Thermalization of a Brownian Particle via Coupling to Low-Dimensional Chaos

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It is shown that a paradigm of classical statistical mechanics—the thermalization of a Brownian particle—has a low-dimensional, deterministic analog: When a heavy, slow system is coupled to fast, deterministic chaos, the resultant forces drive the slow degrees of freedom toward a state of statistical equilibrium with the fast degrees. This illustrates how concepts useful in statistical mechanics may apply in situations where low-dimensional chaos exists.

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Since the study of chaotic dynamics has clarified fundamental issues in classical statistical mechanics [1], it is worthwhile to consider the converse: When does intuition from statistical mechanics carry over to *low-dimensional* chaos? We all know, for instance, that a heavy particle immersed in a heat bath—a Brownian particle—is subject to both an average frictional force and stochastic fluctuations around this average, and that the balance between these two *thermalizes* the particle. Now suppose the "Brownian" particle is coupled to a fast, low-dimensional, chaotic trajectory, rather than to a true heat bath. It is known that the particle then feels a dissipative force [2–4]. Does the particle also (in some sense yet to be defined) "thermalize" with the chaotic trajectory? That is, does the fast chaos behave as a kind of "miniature heat reservoir," exchanging energy with the particle in a way that brings the two into statistical equilibrium? In this paper, we pursue this question by considering the reaction forces acting on a heavy, slow system (our Brownian particle) due to its coupling to a light, fast trajectory. When the fast motion is chaotic, the forces on the particle include a conservative force, and two velocity-dependent forces, one magneticlike, the other dissipative [4]. However (as in the case of coupling to a true thermal bath), there also exists a rapidly fluctuating, effectively *stochastic* force, which has not been studied in detail. We describe an approach which incorporates this force, with the others, into a unified framework. It is shown that the inclusion of this stochastic force—related to the frictional force by a fluctuation-dissipation relation [4]—causes the slow Brownian particle and the fast chaotic trajectory to evolve toward statistical equilibrium.

This result provides some justification for applying statistical arguments (involving, e.g., relaxation toward equipartition of energy) to physical situations of only a few degrees of freedom. A discussion of examples—including one-body dissipation in nuclear dynamics [5], the Fermi mechanism of cosmic ray acceleration [6], and the diffusive transport of comets [7]—where such "thermal" arguments may provide insight into the physics behind more explicit calculations, will be presented in Ref. [8].

As a starting point for our discussion, we consider the framework of Ref. [4], where the position $\mathbf{R}$ of the slow particle parametrizes the Hamiltonian h governing the fast motion: $h = h(\mathbf{z}, \mathbf{R})$, where $\mathbf{z}$ denotes the fast phase space coordinates. (The nature of the fast system will remain unspecified, but we take it to have *a few*, $N \sim 2$, degrees of freedom.) This classical version of the Born-Oppenheimer framework has received considerable interest in recent years [3,4,9]. We assume that if $\mathbf{R}$ were held *fixed*, then a fast trajectory evolving under h would ergodically and chaotically explore its *energy shell* (surface of constant h) in the fast phase space. This sets a fast time scale τ_f which we may take to be the Lyapunov time associated with the fast chaos. A slow time scale τ_s is set by the motion of the slow particle: it is the time required for the Hamiltonian h to change significantly. We assume $\tau_f \ll \tau_s$; thus the fast trajectory $\mathbf{z}(t)$ evolves under a slowly time-dependent Hamiltonian h. The full Hamiltonian for the combined system of slow and fast degrees is given by $H(\mathbf{R}, \mathbf{P}, \mathbf{z}) = P^2/2M + h(\mathbf{z}, \mathbf{R})$, where $\mathbf{P}$ is the momentum of the slow particle, and M is its mass. $(\mathbf{R}, \mathbf{P}, \mathbf{z})$ thus specifies a point in the full phase space of slow and fast variables. It is assumed that surfaces of constant H are bounded in the full phase space.

