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Convection in a Gravitational Field

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We set up a classical stochastic model for the irreversible dynamics of a lattice gas under gravity. We show that for a class of initial states the system converges to equilibrium, which obeys the laws of thermostatics.

KEY WORDS: Lattice gas; convection; gravity.

1. INTRODUCTION

In a challenging article, Dunning-Davies *et al.*[1] have computed the entropy of an ideal gas in a gravitational field; they find that it can become negative, and note that this point is not clear in the literature. The difficulty is traced to one step in the calculation, where a sum in a discrete approximation to the continuum is replaced in the limit by an integral. It is to be expected that a discrete model will not give rise to negative entropies, and it is the purpose of the present work to give a consistent and computable model of a gas in a gravitational field.

We use the field description of the configuration space; thus, we name the points in space, and fix the configuration by listing how many particles sit at each point. The field description automatically treats the particles as indistinguishable, even though classical (Kolmogorovian) probability has been used. The configuration space associated with the union of two regions is the product set of the configuration spaces associated with the two regions. As a result, entropy is an extensive variable, and the theory does not suffer from the Gibbs paradox.

For simplicity we take the system to be noninteracting, the gravitational field to be constant, space to have one dimension, and space-time

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and kinetic energy to be discrete. Thus we are looking at the statistical dynamics of the lattice gas. Each site is either empty or occupied by one particle. This expresses a hard-core repulsion, and is the reason why the equilibrium state turns out to be the Fermi–Dirac ensemble. To describe the dynamics, we use the formalism of ref. 2: if Ω denotes the space of field configurations, then the states make up the convex set $\Sigma(\Omega)$ of probability measures on Ω, and one time-step in the dynamics is given by a possibly nonlinear map τ on $\Sigma(\Omega)$. There are two parts to the dynamics. The first part is a symmetric stochastic map T^* which is affine and describes diffusion in the gravitational field. This map conserves energy, in that it permits transitions only between configurations of the same energy, kinetic + gravitational. The diffusing particles carry some kinetic energy with them, and so heat is transported by convection. The action of T^* thus conserves mean energy. It also conserves mean total number of particles, and is entropy-nondecreasing. On its own, this part of the dynamics cannot be fully mixing, since it does not redistribute the probability between different energy shells; the best it can do is to drive a state with a sharp energy toward the microcanonical state. In particular, we see that if the state of lowest energy is unique, then it cannot be involved in any energy-conserving transitions at all; it forms an energy shell consisting of just one point. Such dynamics makes up a very special subclass of the general type advocated by Penrose.[3] In our model there is a second part to the dynamics, which represents pure dissipation. This implements the idea of *local thermodynamic equilibrium* (LTE) and stems from the remark in ref. 4 that the local dissipative forces in a liquid act many millions of times faster than diffusion or chemical reactions. So to all intents and purposes the local state at each instant must be a grand canonical state, fully described by a local density and beta. Thus, after a particle has diffused, its kinetic energy is instantly redistributed among its modes without net loss or gain in the mean. After redistribution, the probability that its kinetic energy is $j\hbar\omega$ is proportional to $e^{-\beta j\hbar\omega}$, $j = 0, 1, 2, \ldots$. The instantaneous, local value of beta is determined by the requirement that the local mean energy and the local density are unchanged by the dissipation. The dissipation also destroys any correlations between different points. The resulting map is nonlinear and is denoted by Q; it is also entropy-nondecreasing. The map Q thus redistributes the probability among the energy shells. One step in the dynamics is then $p \mapsto \tau p$, where $\tau = Q \circ T^*$. We should not confuse τ with mean-field dynamics, which replaces a field, such as a density, by its mean value, which has no fluctuations. For the same reason, the dynamics is not the same as the deterministic limit.[5,6] The map τ defines by iteration an orbit through the class of local grand canonical states with the same mean total energy and particle number as the initial state. This class is a finite-dimensional compact manifold, and because entropy is a strict Lyapunov function with a unique fixed point, it follows from Lyapunov's direct method that for large times the system converges. It will be shown that the limit is a state of uniform beta and chemical potential, and so obeys the equilibrium condition of thermostatics. At equilibrium the density therefore obeys an approximately exponential law as a funcion of depth (but exhibits a correction at high densities caused by the hard core). The pressure at height x is related to $\log Q_x$ in the usual way, where Q_x is the *local* grand partition function.

