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Entropy and *P*-Particle Observables. I. The General Program

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An information-theoretic notion of entropy is proposed for a system of N interacting particles which assesses an observer's limited knowledge of the state of the system, assuming that he or she can measure with arbitrary precision all one-particle observables and correlations involving some number p of the particles but is completely ignorant of the form of any higher-order correlations involving more than p particles. The idea is to define a generic measure of entropy $S[\tilde{\mu}] = -\mathrm{Tr}\,\tilde{\mu}\log\tilde{\mu}$ for an arbitrary density matrix or distribution function $\tilde{\mu}$, and then, given the "true" N-particle μ, to define a "reduced" μ_R^p which reflects the observer's partial knowledge. The result, at any time t, is a chain of inequalities $S[\mu_R^1] \geq S[\mu_R^2] \geq \cdots \geq S[\mu_R^N] \equiv S[\mu]$, with true equality $S[\mu_R^p] = S[\mu_R^{p+1}]$ if and only if the true μ factorizes exactly into a product of contributions involving all possible p-particle groupings. It follows further than (1) if, at some initial time t_0, the true μ factorizes in this way, then $S[\mu_R^p(t)] \geq S[\mu_R^p(t_0)]$ for all finite times $t > t_0$, with equality if and only if the factorization is restored, and (2) the initial response of the system must be to increase its p-particle entropy.

1. MOTIVATION

The object of this paper is to introduce measures of time-dependent nonequilibrium entropy $S(t)$ for a collection of N interacting particles which (1) are reasonable mathematically and (2) accord with the physical intuition that S should increase as the system becomes "more random" or an observer's knowledge of its state becomes "more imperfect."

The underlying assumption of the analysis is that the state of the system can be characterized by an object $\mu(x_1, p_1, \ldots, x_N, p_N; t) \equiv \mu(1, \ldots, N)$, the evolution of which is governed by a linear Liouville equation

$$\partial\mu/\partial t = -L\mu \tag{1}$$

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For a classical system, μ is an N-particle distribution function which depends at each instant of time on the canonical coordinates and momenta x_i and p_i, and L is the Poisson bracket associated with the Hamiltonian $H(t)$, i.e., $L=\{H,\ldots\}$. In the corresponding quantum description, μ is an N-particle density matrix, the x_i and p_i are reinterpreted as operators, and L denotes instead a commutator, so that $L=i[H,\ldots]$.

Given the form of μ at some time t, one can construct reduced distribution functions or density matrices, such as the one-particle $f(i)$ or the two-particle $g(i,j)$, via partial traces; and, by combining algebraically the $f(i)$, the $g(i,j)$, and so forth, one can generate objects $\sigma(1,\ldots,N)$. It will be assumed throughout this paper that any reasonable measure of entropy S is "local in time" in the sense that it can be expressed as the trace of some $\sigma(t)$:

$$S(t)=\prod_{j=1}^{N}\mathrm{Tr}_j\,\sigma(1,\ldots,N;t)\equiv\mathrm{Tr}\,\sigma(1,\ldots,N;t) \tag{2}$$

where Tr_j denotes a trace over the degrees of freedom of the jth particle at time t (so that, e.g., for a classical system, Tr_j is a six-dimensional phase space integral).

The "ordinary" entropy $\mathcal{S}$ is of this form, corresponding to the choice $\sigma=-\mu\log\mu$. It is, however, clear that $\mathcal{S}$ does not accord completely with one's intuition as to the behavior of an entropy. The fact that L is linear and, more importantly, satisfies the Leibnitz rule implies trivially that $d\mathcal{S}/dt\equiv 0$. Even if the system "appears to become more random," $\mathcal{S}$ cannot change with time.

From the information-theoretic point of view, this is easy to understand. If one in fact knows the form of μ at all times, which is necessary to evaluate $\mathcal{S}$, one knows everything about the system, so that there can be no sense in which information is lost as time goes by. If one is to obtain a measure of entropy which exhibits a nontrivial time dependence, one must introduce a σ which contains less information than the total μ. The definition of S must entail some "coarse graining."

The "appropriate" or "natural" coarse graining will of course reflect the actual sorts of measurements which an observer can perform on the system. If, for example, one can measure correlations between pairs of particles, as encapsulated in the full $g(i,j)$, he or she can clearly know more about the system than if only the one-particle $f(i)$ are accessible. And, similarly, if one can locate particles only within an accuracy of ± 1 mm, he or she can know less about the state than if measurements can be made to an accuracy of ± 1 Å.

Given this observation, one might therefore ask: What is really meant when one says that some system has become "more random?" And at least

one reasonable answer to this seems obvious: As a practical matter, an experimenter measures one-particle observables such as the average position or momentum of some particle, and perhaps correlations between pairs of particles, and then says that the system becomes "more random" if the distribution of positions or momenta, or correlations between pairs, become "more random." "Loss of information" and "increasing randomness" can arise because, as a practical matter, one does not follow the evolution of all the higher-order correlations buried in the full density matrix or distribution function μ. One can measure only some "piece" μ_R of the total μ.

From this point of view, one might argue that the prescription to define the entropy should entail a twofold process.

1. Given the sorts of measurements accessible to the observer, construct a "relevant" or approximate μ_R which constitutes the "best guess" as to the form of the total μ. If the physical coarse-graining corresponds to an ignorance of all interparticle correlations, μ_R must involve only the one-particle $f(i)$. If, alternatively, the observer can measure everything about the system, μ_R should coincide with the total μ.

2. Given this reduced μ_R, define an entropy $S[\mu_R(t)]$ by some prescription

$$S[\mu_R(t)] = \mathrm{Tr}\, \sigma(\mu_R(t)) \tag{3}$$

supposing that σ is not some arbitrary function of μ and all the reduced density matrices, but, instead, is a function only of the reduced μ_R.

Ideally, one would also like to demand that the rule to generate S be independent of the specific coarse graining or, more precisely, of the rule to generate μ_R. This would mean, for example, that one has a "natural" way of comparing the entropies associated with two different coarse grainings, and, in particular, of comparing the entropy of some given coarse-grained description with the "total" entropy $S[\mu]$. Thus, in principle, by restricting attention first to one-particle observables, then to two-particle observables, and so forth, one could hope to generate a succession of approximate density matrices $\mu_R^1, \mu_R^2, \ldots$, and use these to construct a collection of entropies $S[\mu_R^1] \equiv S_1, S[\mu_R^2] \equiv S_2, \ldots$. And, if the information-theoretic interpretation of these entropies were to be valid, one would then be able to show a chain of inequalities $S_1 \geq S_2 \geq \cdots \geq S_N$ connecting the p-particle entropies.