Given this formulation, the force on the slow particle is $\mathbf{F}(t) = -\partial h/\partial \mathbf{R}$, evaluated along the trajectory $\mathbf{z}(t)$. From the point of view of the slow particle, this force fluctuates rapidly, so it is natural to separate $\mathbf{F}(t)$ into a slowly changing *average* component and rapid fluctuations $\tilde{\mathbf{F}}(t)$ around this average. In Ref. [4], Berry and Robbins introduce an approximation scheme for obtaining the net *average* reaction force. At leading (zeroth) order of approximation, the *ergodic adiabatic invariant* [2] dictates the energy of the fast system as a function of the slow coordinates, and this energy in turn serves as a potential for the slow system, giving rise to a conservative "Born-Oppenheimer" force $\mathbf{F}_0$. At next order, the Berry-Robbins framework yields two velocity-dependent reaction forces: *deterministic friction* ($\mathbf{F}_{\mathrm{df}}$) and *geometric magnetism* ($\mathbf{F}_{\mathrm{gm}}$) [10]. Geometric magnetism is a gauge force related to the geometric phase; deterministic friction (see also Ref. [3]) describes the irreversible flow of energy from the slow to the fast variables. Thus, while at leading order the fast degrees of freedom create a poten-

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tial well for the slow degrees, at first order the fast motion effectively adds a magnetic field, and drains the slow system of its energy.

What about the effects of the rapidly fluctuating component $\tilde{\mathbf{F}}(t)$? If the analogy with ordinary Brownian motion is correct and some sort of statistical equilibration occurs, then $\tilde{\mathbf{F}}(t)$ ought to play a central role in the process. We now describe a framework which incorporates the effects of $\tilde{\mathbf{F}}(t)$ into a description of the slow particle's evolution.

In our framework we consider an *ensemble* of systems. Each member of the ensemble consists of a single slow particle coupled to a single fast trajectory, and represents one possible realization of the combined system of slow and fast variables. Representing this ensemble by a density ϕ in the full phase space, Liouville's equation is

$$\frac{\partial \phi}{\partial t} + \frac{\mathbf{P}}{M} \cdot \frac{\partial \phi}{\partial \mathbf{R}} - \frac{\partial h}{\partial \mathbf{R}} \cdot \frac{\partial \phi}{\partial \mathbf{P}} + \{\phi, h\} = 0, \quad (1)$$

where $\{\cdot,\cdot\}$ denotes the Poisson bracket with respect to the fast variables $\mathbf{z}$. Henceforth, we will ignore all information about the fast trajectory except its energy $E(t) \equiv h[\mathbf{z}(t), \mathbf{R}(t)]$ (which evolves on the slow time scale [2]). Thus what we are really after is the evolution of $W(\mathbf{R}, \mathbf{P}, E, t)$; the distribution of our ensemble in the reduced space where all fast variables other than E have been projected out. In this reduced space, $\tilde{\mathbf{F}}(t)$ is *stochastic*, which in turn suggests that W evolves *diffusively*.

The derivation of an evolution equation for W is somewhat involved, and is sketched in the Appendix. Here we simply state the result

$$\frac{\partial W}{\partial t} = -\frac{\mathbf{P}}{M} \cdot \frac{\partial W}{\partial \mathbf{R}} + \hat{\mathbf{D}} \cdot (\mathbf{u} W) + \frac{\epsilon}{2} \hat{D}_i \left[\Sigma L_{ij} \hat{D}_j \left(\frac{W}{\Sigma} \right) \right]. \quad (2)$$

(Summation over repeated indices is implied.) To explain notation, we first define $\Omega(E, \mathbf{R}) = \int d\mathbf{z}\, \theta[E - h(\mathbf{z}, \mathbf{R})]$. Then $\Sigma \equiv \partial \Omega / \partial E$, and $\mathbf{u} \equiv -(1/\Sigma) \partial \Omega / \partial \mathbf{R}$. Next,

$$\hat{\mathbf{D}} \equiv \frac{\partial}{\partial \mathbf{P}} - \frac{\mathbf{P}}{M} \frac{\partial}{\partial E}. \quad (3)$$

$L_{ij}(E, \mathbf{R})$ is an integrated correlation function defined by Eq. (20). Finally, $\epsilon \sim \tau_f / \tau_s \ll 1$ is an ordering parameter; Eq. (2) is valid to $O(\epsilon)$.

