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Entropy and *P*-Particle Observables. II. The Two-Particle Entropy S_2

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This paper defines, and then evaluates perturbatively, an information-theoretic notion of entropy S_2 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 pairs of particles, but is completely ignorant of the form of any higher-order correlations involving three or more particles. By construction, this $S_2(t)$ involves only the reduced two-particle distribution functions, or density matrices, $f_2(i, j)$ at time t, and, though the implementation of a "subdynamics," $dS_2(t)/dt$ can be realized in terms of the $f_2(i, j)$'s at retarded times $t - \tau$. A similar line of reasoning demonstrates that the "most probable" three-particle $f_3(i, j, k)$ consistent with a knowledge of the f_2's is precisely that f_3 suggested by the Kirkwood, or cluster, decomposition.

1. RECAPITULATION AND MOTIVATION

The objective of this and a companion paper (Kandrup, 1988*a*, henceforth denoted Paper I) is to define information-theoretic measures of entropy appropriate for an observer who, in probing the state of some N-particle system, can measure with arbitrary precision the expectation values of all one-particle observables, and correlations involving some number p of the particles, but is totally ignorant of the form of any correlations involving more than p particles.

It is assumed that the system under consideration is characterized by an N-particle distribution function, or density matrix, μ, the evolution of which is governed by a Liouville equation

$$\partial\mu/\partial t = -L\mu \tag{1.1}$$

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The restriction to p-particle observables means, however, that one can only access the reduced p-particle density matrices

$$f_p(i_1, \ldots, i_p) \equiv \prod_{j \neq i_1, \ldots, i_p} \mathrm{Tr}_j \, \mu(1, \ldots, N) \tag{1.2}$$

where Tr_j denotes a trace over the degrees of freedom of the jth particle. The object is to construct from these f_p's a suitable measure of entropy S_p.

The intuition is the following. If the system is characterized by only minimal correlations involving more than p particles, a knowledge of the f_p's provides an excellent characterization of the state of the system, so that the p-particle entropy S_p should be small. Alternatively, if significant higher-order correlations are present, a knowledge of the f_p's provides only a mediocre characterization of the system, so that S_p should instead be large. The evolution of many realistic systems leads typically to a systematic growth of correlations and, as such, this measure of entropy can be expected often to increase as time goes on.

The prescription for constructing the S_p's is straightforward. Suppose that one has access to the p-particle reduced distribution functions, or density matrices, f_p for some $p < N$, but that nothing else about the system is known. There exist then infinitely many candidate N-particle $\tilde{\mu}$'s consistent with the f_p's. For arbitrary $\tilde{\mu}$'s of this form, consider the functional

$$S[\tilde{\mu}] = -\mathrm{Tr}\, \tilde{\mu} \log \tilde{\mu} \tag{1.3}$$

where $\mathrm{Tr} \equiv \prod_j \mathrm{Tr}_j$. Now find that $\tilde{\mu}$ which maximizes the functional $S[\tilde{\mu}]$ and define for this maximizing μ_R^p an entropy

$$S_p \equiv S[\mu_R^p] = -\mathrm{Tr}\, \mu_R^p \log \mu_R^p \tag{1.4}$$

It follows immediately from a Lagrange multiplier argument that μ_R^p must factorize into a product of contributions $z_p(i_1, \ldots, i_p)$ involving all possible p-particle groupings, i.e., that

$$\mu_R^p = \prod_{i_1 < \cdots < i_p} z_p(i_1, \ldots, i_p) \tag{1.5}$$

where the z_p's are chosen to satisfy the constraints

$$\prod_{j \neq i_1, \ldots, i_p} \mathrm{Tr}_j \, \tilde{\mu} = f_p(i_1, \ldots, i_p) \tag{1.6}$$

When $p = N$, $z_p = \mu$, so that one recovers the Gibbs entropy $S_N = -\mathrm{Tr}\, \mu \log \mu$. Alternatively, when $p = 1$, $z_p(i) = f_1(i)$, so that one recovers the Boltzmann entropy

$$S_1 = -\mathrm{Tr}\, \mu_R^1 \log \mu_R^1 = -\sum_i \mathrm{Tr}_i \, f_1(i) \log f_1(i) \tag{1.7}$$

This latter limit is "natural" since, working solely at the level of a one-particle kinetic theory, one can often derive perturbatively an H-theorem inequality $dS_1/dt \geq 0$.

