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Approach to Equilibrium in Models of a System in Contact with a Heat Bath*

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We investigate simple model systems in contact with an infinite heat bath. The former consists of a finite number of particles in a bounded region Λ of $\mathbb{R}^d$, $d=1, 2$. The heat baths are infinite particle systems which can penetrate Λ and interact with the system via elastic collisions. Outside Λ the particles move freely and have a Gibbs probability measure prior to entering Λ. We show that starting from almost any initial configuration, the system approaches, as $t \to \infty$, the appropriate Gibbs distribution. The combined system plus bath is Bernoulli.

KEY WORDS: Heat bath; approach to equilibrium; infinite particle system; Markov process.

1. INTRODUCTION

We consider three infinite particle systems which model a system in contact with a heat bath. The system is modeled by N particles of mass M (molecules) restricted to move in a finite region ($[0, 1]$ or $[0, 1]^2$) by reflecting walls. The heat bath is modeled by an infinite ideal gas of point particles (moving in $\mathbb{R}$ or $\mathbb{R}^2$) of mass $m \leqslant M$ (atoms). The walls are permeable to the atoms and the atoms interact with the molecules. Let Ω denote the phase space of the infinite composite system of the molecules and the bath, and ϕ_t the (mechanical) evolution of this system. (One of the models is stochastic.) Under this infinite system evolution the motion of the finite system (molecules) will not be deterministic, since it depends on the

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position and velocity of atoms. If we specify an initial probability distribution for the bath, then we obtain a stochastic process

$$Z(t) = \{Q_i(t), V_i(t)\}_{t \in \mathbb{R}, 1 \leqslant i \leqslant N}$$

which describes the motion of the molecules. If we choose this probability distribution to be the Gibbs measure on the bath (at some temperature and density) conditioned on the position and velocity of the molecules Z_0, we obtain a process starting Z_0. Let us denote the distribution of this process at time t by $\nu^t_{Z_0}$, where $Z_0 = [Q_i(0), V_i(0)]_{1 \leqslant i \leqslant N}$ denotes the initial position and velocity of the molecules. Let $\nu(dQ_1, ..., dQ_N, dV_1, ..., dV_N)$ denote the equilibrium distribution of the molecules, that is, the distribution of position and velocity of molecules inherited from the Gibbs measure μ for the (composite) infinite system. If the process $Z(t)$ starts with initial distribution ν, we obtain a stationary process. We denote this process by $\mathscr{B}$.

We show that $\nu^t_{Z_0}$ converges to the equilibrium distribution ν, $\|\nu^t_{Z_0} - \nu\| \to 0$ as $t \to \infty$, where $\|\cdot\|$ is the variation norm on measures, [(6.5) Eq. 2 of Ref. 4]. Using this result we show that the composite infinite system (Ω, μ, ϕ_t), denoted by α, is isomorphic to a Bernoulli flow.[2]

These results were proved for one molecule in [0, 1] in contact with a heat bath in Ref. 1. This paper extends the results of that work to more general models.

2. THE MODELS

Model I

We consider N (unlabeled) molecules of mass M moving in the unit interval [0, 1]. The molecules are in contact with a heat bath of atoms, an ideal gas of point particles of mass $m < M$ on the line. The molecules interact with the atoms through elastic collisions. The molecules exchange velocities when they collide with each other and are reflected when they collide with the wall at 0 or 1. The walls are permeable to the atoms. In between collisions all particles move freely. Let Ω be the phase space of the composite infinite system with no atoms between molecules, μ the infinite volume Gibbs state on Ω at some temperature T and bath density ρ, and ϕ_t the mechanical evolution of this system. (There exist configurations $\omega \in \Omega$ such that $\phi_t \omega$ is not well defined for all $0 < t < \infty$. Our prescription is rendered ambiguous by the occurrence of an infinite number of collisions in a finite time or multiple collisions. However, we can show that there exists a set $\hat{\Omega} \subset \Omega$ with $\mu(\hat{\Omega}) = 1$ on which these events do not occur. The arguments are similar to those for the case of one molecule.[1])

Model II

This is a stochastic version of Model I. Again we start with N molecules of mass M constrained to move in $[0, 1]$, in contact with an ideal gas heat bath of particles of mass $m < M$ on the line. Let μ be the Gibbs state for the composite system for some temperature T, bath density ρ, and no interaction between particles (atoms and molecules), i.e., atoms can lie between molecules. When an atom collides with a molecule it undergoes an elastic collision with probability p and goes through the molecule with probability $1-p$. All particles move freely between collisions. This defines a Markov process with state space Ω consisting of configurations of atoms and molecules (including those with atoms between molecules), and transition probability Q_t. In the Appendix we show that μ is an invariant measure for this process. We denote this process by α and call $\mathscr{B}$ the process obtained by observing only the molecules.

