

# A New Approach for the Justification of Ensembles in Quantum Statistical Mechanics—II

Joel E. Keizer<sup>1</sup>

*Received April 23, 1970*

---

The results of the first paper in this series are generalized to include spin, permutation symmetry, and time dependence. In particular, the question of time invariance of localness in the Heisenberg picture is discussed and it is conjectured that an operator that is initially local will remain local over time. In order to treat macroscopic systems, it is shown that the ensemble decomposition of the previous paper can be used to “coarse-grain” configuration space. Finally, a physical interpretation of the ensemble decomposition in terms of “redundant macroscopic information” is used to give a derivation of the generalized microcanonical average.

---

**KEY WORDS:** Local operators; coarse-graining; microcanonical ensemble; foundations of statistical mechanics.

## 1. INTRODUCTION

In the first paper in this series<sup>(1)</sup> (hereafter referred to as I), the idea was introduced that measurements on large systems are actually ensemble averages. The essence of this idea is that values of observables measured in disjoint regions of three-space arise from independent “portions” of the wave function. In other words, measurements in disjoint spatial regions are independent, although this independence is obvious only when the underlying configuration space is examined. The mathematical developments

---

This work was supported in part by research grants from the National Science Foundation and the U.S. Public Health Service. Some of the material in this paper is contained in a doctoral dissertation submitted by the author to the University of Oregon (1969).

<sup>1</sup> Division of Natural Science, University of California, Santa Cruz. Present address: Battelle Memorial Institute, Columbus, Ohio.

in I are an attempt to give a formal basis for this notion. In particular, it is shown in I that expectation values for a pure state  $\psi$  have a natural decomposition into an ensemble average and that the wave functions in this average are derived from the projection of  $\psi$  on disjoint regions of configuration space.

To see what connection this formal ensemble has with statistical mechanics, it is important to look at the decomposition physically. Since the ensemble of "independent systems" arises in configuration space, the physics will be examined at that level. The configuration-space picture of a physical state is a wave function  $\psi$  which carries with it all of the information relevant to a physical system. However, for large systems, not all of the information in  $\psi$  is required since only measurements of a "coarse," i.e., macroscopic, nature are made. Indeed, it is plausible that  $\psi$  contains a great deal of redundant information for macroscopic purposes. By this it is meant that the projections of  $\psi$  onto disjoint regions of configuration space  $A$  and  $B$ , i.e.,  $\xi_A\psi$  and  $\xi_B\psi$ , may contain the same *macroscopic* information, but very different *microscopic* information.<sup>2</sup> In other words, for large systems, it is expected that the state  $\psi$  itself carries with it an ensemble of redundant macroscopic information. Furthermore, it is possible that for *certain initial preparations* the redundant information carried by  $\psi$  is essentially the same for all initial states. In this case, all of the initial states would have the same macroscopic behavior given by their common redundant "ensemble."

It is obvious that the ensemble decomposition obtained in I, namely

$$(\psi, A\psi) = \sum_{j=1}^{\Omega} P_j(\varphi_j, \bar{A}\varphi_j)$$

is of just the right form to be examined from this point of view. Thus, for some partition of configuration space  $\{\sigma_j\}$ , all the states  $\varphi_j = \xi_{\sigma_j}\psi / \|\xi_{\sigma_j}\psi\|$  might carry the same macroscopic information—in the sense that initially each  $\varphi_j$  has the same expectation values as  $\psi$ . That is, the information contained in the  $\varphi_j$ 's would be redundant information. This, in fact, is a very general property of quantum systems and a result of this form is given below.

In addition to the macroscopic information contained in the "ensemble" of functions  $\{\varphi_j\}$ , each function  $\varphi_j$  contains *microscopic* information. In general, these microscopic details are very specific and are not representative of the initial preparation of the system. However, for *certain preparations* it is possible that the microscopic information in the ensemble  $\{\varphi_j\}$  is a random sample of the microscopic information contained in all the states compatible with the preparation. In other words, for a given  $\psi$ , the ensemble  $\{\varphi_j\}$  might embrace all conceivable states of the system compatible with the initial preparation. If the "probabilities"  $P_j$  for such a decomposition were equal, then the decomposition would be equivalent to the microcanonical ensemble average of Gibbs'.

In this paper, these ideas are expanded in order to give a new approach for justifying ensembles. Although the results presented here do not give an explicit justifica-

<sup>2</sup> The possibility of redundant information being contained in a pure state is a direct result of the state of the system being a function on configuration space and not a single point in phase space. Thus, it does not seem possible to carry out a similar argument in a classical setting.

tion of ensembles, they do provide a new point of view from which the problem may be understood physically and attacked mathematically.

**2. SYMMETRY AND SPIN**

Before proceeding with the main argument, it is necessary to introduce two important physical restrictions into the ensemble decomposition, namely symmetry and spin. If the ensemble decomposition is relevant to physics, it should be easy to introduce these complications.

The symmetrization postulate of quantum mechanics<sup>(2)</sup> asserts that the only acceptable wave functions are those which are completely symmetric or completely antisymmetric for sets of identical particles—the kind of symmetry depending on the nature of the particle. The process of subdividing configuration space by partitions will not, in general, preserve this symmetry, as is easily seen. For example,  $\varphi_j = \xi_{\sigma_j} \psi / \|\xi_{\sigma_j} \psi\|$ , where  $\psi$  has one of the two symmetry properties. Now, the symmetric projection operator is  $S = (1/N!)^{1/2} \sum_P P$  and the antisymmetric operator is  $S = (1/N!)^{1/2} \sum_P (-)^P P$ , where  $(-)^P$  is the sign of the permutation and the sum is over all  $N!$  permutations. If  $D$  represents either  $S$  or  $A$ , then it is necessary, for symmetry to be preserved, to have  $D\varphi_j = \varphi_j$ . This means it suffices to have  $P\xi_{\sigma_j} = \xi_{\sigma_j}$  for all  $P$  and so  $\sigma_j$  must be symmetric with respect to the origin.