2. THE KINEMATICS OF THE MODEL

Let $\Lambda = \{0, 1, 2, ..., N\}$ be space, interpreted as lying in the vertical direction with a distance d between points. At each $x \in \Lambda$ define the local sample space to be

$$\Omega_x = \{\emptyset, 0, 1, 2, ...\} \qquad \text{for each} \quad x \in \Lambda$$

The total sample space is then

$$\Omega = \prod_{x \in \Lambda} \Omega_x$$

A sample point is thus a function $\omega: \Lambda \to \{\emptyset, 0, 1, ...\}$. We interpret the sample point ω as follows: if, for an x, $\omega(x) = \emptyset$, then there is no particle at x. If $\omega(x) = j$, where $j = 0, 1, 2, ...$, then there is one particle at x, its kinetic energy is $j\hbar\omega$, and its potential energy is $dmgx$. Here, g is the acceleration due to gravity and m is the mass of the particle.

We are going to consider diffusion which occurs by the hopping of a particle from an occupied site to an unoccupied site next to it. To enable this to occur with the conservation of energy, we take $\hbar\omega = mgd$. This enables a particle of kinetic energy $j\hbar\omega$ at x to hop to $x+1$, its kinetic energy being reduced to $(j-1)\hbar\omega$. Similarly, a particle can fall one step and gain kinetic energy. If $j > 1$, some kinetic energy is carried with the particle. The model therefore describe the convection of heat.

A state of the system is a probability measure p on Ω: for each configuration ω we are given $p(\omega) \geqslant 0$ such that $\Sigma_\omega p(\omega) = 1$. The set of states on Ω is denoted $\Sigma(\Omega)$. Each state $p \in \Sigma(\Omega)$ defines for each x a local state

$$p_x \in \Sigma(\Omega_x)$$

thus: for $j \in \{\emptyset, 0, 1, ...\}$, put

$$p_x(j) = \sum_{\omega \in \Omega: \omega(x) = j} p(\omega) \qquad (1)$$

This is the marginal distribution of p onto the factor Ω_x. We say that a state p is *independent over* Λ if, writing $\omega = (\omega(0), \omega(1), \ldots, \omega(N))$, we have

$$p(\omega) = \prod_{x \in \Lambda} p_x(\omega(x)), \qquad \text{also written} \quad p = \bigotimes_{x \in \Lambda} p_x \tag{2}$$

We say that a state $p_x \in \Sigma(\Omega_x)$ is a grand canonical state with inverse temperature β and chemical potential μ if the ratio of the probability that the occupied site has kinetic energy $jh\omega$ to the probability that the site is unoccupied is given by the usual Boltzmann factor:

$$p_x(j)/q_x = e^{-\beta(jh\omega + mxdg - \mu)} \qquad \text{for} \quad j = 0, 1, 2, \ldots \tag{3}$$

In (3) we have used the notation q_x for $p_x(\varnothing)$, the probability that the site x is empty. Then $\rho(x) = 1 - q_x \leqslant 1$ is the scaled density. The upper limit, 1, corresponds to the close packing of particles. We denote the grand canonical state at x by p_{β_x, μ_x}.

If the state at x is p_{β_x, μ_x}, then

$$q_x = Q^{-1} = \left(1 + \frac{\exp(-\beta_x mdgx + \beta_x \mu_x)}{1 - \exp(-\beta_x h\omega)}\right)^{-1} \tag{4}$$

Whereas every state has bounded density, there are some states with infinite mean kinetic energy: $\langle \mathcal{T}_x \rangle = \sum_{j=0}^{\infty} jp_x(j)\, h\omega$. Let $\mathcal{D}$ be the affine subspace of $\Sigma(\Omega)$ consisting of states of finite mean kinetic energy at each x. We define the *LTE* map $Q: \mathcal{D} \to \mathcal{D}$ by

$$Qp = \bigotimes_x p_{\beta_x, \mu_x}$$

where μ_x and β_x are uniquely determined by the requirement that $(Qp)_x$ have the same mean density and kinetic energy as p_x. It is known from equilibrium theory that $(Qp)_x$ is the state of greatest entropy among all states with this property, and that the state Qp, which is independent over Λ, is the state of greatest entropy among all states with the given marginals. It follows that Q is entropy-nondecreasing. Recall that the Shannon entropy

$$S(p) = -\sum_{\omega \in \Omega} p(\omega) \log p(\omega)$$

is finite for any state in $\mathcal{D}$, since it is not greater than

$$S(p_{\beta_x, \mu_x}) = \sum_{x \in \Lambda} S(p_{\beta_x, \mu_x})$$

3. THE DYNAMICS OF THE MODEL

The diffusive part of τ is determined by a stochastic map T on the (Abelian) W^*-algebra $\mathscr{A}$ of bounded functions on Ω. The motion of the states is then the dual to this, given by the map T^*: $\Sigma \to \Sigma$ determined by

$$\langle T^*p, f \rangle = \langle p, Tf \rangle, \qquad f \in \mathscr{A}, \qquad p \in \Sigma \subseteq \mathscr{A}^*$$