Model III

We consider N nonoverlapping hard squares (molecules) of width $d > 0$ and mass M moving in the unit square $[0, 1]^2 \subset \mathbb{R}^2$. The molecules interact with an infinite ideal gas of point particles (atoms) of mass $m < M$ in the plane. The atoms cannot penetrate into the unit square beyond a boundary layer of width $W < d$, from whose internal walls they are reflected. We assume that the hard squares are oriented with their sides parallel to the sides of the box and that they move freely without rotation between collisions. When two hard squares collide they exchange the component of velocity in the direction normal to the side of collision while the component parallel to the side of collision remains unchanged. When an atom collides with a molecule the component of velocity normal to the face of collision is transformed according to the elastic collision equations

$$V'_N = \frac{M-m}{M+m} V_N + \frac{2m}{M+m} U_N$$

$$U'_N = \frac{2M}{M+m} V_N - \frac{M-m}{M+m} U_N$$

where V_N U_N are the normal components of the velocity of the molecule and atom, respectively. The velocity in the tangential direction remains unchanged. When a hard square collides with the outer walls of the box the component of velocity normal to the wall is reflected while the component parallel to the wall remains unchanged. The phase space Ω of the com-

posite system consists of configurations of *unlabeled* molecules and atoms. Let μ be the infinite volume Gibbs measure at some temperature T and bath density ρ. We assume that $N \leqslant \{d^{-1}\}^2$ where $\{d^{-1}\} = d^{-1} - 1$ if d^{-1} is an integer and $= [d^{-1}]$, the integer part of d^{-1}, otherwise, so that μ is locally absolutely continuous.

(Clearly the above prescription for the time evolution is not sufficient if events such as an infinite number of collisions in a finite time or multiple collisions or an atom colliding at the corner of a hard square occur. It can be shown, using arguments similar to those for the one-dimensional case, that there exists a set $\hat{\Omega} \subset \Omega$, $\mu(\hat{\Omega}) = 1$, on which such events do not occur. We will not supply the arguments here.)

In all three models we obtain our results by considering a system process $\mathscr{M}$ intermediate between α and $\mathscr{B}$. The reason for considering a third process is the following. For a Markov process in which "sufficient spreading" (in the sense indicated later) occurs, convergence to equilibrium can be established. The process α in each model is Markov but does not have sifficient spreading. This is because α is either deterministic or close to being deterministic. The process $\mathscr{B}$ in each model has enough spreading, but is not Markov due to recollisions. The process $\mathscr{M}$ is obtained by observing all the particles in the finite region ($[0, 1]$ or $[0, 1]^2$), not just the molecules. $\mathscr{M}$ is the process $\{Y(t)\}_{t \in \mathbb{R}}$ where $Y(t)$ is the configuration of particles in the finite region at time t. The state space of $\mathscr{M}$ is Ω^F, the set of configurations in the finite region.

That the process $\mathscr{M}$ is Markov follows from the fact that the atoms entering the finite region after time t_0 are independent of atoms which left the finite region before time t_0.[1]

$\mathscr{M}$ has the stationary distribution $\sigma(dy) = \mu(Y(0) \in dy)$. The main problem of this paper is to show that $\mathscr{M}$ has sufficient spreading. Once this is shown we will have convergence to equilibrium (σ) for $\mathscr{M}$. From this it will follow (Ref. 1, Appendix B) that the shift on $\mathscr{M}$ is Bernoulli. Now in Models I and II both $\mathscr{M}$ and $\mathscr{B}$ are isomorphic in the sense of dynamical systems to α. (For Model II the dynamical system α is a Markov shift.) This is true since the knowledge of $\{Y(t)\}_{t \in \mathbb{R}}$ is sufficient to recover the configuration $\omega \in \Omega$ in Model I and the path $\{\omega(t)\}_{t \in \mathbb{R}}$ in Model II. In Model III the knowledge $\{Y(t)\}_{t \in \mathbb{R}}$ is sufficient to recover only that part of the configuration $\omega \in \Omega$ describing atoms which enter $[0, 1]^2$ at some time. However the other atoms move freely. Therefore, in Model III α is isomorphic to the product of $\mathscr{M}$ and an infinite "ideal gas." Thus, that $\mathscr{M}$ is Bernoulli will imply that both α and $\mathscr{B}$ are also Bernoulli. Since the process $\mathscr{B}$ is a factor of $\mathscr{M}$, convergence to equilibrium for $\mathscr{B}$ follows from convergence to equilibrium for $\mathscr{M}$ (Ref. 1, Theorem 2).