This paper will in fact implement this program abstractly, and then consider explicitly the form and evolution of the one-particle S_1. This entails (1) defining a generic rule for the construction of $\sigma(\mu_R)$, (2) ascertaining an appropriate μ_R for the p-particle description, and then (3) showing that these rules lead to a picture in accord with physical intuition. The form and evolution of the two-particle S_2 is considered explicitly in a companion

paper (Kandrup, 1988). At this stage, one can therefore ask what further demands one should impose on these entropies.

One natural requirement to impose is that the N-particle entropy S_N assume the Gibbs (1902) form, i.e., that, given a knowledge of the full N-particle μ, one identify an entropy

$$S_N = -\mathrm{Tr}\, \mu \log \mu \tag{4}$$

This is, e.g., in full accord with the intuition provided by information theory (see, e.g., Khinchin, 1953; Shannon, 1948).

In the absence of correlations, the full many-particle μ factorizes into a product of one-particle contributions $f(i)$ where, explicitly,

$$f(i;t) \equiv \prod_{j\neq i=1}^{N} \mathrm{Tr}_j\, \mu(1,\ldots,N;t) \tag{5}$$

so that the Gibbs entropy reduces to the Boltzmann (1872) form

$$S_{\mathrm{B}} = -\sum_{i=1}^{N} \mathrm{Tr}_i\, f(i) \log f(i) \tag{6}$$

If one knows nothing about any interparticle correlations, it seems natural to suppose that

$$\mu_{\mathrm{R}}^{1}(t) = \prod_{i=1}^{N} f(i;t) \tag{7}$$

i.e., to assert that one's "best guess" is that no correlations are present, and then define a one-particle

$$S_1 = -\mathrm{Tr}\, \mu_{\mathrm{R}}^{1} \log \mu_{\mathrm{R}}^{1} \tag{8}$$

which agrees with Boltzmann's S_{B}.

Another obvious demand is that the entropies S_p increase as interparticle correlations grow. In general, the statement that one state has "more correlations" than another is difficult to quantify, but there is at least one criterion that is easy to impose. If, initially, at some time t_0, the system is totally free of correlations, any interactions among the particles will induce correlations; consequently, if such interactions are present, the initial response of an uncorrelated state should be to increase its entropy. The dynamics should induce a "spontaneous generation of entropy," implying that, for $p \neq N$, $S_p(t_0+\Delta t) > S_p(t_0)$.

If, alternatively, there are no interactions among the particles, an initially uncorrelated state will remain uncorrelated and the entropy should

remain unchanged as the system evolves. More generally, even if there do exist initial correlations, these will evolve trivially in the absence of interactions; consequently, one can demand that dS_p/dt vanish identically for arbitrary initial conditions in the absence of particle interactions.

It should be stressed that, from this point of view, S need not accord completely with the intuition that it increases as the system becomes "more random." A clump of classical noninteracting particles confined initially to some small region in space and then released will eventually spread out to occupy a larger area, and one might argue legitimately that this spreading makes the system "more random." Nevertheless, the measure of entropy S_p defined here will not change during this spreading process. The important point is that S_p makes a distinction between "phase mixing" and "dissipation," or, more precisely, between linear and nonlinear (or nonlocal) evolutions.

In the absence of interactions, each $f(i)$ will satisfy a free Liouville equation

$$\partial f(i)/\partial t = -L_i^0 f(i;\, t) \tag{9}$$

which, at least for a time-independent Hamiltonian H, is time-reversal invariant. Formally, therefore, the Liouville equation predicts that the initially clumped configuration will diffuse over larger areas both as $t \to \infty$ and as $t \to -\infty$. This diffusion represents a type of phase mixing akin to Landau damping in an electrostatic plasma (Case, 1959; Habib *et al.*, 1986) or to the spreading of a wave packet in ordinary quantum mechanics.

When interactions are present, however, the physics is fundamentally different. In this case, the time derivative $\partial f(i)/\partial t$ involves not only $f(i)$, but also (for two-body interactions) the pair correlation $g(i,j)$, and, consequently, one cannot extract a local and linear time-reversible dynamics involving only the $f(i)$. As discussed in Section 5, one *can* solve formally for the evolution of $g(i,j;t)$ in terms of the $f(i)$ at retarded times $t-\tau$, obtaining thereby closed equations for the evolution of the $f(i)$, but this fundamentally nonlocal and nonlinear description leads to an effective "dissipation." Indeed, it is precisely this nonlocal and nonlinear character which induces a nontrivial dS_1/dt.

The notion of entropy S_p developed here treats the evolution of higher-order correlations as fundamental. Processes which generate these correlations may also make the system appear more random at the p-particle level, but this evolution toward a "more random state," albeit important, is considered less fundamental than the concept of information loss.

One principal intuition regarding an entropy is that it should increase monotonically, satisfying an H-theorem $dS/dt \geq 0$. It is therefore important to indicate two physical effects which could destroy this monotonicity.

The more obvious of these is that the system under consideration could be periodic, or very nearly so. Indeed, Poincaré recurrence (Zermelo, 1896) says that most realistic systems are in fact nearly so (although the period may be extremely long!). This is, for example, certainly true for a collection of linearly coupled oscillators if the natural frequencies ω_i and couplings c_{ij} are chosen appropriately. And, if a system is totally periodic, with period T, it follows immediately that $\mu(t_0+T)=\mu(t_0)$. This means that if one starts with an uncorrelated configuration at time t_0, so that $\mu(t_0)=\prod_i f(i;t_0)$, and the entropy initially increases from some S_0, it must eventually reach some maximum value $S_{\max}$ and then decrease to the initial S_0 by time t_0+T. This, however, is hardly surprising. An initially uncorrelated configuration will immediately develop correlations—so that S will increase—but, eventually, if the system is periodic, the correlations will decay, and S must decrease to reflect this fact.

Related to this is another important effect. If, initially, the system is endowed with nontrivial correlations among the particles, it may well be true that $dS(t_0)/dt$ is negative. By endowing the system with "special" initial conditions, one can (at least in principle) induce a "stimulated decrease in the entropy." The physical expectation underlying the notion that the S_p should increase is that no significant initial correlations can exist. When preparing a system initially, one may endow the particles with specified $f(i)$, but, typically, one cannot specify nontrivial correlations among the particles. This is indeed the intuition underlying Boltzmann's (1872) assumption of "initial molecular chaos." In any case, one may argue that, in this sense, the fact that S_p increases reflects initial conditions as well as (or instead of) dynamics. Moreover, even allowing for nontrivial initial conditions, the time derivative dS_p/dt can always be decomposed into a sum of two contributions, one reflecting the initial correlations, which is of indeterminate sign, and another, reflecting the systematic generation of correlations, induced by interactions, which must increase at least initially.