In order to show the existence of such partitions and for later use, an example of such a symmetric partition is given here. To decompose  $V = V_3 \times \dots \times V_3$ , where  $V_3$  is the three-dimensional region available to a particle, consider the open region  $U_1 = \{q \in V: x_1 > x_2 > \dots > x_N\}$ . Then, form the  $N!$  disjoint regions  $U_P = PU_1$ , where  $P$  is an element of the symmetric group  $\zeta$ . Thus,

$$U_P = \{q \in V: x_{P1} > x_{P2} > \dots > x_{PN}\}$$

and, clearly,  $U_P \cap U_{P'} = \emptyset$  if  $P \neq P'$ . Also,  $\lambda(\bigcup_{P \in \zeta} U_P) = \lambda(V)$  because the only points in  $V$  and not in  $\bigcup_{P \in \zeta} U_P$  come from a countable number of hyperplanes defined, for example, by  $x_1 = x_2$ .

In order to construct  $\sigma_j$ , first find a partition  $\{\sigma_j^*\}_{j=1}^Q$  of  $U_1$ . Then, let  $\sigma_j = \bigcup_{P \in \zeta} P\sigma_j^*$ . Since  $\sigma_j^*$  is open,  $\sigma_j$  is open. Also, because  $\sigma_j^* \cap \sigma_k^* = \emptyset$  for  $j \neq k$  and because  $P\sigma_j^* \subset U_P$ , it follows that  $\sigma_j \cap \sigma_k = \bigcup_{P \in \zeta} \bigcup_{Q \in \zeta} P\sigma_j^* \cap Q\sigma_k^* = \emptyset$  for  $j \neq k$ . Finally,

$$\begin{aligned} \lambda\left(\bigcup_j \sigma_j\right) &= \lambda\left(\bigcup_{Q \in \zeta} Q \bigcup_j \sigma_j^*\right) = \sum_{Q \in \zeta} \lambda\left(Q \bigcup_j \sigma_j^*\right) = \sum_{Q \in \zeta} \lambda\left(\bigcup_j \sigma_j^*\right) \\ &= N! \lambda\left(\bigcup_j \sigma_j^*\right) = N! \lambda(U_1) = \lambda(V) \end{aligned}$$

where the third and sixth equalities follow from the invariance of Lebesgue measure under coordinate permutations.<sup>(3)</sup> Thus  $\{\sigma_j\}_{j=1}^Q$  is a partition and, since

$$P\sigma_j = \bigcup_{Q \in \zeta} PQ\sigma_j^* = \bigcup_{Q \in \zeta} Q\sigma_j^* = \sigma_j$$

it is symmetric.

The introduction of spin also presents no difficulties of principle. The Hilbert space  $H_s$  for such systems is the tensor product of  $\mathcal{L}_2$  with various  $m$ -dimensional Hilbert spaces.<sup>(4)</sup> Thus, a vector  $\psi$  and an operator  $\hat{A}$  on  $H_s$  are of the form

$$\psi = \begin{pmatrix} \psi^1(q) \\ \psi^2(q) \\ \vdots \\ \psi^T(q) \end{pmatrix}$$

$$\hat{A} = \begin{pmatrix} a_{11}(q, \nabla_q) & \cdots & a_{1T}(q, \nabla_q) \\ \vdots & & \vdots \\ a_{T1}(q, \nabla_q) & \cdots & a_{TT}(q, \nabla_q) \end{pmatrix}$$

$\hat{A}$  will be called a local operator if all the  $a_{ij}(q, \nabla_q)$  are local operators. The scalar product is  $\sum_{n=1}^T (\varphi^n, \psi^n) = \varphi \cdot \psi$  and the expectation value of  $\hat{A}$  is  $\psi \cdot \hat{A}\psi = \sum_{n,m=1}^T (\psi^n, a_{nm}\psi^m)$ . The following manipulations verify that the ensemble decomposition still holds:

$$\begin{aligned} (\psi^n, a_{nm}\psi^m) &= \left( \sum_{j=1}^{\Omega} \xi_{\sigma_j} \psi^n, a_{nm}\psi^m \right) = \sum_{j=1}^{\Omega} (\xi_{\sigma_j} \psi^n, a_{nm}\psi^m) \\ &= \sum_{j=1}^{\Omega} (\xi_{\sigma_j} \psi^n, a_{nm} \xi_{\sigma_j} \psi^m) = \sum_{j=1}^{\Omega} (\psi_j^n, a_{nm} \psi_j^m) \end{aligned}$$

Thus,

$$\begin{aligned} \psi \cdot \hat{A}\psi &= \sum_{n,m=1}^T \sum_{j=1}^{\Omega} (\psi_j^n, a_{nm} \psi_j^m) = \sum_{j=1}^{\Omega} \left( \sum_{n,m=1}^T (\psi_j^n, a_{nm} \psi_j^m) \right) \\ &= \sum_{j=1}^{\Omega} \psi_j \cdot \hat{A}\psi_j \end{aligned}$$

and, writing  $P_j = \psi_j \cdot \psi_j$  and  $\varphi_j = \psi_j/P_j^{1/2}$ , we obtain

$$\psi \cdot \hat{A}\psi = \sum_{j=1}^{\Omega} P_j \varphi_j \cdot \hat{A}\varphi_j$$

It is clear from the above that, for an open set  $\sigma$  with zero-measure boundary,  $\xi_{\sigma} \hat{A}\psi = \hat{A}\xi_{\sigma}\psi$ . The symmetry considerations follow in an exactly similar manner to that described in the spin-free case.

Thus, the results of the previous work are completely general in the sense that they apply to all systems that satisfy the Pauli spinor formulation of nonrelativistic quantum mechanics.

### 3. LOCAL OPERATORS IN THE HEISENBERG PICTURE

It is useful at this point to discuss the quantum mechanical "picture" that will be used below. The Heisenberg picture<sup>(5)</sup> has certain advantages over the Schrödinger picture and is the one that will be used.