3. DEFINITION AND THEOREMS

The notion of sufficient spreading which is relevant to our purposes is provided by an ergodic, aperiodic, Harris chain.

Let (Γ, π, P) be an ergodic, aperiodic Markov chain, with a transition probability P and a stationary distribution π. (For definition see Ref. 6.) (Γ, π, P) is called a Harris chain if for π a.e. $x \in \Gamma$ there exists a positive integer $n = n(x)$ such that $P^n(x, dy)$ has a component absolutely continuous w.r.t. π. The following is the central result used in obtaining convergence to equilibrium.

Proposition(s). Let (Γ, π, P) be an ergodic, aperiodic Harris chain. Then, for π a.e. $x \in \Gamma$,

$$\|P^n(x, \cdot) - \pi(\cdot)\| \to 0 \qquad \text{as} \quad n \to \infty$$

where $\|\cdot\|$ denotes variation norm for measures.[4]

Let $P^t(y, dy') = \mu(Y(t) \in dy' \mid Y(0) = y)$ be the transition probability for the process $\mathscr{M}$. (The definition can be extended to all y.) For each $\tau > 0$ let $\mathscr{M}_\tau$ be the Markov process obtained by observing Y only at times which are multiples of τ. $\mathscr{M}_\tau = (\Omega^F, \sigma, \bar{P})$ is a stationary Markov chain with $\bar{P} \equiv P^\tau$. We will show that $\mathscr{M}_\tau$ is an ergodic aperiodic Harris chain. We will need the concept of overlapping measures which we define now. Two probability measures μ_1 and μ_2 on the same measure space overlap if they are not mutually singular (i.e., if μ_1 has a component absolutely continuous with respect to μ_2). Let $\mathbb{P}$ denote the measure on the path space (process measure) for the $\mathscr{M}$ process and for any $y \in \Omega^F$, let $\mathbb{P}_y$ denote the process measure and $\mathscr{M}_y$ the process starting from y.

Lemma 1. Let (Γ, π, P) be a stationary Markov chain, with invariant (probability) measure π. Let $\tilde{P}$ be (a realization of) the transition probability for the time reversed process.

Let $\Delta \subset \Gamma$ be a nonempty subset of the state space with the following properties: (i) For π a.e. $\tilde{z} \in \Gamma - \Delta$, there exists an $N(\tilde{z}) \in \mathbb{N}$ such that $P^{N(\tilde{z})}(\tilde{z}, \Delta) > 0$. (ii) Δ admits a topology in which it is connected, open sets are measurable, and if $A \subset \Delta$ is a nonempty open set then $\pi(A) > 0$. (iii) For all $z \in \Delta$ there exist natural numbers $N = N(z)$ and $N^* = N^*(z)$ and a neighborhood $B_z \subset \Delta$ of z such that (a) $P^N(z, \cdot)$ and π overlap for π a.e. $z \in \Delta$ and (b) for π a.e. $y_1, y_2 \in B_z$ either $P^N(y_1, \cdot)$ and $P^N(y_2, \cdot)$ or $\tilde{P}^{N^*}(y_1, \cdot)$ and $\tilde{P}^{N^*}(y_2, \cdot)$ overlap.

Then (Γ, π, P) is an ergodic Harris chain.

Proof. Since $P^{N(\tilde{z})}(\tilde{z}, \Delta) > 0$ for π a.e. $\tilde{z}$ and $P^{N(z)}(z, \cdot)$ overlaps π for π a.e. $z \in \Delta$, for a.e. $\tilde{z} \in \Gamma$ there exists, by stationarity, a $K(\tilde{z}) \in \mathbb{N}$ such that

$P^{K(\tilde{z})}(\tilde{z}, \cdot)$ overlaps π. This proves that (Γ, π, P) is a Harris chain. (iii) implies that π a.e. point of B_z belongs to the same ergodic component of (Γ, π, P). [(Γ, π, P) and $(\Gamma, \pi, \tilde{P})$ have the same ergodic components.] We use the connectivity of Δ to show that π a.e. point in Δ belongs to the same ergodic component. Let γ_i, $i = 1, 2, \ldots, n \leqslant \infty$ be the (nontrivial) intersections with Δ of the ergodic components of (Γ, π, P). Let $\hat{\gamma}_i = \{z \in \Delta \mid B_z \subset \gamma_i (\mathrm{mod}\, 0)\}$. Clearly $\hat{\gamma}_i$ is open, $\{\gamma_i\}_{i=1}^n$ are mutually disjoint, and $\bigcup_{i=1}^n \hat{\gamma}_i = \Delta$. Since Δ is connected we conclude that $n = 1$. This conclusion together with property (i) implies that (Γ, π, P) is ergodic. This completes the proof of the proposition.