Ω, Σ, and $\mathbf{u}$ have simple interpretations in terms of the *energy shell* $(E, \mathbf{R})$ [the surface *in* $\mathbf{z}$ *space* defined by $h(\mathbf{z}, \mathbf{R}) = E$]. $\Omega(E, \mathbf{R})$ is the volume of $\mathbf{z}$ space enclosed by this shell. $\Sigma(E, \mathbf{R}) = \int d\mathbf{z}\, \delta(E - h)$ represents the statistical weight of the shell—i.e., the amount of fast phase space occupied by this shell—and is useful for evaluating energy shell averages:

$$\langle Q \rangle_{E,\mathbf{R}} = \frac{1}{\Sigma(E, \mathbf{R})} \int d\mathbf{z}\, \delta(E - h)\, Q(\mathbf{z}), \quad (4)$$

where $\langle Q \rangle_{E,\mathbf{R}}$ denotes the average of $Q(\mathbf{z})$ over the energy shell $(E, \mathbf{R})$. Finally, $\mathbf{u}(E, \mathbf{R}) = \langle \partial h / \partial \mathbf{R} \rangle_{E,\mathbf{R}}$.

What does Eq. (2) reveal about the reaction forces on the slow particle? Below, we outline calculations behind the following assertions regarding the content of Eq. (2): (1) it reproduces the average reaction forces $\mathbf{F}_0$, $\mathbf{F}_{\mathrm{df}}$, and $\mathbf{F}_{\mathrm{gm}}$; (2) it describes the effects of the rapidly fluctuating force $\tilde{\mathbf{F}}(t)$; and (3) it predicts that the Brownian particle does indeed thermalize with the fast trajectory. For a more detailed treatment of this problem, see Ref. [8].

First, letting $\mathcal{E} = P^2/2M + E$ denote the total energy of the system, note that $\hat{\mathbf{D}} \mathcal{E} = 0$. Thus $\hat{\mathbf{D}}$ is a constrained derivative: $\hat{\mathbf{D}} = (\partial / \partial \mathbf{P})_{\mathcal{E}}$, where the notation indicates that $\mathcal{E}$, not E, is held fixed. This means that the evolution depicted by Eq. (2) takes place along surfaces of constant $\mathcal{E}$ in $(\mathbf{R}, \mathbf{P}, E)$ space; this is simply a statement of energy conservation.

Next, if we explicitly separate drift terms from diffusion terms, Eq. (2) becomes

$$\frac{\partial W}{\partial t} = -\frac{\partial}{\partial \mathbf{R}} \cdot \left(\frac{\mathbf{P}}{M} W \right) - \frac{\partial}{\partial \mathbf{P}} \cdot (\mathbf{f} W) + \frac{\epsilon}{2} \frac{\partial^2}{\partial P_i \partial P_j} (L_{ij} W). \quad (5)$$

Here, the derivatives with respect to $\mathbf{P}$ are the constrained derivatives $(\partial / \partial \mathbf{P})_{\mathcal{E}}$, and

$$\mathbf{f} = -\mathbf{u}(E, \mathbf{R}) - \epsilon K \cdot \frac{\mathbf{P}}{M}, \quad (6)$$

$$K_{ij}(E, \mathbf{R}) = \frac{1}{2\Sigma} \frac{\partial}{\partial E} (\Sigma L_{ij}). \quad (7)$$

In Eq. (5), $\mathbf{f}$ plays the role of a *drift coefficient* for the slow momentum, and thus represents the *average force acting on the Brownian particle*. A comparison with Ref. [4], Sec. 2 reveals that the first term of $\mathbf{f}$ is the leading (Born-Oppenheimer) force $\mathbf{F}_0$; the second is a sum of the two velocity-dependent forces, $\mathbf{F}_{\mathrm{df}}$ and $\mathbf{F}_{\mathrm{gm}}$: If we express the matrix K in Eq. (6) as the sum of its symmetric and antisymmetric components, then the former gives us $\mathbf{F}_{\mathrm{df}}$, the latter $\mathbf{F}_{\mathrm{gm}}$. Equation (5) thus reproduces the *average* forces $\mathbf{F}_0$, $\mathbf{F}_{\mathrm{df}}$, and $\mathbf{F}_{\mathrm{gm}}$ acting on the Brownian particle.