The advantage of the Heisenberg picture is that the Hilbert-space properties of quantum mechanics are separated from dynamical properties. In the Heisenberg picture, the state of a closed system is described by an element of  $\mathcal{L}_2$  and a set of operators. Over time, the wave function remains unchanged and the operators evolve according to

$$dA/dt = i[H, A]$$

where  $H$  is the Hamiltonian and the units are such that  $\hbar = 1$ . Now, statistical mechanics deals with systems that are identical in their composition—that is, dynamical nature—but that are in possibly different *initial* states. In order to utilize this feature in examining the expectation value, it is important to have this represented explicitly. For this purpose, the Heisenberg picture is ideal since the expectation value is  $(\psi, A(t)\psi)$  and the initial state  $\psi$  is clearly exposed.

Because the localness of quantum operators is essential in the following results, it is important to see under what conditions  $A(t)$  is a local operator if  $A(0)$  is. That is, to see when localness is a time-invariant property of observables. It is easy to see why this might be true. The Heisenberg equations of motion are a direct analog of the classical equations of motion for functions of coordinates and momenta.<sup>(6,7)</sup> The difference is that  $\sqrt{-1}$  times the commutator replaces the Poisson bracket that occurs in the classical formulation. Moreover, the classical observables are given at each later time by a function of the coordinates and momenta, and so it might be expected in quantum mechanics that  $A(t)$  is an operator that can be written as a function of the operators  $r$  and  $p = -i\nabla$ . Under these conditions, Theorem 6c-I<sup>3</sup> indicates that  $A(t)$  is a local operator if  $A(0)$  is an analytic function of these fundamental operators.

On the other hand, the general solution to the Heisenberg equations of motion<sup>(8)</sup> is  $U^\dagger(t) A(0) U(t) = A(t)$ , where  $U(t)$  is the unitary time evolution operator determined by the equation

$$i dU(t)/dt = HU(t)$$

with  $H$  the Hamiltonian. Since  $U(t)$  is a unitary, it is a bounded operator, and so, by Theorem 3-I,  $U(t)$  is a local operator if and only if it is a multiplicative operator. Thus, quite generally,  $U(t)$  is a nonlocal operator and it would appear unlikely that  $A(t)$  would be local even if  $A(0)$  is.

Consider, however, the simple case of a free particle. It is well known<sup>(9)</sup> that the evolution operator can be written as

$$\left(\frac{m}{2\pi t}\right)^{3/2} \int dr' \dots \exp\left(-\frac{i3\pi}{4} + \frac{m|r-r'|^2}{2t}\right)$$

which is an integral operator and certainly nonlocal. Yet the Heisenberg equations of motion for the operators  $r$  and  $p$  have solutions

$$r(t) = r - (it/m)\nabla, \quad p(t) = -i\nabla$$

<sup>3</sup> The notation “-I” refers to the corresponding result in Ref. 1.

These are clearly local operators and are direct analogs of the classical equations of motion. A comparable result holds true for a one-dimensional harmonic oscillator, which is solved by

$$r(t) = r \cos \omega t - (i\nabla/m\omega) \sin \omega t, \quad p(t) = -rm\omega \sin \omega t - i\nabla \cos \omega t$$

A number of other examples in which locality is preserved could be given, including the  $N$ -particle generalizations of these examples. Furthermore, if  $A(0) = \sum_n P_n$ , where  $P_n$  is a sum of products of the operators  $r$  and  $p$ , then, since  $U(t)$  is unitary,

$$A(t) = U^\dagger(t) A(0) U(t) = U^\dagger(t) \sum_n (P_n U(t)) = \sum_n U^\dagger(t) P_n U(t)$$

By inserting  $U^\dagger(t) U(t) = I$  between the products in  $P_n$ ,  $A(t)$  can be written

$$A(t) = \sum_n P_n(t)$$

where  $P_n(t)$  is a product indicated by  $P_n$  but involving  $r(t)$  and  $p(t)$ . Thus, in the examples above,  $P_n(t)$  is a local operator, and because of Theorem 6c-I, so is  $A(t)$ . This means that, to see that  $A(t)$  is local when  $A(0)$  is an analytic function in the operators  $r$  and  $p$ , it suffices to see that  $r(t)$  and  $p(t)$  are local. But  $dr(t)/dt = p(t)/m$ , so it suffices to have  $r(t)$  a local operator.

With this discussion as a basis, the following is presented as a conjecture.

**Conjecture.** If  $H$  is the Hamiltonian for a physical system and  $A(0)$  is a local operator corresponding to an observable, then  $A(t)$  determined by the Heisenberg equations of motion is a local operator.

The theorem is not true for  $H$  and  $A(0)$  arbitrary local Hermitian operators, as the following example shows.<sup>4</sup> Let

$$H = \begin{pmatrix} i \partial/\partial x & 0 \\ 0 & -i \partial/\partial x \end{pmatrix} \quad \text{and} \quad A(0) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Then,

$$U^\dagger(t) A(0) U(t)(y_1(x), y_2(x)) = (y_2(x - 2t), y_1(x + 2t))$$

so that  $A(t)$  is certainly nonlocal.<sup>5</sup>

It might be pointed out that the solutions for the free particle and harmonic oscillator given above are of the form

$$A(t) = \sum_{n=0}^{\infty} \frac{t^n \mathcal{L}^n A(0)}{n!}$$

where  $\mathcal{L}$  is the so-called Liouville operator<sup>(10)</sup> defined by  $\mathcal{L}A = i[H, A]$ . In fact,

<sup>4</sup> I am indebted to Professor R. S. Phillips for suggesting this counterexample.

<sup>5</sup> This is *not* a general property for "spin systems," and examples for systems with spin for which locality is preserved are easily constructed.

the convergence to  $A(t)$  of this formal series solution is a sufficient condition for localness to be preserved, since  $\mathcal{L}^n A(0)$  is a local operator if  $H$  and  $A(0)$  are.

It must be stressed that, while quantum mechanical operators are local, they are not, in general, extended local operators. Indeed, it is easy to see that the natural extension of a local Hermitian operator is not necessarily Hermitian. The Hermiticity of the differential operator, for example, depends critically on an application of Gauss' theorem. A function of the form  $\xi_E \psi$ , where  $E$  is an open set and  $\psi$  allows an application of Gauss' theorem, will not generally satisfy the hypothesis of the theorem. This is so because  $\xi_E \psi$  will in general be discontinuous across the boundary of  $E$ .