In Section 4 we apply Lemma 1 to establish in all three models that $\mathscr{M}_\tau$ is an ergodic Harris Chain for all $\tau > 0$, which implies that $\mathscr{M}_\tau$ is also aperiodic. We thus have:

Theorem 1. The Markov chain $\mathscr{M}_\tau$ (in each of the three models) is an aperiodic ergodic Harris chain for all $\tau > 0$.

Corollary 1. (Convergence to equilibrium for $\mathscr{M}$.) (i) $\|P^t(y, \cdot) - \sigma(\cdot)\| \to 0$ as $t \to \infty$ for σ a.e. $y \in \Omega^F$. (ii) More generally, there exists a set $\tilde{\Omega}^F \subset \Omega^F$ with $\sigma(\tilde{\Omega}^F) = 1$ such that $\|\gamma P^t - \sigma\| \to 0$ as $t \to \infty$, for any probability measure γ on Ω^F with $\gamma(\tilde{\Omega}^F) = 1$. Here $\gamma P^t(\cdot) = \int \gamma(dy)\, P^t(y, \cdot)$ is the distribution at time t starting from γ.

Corollary 2. $\mathscr{M}$ and hence α and $\mathscr{B}$ are Bernoulli.

Theorem 2. $\|\nu_{Z_0}^t - \nu\| \to 0$ as $t \to \infty$ for ν—a.e. molecular configuration Z_0.

Corollary 1, Corollary 2, and Theorem 2 follow easily from Theorem 1 in the same manner as Ref. 1.

4. VERIFICATION OF THE CONDITIONS FOR $\mathscr{M}_\tau$

Model I

Let $\bar{\Delta}$ be the set of configurations in Ω^F which contain no atoms (N unlabeled particles in $[0, 1]$). We identify the precollision and postcollision velocities of pairs of molecules in contact with each other and molecules in contact with a wall. Equip $\bar{\Delta}$ with the Euclidean topology with the above identifications. Let $B_1^+ \subset \bar{\Delta}$ be the set of configurations for which at least two molecules have their first collision with $\{0, 1\}$ at the same time, under the evolution arising when no atoms enter $[0, 1]$. Similarly define B_1^- for the time reversed evolution and let $B_1 = B_1^+ \cap B_1^-$. B_1 is contained in a finite union of submanifolds of codimension greater than or equal to 2. Let $B_2 \subset \bar{\Delta}$ be the set of configurations which contain at least

one molecule with velocity zero. Then $\Delta \equiv \bar{\Delta} - (B_1 \cup B_2)$ is connected. (Removal of B_2 does not disconnect because of the identifications at the boundary.)

Since σ (the stationary measure for $\mathscr{M}_t$) is equivalent to Lebesgue measure, it follows that if A is a nontrivial open subset of Δ, then $\sigma(A) > 0$. We have thus verified condition (ii) of Lemma 1. By sending in a fast atom we can push all the atoms out of $[0, 1]$. We leave the details of this argument to the reader. This verifies condition (i) of Lemma 1.

Now for the verification of condition (iii) a special role is played by the evolution of configurations in $\bar{\Delta}$ when no atoms enter $[0, 1]$, which we denote by $\bar{\phi}_t$. Since the molecules exchange velocities when they collide, if we observe the motion, under $\bar{\phi}_t$, of the velocities (velocity *pulses*), ignoring the identity of the molecules which carry them, we obtain free motion, except for reflections at 0 and 1. If collisions with atoms do occur, the evolution of pulses is defined in the obvious way: when a pulse collides with an atom its velocity changes to the post-collision velocity of the corresponding molecule. Moreover, a pulse configuration uniquely determines an (unlabelled) molecular configuration.

For $z \in \bar{\Delta}$, let T_i, $i = 1, 2, \ldots, N$, be the first time the ith pulse hits a wall under the evolution $\bar{\phi}_t$. For $z \in \Delta$, $T_i < \infty$. Let us denote the corresponding wall by W_i (0 or 1). Moreover, the T_i's are distinct for $z \notin B_1^+$, which we may assume: for $z \notin B_1^-$ we need only time reverse our argument. We may also assume that the pulses are so labeled that $T_1 < T_2 < \cdots < T_N$. Let $\bar{T} = \max_{1 \leqslant i \leqslant N} \{T_i\}$ and let T be the smallest multiple of $\tau \geqslant \bar{T}$. Let $E \subset (\mathbb{R}_+ \times \mathbb{R})^N$ be the set of entry times and velocities of the first N atoms entering $[0, 1]$ starting at time 0. We represent a typical element of E by $(\theta_i, U_i)_{i=1}^N$, $\theta_1 < \theta_2 < \cdots < \theta_N$.

