heat transport in systems of confined hard disks with rare interactions reduces to a stochastic process of energy exchanges which obeys Fourier’s law of heat conduction and constitutes a stochastic system and computing its transport properties in the hydrodynamic scaling limit, can be successfully achieved in a class of chaotic billiard systems composed of many hard disks trapped in a semi-porous material which prevents mass transfer and yet allows energy transfer through elastic collisions among neighboring disks.

As emphasized in earlier papers, the following two-step program, which consists of (i) identifying an intermediate level of description—a mesoscopic scale—where the Newtonian dynamics can be consistently approximated by a set of stochastic equations, and (ii) subsequently analyzing the statistical properties of this stochastic system and computing its transport properties in the hydrodynamic scaling limit, can be successfully achieved in a class of chaotic billiard systems composed of many hard disks trapped in a semi-porous material which prevents mass transfer and yet allows energy transfer through elastic collisions among neighboring disks.

Under the assumption that collisions among moving disks are rare compared to wall collision events, the global multi-particle probability distribution of the system typically reaches local equilibrium at the kinetic energy of each individual particle before energy exchanges proceed. This mechanism naturally yields a stochastic description for the process of energy exchanges in the system. In a subsequent paper, it was shown that the same reduction applies to systems of confined hard spheres.

Our purpose in this paper is twofold. Our main objective is to establish a comparison between the process of energy transfer in models of interacting hard spheres with local confinement rules, on the one hand, and the diffusive motion of tracer particles in low-dimensional billiard tables such as the finite-horizon periodic Lorentz gas, on the other. Specifically, we show that the two systems, under equivalent assumptions of local equilibration, whose accuracy can be precisely controlled by tuning the systems’ parameters down to a critical geometry, are both amenable to stochastic descriptions in the form of master equations, whether for the distribution of energies in the case of the former systems, or that of mass in the...
latter. Taking the hydrodynamic limit of these stochastic systems, we obtain explicit values of the transport coefficients of heat conduction and diffusion respectively, which turn out to share the remarkable property that they are given by simple dimensional formulae, i.e., by the square of the mesoscopic length scale multiplied respectively by the rates of energy or mass transfer.

Turning back to the billiard dynamics, we address our second objective, which is to show that, under the assumption of separation of two characteristic timescales, one associated with the local dynamics, the other with energy transfers, the process of heat transport in three-dimensional billiard systems of confined hard spheres is well-approximated by the corresponding stochastic process of energy exchanges. We do so by considering the Helfand moment of thermal conductivity and compute the linear divergence in time of its mean squared change. Plotting our results as functions of the system’s sizes for different parameter values, we compute the infinite-size extrapolations to obtain the heat conductivity and observe a very good convergence to the value obtained for the stochastic systems for parameter values where an effective separation of timescales is observed.

The paper is organized as follows. The problem of mass transport in a spatially periodic billiard table is considered in Sec. II. Starting from the pseudo-Liouville equation for the billiard dynamics, we derive a continuous-time random walk which describes the stochastic jumps of particles across a lattice, and analyze its transport properties, comparing it to that of the billiard. The same procedure is applied in Sec. III to two-dimensional billiards of confined hard disks. In Sec. IV, we turn to a three-dimensional billiard system and discuss our numerical results. Conclusions are drawn in Sec. V.

II. A CONTINUOUS-TIME RANDOM WALK APPROACH TO MASS TRANSPORT

We consider for the sake of the example a periodic array of two-dimensional semi-dispersing Sinai billiard tables in the form of square billiard cells bounded by flat walls of sizes $l$, and connected to each other by small openings of relative widths $\delta$. All the cells are identical and contain circular obstacles arranged so that there are no periodic trajectory that avoid these obstacles. Independent pointwise tracer particles move across this array, performing elastic collisions on the obstacles and walls. An example is shown in figure 1. The diffusive properties of this model were studied in some details in Ref. [12]. There the attention was on memory effects and their impact on the value of the diffusion coefficient. Here we will focus on the derivation of the kinetic prediction of this coefficient, which yields the aforementioned dimensional formula, disregarding the memory effects. The conclusions are similar to those obtained by Machta and Zwanzig in the framework of the periodic Lorentz gas. The continuous-time approach we present below is somewhat similar to that of Zwanzig.