This lack of Hermiticity, however, is unimportant because the natural extension of the local quantum operator  $A$  will occur only formally in the work which follows. What is important is that  $\bar{A} = A$  on the domain of  $A$  and that  $\bar{A}$  is Hermitian on this domain.

#### 4. MICROCANONICAL PARTITIONS

In order to connect the ensemble decomposition of the previous paper with physical ensembles, it is necessary to introduce an initial condition for the functions  $\varphi_j = \xi_{\sigma_j} \psi / \|\xi_{\sigma_j} \psi\|$ . This means, in terms of the discussion in the introduction, that it is necessary to guarantee that each function  $\varphi_j$  contains the same macroscopic information as  $\psi$ . Thus, it must be true at time  $t = 0$  that  $(\varphi_j, \bar{A}(0)\varphi_j) \approx (\psi, A(0)\psi)$  for all  $j$  and all operators  $A$  referring to macroscopic properties. This is the usual physical requirement that an ensemble be composed of systems that have the same initial preparation, i.e., that the ensemble be representative. In order to obtain this initial condition, special partitions, called microcanonical partitions, are introduced.

**Definition.** A *microcanonical partition* is a partition formed in the following manner. Let  $\{A_k\}_{k=1}^\infty$  be a countable partition of  $V$  into open cubes.<sup>6</sup> Divide each set  $A_k$  into  $\Omega$  congruent subcubes called  $B_{kj}$ ,  $j = 1, 2, \dots, \Omega$ . Define  $\sigma_j = \bigcup_{k=1}^\infty B_{kj}$ .

It is clear that a microcanonical partition is a partition, since each  $\sigma_j$  is open,

$$\sigma_j \cap \sigma_k = \bigcup_{r=1}^\infty \bigcup_{r'=1}^\infty B_{rj} \cap B_{r'k} = \emptyset \quad \text{for } j \neq k$$

and

$$\lambda \left( \bigcup_j \sigma_j \right) = \sum_{k=1}^\infty \lambda \left( \bigcup_j B_{kj} \right) = \sum_{k=1}^\infty \lambda(A_k) = \lambda \left( \bigcup_k A_k \right) = \lambda(V)$$

The microcanonical partition has two properties that are of interest for a large system. First,  $\lambda(\sigma_j) = \lambda(V)/\Omega$ , which is true by construction. Second, for every macroscopic subset  $S$  of  $V$  and each  $j$ , it is approximately true that  $\lambda(S \cap \sigma_j) = \lambda(S)/\Omega$ . This means that (in a coarse-grained sense) the points of each set  $\sigma_j$  are dispersed in an unbiased fashion throughout  $V$ . Indeed, it seems plausible for any function  $f \in \mathcal{L}_2$  that  $\int \xi_{\sigma_j} f d\lambda \approx \int f d\lambda/\Omega$ , for some microcanonical partition. The truth of this con-

<sup>6</sup> Such a partition exists by corollary 1-I.

jecture is the content of Theorems 1 and 2 and it is precisely this result which allows an initial condition to be placed on the ensemble  $\{\varphi_j\}$ . In other words, when constructed from such a partition, each function  $\varphi_j$  contains all the initial macroscopic information contained in  $\psi$ .

Before proving Theorems 1 and 2, it is necessary to define a refinement of a microcanonical partition.

**Definition.** Consider the collection of sets  $\{A_k\}$  which occurs in the definition of a microcanonical partition  $\{\sigma_j\}$ . Another microcanonical partition  $\{\sigma_j^*\}_{j=1}^\Omega$  is called a refinement of  $\{\sigma_j\}_{j=1}^\Omega$  if the collection  $\{A_k^*\}$  used to define  $\{\sigma_j^*\}$  has the property that  $A_k^* \subset A_r$  for one and only one  $A_r \in \{A_k\}$ .

**Theorem 1.** For any measurable set  $B \subset V$ , any  $\epsilon > 0$ , and any microcanonical partition  $\{\sigma_j\}_{j=1}^\Omega$ , there exists a refinement of  $\{\sigma_j\}$ , called  $\{\sigma_j^*\}_{j=1}^\Omega$ , with the property that  $|\lambda(B)/\Omega - \lambda(\sigma_j^* \cap B)| < \epsilon$ . Furthermore, if  $\{\sigma_j^{**}\}_{j=1}^\Omega$  is any refinement of  $\{\sigma_j^*\}$ , then  $|\lambda(B)/\Omega - \lambda(\sigma_j^{**} \cap B)| < \epsilon$ .

**Theorem 2.** Let  $\{f_i\}_{i=1}^m$  be any finite collection of functions in  $\mathcal{L}_p(V)$ ,  $1 \leq p < \infty$ . Then, for any  $\epsilon > 0$ , there exists a microcanonical partition  $\{\sigma_j\}_{j=1}^\Omega$  such that

$$\left| \int \xi_{\sigma_j} f_i d\lambda - (1/\Omega) \int f_i d\lambda \right| < \epsilon$$

for  $j = 1, 2, \dots, \Omega$  and all  $f_i$ .

The proofs of these theorems are long and technical and are given in the appendix. The importance of Theorem 2 is that it asserts the existence of a partition that “coarse-grains” any *finite* collection of functions in the sense that

$$\int \xi_{\sigma_j} f_k d\lambda \approx \int f_k d\lambda/\Omega$$

for all  $j$  and  $k$ .

Since it has been shown earlier that only symmetric partitions are of physical interest, it is necessary to prove an analog of Theorem 2 for symmetric partitions. Actually, Theorem 2 is almost sufficient by itself, since only expressions of the form  $\int \psi^* A_i \psi d\lambda$ , where  $A_i$  is a symmetric operator, are needed in quantum mechanics. But  $f_i = \psi^* A_i \psi$  is symmetric under permutations for both fermions and bosons, and so only the analog of Theorem 2 for symmetric functions is needed.

**Corollary 1.** If the functions in Theorem 2 are symmetric, then there exists a *symmetric* partition such that the conclusions of Theorem 2 hold.