where $\mathscr{A}^*$ is the dual of $\mathscr{A}$. We note that $\mathscr{A}$ is the completion of Span Ω, the complex vector space with the elements of Ω as a natural basis. This is also a pre-Hilbert space, with scalar product

$$\left\langle \sum c_i f_i, \sum c_j' f_j \right\rangle = \sum c_i^* c_i'$$

The map T acts locally, its matrix elements in the natural basis being zero except between neighboring sites, and kinetic energies differing by one unit. T is a convex sum of terms $T_x(j)$, which acts on Span$(\Omega_x \times \Omega_{x+1})$ and is the identity on the remaining factors. We arrange that $T_x(j)$ causes a hop, with probability $\lambda < 1$, by a particle at x with kinetic energy $(j+1)\hbar\omega$ to $x+1$ with kinetic energy $j\hbar\omega$, provided that the site $x+1$ is empty. It also causes the inverse jump, as it is a symmetric matrix. Thus, we may present $T_x(j)$ as the stochastic matrix

$$T = \begin{array}{c} \\ \omega_1 \\ \omega_2 \end{array} \!\!\begin{array}{c} \begin{array}{cc} \omega_1 & \quad\omega_2 \end{array} \\ \begin{pmatrix} 1-\lambda & \lambda \\ \lambda & 1-\lambda \end{pmatrix} \end{array} \tag{5}$$

In this matrix, the first row and column are labeled by a point $\omega_1 \in \Omega$ such that $\omega_1(x) = j+1$, $\omega_1(x+1) = \varnothing$ and the second row and column are labeled by a point $\omega_2 \in \Omega$ such that $\omega_2(x) = \varnothing$, $\omega_2(x+1) = j$. For simplicity we have chosen λ to be independent of j. The sample point ω_1 is connected to only finitely many points by such matrices. So by forming a convex sum of all the matrices involving ω_1 we get a stochastic matrix taking care of all its possible transitions. Similarly for any other element of Ω. Thus we get an infinite stochastic matrix, any of whose rows or columns has only finitely-many nonzero elements. It therefore acts on Span Ω (the algbraic sum) in a well-defined way. Its adjoint (equal to it) acts on $\mathscr{D} \subseteq \Sigma(\Omega)$ and preserves the mean total energy and total particle number. This follows from the fact that T connects only states with the same number of particles and the same energy. We shall see this explicitly in a while. It follows that T maps $\mathscr{D}$ into $\mathscr{D}$. To find the fixed points of $\tau = Q \circ T$, note that entropy is a strict Lyapunov function for each $T_x(j)$ and is strictly convex, so a fixed point of a convex sum of these stochastic maps is a fixed point of each of them (Tolman's principle of detailed balance is true here). So a fixed point of τ is a grand canonical state that is left unchanged by all the $T_x(j)$.

Take $p \in \Sigma(\Omega)$ to be independent over Λ, and consider the action of $T_x(j)$ on the relevant part of p, namely $p_x \otimes p_{x+1} \in \Sigma(\Omega_x \times \Omega_{x+1})$. As before, put

$$p_x = (q_x, p_x(j)), \qquad p_{x+1} = (q_{x+1}, p_{x+1}(j))$$

Let $p' \in \Sigma(\Omega_x \times \Omega_{x+1})$ be the relevant part of $T_x^*(j)\, p$. Then p' differs from p at only two points, as we see from Eq. (5):

$$p'(j+1, \varnothing) = (1-\lambda)\, p_x(j+1)\, q_{x+1} + \lambda q_x\, p_{x+1}(j)$$
$$p'(\varnothing, j) = \lambda p_x(j+1)\, q_{x+1} + (1-\lambda)\, q_x\, p_{x+1}(j)$$

Now

$$p'_x(j+1) = p'(j+1, \varnothing) + \sum_{l=0}^{\infty} p'(j+1, l)$$
$$= p'(j+1, \varnothing) + \sum_{l=0}^{\infty} p_x(j+1)\, p_{x+1}(l) \tag{6}$$

since $T_x(j)$ does not alter $p(j+1, l) = p_x(j+1)\, p_{x+1}(l)$. Thus

$$p'_x(j+1) = p'(j+1, \varnothing) + p_x(j+1) \sum_{l=0}^{\infty} p_{x+1}(l)$$
$$= (1-\lambda)\, p_x(j+1)\, q_{x+1} + \lambda q_x\, p_{x+1}(j) + p_x(j+1)(1 - q_{x+1})$$
$$= p_x(j+1) - \lambda(p_x(j+1)\, q_{x+1} - p_{x+1}(j)\, q_x) \tag{7}$$

