REDUCED DESCRIPTION IN NONEQUILIBRIUM STATISTICAL MECHANICS*

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INTRODUCTION

I shall present here some general considerations, as well as two specific recent results, in the mathematically rigorous study of nonequilibrium statistical mechanics. The results were obtained jointly with different colleagues whose names will be given in the appropriate sections. Since this paper is, of necessity, very brief, let me direct the reader's attention to a few recent review articles and books on this subject that are of a kindred spirit.[1-5]

The unifying thread of this subject, which I want to emphasize in this talk, is the derivation of a suitable time evolution for a reduced, or contracted, description of a macroscopic system. To be precise, we assume that the microscopic state of our system—which corresponds, in the classical mechanical framework we shall use, to specifying the coordinates and velocities of all the particles in the system—has a well-defined deterministic evolution given by Hamiltonian dynamics. This microscopic state is, however, not what is measured (or even measurable) experimentally. Rather, one looks at some special, smaller set of variables, suitably defined in each case, which give a more coarse-grained, contracted, or reduced description of the system. It is the behavior of these variables that is the subject of our study.[2,5,6]

It is worth noting that we are making the explicit assumption that our system is isolated. While this is never absolutely true in practice, the relevant question is, can a reasonably simple system, such as a container of fluid, in reality be sufficiently well-isolated from its surroundings for the effects of the latter on the observations made during the course of an experiment to be negligible? We take the point of view that this is indeed the case and that it is, therefore, relevant to one's understanding of the nonequilibrium behavior of real systems to study what happens to observables in isolated, idealized, macroscopic model systems.

Of course, the observables, i.e., the reduced set of variables, will not obey a Hamiltonian time evolution. Rather, they will, in general, have to be described by probabilistic laws and only their distribution will satisfy kinetic equations. There are some limits, however, in which suitably defined reduced variables, the so-called macroscopic variables, have such narrow distributions that they themselves obey autonomous deterministic equations.[5,6] These equations will generally be of the dissipative type, e.g., the Navier-Stokes equations of hydrodynamics, which have been so much discussed at this conference. In this sense, the statistical mechanics of nonequilibrium processes may be considered to be a study of the transition from

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Hamiltonian to dissipative dynamics. Unfortunately, we are still very far from even a good understanding of the appropriate physical and mathematical ingredients of such a transition, not to speak of rigorous proofs. We must, therefore, be satisfied with these modest results—results that, I believe, are steps in the right direction.

Formulation of the Problem

Let z represent the microscopic state of a system that evolves according to Hamiltonian dynamics, $z \in \Gamma$, the phase space (or energy surface). Let T^t, $t \in \mathbf{R}$, describe the flow on Γ,

$$z \to T^t z = z_t(z), \tag{1}$$

i.e., a microscopic state z at time t_0 evolves into $T^t z$ at time $t_0 + t$. We now wish to split z into an observable part x and a background part y, $z = (x, y)$ and study the time evolution of the observables, x.

This splitting is to be taken in a very general sense. Thus, x could represent the coordinates, or the coordinates and velocity, of a test particle in a fluid, which could be either a particle dynamically similar to the other particles of the fluid—which has been given a special marker[7] ("painted red")—or a more massive Brownian particle in the fluid.[10] We could also have x represent the coordinates and velocities of all the particles in a given spatial region, or even have x represent the hydrodynamical variables; i.e., we could divide up space into cells and let x represent the particle number, momentum, and energy of each cell.[5]

Generally, the time evolution of x will not be autonomous but will depend also on the initial state of the (hidden) y variables,

$$z_t(z) = (x_t(x, y), \quad y_t(x, y)). \tag{2}$$

We, therefore, have to specify what we mean by "deriving an equation" for the time dependence of the observables (see the appendix).

The appropriate answer to this question is to consider x_t as a stochastic process on the phase space Γ and ask for transition probabilities. Thus, if X is the space of the observables, and A_i, $i = 1, \ldots n$, are some subsets of X, $A_i \subset X$, then we ask for

$$P_n[(A_n, t_n), \ldots (A_1, t_1)/(x_0, t_0)], \qquad t_n \geq t_{n-1} \geq \ldots t_1 \geq t_0, \tag{3}$$

the probability of finding $x_{t_i} \in A_i$, $i = 1, \ldots n$, given that $x_{t_0} = x_0$. Even such transition probabilities can only be specified meaningfully if we are given, a priori, some conditional distribution of the background $y \in Y$ at time t_0, given that $x_{t_0} = x_0$. Let $\hat{\mu}(\mathrm{d}y/x_0)$ be such a conditional distribution; then, for $t_1 = t_0 + t$, the one-time transition probability is given by

$$\begin{aligned} P_1[(A_1, t_1)/(x_0, t_0)] &= \int_{A_1} \mathrm{d}x \int_Y \mathrm{d}y\, \delta[x - x_t(x_0, y)]\hat{\mu}(\mathrm{d}y/x_0) \\ &\equiv \int_{A_1} P_1(\mathrm{d}x, t/x_0), \end{aligned} \tag{4}$$

and there are similar expressions for P_n, $n > 1$.