It also follows that $S_{p+1}(t) \leq S_p(t)$ for all times t, with equality holding if and only if z_{p+1} factorizes into a product of p-particle $\tilde{z}_p$'s. In particular, this equality requires that no "irreducible" $(p+1)$-particle correlations be present, so that z_{p+1} or f_{p+1} can be realized in terms of the f_p's. In the absence of interactions, the "amount" of correlations cannot change, so that the Liouville equation (1.1) implies that $dS_p/dt \equiv 0$. If, however, interactions are present, dS_p/dt need not vanish except for $p = N$. Indeed, suppose that, at some time t_0, $\mu(t_0) = \mu_R^p(t_0)$. It then follows that, for all later times, $S_p(t) \geq S_p(t_0)$, with equality holding if and only if, at time t, once again $\mu(t) = \mu_R^p(t)$. If no correlations are present initially, interactions can only generate correlations, so that S_p can only increase.

It is clear that, in the presence of interactions, dS_p/dt, unlike S_p itself, cannot be expressed as a local functional of μ_R^p. Thus, e.g., for two-body interactions the BBGKY hierarchy (see, e.g., Balescu, 1975) implies that $dS_p(t)/dt$ involves $\mu_R^{p+1}(t)$. What one can, however, hope to show is that μ_R^p satisfies a closed "subdynamics" whereby $\partial\mu_R^p(t)/\partial t$, and hence $dS_p(t)/dt$, can be realized as a functional of $\mu_R^p(t-\tau)$. This is, e.g., possible for $p = 1$.

Changes in S_p are by construction related to changes in the "amount" of correlations and, as such, S_p will increase only when correlations grow. When, as required by the Poincaré recurrence theorem (Zermelo, 1896), the correlations eventually decay, S_p must decrease correspondingly. The periodicities or near periodicities manifesting this recurrence will, however, be lost in any perturbation theory analysis, and it is for this reason that one can nevertheless derive perturbatively an H-theorem $dS_1/dt \geq 0$.

Paper I examined most of the aforementioned properties of S_p for the special case $p = 1$, where one recovers the Boltzmann entropy. The object here is to generalize the analysis to the case $p = 2$. This is an important test of the entire program, since the case $p = 1$ is in many respects well nigh trivial. Thus, e.g., the Boltzmann entropy S_1 is a well-known object, whereas the corresponding S_p's for $p > 1$ have not yet been considered.

This is, however, also an issue of some practical importance, since there exist physically interesting situations in which the two-particle $f_2(i,j)$'s, and hence presumably S_2, are natural objects to consider. Thus, e.g., it is well known (see, e.g., Peebles, 1980, and references therein) that the large-scale clustering of galaxies is characterized by two- and three-particle correlation functions which satisfy striking scaling and symmetry properties. One natural question to ask, therefore, is whether the observed clustering corresponds to a low- or high-entropy state (Kandrup, 1988*b*).

Section 2 of this paper uses perturbative techniques to obtain approximate formulas for μ_R^2 and S_2. Section 3 then demonstrates that $dS_2(t)/dt$ can be expressed nonlocally in terms of the f_2's at retarded times $t-\tau$.

Section 4 turns to the related issue of determining the "most likely" or "best guess" reduced objects $f_3, f_4, \ldots$ consistent with a knowledge of the f_2's. All of this, like the contents of Paper I, makes sense for systems either classical or quantum mechanical. Section 5 concludes by showing that the classical and quantum descriptions differ fundamentally in the form of the S_p's which they would assign to a pure state.

2. THE FORM OF THE TWO-PARTICLE ENTROPY

The object here is to realize $S_2(t)$ explicitly as a functional of the two-particle f_2's at time t. To avoid superfluous subscripts, Sections 2 and 3 will implement a change of notation, namely $f_1(i) \equiv f(i)$ and $f_2(i,j) \equiv g(i,j)$.