*Proof.* Since  $f_i$  is symmetric

$$\int_V f_i d\lambda = \int_{\cup_{P \in \zeta} U_P} f_i d\lambda = \sum_{P \in \zeta} \int_{U_P} f_i d\lambda = N! \int_{U_1} f_i d\lambda$$



where  $U_p$  is defined in the section on symmetry. Thus, apply Theorem 2 to find a partition  $\{\sigma_j^*\}_{j=1}^{\Omega}$  such that

$$\left| N! \int_{U_1} \xi_{\sigma_j^*} f_i d\lambda - (N!/\Omega) \int_{U_1} f_i d\lambda \right| < \epsilon$$

But  $f_i$  is symmetric, so

$$\int_{U_1} \xi_{\sigma_j^*} f_i d\lambda = \int_{U_p} \xi_{P\sigma_j^*} f_i d\lambda$$

and

$$\begin{aligned} N! \int_{U_1} \xi_{\sigma_j^*} f_i d\lambda &= \sum_{P \in \zeta} \int_{U_p} \xi_{P\sigma_j^*} f_i d\lambda = \sum_{P \in \zeta} \int_V \xi_{P\sigma_j^*} f_i d\lambda \\ &= \int_V \xi_{\cup_{P \in \zeta} P\sigma_j^*} f_i d\lambda \end{aligned}$$

since  $P\sigma_j^* \cap P'\sigma_j^* = \emptyset$  if  $P \neq P'$ . Letting  $\sigma_j = \cup_{P \in \zeta} P\sigma_j^*$ , it follows that

$$N! \int_{U_1} \xi_{\sigma_j} f_i d\lambda = \int_V \xi_{\sigma_j} f_i d\lambda$$

and similarly that

$$(N!/\Omega) \int_{U_1} f_i d\lambda = (1/\Omega) \int_V f_i d\lambda$$

Thus,

$$\left| \int \xi_{\sigma_j} f_i - (1/\Omega) \int f_i d\lambda \right| < \epsilon$$

and  $\{\sigma_j\}_{j=1}^{\Omega}$  is a symmetric partition as verified above.  $\square$

The utility of this result in coarse-graining the ensemble decomposition to give an equally weighted average and the appropriate initial condition is shown in the next section.

## 5. A JUSTIFICATION OF ENSEMBLES IN STATISTICAL MECHANICS

The problem to which this series of papers is addressed is the nature of macroscopic states in statistical mechanics. A state, of course, is some mathematical construct which contains sufficient information to give a characterization of a system of interest. Although it has been assumed that every closed system is described by a wave function  $\psi$  in an  $\mathcal{L}_2$  space, this is useless for predictive purposes since  $\psi$  is unknown. What is known is only that  $\psi$  is an element of a collection of wave functions in  $\mathcal{L}_2$  all of which describe systems which *at an initial time* are identical to the system of interest. This characterization for a large system can be formalized in the following fashion.

Consider a large, closed,  $N$ -particle system initially in the state  $\psi$ . It is assumed that, since the system is large, it can be characterized initially by a collection of operators  $\{A_i\}_{i=1}^m$  with expectation values  $(\psi, A_i\psi) = a_i$ . The characterization is taken to be detailed enough so that, if a similar system is in the state  $\varphi$  and  $(\varphi, A_i\varphi) \approx a_i$  for all  $i$ ,<sup>7</sup> then the two systems cannot be distinguished macroscopically. This means that the collection of operators  $\{A_i\}_{i=1}^m$  describes all the macroscopic properties of the system, and is reasonably called a complete macroscopic description. The set of all initial states<sup>8</sup> compatible with such a complete description is called  $S_N$ .

It is clear that the macroscopic state of a system is bound up in the collection  $S_N$ , since all systems described by a vector in  $S_N$  are initially indistinguishable. It is possible that no such "state" can be attributed to the collection  $S_N$ . This would occur, for example, if systems which were initially identical evolved over time into distinguishable systems. On the other hand, the characterization by  $S_N$  may be complete enough so that no essential differences can be observed in the temporal behavior of systems with wave functions in  $S_N$ . These kinds of preparations have the important characteristic that the macroscopic behavior is independent of the microscopic behavior of the systems and are preparations that are useful experimentally.

The developments which follow use the mathematical ideas of the previous sections to obtain a density operator "state" for a large system characterized by certain collections  $S_N$ . While the method of attack involves the notion of local operators, the physical idea involved in the mathematics should not be forgotten. The idea, again, is that a single measurement of a *macroscopic* property is essentially a measurement on an ensemble of systems derived from local portions of the wave function. The ensemble arises, not from separate collections of particles in three-space, but disjoint portions of configuration space.

### 5.1. Ensembles for Large Systems

Two complete descriptions will be required in the developments below. The first description is defined by  $\{A_i\}_{i=1}^m$ ,  $\{a_i\}_{i=1}^m$ , and  $S_N$  as described above for the  $N$ -particle system. The second description is fictitious, and for it,  $\tilde{S}_N$  is the set of all states of the  $N$ -particle system that verify  $(\psi, \tilde{A}_i\psi) \approx a_i$ .

In order to write down the ensemble decomposition in general form, it is necessary to use the conjecture concerning the time preservation of localness. Since the conjecture has not been proved, what follows is strictly valid only when localness is a time invariant. With this in mind, it is possible to write the expectation value of any of the operators  $A_i$  for any state  $\psi$  in  $S_N$  as

$$(\psi, A_i(t)\psi) = \sum_{j=1}^{\Omega} (\varphi_j, \tilde{A}_i(t)\varphi_j) P_j$$

where  $P_j = \|\xi_{\sigma_j}\psi\|^2$  and the functions  $\varphi_j = \xi_{\sigma_j}\psi/\|\xi_{\sigma_j}\psi\|$  depend only on the parti-

<sup>7</sup> The symbol  $\approx$  means equality within experimental error.