The phase-space configuration of this system refers to a single tracer particle and is specified by the triplet $\{n, r, v\}$, where $n = (n_x, n_y) \in \mathbb{Z}^2$ denotes the lattice index of the cell where the tracer is located, $r$, its position within the cell and $v$ its velocity.

Let $p(n, r, v, t)$ denote the probability distribution of the tracer. Its time evolution is determined by the pseudo-Liouville operator, which comprises four different types of contributions, corresponding to as many different types of events:

1. Free advection of the tracer inside the cell is accounted for by the term $-v \cdot \partial_t$;

2. Collisions of the tracer with any of the circular obstacles inside the cell are determined by the operators $K^{(d)}$, where $d$ refers to a specific disk of radius $\rho_d$ at position $q^d$:

$$K^{(d)} p(n, r, v, t) = \rho_d \int_{e \cdot v > 0} \delta(e \cdot v) e \cdot v,$$

$$\times \left[ \delta(r - q^d - \rho e) p(n, r, v - 2\hat{e} \cdot v, t) - \delta(r - q^d + \rho e) p(n, r, v, t) \right];$$

3. Collisions of the tracer with any of the flat walls of cell $n$, with operator $W^{(j)}$, where $j$ takes on the values $j = 1, \ldots, 4$, corresponding to the right, bottom, left and top walls: letting $r_x$ and $v_x$ denote the position and velocity components of the tracer along the horizontal axis, wall #1 is the right wall

![FIG. 1. Periodic billiard table on a square lattice with a typical trajectory. Here the central disks in the initial and final cells are color-filled. One considers the process of mass transport across the periodic cells. The model has several parameters in terms of which a dimensional formula of the diffusion coefficient is computed.](image-url)
at position \( l/2 \) so that, if the wall is continuous with respect to the vertical axis, i.e. \( \delta = 0 \), the collision operator acts according to

\[
W^{(1)} p(\mathbf{r}, \mathbf{v}, t) = |v_x| \delta(r_x - l/2) \tag{2}
\]

\[
\times \left[ \theta(-v_x) p(\mathbf{r}, v_x, v_y, t) - \theta(v_x) p(\mathbf{r}, -v_x, v_y, t) \right],
\]

with similar expressions for \( W^{(2)} \), \( W^{(3)} \), and \( W^{(4)} \).

4. Jump events between neighboring cells take place when a wall collision event occurs at a position where the wall is actually open, which amounts to subtracting the action of the wall operator \( J^{(1)} \) above, keeping track of the cell indices: using the same set of four indices as above for every wall and assuming that wall \#1 has a slit of width \( \delta \) centered about \( y = 0 \), the jump operator \( J^{(1)} \) is

\[
J^{(1)} p(\mathbf{r}, \mathbf{v}, t) = |v_x| \delta(r_x - l/2) \Theta_\delta(r_y) \theta(-v_x) \tag{3}
\]

\[
\times \left[ p(\mathbf{r} + (1, 0), \mathbf{v}, t) - p(\mathbf{r}, \mathbf{v} - v_x, v_y, t) \right],
\]

where \( \Theta_\delta(x) = 1 \) if \( |x| \leq \delta/2 \) and 0 otherwise.

Collecting these terms together, we obtain the time evolution of \( p(\mathbf{r}, \mathbf{v}, t) \), given by the pseudo-Liouville equation:

\[
\partial_t p(\mathbf{r}, \mathbf{v}, t) = \left\{-v \cdot \partial_r + \sum_j \lambda R^{(d)} + \sum_j W^{(j)} \right\} p(\mathbf{r}, \mathbf{v}, t) + \sum_j J^{(j)} p(\mathbf{r}, \mathbf{v}, t).
\]

The terms on the right-hand side of this equation are grouped so as to distinguish the local terms, which do not act on the cell index in the distribution, from the non-local ones, i.e. the jump terms, which act on the cell index. Also note that the velocity amplitude is invariant under every term of this equation and is therefore a conserved quantity which plays no role once it has been fixed by the initial condition.