The last term in Eq. (5) describes the *diffusion of slow momenta* due to the fluctuating force $\tilde{\mathbf{F}}(t)$. The diffusion coefficient is the matrix L, or, more precisely, its symmetric component L^{sym}. By Eq. (7), however, L^{sym} is related to K^{sym}, which, as mentioned, is responsible for the *dissipative* force acting on the slow particle. Equation (7) thus emerges as a fluctuation-dissipation relation. This relation was first noted by Berry and Robbins [4].

Finally, do the forces acting on the slow Brownian particle cause it to thermalize with the fast trajectory? To answer, we must first define what we mean by "thermalization" in the context of the present problem (where temperature plays no role). In ordinary statistical mechanics, *thermalization* means, fundamentally, a *statistical sharing of the total energy X*: After a Brownian particle has long been in contact with a heat bath, the probability for finding it in some state of energy x is simply proportional to the amount of phase space available for the bath to have the remaining energy $X - x$. [This leads to the Boltzmann factor $P \propto \exp(-x/k_B T)$.] Similarly, in the present context, we take the thermalization of slow and fast degrees to mean a statistical sharing of the total energy $\mathcal{E}$: The slow and fast variables have *thermalized*, if the probability for finding the former in a state $(\mathbf{R}, \mathbf{P})$ is simply proportional to the amount of phase space available for the latter to have energy $E = \mathcal{E} - P^2/2M$, namely, $\Sigma(E, \mathbf{R})$. [Thus, $\Sigma(E, \mathbf{R})$ plays the role of the Boltzmann factor here.] For our *ensemble*, this condition implies that an initial distribution $W(\mathbf{R}, \mathbf{P}, E, t_0)$ evolves toward one that has the form

$$W(\mathbf{R}, \mathbf{P}, E, t_\infty) = G(\mathcal{E})\, \Sigma(E, \mathbf{R}) . \tag{8}$$

[$G(\mathcal{E})$ is determined by the distribution of total energies $\eta(\mathcal{E})$ which remains constant.]

We now make some formal arguments to show that Eq. (8) indeed represents the ultimate fate of a distribution W evolving under Eq. (2). Consider an *entropy* $S[W] \equiv -\int W \ln(W/\Sigma)$, where $\int \equiv \int d^3R \int d^3P \int dE$. Using the identity $\partial\Sigma/\partial\mathbf{R} = -(\partial/\partial E)\Sigma\mathbf{u}$, Eq. (2) gives

$$\frac{dS}{dt} = \frac{\epsilon}{2} \int \frac{\Sigma^2}{W} L_{ij} \Gamma_i \Gamma_j \geq 0 , \tag{9}$$

where $\mathbf{\Gamma} = \hat{\mathbf{D}}(W/\Sigma)$. (The inequality follows from the fact that the eigenvalues of L^{sym} are non-negative. A proof of the latter is given in Ref. [8]; less formally, recall that the eigenvalues of L^{sym} are diffusion coefficients, and as such have no business being negative.) Now, the distribution of total energies $\eta(\mathcal{E})$ is conserved as W evolves with time. However, within the set of all densities W corresponding to a particular $\eta(\mathcal{E})$, $S[W]$ is bounded from above [8]. Thus as W evolves with time, the value of $S[W]$ never exceeds a certain upper limit. Since $dS/dt \geq 0$, the entropy must eventually *saturate*, i.e., $\mathbf{\Gamma} \to 0$ as $t \to \infty$ [11]. This in turn implies that

$$W(\mathbf{R}, \mathbf{P}, E, t) \to g(\mathcal{E}, \mathbf{R}, t)\, \Sigma(E, \mathbf{R}) . \tag{10}$$

However, Eq. (10) is a solution of Eq. (2) only if g is independent of both $\mathbf{R}$ and t, so we finally conclude that $W \to G(\mathcal{E})\, \Sigma(E, \mathbf{R})$ asymptotically with time. Thus the ensemble *thermalizes* in the sense defined in the previous paragraph; this is our central result.

This result may be restated as follows [8]. If we start with a fast chaotic, ergodic system, which we then enlarge by coupling a few slow degrees of freedom to the fast ones, then the combined system is itself ergodic (over the surface of constant H) in the enlarged phase space. Thus the property of ergodicity is promoted from the fast phase space to the full phase space of slow and fast variables.