To summarize: The physical intuition that S_p should increase monotonically is based on two assumptions: (1) that the contributions to dS_p/dt reflecting nontrivial initial correlations may be ignored, and (2) that, for many realistic systems, the time scale T associated with any true or approximate periodicity is much longer than any other time scale of interest.

Section 2 of this paper presents a concrete prescription for constructing the p-particle "entropies" S_p, and then shows that they do indeed satisfy most of the aforementioned demands as to the behavior of an entropy. Section 3 discusses explicitly the case when $p=1$. Section 4 considers abstractly the possibility of expressing dS_p/dt, like S_p itself, as a functional of μ_R^p, and Section 5 demonstrates explicitly that this can be done when $p=1$. Section 6 uses the one-particle S_1 to study a system of two linearly

coupled oscillators, and Section 7 uses the results of this model calculation to motivate several general conjectures as to the generic evolution of dS_1/dt.

2. THE *P*-PARTICLE ENTROPIES

Given the true N-particle density matrix or distribution function μ, one can of course compute the observable reduced p-particle quantities

$$f_p(i_1, \ldots, i_p) \equiv \prod_{j \neq i_1, \ldots, i_p} \mathrm{Tr}_j \, \mu(1, \ldots, N) \tag{10}$$

The obvious point, however, is that there are many different N-particle $\tilde{\mu}$'s which would yield the same f_p. The key idea, therefore, is to start with the f_p as the only given observable quantities, and, from these f_p, to construct a "most likely" or "best guess" μ_{R}^p in terms of which to define the p-particle entropy S_p. The proposal here is that one choose that particular μ_{R}^p constructed only from the f_p which maximizes the entropy functional

$$S[\tilde{\mu}] \equiv -\mathrm{Tr} \, \tilde{\mu} \log \tilde{\mu} \tag{11}$$

subject only to the constraints that

$$\prod_{j \neq i_1, \ldots, i_p} \mathrm{Tr}_j \, \tilde{\mu}(1, \ldots, N) = f_p(i_1, \ldots, i_p) \tag{12}$$

[For $p = 2$, $f_2(i, j)$ corresponds to the $g(i, j)$ of Section 1.]

This prescription is a very natural one from the standpoint of information theory, at least for a classical system where μ admits to an unambiguous interpretation as a probability density. Thus, if one discretizes the N-particle phase space into some set of cells Γ_i and considers probabilities p_i that each cell is occupied, simple combinatorics shows that

$$S = -\sum_i p_i \log p_i \tag{13}$$

is essentially the logarithm of the number of states consistent with the probabilities p_i. Maximizing S corresponds, therefore, to choosing the "most likely" μ.

The form of the desired μ_{R}^p is obtained most easily by introducing Lagrange multipliers $\gamma_p(i_1, \ldots, i_p)$ which enforce the constraints (12). Assume for simplicity that the particles under consideration are distinguishable, so that one need not worry about complications associated with Bose or Fermi statistics. It is then natural to demand that f_p be symmetric under particle interchange, so that one is led to consider the quantity

$$S^* = -\mathrm{Tr} \, \tilde{\mu} \log \tilde{\mu} + \sum_{i_1 < \cdots < i_p} \sum \mathrm{Tr} \, \gamma_p(i_1, \ldots, i_p) \tilde{\mu}(1, \ldots, N) \tag{14}$$

The condition that the first variation $\delta^{(1)}S^* = 0$ then implies that

$$1 + \log \mu_R^p = \sum_{i_1 < \cdots < i_p} \gamma_p(i_1, \ldots, i_p) \tag{15}$$

or, with an obvious redefinition of the Lagrange multipliers, that

$$\mu_R^p = \prod_{i_1 < \cdots < i_p} z_p(i_1, \ldots, i_p) \tag{16}$$

In other words, any extremizing μ_R^p must factorize exactly into a product of p-particle groupings.

To verify that there is a unique extremizing μ_R^p factorizing in this fashion and that this μ_R^p is also an entropy maximum is completely trivial. Because the constraints (12) are linear, it suffices to observe that

$$\delta^{(2)}S = -\tfrac{1}{2}\,\mathrm{Tr}(\mu_R^p)^{-1}(\delta\tilde{\mu})^2 < 0 \tag{17}$$

To express the z_p in terms of the f_p so as to evaluate the S_p explicitly is a much more difficult task. When $p = N$, it is clear that $z_p = \mu$, so that S_N coincides with the Gibbs entropy, but, aside from this trivial case, only μ_R^1 is known analytically. However, even without solving for the z_p as functions of the f_p, one can in fact conclude a great deal.

Most obvious is the fact that μ_R^p can coincide with the true $\mu = \mu_R^N$ only if that true N-particle μ has no "irreducible" $(p+1)$-particle correlations. If μ, and hence f_{p+1}, cannot be expressed solely in terms of the f_p, the desired factorization into p-particle pieces is clearly impossible. It thus follows that $S_p \geq S_N$, with equality possible only if μ itself can be realized in terms of the f_p. More generally, since the $(p+1)$-particle description must imply all the results of the p-particle description, a similar logic dictates that

$$S_1 \geq S_2 \geq \cdots \geq S_{N-1} \geq S_N \tag{18}$$

with $S_p = S_{p+1}$ if and only if z_{p+1} factorizes into a product of $p+1$ contributions $\tilde{z}_p$. This means, in particular, that S_p must be strictly greater than S_{p+1} unless the $(p+1)$-particle f_{p+1} can be expressed as combinations of the f_p.

It follows further that if, at some time t_0, μ factorizes into the desired product of p-particle groupings, then, for all $t > t_0$,

$$S_p(t) \geq S_p(t_0) \tag{19}$$

with equality holding if and only if, at time t, the factorization has been restored. To see this is trivial. It follows from (1) that $dS_N/dt \equiv 0$, and thus, by virtue of (18) and the special choice of initial condition, $S_p(t) \geq S_N(t) = S_N(t_0) = S_p(t_0)$. If, in particular, the system is completely free of correlations at time t_0, one knows that $S_1 = S_2 = \cdots = S_N$ initially and that, later, each of the S_p will satisfy the inequalities (18) and (19). One has the further

intuition that, at least initially, S_p will grow faster than S_{p+1}. The sense in which this is true will be discussed for S_2 and S_1 in Kandrup (1988).