It is an immediate consequence of the ergodicity of the local dynamics that the following distribution,

\[
P^{(\text{leq})}(\mathbf{r}, t) = \int d\mathbf{r} \int d\mathbf{v} \delta(v^2 - v_0^2) p(\mathbf{r}, \mathbf{v}, t),
\]

is invariant under the local terms of the pseudo-Liouville equation \( \partial_t \). We thus refer to \( P^{(\text{leq})}(\mathbf{r}, t) \) as the local equilibrium distribution. Its time evolution occurs through jump events only:

\[
\partial_t P^{(\text{leq})}(\mathbf{r}, t) = \sum_j \int d\mathbf{r} \int d\mathbf{v} \delta(v^2 - v_0^2) J^{(j)} p(\mathbf{r}, \mathbf{v}, t).
\]

In order to close this equation for \( P^{(\text{leq})}(\mathbf{r}, t) \), we make the local equilibrium approximation,

\[
p(\mathbf{r}, \mathbf{v}, t) = \frac{1}{\pi A} \delta(v^2 - v_0^2) P^{(\text{leq})}(\mathbf{r}, t),
\]

where \( A \) is the area of the billiard, e.g. \( A = l^2 - \pi (\rho_1^2 + \rho_2^2) \) in the case of figure \( \Pi \) (where \( \rho_1 \) denotes the radius of the disk at the center of the cell and \( \rho_2 \) that of the disks at the cell corners).

Plugging Eq. \( 7 \) into \( 6 \), the pseudo-Liouville equation \( \partial_t \) reduces to the following continuous-time random walk

\[
\partial_t P^{(\text{leq})}(\mathbf{r}, t) = \sum_j \frac{\nu_0 \delta}{\pi A} \left[ P^{(\text{leq})}(\mathbf{r} + \mathbf{e}_j, t) - P^{(\text{leq})}(\mathbf{r}, t) \right],
\]

where \( \mathbf{e}_j \in \{ \pm 1, 0 \}, (0, \pm 1) \} \).

In the continuum scaling limit, \( \mathbf{r} = \mathbf{l} n, l \to 0, v_0 \sim t^{-2} \), this reduces to a diffusion equation,

\[
\partial_t P(\mathbf{r}, t) = D \nabla^2 P(\mathbf{r}, t),
\]

with diffusion coefficient

\[
D = \mu^{(J)},
\]

here written in terms of the frequency \( \nu^{(J)} \) of a jump event in a specific direction, identical for all four directions,

\[
\nu^{(J)} = \frac{\nu_0 \delta}{\pi A}.
\]

Equation \( 10 \) is what we refer to as a dimensional formula: the diffusion coefficient associated with the continuous-time random walk process \( \partial_t \) is the product between the scale of displacements squared and hopping rate. The fact that it is an exact property of the stochastic process is remarkable.

As far as the transport properties of the billiard table go, Eq. \( 10 \) is a mere approximation: its validity relies on the local equilibrium approximation \( \partial_t \). In contrast, Eq. \( 11 \) is an exact result for the billiard dynamics as well—valid for all parameter values—as it relies solely on the ergodicity of the billiard table \( \Pi \).

The closure approximation \( \partial_t \) is expected to be exact in the limit of vanishing window widths, \( \delta \to 0 \), whereby the hopping rate \( \nu^{(J)}(\Pi) \) diverges and the diffusion coefficient \( \nu^{(J)} \) vanishes. In practice however, we may expect \( p(\mathbf{r}, \mathbf{v}, t) \) to converge to the local equilibrium distribution \( P^{(\text{leq})}(\mathbf{r}, t) \) between successive jumps so long as the typical number of disk collision events within a cell is large. This can be verified numerically, as shown on the top panel of figure \( 2 \). These numerical results were already reported in Ref. \( 12 \). Similar results are equally obtainable for three dimensional billiard systems such as the three-dimensional periodic Lorentz gas \( 13 \).

### III. Heat Transport in Two-Dimensional Confining Billiards

Similar considerations apply to models of heat transport with mass confinement \( 14 \). Classes of such models were initially introduced by Bunimovich et al in
Ref. [16]. There, the authors proved the ergodicity of two-dimensional billiard tables consisting of an arbitrary large number of unit cells placed side by side, each containing a single disk trapped within the cell’s boundaries, but in such a way that collisions may still take place between disks belonging to neighboring cells.

Figure 3 shows an example of such a system. In Ref. [7], we introduce the following parametrization of the model in terms of two parameters: $\rho$, which characterizes the timescale of wall collision events, and $\rho_m$, which characterizes that of binary collisions.