If $g(i,j) \equiv f(i)f(j)$, i.e., if no correlations are present, it is clear that one should pick

$$z_2(i,j) = [f(i)f(j)]^{1/(N-1)} \tag{2.1}$$

so that $\mu_R^2 = \mu_R^1$ and $S_2 = S_1$. If, alternatively, correlations do exist, $z_2(i,j)$ will assume a more complicated form. Indeed, it seems difficult, if not impossible, to obtain a closed-form expression for z_2 in terms of the $g(i,j)$'s. What is, however, straightforward is to evaluate z_2 perturbatively in the limit that the two-particle correlations are weak.

Thus, writing

$$g(i,j) = f(i)f(j)[1+\lambda\gamma(i,j)] \tag{2.2}$$

where $|\lambda| \ll 1$, one finds that, working to $O(\lambda)$,

$$z_2(i,j) = g(i,j)/[f(i)f(j)]^{(N-2)/(N-1)} \tag{2.3}$$

whence

$$\mu_R^2 = \left[\sum_{k=1}^{N} f(k)\right]^{2-N} \prod_{i<j=1}^{N} g(i,j) \simeq \prod_{k=1}^{N} f(k)\left[1+\lambda \sum_{i<j=1}^{N} \gamma(i,j)\right] \tag{2.4}$$

That this μ_R^2 really is an approximate solution follows trivially from the observation that

$$\mathrm{Tr}_j f(k)f(j)\gamma(j,k) = \mathrm{Tr}_j g(j,k) - \mathrm{Tr}_j f(j)f(k) \equiv 0 \tag{2.5}$$

This μ_R^2 implies a three-particle

$$h(i,j,k) = f(i)f(j)f(k)[1+\lambda\gamma(i,j)+\lambda\gamma(i,k)+\lambda\gamma(j,k)] \tag{2.6}$$

What equation (2.6) says is that the only correlations manifest in the three-particle distribution function, or density matrix, $h(i,j,k)$ are those induced by the presence of two-particle correlations. It is in this sense that

$h(i,j,k)$ contains no "irreducible" three-particle correlations. Note also that the form of h predicted by (2.6) is nothing other than that suggested by a Kirkwood (1935), or cluster, decomposition, truncated at $O(\lambda)$.

This expression is not, however, valid to $O(\lambda^2)$. Rather, one computes that, to this order,

$$\mu_R^2 = \left[\prod_{l=1}^{N} f(l)\right]^{2-N} \prod_{i<j=1}^{N} f(i)f(j) \times \left[1+\lambda\gamma(i,j)-\lambda^2 \sum_{k\neq i,j} \mathrm{Tr}_k\, f(k)\gamma(i,k)\gamma(j,k)\right] \tag{2.7}$$

or, in terms of the $g(i,j)$'s, that

$$\mu_R^2 = \left[\prod_{l=1}^{N} f(l)\right]^{2-N} \prod_{i<j=1}^{N} \{g(i,j) - \sum_{k\neq i,j} [\mathrm{Tr}_k\, g(i,k)g(j,k)f^{-1}(k) - f(i)f(j)]\} \tag{2.8}$$

This again seems reasonable, since it implies a three-particle

$$\begin{aligned} h(i,j,k) = f(i)f(j)f(k)[&1+\lambda\gamma(i,j)+\lambda\gamma(i,k)+\lambda\gamma(j,k) \\ &+\lambda^2\gamma(i,j)\gamma(j,k)+\lambda^2\gamma(i,k)\gamma(j,k)+\lambda^2\gamma(i,j)\gamma(i,k) \\ &-\lambda^2\,\mathrm{Tr}_j\, f(j)\gamma(i,j)\gamma(j,k)-\lambda^2\,\mathrm{Tr}_k\, f(k)\gamma(i,k)\gamma(j,k) \\ &-\lambda^2\,\mathrm{Tr}_i\, f(i)\gamma(i,j)\gamma(i,k)] \end{aligned} \tag{2.9}$$

The first seven terms here correspond to the Kirkwood expansion truncated at $O(\lambda^2)$, and the last three implement corrections which ensure that

$$\mathrm{Tr}_k\, h(i,j,k) \equiv g(i,j) \tag{2.10}$$

These corrections can be neglected only if one assumes that the quantity $\mathrm{Tr}_i\, f(i)\gamma(i,j)\gamma(i,k)$ is somehow small. As will be discussed in Section 4, this can in fact be justified in a thermodynamic limit where the volume V of the system $\to \infty$.