One might naively like to conclude further that, whenever the true μ is constructed solely from the f_p, $S_p = S_{p+1} = \cdots = S_N$. However, this is quite false! Consider, e.g., the case when $N=4$ and $p=2$. One then verifies immediately that the density matrix

$$\tilde{\mu}_p = f_2(1,2)f_2(3,4) + f_2(1,3)f_2(2,4) + f_2(1,4)f_2(2,3) - 2f_1(1)f_1(2)f_1(3)f_1(4) \tag{20}$$

built only from the f_2's does indeed satisfy the constraints (12), but, since it is not of the form (16), one knows that $S[\tilde{\mu}_p] > S[\mu_{\mathrm{R}}^2]$. This inequality should reflect the fact that the state $\tilde{\mu}_p$ is "less probable" than μ_{R}^2, reflecting, e.g., a more specialized preparation. This, however, seems reasonable. There can exist many $\tilde{\mu}$'s constructed only from the f_2's that satisfy the constraints (12), and some of them will certainly be "stranger" than others. As illustrated in Kandrup (1988), what makes the special choice μ_{R}^2 "less strange," at least intuitively, is that it corresponds precisely to the "approximate" form of μ suggested by a Kirkwood (1935), or cluster, decomposition.

3. THE SPECIAL CASE $p=1$

As noted already, $z_N = \mu$, so that, given a complete knowledge of the state of the system, one recovers the Gibbs entropy $S_N = -\mathrm{Tr}\,\mu \log \mu$. Alternatively, at the other extreme, when $p=1$, it is easy to see that $z_1(i) = f_1(i)$, so that $\mu_{\mathrm{R}}^1 = \prod_i f_1(i)$ and one recovers the Boltzmann S_{B} of equation (6). Unfortunately, the situation is more complicated for $1 < p < N$, so that, hitherto, exact formulas for the S_p have not been derived. Thus, e.g., choosing each $z_p(i_1, \ldots, i_p)$ to equal $f_p(i_1, \ldots, i_p)$ overcounts the particles in the product μ_{R}^p, and the most naive modifications that one might envision all prove unsatisfactory. Approximate results can, however, be derived perturbatively in the limit of "weak" correlations. Thus, e.g., as described in Kandrup (1988), one can compute S_2 as a power series in λ if one supposes that the two-particle

$$f_2(i,j) = f_1(i)f_1(j)[1 + \lambda\gamma(i,j)] \tag{21}$$

In any event, though, given an analytic expression for S_1, one can evaluate the time derivative dS_1/dt so as to study how S_1 grows from an initially uncorrelated state with $\mu(t_0) = \mu_{\mathrm{R}}^1(t_0)$. Suppose, for specificity, that μ is a classical distribution function and that the particles interact via two-body forces $F(j \to i)$ which derive from a potential $\Phi(|x_{ij}|)$. In this case, as is well known (Bogoliubov, 1946), the Liouville equation implies that

$$\partial f_1(i)/\partial t + (p_i/m)\,\partial f_1(i)/\partial x_i + \sum_{j \neq i} \mathrm{Tr}_j\, F(j \to i)\,\partial f_2(i,j)/\partial p_i = 0 \tag{22}$$

and analogous relations connecting $\partial f_2(i,j)/\partial t$ with all the $f_3(i,j,k)$. These are nothing other than the first two equations of the BBGKY hierarchy.

It follows immediately from (22), with some straightforward integrations by parts, that

$$dS_1(t)/dt = -\sum_i \mathrm{Tr}_i[1+\log f_1(i)]\,\partial f_1(i)/\partial t$$

$$= -\sum_{i\neq j}\sum \mathrm{Tr}_i\,\mathrm{Tr}_j \log f_1(i) F(j\to i)\,\partial f_2(i,j)/\partial p_i \tag{23}$$

an equality which demonstrates explicitly that dS_1/dt cannot be realized as a local functional of μ_R^1. One can, however, evaluate $dS_1(t_0+\Delta t)/dt$ perturbatively for an initial state free of correlations. Thus, by exploiting the fact that

$$f_3(i,j,k;t_0) = f_1(i;t_0)f_1(j;t_0)f_1(k;t_0) \tag{24}$$

one can solve the equation for $\partial f_2(i,j)/\partial t$ to obtain $f_2(t_0+\Delta t)$, and, by inserting that solution into (23), one concludes that

$$dS_1(t_0+\Delta t)/dt = \Delta t\,\mathrm{Tr}[\mu_R^{-1}(t_0)]\,\zeta^2(t_0) > 0 \tag{25}$$

Here

$$\zeta = \sum_{i\neq j}\sum \mathscr{F}(j\to i)\,\partial\mu_R^1/\partial p_i \equiv \mathscr{L}\mu_R \tag{26}$$

where

$$\mathscr{F}(j\to i) \equiv F(j\to i) - \mathrm{Tr}_j f(j) F(j\to i) \tag{27}$$

Analogous results are obtained for a quantum system, provided that $\mathscr{L}$ is appropriately reinterpreted as the difference between the "true" quantum Liouville operator and an "average" $\langle L\rangle$ (Hu and Kandrup, 1987, Section 3).

The obvious point to observe is that

$$S_1(t_0+\Delta t) - S_1(t_0) \propto (\Delta t)^2 \tag{28}$$

a proportionality that reflects the fact that an uncorrelated $\mu_R(t_0)$ at time t_0 maximizes $S_1(t_0)$.

4. NONLOCAL p-PARTICLE SUBDYNAMICS

Equation (23) illustrates an important point, true more generally, namely that in the presence of interactions the time derivative dS_p/dt, unlike $S_p(t)$ itself, cannot be expressed as a functional of $\mu_R^p(t)$. This means that, even though S_p involves only the "physically accessible" pieces of the total μ, dS_p/dt appears to involve other pieces of μ (namely the full f_{p+1}), which, by assumption, are physically inaccessible. This would seem a serious

blemish for a theory of entropy which purports to focus exclusively on accessible quantities; as such, it is natural to ask whether there is any sense in which dS_p/dt can be expressed solely in terms of the f_p.

The answer to this query is a qualified yes. Specifically, to the extent that the "relevant" μ_R^p and the "irrelevant" remainder $\mu_I^p \equiv \mu - \mu_R^p$ are orthogonal in an appropriate sense, μ_R^p may be shown to satisfy a nonlocal "subdynamics," whereby $\partial \mu_R^p(t)/\partial t$ is expressed as a nonlinear functional of μ_R^p at retarded times $t-\tau$. Given such an equation, $dS_p(t)/dt$ can also be realized in terms of $\mu_R^p(t-\tau)$.

It should perhaps be observed that the notion of a "subdynamics" has been interpreted by various authors as meaning different things. Here it is meant simply that, given a "complete" dynamical description, encapsulated in a density matrix μ which satisfies a closed evolution equation like (1), one can construct a "less complete" reduced μ_R which again satisfies a closed (albeit not necessarily local or linear) equation with no explicit reference to $\mu_I \equiv \mu - \mu_R$ except through the propagation of an initial condition $\mu_I(t_0)$. More sophisticated and refined formulations are certainly possible, as exemplified by the approach developed by the so-called Brussels school (Balescu, 1975), but these are superfluous for what follows. The specific implementation described here generalizes the approach of Willis and Picard (1974).