On the one hand, the dynamics within an isolated cell of width $l$ boils down to the motion of a point particle in an area bounded by the exterior intersection of four disks of radius $\rho$, $l/2 \leq \rho < l/\sqrt{2}$. In the absence of interaction with neighboring particles, the mean free path of a particle is given by $\ell = \pi |B_\rho|/|\partial B_\rho|$, where $B_\rho$ and $\partial B_\rho$ denote respectively the area and perimeter of the billiard cell. The corresponding wall collision timescale is obtained by multiplying the mean free path by the speed of the particle.

Interactions among neighboring particles on the other hand take place provided the radius of the moving particles $\rho_m$ is larger than a critical value, $\rho_m > \rho_c = \sqrt{\rho^2 - l^2/4}$. The corresponding timescale can be computed and shown to diverge with $(\rho_m - \rho_c)^{-3}$. Letting $\nu^{(W)}(T)$ and $\nu^{(B)}(T)$ respectively denote the frequencies of wall collision and binary collision events measured at equilibrium temperature $T$, the following separation of timescales is assumed,

$$\nu^{(B)}(T) \ll \nu^{(W)}(T),$$

which occurs when $\rho_m \rightarrow \rho_c$.

Under this assumption, we showed that the heat conductivity of spatially extended billiard systems, which are infinite size limits of systems such as depicted in Fig. 3, reduces, up to a dimensional factor $l^2$, to the frequency of binary collisions,

$$\kappa^{(B)}(T) = l^2 \nu^{(B)}(T).$$

Furthermore the heat conductivity scales with the thermal speed, $\kappa^{(B)}(T) \sim \sqrt{T}$.

Although Eqs. [10] and [13] are very much alike, the derivation of the latter is much more involved than that of the former.

Proceeding as in Sec. II the first part of the program, which is to reduce the pseudo-Liouville equation describing the time evolution of the billiard system to a
continuous-time stochastic process of energy exchanges, follows closely along lines which led from Eqs. [4] to [5]. Indeed, considering the time evolution acting on the $N$-particle phase-space distribution $p_N(\{r_i, v_i\}, t)$, one readily notices that the local equilibrium distribution

$$P^{(\text{leq})}_N(\epsilon_1, \ldots, \epsilon_N, t) \equiv \int \prod_{a=1}^{N} \diff r_a \diff v_a \delta(\epsilon_a - m v_a^2/2) p_N(\{r_i, v_i\}, t)$$

is left unchanged by the advection and wall collision

$$\partial_t P^{(\text{leq})}_N(\epsilon_1, \ldots, \epsilon_N, t) = \frac{1}{2} \sum_{a,b=1}^{N} \int \diff \eta \left[ W(\epsilon_a + \eta, \epsilon_b - \eta|\epsilon_a, \epsilon_b) P^{(\text{leq})}_N(\ldots, \epsilon_a + \eta, \ldots, \epsilon_b - \eta, \ldots, t) \right. \left. - W(\epsilon_a, \epsilon_b|\epsilon_a - \eta, \epsilon_b + \eta) P^{(\text{leq})}_N(\ldots, \epsilon_a, \ldots, \epsilon_b, \ldots, t) \right],$$

where the expression of $W$ can be obtained by direct computation of the collision integrals, which, after rescaling the time variable to the units of the frequency of binary collision events and thus absorbing all the parameters into the time scale, yields the universal function

$$W(\epsilon_a, \epsilon_b|\epsilon_a - \eta, \epsilon_b + \eta) = \sqrt{\frac{2}{\pi^3}} \times \begin{cases} \sqrt{\frac{1}{\epsilon_a} K \left( \frac{\epsilon_a + \eta}{\epsilon_a} \right)} & \text{if } \epsilon_a > \epsilon_b \geq \eta, \\ \sqrt{\frac{1}{\epsilon_b} K \left( \frac{\epsilon_b + \eta}{\epsilon_b} \right)} & \text{if } \epsilon_b > \epsilon_a \geq \eta, \\ \sqrt{\frac{1}{\epsilon_a} K \left( \frac{\epsilon_a - \eta}{\epsilon_a} \right)} & \text{if } \epsilon_a > \eta > \epsilon_b, \\ \sqrt{\frac{1}{\epsilon_b} K \left( \frac{\epsilon_b - \eta}{\epsilon_b} \right)} & \text{if } \epsilon_b > \eta > \epsilon_a, \end{cases}$$

(16)

whose definition intervals correspond respectively to $-\epsilon_b < \eta < -\max(\epsilon_a - \epsilon_b, 0)$, $-\max(\epsilon_a - \epsilon_b, 0) < \eta < 0$, $0 < \eta < \max(\epsilon_a - \epsilon_b, 0)$, and $\max(\epsilon_a - \epsilon_b, 0) < \eta < \epsilon_a$. Here $K(m)$ denotes the complete elliptic integral of the first kind.