More generally, one can calculate $z_2(i,j)$ to $O(\lambda^n)$, obtaining thereby an expression of the general form

$$\begin{aligned} \mu_R^2 &= \left[\prod_{l=1}^{N} f(l)\right]^{2-N} \prod_{i<j=1}^{N} f(i)f(j)\left[1+\sum_{n=1}^{\infty} \lambda^n \chi_n(i,j)\right] \\ &\equiv \left[\prod_{l=1}^{N} f(l)\right]^{2-N} \prod_{i<j=1}^{N} g(i,j)[1+\psi(i,j)] \end{aligned} \tag{2.11}$$

this corresponding to

$$z_2(i,j) = g(i,j)[1+\psi(i,j)]/[f(i)f(j)]^{(N-2)/(N-1)} \tag{2.12}$$

where $\psi(i,j)$ is itself $O(\lambda^2)$.

It follows that

$$S_2 = -\mathrm{Tr} \prod_{i<j} z_2(i,j) \left[\prod_{k<l} \log z_2(k,l) \right]$$

$$= -\sum_{i<j} \mathrm{Tr}_i \, \mathrm{Tr}_j \, g(i,j) \log z_2(i,j) \tag{2.13}$$

or, to $O(\lambda^2)$, that

$$S_2 = S_1 - (\lambda^2/2) \sum_{i<j} \mathrm{Tr}_i \, \mathrm{Tr}_j \, f(i) f(j) \gamma^2(i,j) \leq S_1 \tag{2.14}$$

where, of course,

$$S_1 = -\sum_{i=1}^{N} \mathrm{Tr}_i \, f(i) \log f(i) \tag{2.15}$$

Equation (2.14) demonstrates explicitly that the one-particle entropy S_1 is in fact a maximum with respect to deviations from a pure product state induced by small pair correlations.

More generally, by inserting into (2.13) the z_2 of (2.12), one can write the two-particle entropy in the form

$$S_2 = -\sum_{i<j=1}^{N} \mathrm{Tr}_i \, \mathrm{Tr}_j \, g(i,j) \log g(i,j)$$

$$+(N-2) \sum_{i=1}^{N} \mathrm{Tr} f(i) \log f(i)$$

$$-\sum_{i<j=1}^{N} \mathrm{Tr}_i \, \mathrm{Tr}_j \, g(i,j) \log[1+\psi(i,j)] \tag{2.16}$$

This admits to a natural interpretation. The first term represents the "entropy of pairs" associated with each pairing of i and j. The second represents a normalization which ensures that, in the absence of correlations, $S_2 = S_1$. And finally, the third term represents the effects of induced correlations involving more than two particles. The key point is that finite two-particle correlations will induce additional correlations involving three or more particles; and these induced correlations will also contribute to the two-particle entropy.

3. THE TIME DERIVATIVE $dS_2(t)/dt$

As discussed in Paper I, one beautiful property of μ_R^1 is that it satisfies a closed "subdynamics" in the sense that $\partial \mu_R^1(t)/\partial t$ can be realized as a nonlocal functional of μ_R^1 at retarded times $t-\tau$. What this means is that $dS_1(t)/dt$, like $S_1(t)$ itself, can be expressed solely in terms of the "physically

accessible" $f(i)$'s. A natural question to ask, therefore, is whether $dS_2(t)/dt$ can be expressed similarly as a functional of the $g(i,j)$'s at retarded times. Given that one is lacking a closed-form expression for μ_R^2, this might seem difficult, but, given the observation that μ_R^2, and hence S_2, is constructed solely in terms of the g's, this in fact proves possible. All that one need do is derive exact equations expressing $\partial g(i,j)/\partial t$ in terms of all the $g(k,l)$'s and then use these relations to evaluate dS_2/dt for the perturbative S_2's generated as in Section 2.