<sup>8</sup> The word "state" loosely refers to a function in  $\mathcal{L}_2$ . Of course, the function must be in the domain of the operators which act upon it and have the appropriate permutation symmetry.

tion  $\{\sigma_j\}$ . To remove some of the arbitrariness from the functions  $\varphi_j$ , a special microcanonical partition is chosen. By Corollary 1, there exists a *symmetric* partition such that

$$\int \xi_{\sigma_j} \psi^* A_i(0) \psi d\lambda \approx (1/\Omega) \int \psi^* A_i(0) \psi d\lambda = a_i/\Omega$$

and

$$\int \xi_{\sigma_j} \psi^* \psi d\lambda \approx (1/\Omega) \int \psi^* \psi d\lambda = 1/\Omega$$

for all  $i$  and  $j$ . But

$$a_i/\Omega \approx \int \xi_{\sigma_j} \psi^* A_i(0) \psi d\lambda = \int \xi_{\sigma_j} \psi^* \tilde{A}_i(0) \psi d\lambda = \|\xi_{\sigma_j} \psi\|^2 (\varphi_j, \tilde{A}_i(0) \varphi_j)$$

and

$$\int \xi_{\sigma_j} \psi^* \psi d\lambda = \|\xi_{\sigma_j} \psi\|^2 \approx 1/\Omega$$

Hence,

$$(\varphi_j, \tilde{A}_i(0) \varphi_j) \approx a_i$$

and  $P_j \approx 1/\Omega$ . For this partition, the ensemble decomposition becomes

$$(\psi, A_i(t) \psi) \approx \sum_{j=1}^{\Omega} (\varphi_j, \tilde{A}_i(t) \varphi_j)/\Omega \tag{1}$$

with the initial condition that  $(\varphi_j, \tilde{A}_i(0) \varphi_j) \approx a_i$ , i.e.,  $\varphi_j \in \tilde{S}_N$ .

Equation (1) is the essential result of this section and expresses the expectation value of any operator  $A_i$  for a pure state  $\psi$  as an equally weighted average of states in  $\tilde{S}_N$ . Since no restrictions have been made of the system, Eq. (1) applies to any system contained in a bounded region of space.

In order to see the relationship between Eq. (1) and the usual microcanonical-type ensemble for large systems, both the nature of the initial preparation  $S_N$  and the structure of the functions  $\varphi_j$  must be examined. In particular, it is necessary that the "initial" sets of wave functions,  $S_N$  and  $\tilde{S}_N$ , be related in some fashion. Since  $\tilde{S}_N$  is strictly larger than  $S_N$ , the only realistic requirement is that there exist a subspace  $X_N \subset S_N$  that is "almost all" of both  $S_N$  and  $\tilde{S}_N$ . By this, it is meant that, if  $\pi$  is the projector on  $X_N$ , then  $\|\pi\psi\| \approx 1$  for  $\psi$  in  $S_N$  or  $\tilde{S}_N$ . It is expected that this condition might hold for large systems and it is roughly equivalent to the notion of "phase cells" commonly used in ergodic theory.<sup>(11)</sup>

If such a large subspace of  $S_N$  and  $\tilde{S}_N$  exists, then Eq. (1) can be reinterpreted as an equally weighted average over states in  $S_N$  since  $\tilde{A}_i(t) = A_i(t)$  on  $S_N$ . However, this is not yet equivalent to the Gibbsian ensemble because there is no certainty that  $\varphi_j$  is appreciably different from  $\psi$ . In other words, by coarse-graining configuration space to ensure that  $\varphi_j$  is in  $\tilde{S}_N$ , it may be necessary to make  $\varphi_j$  essentially the same as  $\psi$ . That is,  $\varphi_j$  and  $\psi$  might have essentially the same components in a basis. Thus, Eq. (1) would be trivial because each  $\varphi_j$  would be *microscopically* identical to  $\psi$ .

To see for large systems that the (1) ensemble average is not necessarily trivial,

it is necessary to look at the construction of the functions  $\varphi_j$  in detail. In particular, the size of the open cubes  $\{A_k\}_{k=1}^\infty$  from which the partition  $\{\sigma_j\}$  is constructed is very important. Since only coarse details are required for a macroscopic preparation, it should suffice (when choosing to partition that makes  $\varphi_j \in \mathcal{S}_N$ ) to take the edge of a cube  $A_k$  to be *microscopically large* but *macroscopically small*. Thus, the cube  $A_k$  can reflect a great deal of microscopic variation, but little variation on the macroscopic scale. Since each function  $\varphi_j$  is constructed from only a small part of  $\psi$  on  $A_k$ , the functions  $\varphi_j$  should be *microscopically distinct* from each other and from  $\psi$ .

To get an idea of the order of magnitudes involved in this construction, take the edge of a cube  $A_k$  to be  $10^{-4}$  cm and divide  $A_k$  into subcubes  $B_{kj}$  with edges  $10^{-6}$  cm. For large systems,  $A_k$  should correspond to uniform macroscopic properties while the cubes  $B_{kj}$  should reflect great microscopic differences. In addition, for this case, the number of members of the partition is  $\Omega = 100^{3N}$ , which is the order of degeneracies for large systems.<sup>(12)</sup> Thus, it is plausible that the coarse-graining of configuration space can be balanced between macroscopic uniformity and microscopic diversity for the functions  $\varphi_j$ .

This discussion can be formalized by making the following assumptions: (i) A set  $X_N$ , as described above, exists with a basis  $\{\theta_n\}_{n=1}^W$  and (ii) for any  $\psi \in S_N$ , a partition exists that randomly distributes the functions  $\varphi_j$  throughout  $\mathcal{S}_N$ . Using these assumptions, Eq. (1) becomes

$$(\psi, A_i(t) \psi) \approx \sum_{m=1}^W \sum_{n=1}^W (\theta_m, A_i(t) \theta_n) \sum_{j=1}^{\Omega} C_{jm}^* C_{jn} / \Omega$$

where  $C_{jm} = (\theta_m, \varphi_j)$  and small terms not in  $X_N$  have been neglected. Because of assumption (ii), the coefficients of the cross terms in this equation vanish and the diagonal coefficients,  $\sum_{j=1}^{\Omega} |C_{jm}|^2 / \Omega$ , are equal. Finally, the approximate normalization condition  $\sum_{j=1}^{\Omega} \sum_{m=1}^W |C_{jm}|^2 = \Omega$  implies that  $\sum_{j=1}^{\Omega} |C_{jm}|^2 / \Omega = 1/W$ , and the above equation reduces to

$$(\psi, A_i(t) \psi) \approx \sum_{m=1}^W (\theta_m, A_i(t) \theta_m) / W$$

which is the generalized microcanonical-type average of Gibbs'.