Abstractly, the notion of a subdynamics can be implemented by the construction of an appropriate "projection operator." The idea is in fact quite simple. Given the full N-particle μ and some time-independent rule to generate a reduced μ_R, one is instructed to construct a linear mapping P_{μ_R}, the form of which depends only on μ_R, which satisfies three fundamental requirements:

1. At any given time,

$$P_{\mu_R}\mu = \mu_R \tag{29}$$

2. For any $\xi(1, \ldots, N)$,

$$P_{\mu_R(t_2)}P_{\mu_R(t_1)}\xi(1, \ldots, N) = P_{\mu_R(t_2)}\xi(1, \ldots, N) \qquad \text{for} \quad t_2 \geq t_1 \tag{30}$$

3. At any given time t,

$$[P_{\mu_R}, \partial/\partial t]\mu \equiv 0 \tag{31}$$

The first of these requirements says that the mapping "projects out" from the full μ the desired μ_R. The second implies that, at any given instant of time, P is idempotent, i.e., that, in terms of its action on an arbitrary $\xi(1, \ldots, N)$, P is a "projection operator." This expresses the sense in which μ_R and μ_I really are orthogonal. However, because the rule to generate P depends on the time-dependent $\mu_R(t)$, the operations of time translation

and projection need not necessarily commute, so that this notion of orthogonality might be inconsistent with the fundamental dynamics. What the third requirement says is that, at least when restricted to their action on μ, these operations do effectively commute, so that

$$P(\partial\mu/\partial t) = \partial(P\mu)/\partial t = \partial\mu_R/\partial t \tag{32}$$

This shows that the notion of orthogonality really is consistent with the dynamics.

Given such a P, one concludes immediately that the single Liouville equation (1) is equivalent to the coupled system

$$\partial\mu_R/\partial t + PL\mu_R = -PL\mu_I \tag{33}$$

$$\partial\mu_I/\partial t + (1-P)L\mu_I = -(1-P)L\mu_R \tag{34}$$

At this stage, however, it is easy to solve (34) in terms of an initial condition $\mu_I(t_0)$ to express $\mu_I(t)$ as a functional of $\mu_R(t-\tau)$; by inserting that formal solution back into (33), one concludes that

$$\partial\mu_R/\partial t + PL\mu_R = C[\mu_R] \tag{35}$$

where

$$C[\mu_R] = -P(t)L(t)\mathcal{G}(t, t_0)\mu_I(t_0) + \int_0^{t-t_0} d\tau\, P(t)L(t)\mathcal{G}(t, t-\tau)[1-P(t-\tau)]L(t-\tau)\mu_R(t-\tau) \tag{36}$$

and

$$\mathcal{G}(t_2, t_1) \equiv T\exp\left\{-\int_{t_1}^{t_2} d\tau\,[1-P(\tau)]L(T)\right\} \tag{37}$$

Here $P(t)$ is a shorthand for the operator P_{μ_R} associated with $\mu_R(t)$, and T denotes a time-ordering operator which explains how one is to interpret the exponential in equation (37). The important point is that, given (35), the time derivative of $S[\mu_R]$ can be expressed in terms of $\mu_R(t-\tau)$, with reference to the physically inaccessible μ_I only through the propagation of an initial condition $\mu_I(t_0)$.

It is important to stress that, for an arbitrary μ_R, there is no guarantee that there will exist any P_{μ_R} which satisfies the three requirements (29)–(31). The existence of such a P_{μ_R} actually constitutes an important check that some choice of μ_R is in fact a "natural" one. The fact that, at least for $p = 1$ and 2, the μ_R^p admit to such a construction is therefore an important additional justification for believing that the S_p are reasonable objects to consider. The comparatively trivial case $p = 1$ is treated in Section 5. The case $p = 2$ is already much more complicated, but, as described by Kandrup

and Hill Kandrup (1984), one can in fact construct an analogous subdynamics at the two-particle level. Kandrup (1988) uses that subdynamics to evaluate dS_2/dt. It appears straightforward, albeit messy, to generalize the analysis to $p > 2$.

5. THE TIME DERIVATIVE $dS_1(t)/dt$

Turn now to evaluating $dS_1(t)/dt$. Here the first order of business is to construct explicitly a "projection operator" P which will generate the desired closed equation for μ_R^1. As noted already, there was no guarantee *a priori* that such a P even exists, and, similarly, there is no guarantee that there need exist at most one such P. It is, however, relatively easy to exhibit one such P and then use it to evaluate dS_1/dt. Specifically, one verifies explicitly (Willis and Picard, 1974) that, for the μ_R^1 of equation (7), equations (29)–(31) are satisfied by an operator

$$P \equiv \sum_{i=1}^{N} \left[\prod_{j \neq i=1}^{N} f(j)\,\mathrm{Tr}_j \right] - (N-1) \prod_{j=1}^{N} f(j)\,\mathrm{Tr}_j \tag{38}$$

Given this form for P, it is easy to see that

$$PL\mu_R^1 = \langle L \rangle \mu_R^1 = \sum_{i=1}^{N} \langle L_i \rangle \mu_R^1 \tag{39}$$

where $\langle L \rangle$ denotes an "average" Liouville operator which decouples into a sum of one-particle contributions $\langle L_i \rangle$ involving only the x_i and p_i of the ith particle. In the absence of particle interactions, L itself will decouple into a sum of one-particle L_i^0, and $\langle L_i^0 \rangle = L_i^0$. If, alternatively, interactions are present, $\langle L_i \rangle$ is the sum of the free L_i^0 and an average interaction Liouvillian defined with respect to μ_R itself. This means in particular that the approximate relation $\partial \mu_R^1(t)/\partial t + PL\mu_R^1 \simeq 0$, which obtains by neglecting the contribution $PL\mu_1^1$, is nothing other than the Vlasov equation appropriate for μ_R^1.