Let S_1 be the last time before T_1 that the first pulse is not the one closest to the wall W_1 for the evolution $\bar{\phi}_t$. (If there is no such time we set $S_1 = 0$). Consider the event $E_1 \subset E$ defined as follows: $S_1 < \theta_1 < T_1$ and the corresponding atom enters through W_1 with velocity U_1 such that for the subsequent free evolution of pulse 1 no collisions with a wall coincide with any T_i. We define E_i, $1 < i \leqslant N$, similarly, the only difference being that S_i for $i > 1$ is defined using the motion induced by the entering atoms (θ_k, U_k), $k < i$. Let E_0 be the event that exactly N atoms enter $[0, 1]$ during $[0, T]$, and let $E_z = \bigcap_{i=0}^N E_i$. We denote a typical element of E_z by γ.

Regarding E_z as a subset of path space, let $\bar{\mathbb{P}}_z = \mathbb{P}_z \restriction E_z$. Let $(\bar{Q}_i(t), \bar{V}_i(t))$, $i = 1, 2, \ldots, N$, be the positions and velocities of the pulses at time t. We claim that $\bar{\mathbb{P}}_z(d\bar{Q}_1(T), \ldots, d\bar{Q}_N(T), d\bar{V}_1(T), \ldots, d\bar{V}_N(T))$ is given by a positive density with respect to Lebesgue measure on a nonempty open set $G_z \subset [0, 1]^N \times \mathbb{R}^N$. Since on E_z each pulse moves freely between the time of collision and T it is enough to show that the conditional dis-

tribution given earlier events of the position and velocity of the ith pulse at time T_i is given by a positive density with respect to Lebesgue measure. This can be easily done by explicitly expressing the position and velocity of the ith pulse at time T_i in terms of γ, $\bar{Q}_i(0)$, and $\bar{V}_i(0)$ and using the equivalence of the distribution of $(\theta_i, U_i)_{i=1}^N$ to Lebesgue measure.[1] We thus have established (iii) (a) of Lemma 1, and now turn to (b).

Let $\Delta_E = \{(z, \gamma) \mid z \in \Delta, \gamma \in E_z\}$ and let $S: \Delta_E \to \Delta$, $S(y, \gamma) = y'$, be the map which maps y onto the configuration y' into which it evolves at time T, if the entry of atoms into $[0, 1]$ during $[0, T]$ is specified by γ. Now $S(y, \gamma)$ and $\partial \mathbf{S}/\partial\gamma$ (y, γ) are continuous (the latter as a matrix valued function), as can be easily seen by explicitly computing $S(y, \gamma)$. Moreover, $\det(\partial \mathbf{S}/\partial\gamma)(y, \gamma)$ is nonzero. We therefore conclude that for every $z \in \Delta$ there exists a neighborhood B_z of z such that for every y, $y' \in B_z$ the measures $\bar{\mathbb{P}}_y(d\bar{Q}_1(T),..., d\bar{Q}_N(T), \quad d\bar{V}_1(T),..., d\bar{V}_N(T))$ and $\bar{\mathbb{P}}_{y'}(d\bar{Q}_1(T),..., d\bar{Q}_N(T), d\bar{V}_1(T),..., d\bar{V}_N(T))$ overlap. We have thus established overlap for the pulse distribution, but this implies overlap for the (unlabeled) molecular distributions.

Model II

Use the same Δ as for Model I. Condition (i) can be verified for configurations for which the atoms in $[0, 1]$ have a nonzero velocity, since with positive probability the atoms pass through the molecules when they collide, and no atoms enter until all the atoms leave $[0, 1]$ in this case. Verification of condition (ii) is the same as for Model I. For checking condition (iii) we define the event E_z as before, except that now it must be explicitly required that the entering atoms defining E_z collide elastically. With this extra condition we are in exactly the same setup as in Model I.

Model III

Let $\bar{\Delta} \subset \Omega^F$ be the set of configurations which contain no atoms in the boundary layer. For convenience we shall regard configurations $z \in \bar{\Delta}$ as labeled for the verification of (iii) of Lemma 1, from which the corresponding result for unlabeled configurations immediately follows. (Only for the verification of (ii) is it necessary to regard configurations as unlabeled.)