It is worth emphasizing that the "derivation" above does not give a direct verification of the equilibrium microcanonical ensemble. Indeed, since a macroscopically complete set of observables has been used to define  $S_N$ , the results are a quantum analog of Lewis' results in classical ergodic theory.<sup>(13)</sup> Thus, to verify that the above ideas lead to the equilibrium microcanonical ensemble, it would be necessary to verify assumptions (i) and (ii) above. This is no easy task and is somewhat like the situation in classical ergodic theory where either metric indecomposibility or a lack of motion constants other than the energy must be shown.<sup>(14)</sup>

## 6. SUMMARY

The developments of this paper are an attempt to carry out the physical idea presented in the introduction; namely that ensemble averages arise in a natural way

from redundant information carried by pure state wave functions. This redundant information is carried by projections  $\varphi_j$  of the function  $\psi$  onto disjoint regions of configuration space. Because operators corresponding to observables are “local,” the projected wave functions  $\varphi_j$  are formally independent of one another and can be used to form an ensemble average. By forming the projected wave functions appropriately, i.e., “coarse-graining,” it is shown that the functions  $\varphi_j$  can be made *macroscopically* the same as  $\psi$  and that the functions can be given equal weights in the average. This is the central result of this paper and provides a new point of view for understanding ensembles. For large systems, a heuristic argument is given which suggests that the coarse-graining can be performed so that the functions in the ensemble  $\{\varphi_j\}$  are *microscopically different* from each other and from  $\psi$ . If for such a decomposition the functions  $\varphi_j$  are “randomly” distributed throughout the state space of the initial preparation, then it is shown that the generalized microcanonical average of Gibbs’ is valid. These arguments make it clear how in specific cases a mathematical attack of the justification of ensembles would proceed.

## APPENDIX

### Proof of Theorem 1

*Case 1.* The proof is in two steps. The first step proves the theorem for any open set  $I$  that has zero-measure boundary, i.e.,  $\lambda(\partial I) = 0$ . For such a set, a stronger statement holds than in the general case, namely equality holds in the conclusion of the theorem.

Let  $\{A_k\}$  be the collection of open disjoint cubes that defines  $\{\sigma_j\}$ . Then, let

$$\begin{aligned} K_1 &= \{A_j \in \{A_k\}: A_j \cap I = \emptyset\} \\ K_2 &= \{A_j \in \{A_k\}: A_j \cap I = A_j\} \\ K_3 &= \{A_j \in \{A_k\}: A_j \notin K_1 \text{ or } K_2\} \end{aligned}$$

Clearly,  $\{A_k\} = K_1 \cup K_2 \cup K_3$  and the collections are disjoint. A collection of open cubes,  $K_4$ , will be constructed from the elements of  $K_3$  such that  $\{A_k^*\} = K_1 \cup K_2 \cup K_4$ .

Let  $A_m \in K_3$ . Since  $I, (I)'$ , and  $\partial I$  are disjoint and  $I \cup (I)' \cup \partial I = V$ , it follows that  $A_m = (A_m \cap I) \cup (A_m \cap (I)') \cup (A_m \cap \partial I)$ . Consider the two disjoint, nonvoid, open sets  $A_m \cap I$  and  $A_m \cap (I)'$ . Each of these can be approximated by collections of open disjoint cubes,  $\{A_{mj}^1\}_j$  and  $\{A_{mj}^2\}_j$ , respectively, as noted in Corollary 1-I. Define  $K_4 = \{A_{mj}^1: A_m \in K_3\} \cup \{A_{mj}^2: A_m \in K_3\}$  and then let  $\{A_r^*\} = K_1 \cup K_2 \cup K_4$ .

Now,  $K_1$  and  $K_2$  are countable collections of open cubes and  $K_4$  is clearly such a collection, so  $\{A_r^*\}$  is a countable collection of open cubes. By construction,  $A_r^* \subset A_k$  for one and only one  $k$  and, moreover,  $A_k^* \cap A_r^* = \emptyset$  if  $k \neq r$ .

The collection  $\{\sigma_j^*\}$  is constructed from the sets  $\{A_k^*\}$  as prescribed in the definition of the microcanonical partition. Thus, to show that  $\{\sigma_j^*\}$  is a microcanonical partition that refines  $\{\sigma_j\}$ , it is only necessary to check that  $\lambda((\cup_r A_r^*)' \cap V) = 0$ , or equivalently, that  $\lambda((\cup_r A_r^*)' \cap \cup_r A_r) = 0$ . But this is clear since the only points in

$\bigcup_r A_r$  that are not in  $\bigcup_r A_r^*$  come from a countable union of zero-measure boundaries of open sets. Thus,  $\{\sigma_j^*\}$  is a microcanonical partition that refines  $\{\sigma_j\}$ .

In order to see that this is the desired refinement, let  $B_{kj}^*$  be the contribution to  $\sigma_j^*$  coming from the cube  $A_k^*$ , i.e.,  $\sigma_j^* = \bigcup_{k=1}^* B_{kj}^*$ . Then, by construction, either (a)  $A_k^* \cap I = \emptyset$  or (b)  $A_k^* \cap I = A_k^*$ , and in all cases (c)  $\lambda(B_{kj}^*) = \lambda(A_k^*)/\Omega$ .