The conceptual question then reduces to the appropriate choice of $\hat{\mu}(\mathrm{d}y/x_0)$. In some cases, such as that of a Brownian particle in a fluid, it is natural to take for $\hat{\mu}$ its "equilibrium value," i.e.,

$$\hat{\mu}(\mathrm{d}y/x) = \mu_{\mathrm{eq}}(\mathrm{d}x\mathrm{d}y) \Big/ \int_y \mu_{\mathrm{eq}}(\mathrm{d}x\mathrm{d}y') \equiv \frac{\mu_{\mathrm{eq}}(\mathrm{d}x\mathrm{d}y)}{\nu(\mathrm{d}x)}, \tag{5}$$

with μ_{eq} a suitable equilibrium distribution of the full system. For a finite system, this could be the microcanonical distribution, while, in the case where z represents an infinite system (thermodynamic limit), μ_{eq} would be the appropriate Gibbs measure. If the measure μ_{eq} is invariant under the time evolution T^t, then the stochastic process described by P_n in (3) would be homogeneous in time with the invariant distribution $\nu(\mathrm{d}x)$, satisfying the equation,

$$\nu(\mathrm{d}x) = \int P_1(\mathrm{d}x, t/x')\nu(\mathrm{d}x'), \qquad \forall t. \tag{6}$$

In the case of a Brownian particle in an infinite fluid, the measure $\nu(\mathrm{d}x)$ is not normalized if x stands for both position and velocity, since, in equilibrium, the particle is spread out uniformly over space, but this presents no problem. (The velocity part would, however, still have a normalized distribution, i.e., the Maxwellian distribution at a given temperature.) A generalization of (5) to nonequilibrium situations will be considered later.

Having formulated our problem, we are now left with precise but extremely difficult mathematical questions about the properties of the "x-process" for different systems. We can obtain some information about this process from knowledge of the ergodic properties of the classical dynamical system (Γ, T^t, μ).[4] Thus, if $f(x)$ and $g(x)$ are square integrable with the stationary measure $\nu(\mathrm{d}x)$, $f, g \in L_2(\nu)$, then we define

$$\langle f(x_t)g(x)\rangle = \langle f(t)g\rangle = \int f(x_1)P_1(\mathrm{d}x_1, t/x_0)g(x_0)\nu(\mathrm{d}x_0), \tag{7}$$

$$\langle f\rangle = \int f(x)\nu(\mathrm{d}x), \tag{8}$$

$$C(t; f, g) = \langle f(t)g\rangle - \langle f\rangle\langle g\rangle. \tag{9}$$

Then, ergodicity, weak mixing, and mixing of the full system imply, respectively, the successively stronger properties,

$$\frac{1}{\tau}\int_0^\tau \mathrm{d}t\ C(t; f, g) \to 0, \qquad \text{as } \tau \to \infty, \tag{10}$$

$$\frac{1}{\tau}\int_0^\tau \mathrm{d}t\,|C(t; f, g)| \to 0, \qquad \text{as } \tau \to \infty, \tag{11}$$

$$C(\tau; f, g) \to 0, \qquad \text{as } \tau \to \infty, \tag{12}$$

We are interested, however, in proving stronger results for the x-process. In particular, we would like to know under what conditions there is a strong approach to equilibrium, e.g.,

$$P_1(\mathrm{d}x, t/x_0) \to \nu(\mathrm{d}x), \qquad \text{for "almost all" } x_0. \tag{13}$$

Also of great interest is the question of whether or not the x-process is Markovian; i.e., for all $n > 1$,

$$P_n(\mathrm{d}x_n, t_n, \ldots /x_0) = P_1(\mathrm{d}x_n, t_n - t_{n-1}/x_{n-1})P_{n-1}(\mathrm{d}x_{n-1}, t_{n-1}, \ldots /x_0). \tag{14}$$

We expect that (13) and (14) would be valid only in some limits; in particular, the number of degrees of freedom in the background should become infinite, in order to provide a reservoir for the dispersion of information necessary in going from the Hamiltonian dynamics of the microscopic states to the dispersive dynamics of the x-process. This will become clearer in the examples we discuss in the following sections.