A system of $N$ isolated cells whose time evolution is specified by the master equation (15) reaches a microcanonical equilibrium state whose total energy can be parametrized in terms of the temperature according to $\epsilon_1 + \ldots + \epsilon_N = NT$. The corresponding energy exchange frequency is

$$\nu_N(T) = \sqrt{T} \left[ 1 + O(1/N) \right],$$

(17)

whose infinite-size limit is simply $\nu(T) = \lim_{N \to \infty} \nu_N(T) = \sqrt{T}$ (in the chosen units of time).

An expression of the heat conductivity of the system described by Eq. (15) is obtained by considering the Einstein-type relation satisfied by the variance of the associated Helfand moment, which measures the spread of energy as a function of time.

For the system of $N$ energy cells aligned along a one-dimensional ring, the Helfand moment is defined accord-

terms. Therefore, and provided binary collision events are rare with respect to wall collision events, we can make a closure approximation similar to Eq. (7) to obtain the time evolution of the local equilibrium distribution in the form of a stochastic process.

The result is a master equation which describes the time evolution of the $N$ cell system with energy variables $\{\epsilon_1, \ldots, \epsilon_N\}$ in terms of energy exchanges between neighboring cells at respective energies $\epsilon_a$ and $\epsilon_b$ of amount $\eta$, specified by a stochastic kernel $W$:

$$H_N(t) = \sum_{i=1}^{N} \epsilon_i(t),$$

(18)

where $\epsilon_i(t)$ is the state of the energy at site $i$ at time $t$. This quantity evolves in time by discrete steps, when energy exchanges occur. Let $\{\tau_n\}_{n \in \mathbb{N}}$ denote the sequence of times at which successive energy exchanges take place. Assuming cells $i$ and $i+1$ exchange some amount of energy at time $\tau_n$, we can write the corresponding change in the Helfand moment as $\epsilon_i(\tau_n - 0) - \epsilon_i(\tau_n + 0)$.

Computing the mean squared change in the Helfand moment as a function of time, we obtain an expression of the thermal conductivity according to

$$\kappa(T) = \lim_{N \to \infty} \kappa_N(T),$$

(19)

where we defined the finite $N$ conductivity to be

$$\kappa_N(T) = \frac{1}{N(\epsilon_B T)^2} \lim_{n \to \infty} \frac{1}{2\tau_n} \left\langle (H_N(\tau_n) - H_N(\tau_0))^2 \right\rangle.$$

(20)

In Ref. [5], it was argued that the infinite $N$ limit of this quantity is determined by the static correlations only, yielding the result

$$\kappa_N(T) = l^2 T \left[ 1 + O(1/N) \right].$$

(21)

Comparing Eqs. (17) and (21), we obtain the announced result

$$\kappa(T) = l^2 \nu(T),$$

(22)

which is an exact result for the stochastic system evolved by the master equation (15) and does not make explicit
use of the form (16), except for some symmetries. The corresponding result (13) for the billiard dynamics is obtained by plugging back the proper timescale of binary collisions and letting $\rho_m \to \rho_c$ so that the separation of timescales (12) is effective.

Unlike mass transport in Sinai billiard tables for which the transport equation (9) follows directly from the continuous-time random walk (8), so that there only remains the problem of comparing the diffusion coefficient of the billiard to the dimension formula (10) in the appropriate parameter regime, the problem of computing the heat conductivity associated with heat transport in billiard systems of many confined particles proceeds in two separate steps.

Having carried out the reduction of the billiard’s pseudo-Liouville equation to a master equation for a stochastic energy exchange system, the first step is to establish the cancellation of dynamical correlations in such a system, which yields the identity $\lim_{N \to \infty} \kappa N / \nu N = l^2$. This is however a delicate result and requires in-depth knowledge of the spectral properties of the master equation (15). The approach we took in Ref. [8], though equivalent, uses different techniques, based on analyzing the first few orders of the gradient expansion of the kinetic equation to obtain the expression of the heat current in terms of the local temperature gradient in a non-equilibrium stationary state, i.e. Fourier’s law.