As a concrete example, consider a quantum mechanical system with particles coupled via an interaction Hamiltonian involving pairs H_{ij}^I. In this case, the true interaction Liouvillian satisfies

$$L_i^I \xi(1, \ldots, N) = i \sum_{j \neq i} [H_{ij}^I, \xi] \tag{40}$$

whereas the "average" $\langle L_i^I \rangle$ entails a replacement

$$H_{ij}^I \to \mathrm{Tr}_j f(j) H_{ij}^I \tag{41}$$

Given that the Vlasov equation conserves the Boltzmann entropy $S_B = S_1$, it follows that the time derivative

$$dS_1/dt = -\mathrm{Tr}(1+\log \mu_R^1)\,\partial\mu_R^1/\partial t = -\mathrm{Tr}(1+\log \mu_R^1)C[\mu_R^1] \qquad (42)$$

reflects only the "deviations from mean field conditions" buried in $C[\mu_R^1] = PL\mu_R^1$. Using equations (36), (38) and (39), it is then straightforward to show [see Kandrup (1987) for a discussion of the corresponding field-theoretic case] that

$$dS_1(t)/dt = -\mathrm{Tr}\,\mu_R^{-1}(t)D(t)\mathcal{G}(t, t_0)\mu_I(t_0) + \int_0^{t-t_0} d\tau\,\mathrm{Tr}\,\mu_R^{-1}(t)\zeta(t)\mathcal{G}(t, t-\tau)\zeta(t-\tau) \qquad (43)$$

where

$$D = L^I\mu_R^1, \qquad \zeta = (L-\langle L\rangle)\mu_R^1 \qquad (44)$$

It follows that, in the absence of initial correlations, $dS_1(t_0)/dt \equiv 0$ but, as correlations evolve after a time Δt, dS_1/dt will be positive and the entropy will begin to increase in the fashion predicted by equation (25). This is the "spontaneous generation of entropy" induced by the evolving dynamics. If, however, $\mu_I^1(t_0) \neq 0$, $dS_1(t_0)/dt$ certainly need not vanish. Rather, one sees that

$$dS_1(t_0)/dt = \mathrm{Tr}\,\mu_R^{-1}(t_0)D(t_0)\mu_I(t_0) \qquad (45)$$

Nontrivial $\mu_I^1(t_0)$ can induce "stimulated changes in the entropy" of indeterminate sign.

6. A SIMPLE EXAMPLE

Three conclusions have been reached regarding the time evolution of $S_p(t)$ from an uncorrelated state at time t_0. (1) For all later times t, $S_p(t) \geq S_p(t_0)$, with equality if and only if, at time t, once again μ factorizes into a product of p-particle groupings. (2) At least when $p = 1$ or 2, $dS_p(t)/dt$ can be realized as a nonlocal functional of $\mu_R^p(t-\tau)$. (3) When $p = 1$, for short times, $S_p(t) - S_p(t_0)$ grows as $(t-t_0)^2$.

However, nothing conclusive has been said about the longer time evolution of the S_p. One has the intuition that S_p will increase "as correlations grow," but one also knows that most realistic systems are periodic, or nearly periodic (although the period may be very large!), so that, eventually, correlations can decay and S_p decrease. The object here is to explore the effects of such periodicities by studying $S_1(t)$ for the simple example

of two classical, linearly coupled oscillators characterized by the time-independent Hamiltonian

$$H = \sum_{i=1}^{2} \tfrac{1}{2}(p_i^2 + \omega^2 q_i^2) + c q_1 q_2, \qquad |c| < \omega^2 \tag{46}$$

Motions derived from this H will be doubly periodic with squared frequencies

$$\Omega_{\pm}^2 = \omega^2 \pm c > 0 \tag{47}$$

The general solution of the particle equations can be written out explicitly. Thus, setting

$$\Delta \equiv (\omega^2 + c)^{1/2} - \omega \tag{48}$$

one concludes that, in terms of initial conditions p_i^0 and q_i^0 at $t_0 = 0$,

$$\begin{aligned} q_i(t) = {} & q_i^0 \cos \omega t \cos \Delta t \\ & + (p_i^0/\Omega_+\Omega_-)(\omega \sin \omega t \cos \Delta t - \Delta \cos \omega t \sin \Delta t) \\ & - q_j^0 \sin \omega t \sin \Delta t \\ & + (p_j^0/\Omega_+\Omega_-)(\omega \cos \omega t \sin \Delta t - \Delta \sin \omega t \cos \Delta t) \end{aligned} \tag{49}$$

and

$$\begin{aligned} p_i(t) = {} & p_i^0 \cos \omega t \cos \Delta t \\ & - q_i^0(\omega \sin \omega t \cos \Delta t + \Delta \cos \omega t \sin \Delta t) \\ & - p_j^0 \sin \omega t \sin \Delta t \\ & - q_j^0(\omega \cos \omega t \sin \Delta t + \Delta \sin \omega t \cos \Delta t) \end{aligned} \tag{50}$$

where $i = 1$ or 2 and $j \neq i$. Given these explicit formulas, one can evaluate the evolution of an initial $\mu(t_0 = 0)$; and, given $\mu(t)$, one can compute $\mu_{\mathrm{R}}^1(t)$ and the associated $S_1(t)$.

As a concrete example, consider an initial state

$$\mu(t_0 = 0) = (\beta\omega/2\pi)^2 \exp(-\beta H_0) \tag{51}$$

which would correspond to equilibrium in the absence of the coupling cq_1q_2. Here one calculates explicitly that

$$S_1(t) = 2 - 2\log(\beta\omega/2\pi) + \log(ab - c^2) \equiv S(0) + \log(ab - c^2) \tag{52}$$

where

$$a = \cos^2 \omega t \cos^2 \Delta t + \sin^2 \omega t \sin^2 \Delta t + \frac{\omega^2(\omega^2+\Delta^2)}{(\omega^2-\Delta^2)^2}(\sin^2 \omega t \cos^2 \Delta t + \cos^2 \omega t \sin^2 \Delta t) - \frac{4\omega^3}{(\omega^2-\Delta^2)^2} \sin \omega t \cos \omega t \sin \Delta t \cos \Delta t \tag{53}$$

$$b = \cos^2 \omega t \cos^2 \Delta t + \sin^2 \omega t \sin^2 \Delta t + (1+\Delta^2/\omega^2)(\sin^2 \omega t \cos^2 \Delta t + \cos^2 \omega t \sin^2 \Delta t) + (4\Delta/\omega) \sin \omega t \cos \omega t \sin \Delta t \cos \Delta t \tag{54}$$

$$c = \frac{\Delta^2}{(\omega^2-\Delta^2)} \sin \omega t \cos \omega t (\sin^2 \Delta t - \cos^2 \Delta t) + \frac{\Delta(2\omega^2-\Delta^2)}{\omega(\omega^2-\Delta^2)}(\cos^2 \omega t - \sin^2 \omega t) \sin \Delta t \cos \Delta t \tag{55}$$

When $t=0$, $ab=1$ and $c=0$, so that one recovers the standard entropy S_0 for two free oscillators, but, for $t>0$, S_1 initially increases and then exhibits a complicated doubly periodic time dependence.