To derive the desired expressions for $\partial g/\partial t$, what one must do is introduce some splitting of the true μ into pieces μ_P and μ_I, for which

$$\prod_{k\neq i,j} \mathrm{Tr}_k\, \mu_P(1,\ldots,N) = g(i,j) \tag{3.1}$$

and then construct explicitly a "projection operator" P which implements the splitting canonically. One such prescription has already been proposed by Kandrup and Hill Kandrup (1984) in their analysis of galaxy clustering.

Suppose, for simplicity, that N is even. There are then $(N-1)!!$ ways in which the N particles can be parceled into pairs, these corresponding to the product $g(1,2)g(3,4)\cdots g(N-1,N)$ and all possible permutations thereof. What one is instructed to do is add up all these permutations, divide through by an overall normalization $(N-3)!!$, and then substract off $(N-2)$ times the uncorrelated μ_R^1:

$$\mu_P = \frac{1}{(N-3)!!}[\text{sum of } (N-1)!! \text{ permutations of } g(1,2)\cdots g(N-1,N)] - (N-2)\prod_{i=1}^{N} f(i) \tag{3.2}$$

The normalizations $(N-3)!!$ and $-(N-2)$ ensure that, to $O(\lambda)$,

$$\mu_P = \prod_{k=1}^{N} f(k)\left[1+\sum_{i<j=1}^{N}\lambda\gamma(i,j)\right] \tag{3.3}$$

in agreement with (2.4). At least to lowest nontrivial order, μ_P coincides with the true μ_R^2.

As discussed in Paper I, the key idea, given such a μ_P, is to construct a linear operator P_{μ_P}, the form of which depends on μ_P (and hence parametrically on time), which satisfies three basic requirements (cf. Willis and Picard, 1974):

1. At any given time,

$$P_{\mu_P}\mu = \mu_P$$

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

$$P_{\mu_P(t_2)}P_{\mu_P(t_1)}\xi(1,\ldots,N) = P_{\mu_P(t_2)}\xi(1,\ldots,N) \qquad \text{for} \quad t_2 \geq t_1 \tag{3.5}$$

3. At any given time t, the commutator

$$[P_{\mu_P}, \partial/\partial t]\mu \equiv 0 \tag{3.6}$$

The crucial fact is that if, at some time t_0, $\mu = \mu_P$, the Liouville equation (1.1) then implies the nonlinear relation

$$\partial\mu_P(t)/\partial t + PL\mu_P(t) = \int_0^{t-t_0} d\tau\, P(t)L(t)\mathcal{G}(t, t-\tau)[1-P(t-\tau)]L(t-\tau)\mu_P(t-\tau) \tag{3.7}$$

where $P(t)$ denotes the operator P_{μ_P} evaluated for $\mu_P(t)$, and $\mathcal{G}$ is an operator built solely from P and L. And, by integrating over any $N-2$ of the particle variables, (3.7) yields an equation for $\partial g(i,j)/\partial t$ in terms of $\mu_P(t-\tau)$ which is, by construction, a function only of the $g(k,l)$'s. An explicit realization of P_{μ_P} is presented in Kandrup and Hill Kandrup (1984), which also discusses in detail the form of the equations for $\partial g/\partial t$.

One knows that if, initially, $\mu(t_0) = \mu_R^1(t_0)$, then $S_1 = S_2 = S_N$. And one knows further that interactions among the particles will generate correlations which induce at least an initial increase in S_1 and S_2. A key piece of intuition, which, however, remains to be understood further, is that S_1 will increase more rapidly than S_2. One of the principal conclusions of Paper I was that, for the special case of (well-behaved) two-body interactions,

$$\left.\frac{dS_1(t)}{dt}\right|_{t_0} = 0 \qquad \text{and} \qquad \left.\frac{d^2S_1(t)}{dt^2}\right|_{t_0} = a^2 > 0 \tag{3.8}$$

so that, for at least short times $(t-t_0)$,

$$S_1(t) = S_1(t_0) + \tfrac{1}{2}a^2(t-t_0)^2 + \cdots \tag{3.9}$$

Equation (3.8) is easy to understand. S_1 will change only by virtue of nontrivial correlations $\gamma(i,j)$; and thus, if initially no correlations are present, dS_1/dt must vanish. Only as these correlations are generated is there a "source" for changes on S_1, so that the initial increase in S_1 can only be of order $(t-t_0)^2$. In a similar sense, one anticipates that S_2 can change only in the presence of three-body correlations; and thus, one expects that