This could have been guessed, since the change in $p_x(j+1)$ can come about from the absence of a particle at x (probability: q_x) and the presence of one at $x+1$ of energy $j\hbar\omega$ [probability: $p_{x+1}(j)$], or from a hole at $x+1$ and a particle of energy $(j+1)\,\hbar\omega$ at x [probability: $p_x(j+1)\, q_{x+1}$]. Our calculation shows that this intuitively natural dynamical law comes from a symmetric stochastic matrix followed by Q, and is therefore entropy-increasing. Similarly we get

$$p'_{x+1}(j) = p_{x+1}(j) + \lambda(p_x(j+1)\, q_{x+1} - p_{x+1}(j)\, q_x) \tag{8}$$

We remark that $p_0(0)$, the ground-state occupation density, does not appear in either equation of motion, and so is a constant of the motion under the Markov chain generated by T^*. It is Q that causes the time dependence of this variable and leads us to equilibrium. We can now verify explicitly that $T_x^*(j)$ conserves the mean energy of the two sites x and $x+1$. For this energy is

$$\begin{aligned}[(j+1)\hbar\omega + dmgx]\,p_x(j+1) + [j\hbar\omega + dmg(x+1)]\,p_{x+1}(j)\\ = (j+x+1)\hbar\omega[p_x(j+1) + p_{x+1}(j)]\end{aligned}$$

and since

$$p_x(j+1) + p_{x+1}(j) = p'_x(j+1) + p'_{x+1}(j)$$

this is conserved; this also shows that the mean number of particles is conserved.

We conclude that $\{\tau'' p\}$ is an orbit in $\Sigma(\Omega)$ with fixed mean energy and particle number, moving through local grand canonical states with entropy as a strict Lyapunov function. The proof of convergence to a fixed point will be complete when we show that there is a unique fixed point. This is done in the next section.

4. THE FIXED POINT

To be stationary, a state must be a fixed point of all $T_x(j)$, and so must satisfy

$$p_x(j+1)\,q_{x+1} = q_x\,p_{x+1}(j) \qquad \text{for all} \quad x, j \geqslant 0 \tag{9}$$

as well as the LTE conditions, Eq. (3):

$$p_x(j+1)/q_x = \exp\{-\beta_x[(j+1)\hbar\omega + mdgx - \mu_x]\} \tag{10}$$

$$p_{x+1}(j)/q_{x+1} = \exp\{-\beta_{x+1}[j\hbar\omega + mgd(x+1) - \mu_{x+1}]\} \tag{11}$$

We note that these conditions do not depend on λ, or on whether λ depends on x or j, as long as $\lambda > 0$. This is usual in statistical dynamics. Combine (9) with (10) and (11) for all j to give $\beta_x = \beta_{x+1}$ and $\mu_x = \mu_{x+1}$, since $mgd = \hbar\omega$. Thus our model of convection is fully mixing, in that it ensures a uniform beta and chemical potential at equilibrium. The value of μ is fixed by the total mean number of particles, provided that it is not greater than $N+1$. We note that beta is fixed by the mean energy, which must be nonnegative. We conclude that there is only fixed point in the set of local grand canonical states with a given mean energy and particle number. This is enough, by Lyapunov's direct method, to establish that the system converges at large time.

It is usual to relate the grand canonical partition function to the pressure; but here the pressure P varies with height. At equilibrium we can, however, relate this to the local grand partition function:

$$P(z) = (\beta d)^{-1} \log Q(x) = (\beta d)^{-1} \log\left(1 + \frac{e^{-\beta(mgz - \mu)}}{1 - e^{-\beta\hbar\omega}}\right) \tag{12}$$

where $z = xd$. In fact, this function is the unique solution to

$$dP(z)/dz = -mg\rho_x/d$$

which takes the value zero when $\rho_x = 0$. For the density, we easily find

$$\rho_x = \rho_0 e^{-\beta mdgx}/[1 - \rho_0(1 - e^{-\beta mdgx})]$$

which is an exponential thinning with height for very small ρ_0. For larger ρ_0 we see a correction to the exponential law caused by the hard core.

5. OUTLOOK

We have constructed a discrete model of a hard-core lattice gas in a gravitational field using the field picture, but remaining within classical probability theory. The discrete-time flow is caused by hopping, followed by local thermalization, without any loss of energy or particles. The entropy is a strict Lyapunov function, as follows from the construction, and the equations for the fixed points are obtained from the principle of detailed balance. It is shown that the fixed point is unique, being determined by the initial values of the mean energy and mean particle number. This is enough to guarantee that the system converges to a fixed point for large times. The fixed point is that given by the usual laws of thermostatics. The usual relationship between the pressure and the grand partition function is shown to lead to the correct relationship between pressure and density in a gravitational field.

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