One obvious point to note is that the total S_1 will itself be strictly periodic if the frequencies Ω_+ and Ω_- are commensurate. Moreover, even if Ω_+ and Ω_- are not commensurate, there will exist times t at which the system has returned arbitrarily close to its initial state, so that $S_1(t) - S_1(t_0)$ is arbitrarily small.

The second important point is that this long-term periodicity would be lost completely if, in the spirit of ordinary kinetic theory, one tried to realize $S_1(t)$ perturbatively in powers of the coupling c. Thus, for example, working to $O(c^2)$, one sees that

$$S \simeq S(0) + (c^2/\omega^4) \sin^2 \omega t \tag{56}$$

In this approximation, the complicated Ω_+ and Ω_- periodicities are lost and S_1 simply oscillates with a period π/ω that reflects the unperturbed motion. If, alternatively, one works to $O(c^4)$, one begins to see deviations from this unperturbed periodicity, although the "true" periodicities $\Omega_\pm$ are still lost.

It is also instructive to obtain (56) directly from equation (43). Working to $O(c^2)$, one concludes quite generally that, if $\mu_1^1(t_0) = 0$,

$$dS(t)/dt = \int_0^t d\tau \, \mathrm{Tr} f^{-1}(1; t) f^{-1}(2; t) \zeta(t) \zeta(t-\tau) \tag{57}$$

where, in terms of the average value

$$\langle q_i \rangle \equiv \mathrm{Tr}_i f(i) q_i \tag{58}$$

one has the quantity

$$\zeta(t) = c[(q_1 - \langle q_1 \rangle)\, \partial/\partial p_2 + (q_2 - \langle q_2 \rangle)\, \partial/\partial p_1] f(1) f(2) \tag{59}$$

and $\zeta(t-\tau)$ is evaluated at retarded time $t-\tau$ in the approximation that the oscillators follow unperturbed $c=0$ periodic trajectories. The special initial condition implies that, to lowest order, $\langle q_i \rangle = 0$, that $f(1;\, t) = f(i;\, 0)$, and that most other expectation values, such as $\langle q_1 p_1 q_2 p_2 \rangle$, vanish identically. Thus, one concludes that

$$dS_1/dt = \beta^2 c^2 (\langle q_1^2 \rangle \langle p_2^2 \rangle + \langle q_2^2 \rangle \langle p_1^2 \rangle) \int_0^t d\tau\, (\cos^2 \omega\tau - \sin^2 \omega\tau)$$

$$= (2c^2/\omega^3) \sin \omega t \cos \omega t \tag{60}$$

in agreement with equations (25) and (56).

This simple calculation reveals two important conclusions. (1) If the coupling c is chosen judiciously, the entire system, and hence $S(t)$, will evidence a periodic behavior. Moreover, even if the coupling is not so chosen, there will exist times t where $S_1(t) - S_1(t_0)$ is arbitrarily small. (2) These long-term effects will be lost completely in a simple perturbation expansion. This long-term (near) periodicity, which manifests Poincaré recurrence, is intrinsically nonperturbative.

These conclusions reflect (1) the true periodicity of the unperturbed $c=0$ trajectories and (2) the fact that the true motion is doubly periodic. It is therefore instructive to consider the special case with $\omega^2 = -c = \lambda^2/2 > 0$, where

$$H = \sum_{i=1}^{2} \tfrac{1}{2} p_i^2 + \frac{\lambda^2}{4} (q_1 - q_2)^2 \equiv H_0 + H_1 \tag{61}$$

Here the "natural" unperturbed H_0 corresponds to free rectilinear motion, so that is it instructive to consider the entropy S_1 associated with an initial

$$\mu(t_0 = 0) = (\beta\Omega/2\pi)^2 \exp\left[\tfrac{1}{2}\beta \sum_{i=1}^{2} (p_i^2 + \Omega^2 q_i^2)\right] \tag{62}$$

This corresponds to an initial Maxwellian distribution of velocities for a system localized in a spatial region of dimensions $\sim(\beta\Omega^2)^{-1}$. In this case,

$$S_1(t) = 2 - 2\log(\beta\Omega/2\pi) + \log(ab - c^2) = S(0) + \log(ab - c^2) \tag{63}$$

where

$$a = \tfrac{1}{2}(1+\cos^2 \lambda t)+\tfrac{1}{2}(\Omega/\lambda)^2(\lambda^2 t^2+\sin^2 \lambda t) \tag{64}$$

$$b = \tfrac{1}{2}(1+\cos^2 \lambda t)+\tfrac{1}{2}(\lambda/\Omega)^2 \sin^2 \lambda t \tag{65}$$

$$c = \tfrac{1}{2}\Omega t - \tfrac{1}{2}(1-\Omega/\lambda) \sin \lambda t \cos \lambda t \tag{66}$$

For small $t \ll \lambda^{-1}$, one sees that

$$S_1 \simeq S(0)+(\lambda^2 t)^2/(2\Omega^2) \tag{67}$$

a result consistent with equation (43), but, in general, as t grows, the time dependence of S_1 becomes more complicated, exhibiting the frequency associated with oscillations about the center of mass. Here, however, although dS_1/dt need not be monotonic, it is clear that $S_1(t)$ can never return to its initial value $S(0)$. Indeed, as $t \to \infty$, $S_1(t)$ actually diverges logarithmically. This does not, however, imply that dS_1/dt is monotonic as $t \to \infty$. Rather, one sees that

$$dS_1(t)/dt \to [2\lambda(\lambda^2-\Omega^2) \sin \lambda t \cos \lambda t]/(\Omega^2 \cos^2 \lambda t+\lambda^2 \sin^2 \lambda t) \tag{68}$$

These general conclusions are altered significantly if one supposes instead that $\lambda^2 \equiv -\eta^2 < 0$. In this case, $S_1(t)$ diverges linearly as $t \to \infty$ and $dS_1(t \to \infty)/dt \to 4\eta$.

These asymptotic forms are both easy to understand. When $\lambda^2 > 0$, the q_i will diverge as t, so that $H_0(t) \sim t^2$ and the entropy $S_1 \sim \log H_0(t) \sim \log t$. Alternatively, when $\lambda^2 < 0$, both the q_i and the p_i will diverge as $\exp(\eta t)$, so that $H_0(t) \sim \exp(2\eta t)$ and $S_1 \sim \log H_0(t) \sim t$. In each case, $q_i(t \to \infty)$ diverges for all finite $q_i(t_0 = 0)$, so that the conditions for the validity of the Poincaré recurrence theorem are not met.