Let us denote the mechanical evolution of the molecules when there are no atoms in the boundary layer by $\bar{\phi}_t$. A configuration $z \in \bar{\Delta}$ is determined by specifying the x and y coordinates of the centers of the N molecules and their velocities. Let us denote this by $(x_i, u_i, y_i, v_i)_{i=1}^N$ where u_i and v_i are the x and y components of the velocity, respectively. We start

with the Euclidean topology on $\bar{\Delta}$ and identify precollision and post-collision configurations.

As in the previous models, we produce "overlapping spreading" by sending in atoms, here $2N$, which collide with molecules in such a way that these atoms can undergo no further collisions with molecules. We therefore consider $\tilde{\phi}_t \equiv \tilde{\phi}_t(z, \xi)$, the evolution of molecules arising from the initial molecular configuration z and atomic configuration ξ (outside of $[0, 1]^2$); here ξ describes $2N$ atoms and the evolution is, for simplicity, defined by stipulating that after colliding with a molecule an atom disappears.

Let us consider the projection of the dynamics of molecules onto the x axis. That is, we observe only the evolution of the x coordinates of the molecules as the whole system evolves. Under $\bar{\phi}_t$, the projected motion corresponds to the motion of N hard rods in $[0, 1]$. When two hard rods in this system collide they either pass through each other or exchange velocities (depending on the location of the y coordinates of the corresponding molecules). If we observe the motion of the velocity pulses (*x pulses*) in this system they move freely between collisions. When two pulses are a distance d apart the pulses either jump a distance d in opposite directions or move freely. Similar properties hold for the projection onto the y axis and y pulses. Under $\tilde{\phi}_t$, the pulse velocities are transformed in the usual way during collisions with atoms. We denote by $\alpha(t) = (x_i(t), u_i(t), y_i(t), v_i(t))_{i=1}^N$ the pulse configuration at time t arising from the initial molecular configuration $z \equiv (x_i, u_i, y_i, v_i) \equiv (x_i(0), u_i(0), y_i(0), v_i(0))$. We will call pulses which have not yet been involved in collisions with atoms *original* pulses.

Let $B_1^+ \subset \bar{\Delta}$ be the set of initial molecular configurations z for which a pair of original x pulses and a pair of original y pulses simultaneously collide at some time $t \geqslant 0$, under the evolution $\tilde{\phi}_t(z, \xi)$ for some ξ. Note that, for example, configurations z for which a pair of molecules undergo a "corner collision" under $\bar{\phi}_t$ at a time $t \geqslant 0$ belong to B_1^+. Note also that if $z \in B_1^+$ then the set of ξ's for which the condition defining B_1^+ is satisfied has nonvanishing Lebesgue measure.

Similarly define B_1^- using the time reversed motion and the time reversed notion of "original pulse."

Let $B_2 = \{z \in \bar{\Delta} \mid \text{either } u_i = 0 \text{ or } v_i = 0 \text{ for some } 1 \leqslant i \leqslant N\}$.

Let $B_3^+ \subset \bar{\Delta}$ be the set of initial molecular configurations z for which a pair of original pulses simultaneously hit a wall or a pair of original pulses collides at the same time that an original pulse hits a wall, at some time $t \geqslant 0$, under the evolution $\tilde{\phi}_t(z, \xi)$ for some ξ.

Similarly define B_3^- using the time reversed evolution.

Let $\Delta = \bar{\Delta} - \{[B_1^+ \cup B_3^+) \cap (B_1^- \cup B_3^-)] \cup B_2\}$. In the Appendix we show that Δ is connected.

Suppose the initial configuration $\tilde{z} \in \Omega^F$ is not in Δ and there are some atoms in the boundary layer. Since the number of atoms in the boundary layer cannot increase if no additional atoms are sent in, it is easy to see that (i) of Lemma 1 is satisfied. Since the Gibbs measure μ on Ω is locally equivalent to Lebesgue measure, its normalized restriction σ to Ω^F is also equivalent to Lebesgue measure. Thus we have verified conditions (i) and (ii) for this model. Now we proceed to verify condition (iii).

Let $z \in \Delta$. We may assume that $z \notin B_1^+ \cup B_3^+$ since for $z \notin B_1^- \cup B_3^-$ we may time reverse the following argument.

We first consider the relationship between the molecular and pulse configurations at time t. At $t=0$ they are, of course, the same, but at later times, because of collisions, x and y pulses will be paired differently than the x and y molecular components. Let $\pi(t)$ be the permutation, on N symbols, relating the pulse and molecular configurations at time t.