The second step of the program is to go back to the billiard dynamics and investigate the convergence of the heat conductivity to the binary collision frequency in the limit $\rho_m \to \rho_c$.

For two-dimensional billiard systems such as the ones shown in Fig. 3, the agreement was found to be rather satisfactory. For the three-dimensional billiard systems we turn to now, this agreement is even better.

**IV. THREE-DIMENSIONAL BILLIARD FOR HEAT TRANSPORT**

Consider a three-dimensional billiard of confined hard spheres such as shown in Fig. 4. The reduction of the pseudo-Liouville equation governing the phase-space evolution of probability densities $p_N(\{\mathbf{r}_i, \mathbf{v}_i\}, t)$ to a master equation similar to Eq. (15) was already carried out in Ref. [9].

The corresponding kernel, in the appropriate time units, is found to have the universal form

$$W(\epsilon_a, \epsilon_b|\epsilon_a - \eta, \epsilon_b + \eta) = \frac{\sqrt{\pi}}{8} \times \begin{cases} \frac{e^{\frac{\epsilon_a + \eta}{\tau_a \epsilon_a}}}{\sqrt{\max(\epsilon_a, \epsilon_b)}} \frac{1}{\sqrt{\max(\epsilon_a, \epsilon_b)}}, & (23) \\
\frac{e^{\frac{\epsilon_a - \eta}{\tau_a \epsilon_a}}}{\sqrt{\max(\epsilon_a, \epsilon_b)}} & \end{cases}$$

whose definition intervals correspond respectively to $-\epsilon_b < \eta < -\max(\epsilon_b - \epsilon_a, 0)$, $-\max(\epsilon_b - \epsilon_a, 0) < \eta < \max(\epsilon_a - \epsilon_b, 0)$, and $\max(\epsilon_a - \epsilon_b, 0) < \eta < \epsilon_a$.

Extensive numerical investigations of the master equation (15) with the stochastic kernel (23) were presented in Ref. [9], supporting with high precision the validity of Eq. (22). Here we focus on the billiard dynamics and consider the mean squared change in time of the Helfand moment associated with the distribution of energy in billiard systems formed by one-dimensional lattices of billiard cells such as shown in Fig. 4.

Let $\{\tau_n\}_{n \in \mathbb{Z}}$ denote the times at successive binary col-
collision events. As we now need to account for the motion of particles within their respective cells, there are two types of contributions to changes in the Helfand moment between two successive binary collision events. The leading contribution arises from the energy exchanges which take place at binary collision events. Thus, when a binary collision occurs between particles \( j \) and \( k \), the Helfand moment changes by the amount \([x_j(\tau_n) - x_k(\tau_n)](\epsilon_j(\tau_n + 0) - \epsilon_j(\tau_n - 0))\), where \( x_j(\tau_n) \) and \( x_k(\tau_n) \) denote the positions of particles \( j \) and \( k \) along the direction of the lattice spatial extension at time \( \tau_n \). The other contribution to the Helfand moment arises from the advection of particles within their respective cells according to \( \sum \|x_a(\tau_n) - x_a(\tau_{n-1})\|\epsilon_a(\tau_{n-1}) \).

The range of allowed parameter values is identical to the two-dimensional case: \( 1/2 \leq \rho < 1/\sqrt{2} \), and \( \rho_c < \rho_m < \rho \), where \( \rho_c \equiv \sqrt{\rho^2 - 1^2/4} \).

Taking \( l = 1 \), we fix \( \rho = 0.50 \) so \( \rho_c = 0 \) and use the six parameter values \( \rho_m = 0.20, 0.25, \ldots, 0.45 \). For each one of them, we fix the total energy to be \( E = 3N/2 \) \( (T = 1) \) and vary the system size from \( N = 3 \) and up to \( N = 100 \) cells. We typically run \( 10^4 \) trajectories, each for a duration of \( 10^3 \times N \) units of the average time between collision events. We compute: (i) the Helfand moment versus time and take the mean and standard deviation of the transport of Eq. \( (20) \) to obtain the conductivities \( \kappa_N^{(B)} \); (ii) the binary and wall collision frequencies \( \nu_N^{(B)} \) and \( \nu_N^{(W)} \) by directly averaging their numbers with respect to time.