$$\left.\frac{dS_2(t)}{dt}\right|_{t_0} = 0 = \left.\frac{d^2S_2(t)}{dt^2}\right|_{t_0} \tag{3.10}$$

whereas

$$\left.\frac{d^3S_2(t)}{dt^3}\right|_{t_0} = b^2 > 0 \tag{3.11}$$

The increase in S_2 from an inital totally uncorrelated state should only be of order $(t-t_0)^3$.

To verify (3.10) is in fact straightforward: given that no initial correlations are present, it suffices to verify these equalities in the weak coupling limit of (2.14), considering S_2 only to $O(\lambda^2)$. Thus, if one defines

$$G(i,j) \equiv \lambda f(i) f(j) \gamma(i,j) \tag{3.12}$$

and observes that, by assumption, $G(i,j;t_0) \equiv 0$, it follows that

$$\left.\frac{dS_2}{dt}\right|_{t_0} = \left.\frac{dS_1}{dt}\right|_{t_0} - \sum_{i<j} \mathrm{Tr}\left\{ \frac{G(i,j)}{f(i)f(j)} \frac{\partial G(i,j)}{\partial t} - \frac{G^2(i,j)}{2f^2(i)f^2(j)} \frac{\partial}{\partial t} f(i)f(j) \right\} \Bigg|_{t_0} \equiv 0 \tag{3.13}$$

Similarly, one computes

$$\left.\frac{d^2S_2}{dt^2}\right|_{t_0} = \left.\frac{d^2S_1}{dt^2}\right|_{t_0} - \sum_{i<j} \mathrm{Tr}_i \, \mathrm{Tr}_j f^{-1}(i) f^{-1}(j) \left(\frac{\partial G(i,j)}{\partial t} \right)^2 \Bigg|_{t_0} \tag{3.14}$$

In this case, d^2S_2/dt^2 is the difference between two terms, each of which is intrinsically nonnegative. One knows, however, from Paper I that, in the absence of initial correlations,

$$\partial \mu_I^1(t_0)/\partial t = -(1-P) L \mu_R^1(t_0) = -\sum_{k<l} \Delta_{kl} \prod_m f(m) \tag{3.15}$$

where Δ_{kl} denotes a "fluctuating" Liouville operator involving particles k and l, so constructed that

$$\mathrm{Tr}_k \, \Delta_{kl} f(k) f(l) \equiv 0 \tag{3.16}$$

Thus, it follows immediately that

$$\partial G(i,j;t_0)/\partial t = -\Delta_{ij} f(i) f(j) \tag{3.17}$$

However, one knows also that

$$\frac{d^2 S_1(t_0)}{dt^2} = \mathrm{Tr}\left[\prod_l f(l) \right]^{-1} \left| \sum_{i<j} \Delta_{ij} \prod_k f(k) \right|^2 = \sum_{i<j} \mathrm{Tr}_i \, \mathrm{Tr}_j [f(i)f(j)]^{-1} |\Delta_{ij} f(i) f(j)|^2 \tag{3.18}$$

where the second equality follows from (3.16). By inserting these last two relations into (3.14), one sees that, in the absence of initial correlations, $d^2S_2/dt^2 \equiv 0$ at time $t = t_0$.

It should perhaps be noted that, strictly speaking, the analysis leading to (3.8)–(3.10) requires well-behaved interactions derived from a Hamiltonian $H^I_{ij}(|x_{ij}|)$ which remains bounded as $|x_{ij}| \to 0$. Consider, e.g., a classical self-gravitating cosmology with $H^I_{ij} \propto |x_{ij}|^{-1}$, for which this criterion is not satisfied. A careful analysis then shows that (Kandrup, 1988*c*), even though $S_1(t_0+\Delta t) > S_2(t_0+\Delta t)$, for short times both $dS_1(t_0+\Delta t)/dt$ and $dS_2(t_0+\Delta t)/dt$ are in fact independent of Δt! The perturbative analysis considered here fails beause

$$\mathrm{Tr}_i \, \mathrm{Tr}_j \, \Delta_{ij}(t_2)\Delta_{ij}(t_1) f(i) f(j) \tag{3.19}$$

diverges in the coincidence limit $t_2 \to t_1$.