7. PERTURBATIVE FORMULAS YIELDING ENTROPY INCREASE

The periodic phenomena observed in Section 6 manifest the fact that a system initially free of correlations will tend immediately to generate correlations, but that, later, there can exist phases of the evolution during which these correlations actually "decay." Such a decay of correlations seems, however, contrary to physical intuition and practical experience; consequently, it is natural to ask why it is that one does not actually see this sort of behavior in realistic large-scale systems. Any answer to this question would appear to involve at least two basic observations.

1. At least in the weak coupling limit, the short-time wiggling that is manifest, e.g., in (56) is only a reflection of the fact that the unperturbed motions are themselves periodic. For many realistic systems, however, the "natural" unperturbed motion is in fact rectilinear rather than oscillatory, so that there is no short-term unperturbed periodicity. The interactions

among the particles may well induce new periodicities, but, at least for weak couplings, these should be very long. Thus, in Section 6, when perturbing about orbits with period $T_0 = 2\pi/\omega$, one acquired an additional periodicity $T_1 = 2\pi/\Delta \simeq 4\pi\omega/|c|$, which, for small $|c|$, is very much larger than T_0. Similarly, when $\omega^2 = -c = \lambda^2/2$, one had no unperturbed periodicity and obtained only an induced $T_1 = 2\pi/\lambda$, which, for small $|\lambda|$, should again be extremely large.

2. For realistic systems, any long-term true or near periodicity manifesting Poincaré recurrence should occur on a time scale t^* much greater than any other time scale of interest. Systems may well evolve back to a nearly uncorrelated state, at least in principle, but the time before this happens will in general be extremely long. This is the essence of Boltzmann's (1896) response to Zermelo's (1896) proof of the Poincaré recurrence theorem. Indeed, one might argue further that if this t^* is sufficiently long, even very weak interactions of a nearly isolated system with its surroundings will tend to accumulate, so that the deterministic statistical evolution embodied in the Liouville equation, which implies the recurrence, must, as a practical matter, be modified somewhat.

As illustrated in Section 6, both Poincaré recurrence and induced multiple periodicities can be lost easily in the context of perturbation theory and consequently one might conjecture that, in the context of such a perturbation expansion, the evolution of many nearly periodic systems will in fact appear to satisfy an H-theorem inequality like $dS_1/dt \geq 0$. Indeed, this is really true! If one views classical two-body interactions as weak, short-range perturbations about free, rectilinear trajectories, it follows that, to lowest nontrivial order, $f_1(t)$ satisfies the standard Landau (1937) equation. As is well known (see, e.g., Balescu, 1975), this Landau equation implies that $dS_1/dt \geq 0$.

That this is the case is relatively easy to see. Simply consider a classical system characterized by an $H_{ij}^{\mathrm{I}} = \lambda_{ij}\Phi(|x_{ij}|)$, where the λ_{ij} are small, and evaluate dS_1/dt consistently in a perturbative expansion to $O(\lambda^2)$. The net result is that

$$dS_1/dt = \tfrac{1}{2}\sum_{i\neq j=1}^{N}\sum (\lambda_{ij})^2 \int d^3x \int d^3p_i \int d^3p_j \int d^3k\, \delta(k\cdot P_{ij})|\xi_{ij}|^2 \quad (69)$$

where, in terms of the Fourier-transformed $\Phi_{ij}(|k|)$ and the quantities

$$P_{ij} \equiv p_i - p_j, \qquad \partial^{ij} \equiv \partial/\partial p_i - \partial/\partial p_j$$

one has

$$\xi_{ij} = \Phi_{ij}(|k|) f^{-1/2}(x, p_i; t) f^{-1/2}(x, p_j; t) \times [k\cdot \partial^{ij} f(x, p_i; t) f(x, p_j; t)] \quad (70)$$

The time derivative dS_1/dt can never be negative.

If, moreover,

$$\lim_{|k|\to 0} [k^4 \Phi_{ij}(|k|)^2] = 0 \tag{71}$$

a condition holding for potentials $\Phi(|r|)$ which, at large r, fall off faster than r^{-1}, equality can obtain in (68) if and only if the term in brackets in equation (70) is proportional to $k \cdot P_{ij}$. Thus, if one demands that the integral $\int d^3p f(x, p, t)$ be finite, it follows that S_1 must be increasing unless it has achieved a special end state with

$$f_0(x, p_i) \propto \exp(-\beta p_i^2/2) \tag{72}$$

where β is independent of i. This is precisely Boltzmann's H-theorem!

Alternatively, if (71) does not hold, the situation is more complicated. In this case, one can still show that S_1 must never decrease, but now there is in fact no special end state (72). For a long-range interaction like gravity, even a naive perturbation expansion precludes the possibility of any "equilibrium" state (Prigogine and Severne, 1966; Kandrup, 1985).

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REFERENCES

Balescu, R. (1975). *Equilibrium and Nonequilibrium Statistical Mechanics*, Wiley, New York.

Bogoliubov, N. (1946). *Problemi Dynamitcheskij Theorie Statisticheskey Physiki* [English transl., *Studies in Statistical Mechanics*, Vol. 1, DeBoer and Uhlenbeck, eds., North-Holland, Amsterdam (1962), p. 5].

Boltzmann, L. (1872). *Wien Berichte*, **66**, 275.

Boltzmann, L. (1896). *Annalen der Physik*, **57**, 773.

Case, K. M. (1959). *Annals of Physics*, **7**, 349.

Gibbs, J. W. (1902). *Elementary Principles in Statistical Mechanics*, Yale University Press, New Haven, Connecticut.

Habib, S., Kandrup, H. E., and Yip, P. F. (1986). *Astrophysical Journal*, **309**, 176.

Hu, B. L., and Kandrup, H. E. (1987). *Physical Review D*, **35**, 1776.

Kandrup, H. E. (1985). *Astrophysics and Space Sciences*, **112**, 215.

Kandrup, H. E. (1987). *Journal of Mathematical Physics*, **28**, 1398.

Kandrup, H. E. (1988). *International Journal of Theoretical Physics*, submitted.

Kandrup, H. E., and Hill Kandrup, S. (1984). *Astrophysical Journal*, **277**, 1.

Khinchin, A. I. (1953). *Uspekhi Matematischeskikh Nauk*, **8**, 3.

Kirkwood, J. G. (1935). *Journal of Chemical Physics*, **3**, 300.
Landau, L. D. (1937). *Soviet Physics-JETP*, **7**, 203.
Prigogine, I., and Severne, G. (1966). *Physica*, **32**, 1376.
Shannon, C. E. (1948). *Bell System Technical Journal*, **27**, 370.
Willis, C., and Picard, R. (1974). *Physical Review A*, **9**, 1343.
Zermelo, E. (1896). *Annalen der Physik*, **57**, 485.