Now it is not hard to see that the motion of the molecules under $\bar{\phi}_t$ is continuous in the following sense. The times $\{C_i(z)\}$ of collision between molecules and between a molecule and a wall are continuous functions of z. Moreover, if z and z' are close enough at time $t=0$, then they remain close (in the Euclidean topology) at later times except for times t between collisions (i.e., $t \in [C_i(z), C_i(z')]$ for $C_i(z) < C_i(z')$). They remain close even at times $t \in [C_i(z), C_i(z')]$ if the precollision and post-collision configurations are identified.) This follows from the continuity of the free motion and the continuity of the transformation relating post-collision to precollision velocities. (Note that if $z \in B_1^+$ the continuity property described above does not hold. Similar continuity properties hold for $z \notin B_1^-$ with reversed time evolution $(\bar{\phi}_t, t \leqslant 0)$.) Similarly, for the molecular motion under $\tilde{\phi}_t$ we have that for a.e. ξ the collision times $C_i(z', \xi')$ and $\tilde{\phi}_t(z', \xi')$ are continuous functions of z' and ξ' for (z', ξ') in a sufficiently small neighborhood of (z, ξ), if t is not a collision time $C_i(z, \xi)$.

It follows that, for a.e. ξ, $\pi(t)$, as well as $n_i(t)$ and $r_i(t)$ (see Eq. (1) of Appendix II.2), are constant on a sufficiently small neighborhood (depending on t) of (z, ξ), provided t is not a collision time $C_j(z, \xi)$. Thus it suffices to check condition (iii) for pulse configurations, which, to all intents and purposes, may be assumed to evolve freely on such a neighborhood.

Since the dynamics of pulses are one-dimensional we proceed as in Model I. We describe the construction of an event E describing the entry of $2N$ atoms into the barrier, which produces the required spreading and overlap in the pulse distribution. We want to hit each pulse (more precisely the molecule that carries it) with an atom when it gets into the barrier. Since a pulse can jump back a distance d when a faster pulse catches up with it, it is not completely clear that a given pulse will eventually reach the

barrier. We define E in such a way that every original pulse reaches the barrier in a finite time. As in Model I, E is defined in terms of events E_i, $0 \leqslant i \leqslant 2N$. Times T_i and S_i are defined as in Model I. The velocity of the atom which enters the barrier between times S_i and T_i is so chosen that the speed of the pulse after collision is less than $\min_i \{|u_i|, |v_i|\}$, ensuring that all pulses reach the barrier in a finite time.

Let $T = \min\{n\tau \mid n\tau \geqslant T_i + 1, 1 \leqslant i \leqslant 2N\}$. For a.e. ξ, T is not a collision time $C_i(z, \xi)$. Call such a ξ *good* (for z) if it is also of the sort arising in the description of the continuity of $\tilde{\phi}_t$. As in Model I, define E_z, now using only γ's corresponding to good ξ's, Δ_E and $S(z, \gamma)$. Then, just as in Model I, the condition (iii) for pulse configurations follows.

APPENDIX I

We prove that the measure μ (Gibbs state with no interaction between any of the particles) on the composite system in Model II is an invariant measure for the Markov process Q_t: $\int_\Omega \mu(dz)\, Q_t(z, A) = \mu(A)$ for any measurable $A \subset \Omega$. Let $\phi_t^{(1)}$ be the deterministic evolution on Ω corresponding to no interaction between particles (free motion). Let $\phi_t^{(2)}$ be the deterministic evolution for which velocities are transformed according to the elastic collision equation when a molecule collides with an atom. Let $B \subset \Omega$ be the set of configurations for which the position of a molecule and atom coincide and their velocities are post-collision velocities. Given $z \in B$, let $f(z)$ be the time of first collision of an atom and a molecule starting from z and evolving under $\phi_t^{(2)}$. Now $\phi_t^{(1)}$ and $\phi_t^{(2)}$ can be represented by the same flow under the function $f(z)$ (Ref. 3) with base B, but with different base transformations T_1 and T_2.

Let μ_B be the measure on the base which corresponds to μ on Ω. That is, μ is isomorphic, up to normalization, to $\mu_B \times$ Lebesgue measure restricted to the region above the base and under the graph of $f(x)$. Now μ_B is preserved by both T_1 and T_2, since $\phi^{(1)}$ and $\phi^{(2)}$ preserve μ.

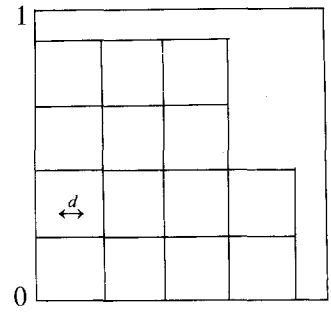
The Markov process α can be similarly represented using f and B, but with the "transformation" on the base now given by a Markov chain rather than a deterministic map. The transition probability for this Markov chain is given as follows:

Given $z \in B$, z goes to $T_1 z$ with probability p, and $T_2 z$ with probability $(1-p)$. Clearly μ_B is an invariant measure for the Markov process on the base, since it is invariant for T_1 and T_2. From this it follows that μ is an invariant measure for α.