Note also that this thermalization proceeds on a time scale much longer than that characterizing the chaotic evolution (τ_f). This is again similar to the case of ordinary Brownian motion—where such a separation of time scales is central [12]—but stands in contrast to the more familiar examples of low-dimensional chaos (e.g., the $N = 2$ Sinai billiard [13]), where the *mixing time* and the Lyapunov time are comparable.

It is no new thing to say that a chaotic, ergodic trajectory offers a low-dimensional ($N \sim 2$) analog for a truly thermal ($N \gg 1$) system. The novelty of the present work is that it extends this analogy to encompass the important paradigm of Brownian motion, where the thermal system or chaotic trajectory is coupled to a few degrees of freedom characterized by a much longer time scale. Then, in either case, the forces acting on the slow system drive it toward a state of genuine *statistical* equilibrium with its environment.

Finally, it would be interesting to study the quantal version of this problem. Srednicki [14] has recently argued that concepts from quantum chaos may provide a solid foundation for quantum statistical mechanics. The focus in Ref. [14] is on genuinely thermal systems ($N \gg 1$), and does not deal specifically with the case when a few degrees of freedom are slower than the rest. Nevertheless, Srednicki's application of *Berry's conjecture* [15] to the quantal evolution of a classically chaotic system might serve as a guide to a quantal analysis of the purely classical problem studied here. (To the best of my knowledge, no one has looked explicitly at the application of Berry's conjecture to a system which classically exhibits two widely separated time scales.)

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Appendix.—Here we sketch the derivation of Eq. (2) from Eq. (1), using what is essentially (though not explicitly) a multiple-time-scale analysis, and is similar to that of Ref. [4].

To begin, we use our adiabaticity parameter $\epsilon \ll 1$ to formally incorporate into Eq. (1) the assumption that $(\mathbf{R}, \mathbf{P})$ is "slow and heavy," whereas $\mathbf{z}$ is "fast and light":

$$\epsilon \frac{\partial\phi}{\partial t} + \epsilon \frac{\mathbf{P}}{M} \cdot \frac{\partial\phi}{\partial\mathbf{R}} - \epsilon \frac{\partial h}{\partial\mathbf{R}} \cdot \frac{\partial\phi}{\partial\mathbf{P}} + \{\phi, h\} = 0 . \tag{11}$$

With this modification, changes in $(\mathbf{R}, \mathbf{P})$ take place over times of order unity, whereas changes in $\mathbf{z}$ occur over times of order ϵ.

Next, we insert the ansatz $\phi = \phi_0 + \epsilon\phi_1 + \epsilon^2\phi_2 + \cdots$ into Eq. (11) and order by powers of ϵ:

$$\{h, \phi_0\} = 0 , \tag{12}$$

$$\{h, \phi_r\} = \left(\frac{\partial}{\partial t} + \frac{\mathbf{P}}{M} \cdot \frac{\partial}{\partial\mathbf{R}} - \frac{\partial h}{\partial\mathbf{R}} \cdot \frac{\partial}{\partial\mathbf{P}}\right) \phi_{r-1} , \tag{13}$$

$r \geq 1$. Since h commutes only with functions of itself under the Poisson bracket (by assumption of ergodicity), the solution to Eq. (12) has the form $\phi_0(\mathbf{R}, \mathbf{P}, \mathbf{z}, t) = A(\mathbf{R}, \mathbf{P}, h(\mathbf{z}, \mathbf{R}), t)$. To solve for the dependence of A on its arguments, we must examine Eq. (13), with $r = 1$:

$$\{h, \phi_1\} = \left(\frac{\partial}{\partial t} + \frac{\mathbf{P}}{M} \cdot \frac{\partial}{\partial \mathbf{R}} - \frac{\partial h}{\partial \mathbf{R}} \cdot \frac{\partial}{\partial \mathbf{P}}\right)\phi_0 . \qquad (14)$$