Mechanical Model of Heat Bath[7]
(With S. Goldstein, E. Presutti, and K. Ravishankar)

Let $\Lambda \subset \mathbf{R}^d$ be a bounded region in d dimensions with some smooth boundary $\partial\Lambda$ in which there are a fixed number, N, of "blue" particles interacting with each other through a pair potential $v(r)$. These blue particles are confined to the box, Λ, by specular reflection at $\partial\Lambda$. Let this box be immersed in an infinite ideal gas heat bath made up of "white" particles that do not interact with each other, have no impedance to crossing the boundary $\partial\Lambda$ and interact with the blue particles by hard sphere collisions; i.e., there is a hard core pair potential $q(r)$ between white and blue particles, $q(r) = \infty$, $r < a$, and $q(r) = 0$, $r > a$. The blue and white particles have masses M and m, respectively. We now let z stand for the coordinates and momenta of both the white and blue particles—a composite infinite system—and take for μ_{eq} the Gibbs measure with reciprocal temperature β.

A natural choice for the observables, x, would be the positions and velocities of the blue particles—the ones whose evolution from some initial state at $t = 0$ we are really interested in. Such a choice leads, however, to a non-Markovian x-process that is very difficult to investigate. One way around this difficulty is to let x stand for the coordinates and velocities of *all* the particles, blue and white, that are inside Λ. While this means that the number of particles represented by x changes with time, it is clear that $x(t)$ is a stationary Markov process, since once a white particle leaves Λ it never returns there and, thus, there are no memory effects. With this choice of x it is then possible to prove (13), under some technical conditions on the interaction $v(r)$, for almost all x_0 with respect to $\nu(\mathrm{d}x)$ (or w.r.t. Lebesgue measure, since $\nu(\mathrm{d}x) = \rho(x)\mathrm{d}x$). The convergence in (13) is in the variation norm, which is the best that can be expected.

It now follows rather directly that the process involving *only* the blue particles also has strong ergodic properties. We thus have a dynamical model of the approach to equilibrium of a system (the blue particles) in contact with a heat bath. The model can be made more "realistic" by restricting the white particles in Λ to a region near the boundary, $\partial\Lambda$. The interaction between the blue system and the heat bath is then a surface effect.

The model can be generalized to the case where the blue particle system interacts

with several ideal heat baths at different tempertures.[8] We imagine that part of the region near $\partial\Lambda$ is accessible only to white particles at temperature T_1 and another part only to white particles at temperature T_2; e.g., two planes σ_1 and σ_2 perpendicular to the x-axis separate Λ into three regions: to the left of σ_1 there is a semi-infinite bath of white particles described at $t = 0$ by a Gibbs measure with temperature T_1, while to the right of σ_2 there is a semi-infinite bath with temperature T_2. The bath particles can cross $\partial\Lambda$ but not planes σ_1 and σ_2, while the blue particles can cross the planes but not $\partial\Lambda$.

If we again call x the positions and momenta of all particles in Λ and call $y = (y_1, y_2)$ the coordinates and momenta of the left and right reservoirs, then the x-process will be homogeneous and Markovian with $\hat{\mu}(\mathrm{d}y/x) = \mu_1(\mathrm{d}y_1/x)\,\mu_2(\mathrm{d}y_2/x)$. μ_1 and μ_2 are the semi-infinite Gibbs states at temperatures T_1 and T_2. For $T_1 = T_2$ we are in the case of a single reservoir and ν is an equilibrium state. For $T_1 > T_2$, we expect the system to approach, as $t \to \infty$, a stationary state ν in which there will be a heat flow through the system. We can show, in some cases, that this is indeed what happens,[1,8] but much remains to be done.

Mechanical Model of the Ornstein-Uhlenbeck Process[10]
(With D. Dürr and S. Goldstein)

The erratic motion of a macroscopically small but microscopically large particle (one visible in a microscope), in an equilibrium fluid, e.g., pollen in a liquid or a smoke particle in air, is a well-known physical phenomena called Brownian motion. The physical explanation and mathematical description of these erratic motions were first given by Einstein: They are due to the fluctuating force exerted on the B-particle by the fluid atoms and the process is described by a diffusion equation for the displacement of the B-particle. The ultimate mathematical idealization of this phenomena is the Ornstein-Uhlenbeck (OU) process for the velocity of the B-particle V_t,

$$\mathrm{d}V_t = -\gamma V_t\,\mathrm{d}t + \mathrm{d}W_t, \qquad \gamma > 0, \qquad W = \text{Wiener process.}$$

This reduces—in appropriate regimes—to the Wiener process describing only the spatial diffusion of the B-particle.

A little thought shows that the Ornstein-Uhlenbeck process for the B-particle alone can be rigorously derived from the Hamiltonian description of the isolated system consisting of the B-particle plus fluid only in a "suitable" limit—one in which the ratio of the mass of the B-particle to the mass of a fluid particle becomes infinitely large. Such a derivation was indeed given by Holley for a one-dimensional system:[11] the "fluid" consists of point particles of mass m, the B-particle has mass M, and the interaction is via elastic collisions. In the B-limit, $m \to 0$, while the density of fluid particles increases as $\rho/\sqrt{m}$. (Equivalently, $M \to \infty$ and position and time are scaled appropriately.)