APPENDIX II

In this appendix we show that Δ in Model III is connected. We first show that (1) the set of configurations $\bar{\Delta} - B_2$ is connected. Then we show that (2) $B_1^+ \cap B_1^-$ is contained in a countable union of submanifolds of $\bar{\Delta}$, each of which has codimension greater than or equal to 2, so that their removal does not disconnect $\bar{\Delta}$. Similar arguments can be given for $B_1^+ \cap B_3^-$, $B_3^+ \cap B_1^-$, and $B_3^+ \cap B_3^-$.

1. $\bar{\Delta}$ consists of unlabeled molecular configurations of nonoverlapping molecules. Moreover, when two molecules are in contact their post- and precollision velocities are identified. Similar identification is made when molecules are in contact with the walls of the box. It is easy to see that any configuration $z \in \bar{\Delta}$ can be taken to a special configuration z^* by changing z continuously. z^* is the configuration in which $|u_i| = |v_i| = 1$ and the molecules are arranged in vertical stacks, starting from the left:



Note that since the molecules touch each other (and some touch the walls), we need specify only the speeds, not velocities, because of the identification of pre- and post-collision velocities. This is important since B_2 has been removed, so that we cannot pass through configurations in which a velocity component is zero in going from z to z^*. Removal of B_2 will disconnect $\bar{\Delta}$ without the identification. Moreover, if the molecules were labeled, connectedness would depend upon the density.

2. For $z \in B_1^+$ or B_1^- two original x pulses (say the ith and jth) are exactly a distance d apart at time t and two original y pulses (say the pth and qth) are exactly a distance d apart at the same time t. Now the position at time t of the ith x pulse, since it is original, can be expressed as follows

$$x_i(t) = \begin{cases} x_i(0) + u_i(0)\,t + \operatorname{sgn}[u_i(0)]\, n_i(t)\, d - \operatorname{sgn}[u_i(0)]\, r_i(t) \\ \qquad \text{if } r_i(t) \text{ is even} \\ 1 - \{x_i(0) + u_i(0)\,t + \operatorname{sgn}[u_i(0)]\, n_i(t)\, d - \operatorname{sgn}[u_i(0)]\, r_i(t)\} \\ \qquad \text{if } r_i(t) \text{ is odd} \end{cases} \tag{1}$$

where $n_i(t)$ is the net number of jumps in the direction of motion that the pulse makes in $(0, t)$ and $r_i(t)$ is the number of times the pulse is reflected at a wall during $(0, t)$. Thus $x_i(t) = l_{[\mathrm{sgn}[u_i(0)], n_i(t), r_i(t), t]}[x_i(0), u_i(0)]$ where

$$l_{\pm,n,r,t}(x, u) = \begin{cases} x + ut \pm nd \mp r & \text{if } r \text{ is even} \\ 1 - (x + ut \pm nd \mp r) & \text{if } r \text{ is odd} \end{cases}$$

is linear in x, u. We have similar equations for y pulses.

Now the condition that the ith and jth x pulses are a distance d apart at time t can be expressed by the equation

$$|l_{\sigma_i, n_i, r_i, t}(x_i, u_i) - l_{\sigma_j, n_j, r_j, t}(x_j, u_j)| = d \tag{2}$$

where $\sigma_i = \mathrm{sgn}[u_i(0)]$, $n_i = n_i(t)$, $r_i = r_i(t)$,.... We would need the details of the molecular dynamics to determine $n_i(t), r_i(t)$,..., so we overestimate by considering the set $C_{t,x}$ of all initial configurations for which (2) is satisfied for some choice of integers n_i, n_j, r_i, r_j; $\sigma_i, \sigma_j = \pm$; and some i, j, $1 \leqslant i, j \leqslant N$, $i \neq j$. $C_{t,x}$ is a countable union of hyperplanes. We may repeat the above analysis for y pulses, obtaining the set $C_{t,y}$. For $t > 0$ and $s < 0$, $C(t, s) \equiv C_{t,x} \cap C_{t,y} \cap C_{s,x} \cap C_{s,y}$ is a countable union of affine sets, each of which is defined by four linearly independent linear functions and hence has codimension 4. Moreover, $C(0, 0)$ has codimension 2. Thus

$$B_1^+ \cap B_1^- \subset C(0, 0) \cup \bigcup_{\substack{t>0 \\ s<0}} C(t, s)$$

and is thus contained in a countable union of submanifolds of codimension at least 2.

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