Taking a phase space average of both sides over some energy shell $(E, \mathbf{R})$ in the fast phase space, we get

$$0 = \frac{\partial A}{\partial t} + \frac{\mathbf{P}}{M} \cdot \frac{\partial A}{\partial \mathbf{R}} - \mathbf{u} \cdot \hat{\mathbf{D}} A , \qquad (15)$$

where the third argument of A is now E, the energy of the shell over which the average is taken. With the identity $\hat{\mathbf{D}} \cdot \Sigma \mathbf{u} = \mathbf{P}/M \cdot \partial\Sigma/\partial\mathbf{R}$, we rewrite Eq. (15) as

$$\frac{\partial}{\partial t}(\Sigma A) = -\frac{\mathbf{P}}{M} \cdot \frac{\partial}{\partial \mathbf{R}}(\Sigma A) + \hat{\mathbf{D}} \cdot \mathbf{u}\Sigma A . \qquad (16)$$

To solve for ϕ_1, we first use Eq. (15) to rewrite Eq. (14):

$$\{h, \phi_1\} = -\left(\frac{\partial h}{\partial \mathbf{R}} - \mathbf{u}\right) \cdot \hat{\mathbf{D}} A \equiv -\frac{\partial \tilde{h}}{\partial \mathbf{R}} \cdot \hat{\mathbf{D}} A , \qquad (17)$$

adopting the notation of Ref. [4]. [The left side of this equation is evaluated at $(\mathbf{R}, \mathbf{P}, \mathbf{z}, t)$; the value of the third argument of A on the right side is $E = h(\mathbf{z}, \mathbf{R})$.] This has the form $\{h, f\} = g$; the general solution [4] consists of both a homogeneous term $\phi_{1H} = B(\mathbf{R}, \mathbf{P}, h, t)$ and an inhomogeneous term

$$\phi_{1I}(\mathbf{R}, \mathbf{P}, \mathbf{z}, t) = \int_{-\infty}^{0} ds \, \frac{\partial \tilde{h}}{\partial \mathbf{R}}(\mathbf{z}_s, \mathbf{R}) \cdot \hat{\mathbf{D}} A , \qquad (18)$$

where $\mathbf{z}_s(\mathbf{z}, \mathbf{R})$ is the point in phase space reached by evolving a trajectory from $\mathbf{z}$, for a time s, under the Hamiltonian $h(\mathbf{z}, \mathbf{R})$. Note that $\langle \phi_{1I} \rangle_{E,\mathbf{R}} = 0$ for any $(E, \mathbf{R})$.

We solve for B much as we did for A: writing Eq. (13), with $r = 2$, we average each side over an energy shell $(E, \mathbf{R})$. After manipulation, this gives

$$0 = \frac{\partial}{\partial t}(\Sigma B) + \frac{\mathbf{P}}{M} \cdot \frac{\partial}{\partial \mathbf{R}}(\Sigma B) - \hat{\mathbf{D}} \cdot (\mathbf{u}\Sigma B) - \frac{1}{2}\hat{D}_i(\Sigma L_{ij}\hat{D}_j A) , \qquad (19)$$

where

$$L_{ij} = 2\int_{-\infty}^{0} ds \left\langle \frac{\partial \tilde{h}}{\partial R_i}\left(\frac{\partial \tilde{h}}{\partial R_j}\right)_s \right\rangle_{E,\mathbf{R}} . \qquad (20)$$

The first factor inside the angular brackets is evaluated at $\mathbf{z}$, the second at $\mathbf{z}_s(\mathbf{z}, \mathbf{R})$; the average is over all points $\mathbf{z}$ on the energy shell $(E, \mathbf{R})$. It is assumed that the integral converges.

Finally, $W(\mathbf{R}, \mathbf{P}, E, t)$ is given by a projection of ϕ from $(\mathbf{R}, \mathbf{P}, \mathbf{z})$ to $(\mathbf{R}, \mathbf{P}, E)$:

$$W = \int d\mathbf{z} \, \delta(E - h)\phi = \Sigma(E, \mathbf{R})\langle \phi \rangle_{E,\mathbf{R}} . \qquad (21)$$

Since $\langle \phi \rangle_{E,\mathbf{R}} = A + \epsilon B$ (to order ϵ), we combine Eqs. (16), (19), and (21) to obtain the desired result, Eq. (2).

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