In our work, we use a model similar to Holley's in three dimensions: The B-particle is a ball of unit radius and unit mass, while the infinite fluid of point particles of mass m are, at $t = 0$, in conditional equilibrium with the density, $\rho/\sqrt{m}$, and have an independent Maxwellian velocity distribution, $m^{3/2} f(\sqrt{m}\,|v|)$. Let $V_m(t)$ be the

velocity of the B-particle at time t. Then, using the analysis given in the second section of this paper, $V_m(t)$ is a well-defined stochastic process. (The position at any time t is obtained from $V_m(t)$ by integration.) The process is non-Markovian due to the possibility of recollisions both real and virtual. (The latter correspond to collisions that are impossible if the past history of the B-particle is known.) We can now prove the following theorem: For any $\tau > 0$, the sequence of processes $V_m(t)$, $0 \leq t \leq \tau$, with $m \to 0$ and ρ fixed, converges (weakly) to $V(t)$, as described by the OU process with the same initial velocity. The stationary distribution of $\mathbf{V}$ is $f(\mathbf{V})$. (This theorem is actually valid even if the fluid particles do not have a Maxwellian distribution.)

The proof of this theorem consists of two parts: (1) construction of a Markov process $U_m(t)$, whose trajectories are close to the non-Markovian $V_m(t)$, approaching it in probability as $m \to 0$, and (2) proof that $U_m(t) \to V(t)$, the OU process. The second part is based on a demonstration that the generator of the $U_m(t)$ process converges to the generator of the OU process as $m \to 0$.

The construction of $U_m(t)$ is a bit more complicated. It is based primarily on the observation, already made by Holley in the one-dimensional case, that the recollisions that spoil the Markov property of $V_m(t)$ are due solely to the slow fluid particles—as long as the speed of the B-particle is itself small. More precisely, there exists an $\alpha(m)$, $\alpha(m) \to 0$ as $m \to 0$, such that, if we "ignore" collisions with fluid particles whose normal velocity component is less than $\alpha(m)$, then , as long as the B-particle speed is less than $\alpha(m)$, there will be no recollisions that are not ignored. This defines, then, a Markov process $\hat{U}_m(t)$. While this is sufficient in one dimension, the greater instability of the motion in higher dimensions requires that $U_m(t)$ be modified to make it close to $V_m(t)$; i.e., we have to continually adjust the fluid so that the indirect effects of the slow collisions do not build up to spoil the closeness of the two processes. This leads to the $U_m(t)$ Markov process used in the proof.

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References

1. Lebowitz, J. L. 1978. Prog. Theor. Phys., Suppl. **64:** 35.
2. Penrose, O. 1979. Rep. Prog. in Phys. **42:** 129.
3. Spohn, H, & J. L. Lebowitz. 1978. Adv. Chem. Phys. **38:** 109; Spohn, H. 1980. Rev. Mod. Phys. **52:** 569.
4. Sinai, Ya. G. 1976. Introduction to Ergodic Theory, Princeton Math Notes, Vol. 18. Princeton University Press. Princeton, N. J.
5. Krylov, N. S. 1979. Works on the Foundations of Statistical Mechanics, Princeton University Press. Princeton, N. J.
6. See, for example, articles by N. van Kampen, G. Nicolis, and others in Prog. Theor. Phys., Suppl. **64**(1978).
7. Goldstein, S., J. L. Lebowitz, E. Presutti & K. Ravishankar. In preparation.
8. Goldstein, S., J. L. Lebowitz & E. Presutti. 1980. Proc. Conf. on Random Fields. Esztergom, 1979. Bolyoi Janos Publications. Hungarian Academy of Sciences.
9. Penrose, O. 1970. Foundations of Statistical Mechanics. Oxford. Pergamon.
10. Dürr, D., S. Goldstein & J. L. Lebowitz. 1980. Commun. Math. Phys. In press.
11. Holley, R. 1971. Z. Wahr. verw. Geb. **17:** 181.

APPENDIX

There are some interesting examples, often used for various illustrative purposes, in which the evolution of x is, at least in the forward time direction, deterministic. The simplest of these is the baker's transformation where Γ is a unit square, $0 \leq x, y \leq 1$, and the discrete transformation $T^t (t \in Z)$ is

$$T(x, y) = \begin{cases} (2x, \tfrac{1}{2} y), & \text{if } 0 \leq x \leq \tfrac{1}{2} \\ (2x - 1, \tfrac{1}{2}(y + 1)), & \text{if } \tfrac{1}{2} < x \leq 1, \end{cases}$$

so that $x_t = x_t(x)$ for t a positive integer. The evolution of x, which is not invertible, yields a monotone approach to equilibrium for any smooth initial distribution—something not available with the complete description.[9]