We then use linear fits in \( 1/N \) for \( N \geq 10 \) of \( \kappa_N^{(B)} \) and \( \nu_N^{(B)} \) to obtain the extrapolation \( \nu_\infty^{(B)} = \lim_{N \to \infty} \nu_N^{(B)} \) and \( \kappa_\infty^{(B)} = \lim_{N \to \infty} \kappa_N^{(B)} \). Here and below, explicit temperature dependencies are dropped.

Measurements of the ratio between \( \nu_N^{(B)} \) and \( \nu_N^{(W)} \), by which we can assess the effectiveness of the separation of timescales \((12)\), are displayed in Fig. 4 for \( N = 25 \) (other system sizes yield similar values). The results of the computations of \( \kappa_\infty^{(B)}/\nu_\infty^{(B)} \) for the different parameter values \( \rho_m \) are displayed in Fig. 5 and are found to be in very good agreement (within two digits) of the dimensional formula \((13)\) for values of \( \rho_m \) as large as 0.30. In Fig. 7, the details of the fitting procedure used to obtain the values of \( \kappa_\infty^{(B)} \) and \( \nu_\infty^{(B)} \) are shown for the different parameter values as functions of \( N \).

V. CONCLUDING REMARKS

By controlling the rate at which a tracer hops from cell to cell in a Sinai billiard table or that of interaction among neighboring disks or spheres in a high-dimensional billiard with local confinement rules, one identifies a limit of vanishing rate where the complicated phase-space dynamics are replaced by stochastic processes which account for the transport of mass in the first case, or (kinetic) energy in the second. Furthermore, the transport coefficients of these stochastic processes have the same simple dimensional expression, given by the length scale of transfers squared multiplied by the corresponding rates.

As emphasized in this paper, the dimensional formulae we obtained for the transport coefficients of the models of mass and heat transport we have considered are but two faces of the same coin. Indeed, in both cases the accuracy of our approximation of the transport coefficients of the billiards in terms of hopping or collision rates relies on the efficient separation of two timescales, namely the timescale of local collision events must be much shorter than that characterizing the transfer of mass or energy. In other words, the relaxation to local equilibrium precedes mass or energy transfers.

We can in fact view the notion of relaxation to local equilibrium as a low-dimensional transposition of that of local thermal equilibrium, which is at the heart of many theories involving hydrodynamic scaling limits and typically assumes a large number of degrees of freedom\((10)\). In our billiards, the relaxation to local equilibrium occurs
on the constant energy surface of a single particle. But one could instead consider systems of trapped gases, in which case the relaxation to local equilibrium would involve transfers of energy among the particles in the same trap. In such a case, provided relaxation to local equilibrium takes place on timescales much shorter than that of energy transfer between neighboring traps, a similar dimensional expression of the heat conductivity of the corresponding stochastic process in terms of the product of length scale squared and rate of energy transfer would yield an accurate approximation of the transport coefficient of the billiard system.

We end with a remark concerning the closure (7) which relies on the ergodicity of the local dynamics on the surface of constant energy. As noted already by Zwanzig, Sinai billiards cannot be replaced by polygonal ones, for which the notion of ergodicity is weaker since the velocity directions take on values in a discrete set. In energy exchange processes, however, ergodicity of the many-particle billiard may be restored through the sole interaction among neighboring particles. As shown in Ref. [20], an elastic string-type interaction between particles trapped in polygonal boxes provides a simple model of a system which, on the one hand, cannot be accurately described by a master equation similar to Eq. (15), even when interactions are rare, but on the other hand, has a well-defined heat conductivity which is well approximated by a dimensional formula. An understanding of

FIG. 7. Heat conductivities \( \kappa_N^{(B)} \) and binary collision frequencies \( \nu_N^{(B)} \) measured as functions of the system size \( N \) for different values of the parameter \( \rho_m \) (\( \rho = 0.50 \)). The solid curves correspond to the linear fits of \( \kappa_N^{(B)} \) and \( \nu_N^{(B)} \) as functions of \( 1/N \). The intercepts yield the infinite size estimates \( \kappa_\infty^{(B)} \) and \( \nu_\infty^{(B)} \).
the transport properties of this system beyond the Boltzmann hypothesis remains to be elucidated.

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For technical reasons pertaining to the probability of direct re-collisions between two particles, this example actually falls out of the class of systems considered in Ref. [16]. This is however unimportant for our own considerations.

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