4. THE "MOST LIKELY" THREE-PARTICLE $f_3(i, j, k)$

The construction of the two-particle S_2 entails first evaluating the "most likely" N-particle μ^2_R consistent with some given $f_2(i, j)$'s. Of more direct physical interest, however, are the most likely three- or four-particle f_q's. Thus, e.g., if one knows both $f_2(i, j)$ and $f_3(i, j, k)$, it is natural to ask whether the observed f_3 is the "most likely" f_3 consistent with f_2 or whether, alternatively, it is somehow "less likely."

The most likely f_3 can be derived by maximizing the functional

$$\zeta[F_3] = -\prod_{i=1}^{3} \mathrm{Tr}_i \, F_3(1, 2, 3) \log F_3(1, 2, 3) \tag{4.1}$$

subject to the constraints

$$\mathrm{Tr}_k \, F_3(i, j, k) = f_2(i, j) \tag{4.2}$$

This leads obviously to the demand that the most likely

$$f_3(i, j, k) = Z_2(i, j) Z_2(i, k) Z_2(j, k) \tag{4.3}$$

where the Lagrange multipliers Z_2 must be chosen to implement the constraints. In this sense, the analysis is completely analogous to that leading to μ^2_R. The crucial difference here is that the Z_2's can in fact be evaluated exactly in a thermodynamic limit.

Suppose now that

$$f_2(i, j) = f_1(i) f_1(j)[1 + \xi(i, j)] \tag{4.4}$$

where $\xi(i, j) \equiv \lambda \gamma(i, j)$. The intuition of Section 2 then suggests that one look for a solution

$$Z_2(i, j) \equiv [f_1(i) f_1(j)]^{1/2} [1 + \xi(i, j)] S(i, j) \tag{4.5}$$

where $S(i,j)$ is a new unknown. And, with this *Ansatz*, (4.2) yields

$$f_2(i,j) = f_2(i,j)S(i,j)\,\mathrm{Tr}_k\, f_1(k)[1+\xi(i,k)][1+\xi(j,k)]S(i,k)S(j,k) \quad (4.6)$$

What remains to be shown is that, for sufficiently large systems, $S(i,j) \simeq 1$.

Specifically, consider the thermodynamic limit in which the number N and the volume V diverge, but the average density $n \equiv N/V$ remains finite. One knows of course [see (2.5)] that

$$\mathrm{Tr}_k\, f_1(k)\xi(i,k) \equiv 0 \quad (4.7)$$

so that, if $S(i,j) = 1$, equation (4.6) reduces to

$$1 = \mathrm{Tr}_k\, f_1(k)[1+\xi(i,k)+\xi(j,k)]$$

or

$$\mathrm{Tr}_k f_1(k)\xi(i,k)\xi(j,k) = 0 \quad (4.8)$$

It is, however, clear that (4.8) holds in this thermodynamic limit provided that the "range" R of any two-particle correlations is finite. Thus, on dimensional grounds, the left-hand side of (4.8) is of order v/V, where $v \sim R^3$; and, in the thermodynamic limit, $v/V \to 0$.

The net result is that, for sufficiently large systems ($v/V \ll 1$), the "most likely" three-particle distribution function, or density matrix, consistent with given $f_2(i,j)$'s takes the form

$$f_3(1,2,3) = \prod_{i=1}^{3} f_1(i)\left[\prod_{j<k=1}^{3} 1+\xi(j,k)\right] \quad (4.9)$$

precisely the "best guess" form suggested by the Kirkwood (1935) expansion. This prescription also generalizes trivially to the most likely f_q for $q = 4, 5, \ldots$. Specifically, for $q \ll N$, one concludes that the most likely

$$f_q(i_1, \ldots, i_q) = \prod_{j=i_1,\ldots,i_q} f_1(j) \prod_{k<l=i_1,\ldots,i_q} [1+\xi(k,l)] \quad (4.10)$$

This argument must, however, fail for $q \to N$. Thus, e.g., from the viewpoint of Section 2, equation (4.10) clearly involves a neglect of certain terms $O(\lambda^2)$, so that, for $q = N$, it would be tantamount to ignoring the final term

$$\lambda^2 \sum_{k \neq i,j} \mathrm{Tr}_k\, f(k)\gamma(i,k)\gamma(j,k) \quad (4.11)$$

in (2.7). This final term is, however, of order $\lambda^2(N-2)v/V \simeq \lambda^2 nv$, which cannot in general be neglected compared to a term like $\lambda^2\gamma(i,j)\gamma(k,l)$.

5. CONCLUSIONS

Together with Paper I, this paper has exploited the ideas of information theory to define measures of entropy S_p appropriate for an observer who, in probing the state of some N-particle system, can measure with arbitrary precision all the information buried in the p-particle reduced distribution functions, or density matrices, but is completely ignorant of any correlations involving more than p particles. On the one hand, this is of interest in that it shows that the (often hazy) notion of "coarse graining" can in fact be implemented in a fashion both reasonable physically and precise mathematically. On the other hand, this is also of interest because of concrete applications to the study of phenomena such as galaxy clustering (Kandrup 1988*b*,*c*) and because the basic approach admits an obvious generalization to a field-theoretic setting (Hu and Kandrup, 1987; Kandrup, 1987).

In accord with the conventional approach to nonequilibrium statistical mechanics, the analysis has been formulated abstractly in a fashion applicable either to a classical N-particle distribution function or a quantum mechanical N-particle density matrix. All that is really assumed is that the N-particle μ satisfies a Liouville equation $\partial\mu/\partial t = -L\mu$, which implies conservation of probability. At least for the case of mixed states, the qualitative results of the analysis are the same in both a classical and a quantum setting. However, one may conclude by observing that, for the special case of a pure state, the classical and quantum descriptions lead to very different physical pictures.

Classically, a pure state corresponds to the specification of a point in the $6N$-dimensional phase space. The N-particle μ then reduces to a $6N$-dimensional delta function, and the reduced f_p's reduce to $6p$-dimensional delta functions. What this means, however, is that, for a pure state, $\mu = \mu_R^p$ for all p. A simple knowledge of where each particle actually is—i.e., the forms of the individual f_1's—constitutes a complete description of the system; and, as such, the p-particle "coarse grainings" considered here entail no information loss. One concludes, therefore, that $S_p = S_N$ for all p and that $dS_p/dt \equiv 0$.

Quantum mechanically, the situation is very different. Working in the Schrödinger picture in a position representation, a pure state corresponds to an N-particle wave function involving $3N$ coordinates, so that the density matrix $\mu(1, \ldots, N)$ has a realization

$$\mu(x_1, x_1', \ldots, x_N, x_N') = \psi^*(x_1, \ldots, x_N)\psi(x_1', \ldots, x_N') \tag{5.1}$$

This means, however, that

$$f(i) = \prod_{j \neq i} \mathrm{Tr}_j\, \psi^*(x_1, \ldots, x_N)\psi(x_1', \ldots, x_N')\big|_{j'=j} \tag{5.2}$$

so that, in general, there is no reason to expect that $\mu = \mu_R^1$. If, as a special case, one were to demand at some instant of time that μ be diagonal in the particle variables, i.e., that

$$\mu(x_1, \ldots, x_N) = \prod_{i=1}^{N} \phi_i(x_i) \tag{5.3}$$

where

$$\mathrm{Tr}_i\, \phi_i(x_i)\phi_i(x_i) = 1 \tag{5.4}$$

it would follow that $\mu = \mu_R^1$, but this is clearly an unreasonable restriction. Even if (5.3) were true at that instant, interparticle correlations would be generated by the evolving dynamics so that the special factorization would be lost.

What this means is that, even if one chooses initial data corresponding to a pure state, the quantum entropies S_p defined here and in Paper I will in fact exhibit a nontrivial time dependence. One expects that, generally, $S_p \neq S_N$ and that S_p is strictly greater than S_{p+1}.

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