If (a) holds, then  $B_{kj}^* \cap I = \emptyset$  and

$$\lambda(B_{kj}^* \cap I) = \lambda(\emptyset) = \lambda(A_k^* \cap I)/\Omega$$

If (b) holds, then  $B_{kj}^* \cap I = B_{kj}^*$  and (c) implies that

$$\lambda(B_{kj}^* \cap I) = \lambda(B_{kj}^*) = \lambda(A_k^*)/\Omega = \lambda(A_k^* \cap I)/\Omega$$

Thus, for all  $k$  and  $j$ ,  $\lambda(B_{kj}^* \cap I) = \lambda(A_k^* \cap I)/\Omega$ . Hence,

$$\begin{aligned} \lambda(\sigma_j^* \cap I) &= \lambda\left(\bigcup_k B_{kj}^* \cap I\right) = \sum_k \lambda(B_{kj}^* \cap I) \\ &= \sum_k \lambda(A_k^* \cap I)/\Omega = \lambda\left(\bigcup_k A_k^* \cap I\right)/\Omega \end{aligned}$$

But  $\lambda((\bigcup_k A_k^*)' \cap I) \leq \lambda((\bigcup_k A_k^*)' \cap V) = 0$ , so (d)  $\lambda(\sigma_j^* \cap I) = \lambda(I)/\Omega$ .

Since for any refinement of  $\{\sigma_j^*\}$  the relationships (a)–(c) hold, it is clear that the refinement verifies (d).

**Case 2.** Let  $B \subset V$  be an arbitrary measurable set. Choose a sequence of open sets,  $\{U_n\}$  with  $B \subset U_n$  and  $\lambda(U_n) < \lambda(B) + \frac{1}{2}^{n+1}$ . Furthermore, for each set  $U_n$ , select a finite collection of open disjoint cubes  $\{\omega_{nm}\}_m$  with  $\omega_{nm} \subset U_n$  for all  $m$  and such that  $\omega_n \equiv \bigcup_m \omega_{nm}$  satisfies  $\lambda(\omega_n' \cap U_n) \leq \frac{1}{2}^{n+1}$ . Thus,  $\lambda(U_n) \leq \lambda(\omega_n) + \frac{1}{2}^{n+1}$  and  $\lambda(\omega_n) \leq \lambda(U_n)$ . The possibility of doing this has been discussed in the proof of Theorem 3-I.

Take any microcanonical partition  $\{\sigma_j\}_{j=1}^\Omega$  and any  $\epsilon > 0$  and choose some  $n$  so that  $\frac{1}{2}^n < \epsilon$ . For  $\omega_n$  select a refinement that satisfies  $\lambda(\sigma_j^* \cap \omega_n) = \lambda(\omega_n)/\Omega$ . This is possible by case 1, since  $\omega_n$  is a finite union of disjoint cubes.

To obtain estimates for  $\lambda(B \cap \sigma_j^*)$ , write first

$$\begin{aligned} B \cap \sigma_j^* \cap U_n &\subset U_n \cap \sigma_j^* = (\omega_n \cup (\omega_n' \cap U_n)) \cap \sigma_j^* \\ &= (\sigma_j^* \cap \omega_n) \cup (\sigma_j^* \cap \omega_n' \cap U_n) \end{aligned}$$

Thus,

$$\begin{aligned} \lambda(B \cap \sigma_j^*) &\leq \lambda(\sigma_j^* \cap \omega_n) + \lambda(\sigma_j^* \cap \omega_n' \cap U_n) \\ &\leq \lambda(\sigma_j^* \cap \omega_n) + \lambda(\omega_n' \cap U_n) \\ &\leq \lambda(\omega_n)/\Omega + \frac{1}{2}^{n+1} \\ &\leq \lambda(U_n)/\Omega + \frac{1}{2}^{n+1} \\ &< (\lambda(B) + \frac{1}{2}^n)/\Omega + \frac{1}{2}^{n+1} \\ &< \lambda(B)/\Omega + \frac{1}{2}^n \end{aligned} \tag{2}$$

A second estimate comes from

$$\omega_n \cap \sigma_j^* \subset U_n \cap \sigma_j^* \subset (B \cup (B' \cap U_n)) \cap \sigma_j^* = (\sigma_j^* \cap B) \cup (\sigma_j^* \cap B' \cap U_n)$$

Thus,

$$\begin{aligned} \lambda(\omega_n \cap \sigma_j^*) &\leq \lambda(B \cap \sigma_j^*) + \lambda(B' \cap U_n \cap \sigma_j^*) \\ &\leq \lambda(B \cap \sigma_j^*) + \lambda(B' \cap U_n) \\ &\leq (B \cap \sigma_j^*) + \frac{1}{2}^{n+1} \end{aligned}$$

or  $\lambda(\omega_n)/\Omega \leq \lambda(B \cap \sigma_j^*) + \frac{1}{2}^{n+1}$ . But  $\lambda(B) - \lambda(\omega_n' \cap B) = \lambda(\omega_n \cap B) \leq \lambda(\omega_n)$ . Therefore,

$$(\lambda(B) - \lambda(\omega_n' \cap B))/\Omega \leq \lambda(B \cap \sigma_j^*) + \frac{1}{2}^{n+1}$$

Thus,

$$\begin{aligned} \lambda(B)/\Omega &\leq \lambda(\omega_n' \cap B)/\Omega + \lambda(B \cap \sigma_j^*) + \frac{1}{2}^{n+1} \\ &\leq \lambda(\omega_n' \cap U_n)/\Omega + \lambda(B \cap \sigma_j^*) + \frac{1}{2}^{n+1} \\ &\leq \frac{1}{2}^{n+1}/\Omega + \lambda(B \cap \sigma_j^*) + \frac{1}{2}^{n+1} \\ &< \lambda(B \cap \sigma_j^*) + \frac{1}{2}^n \end{aligned} \tag{3}$$

Hence, it follows from Eqs. (2) and (3) that

$$|\lambda(B)/\Omega - \lambda(B \cap \sigma_j^*)| < \frac{1}{2}^n < \epsilon$$

Moreover, for any refinement of  $\{\sigma_j^*\}_{j=1}^{\Omega}$ , it is true by case 1 that  $\lambda(\omega_n \cap \sigma_j^{**}) = \lambda(\omega_n)/\Omega$ . Thus, the equalities and inequalities above are valid for the refinement and it remains true for  $\{\sigma_j^{**}\}_{j=1}^{\Omega}$  that  $|\lambda(B)/\Omega - \lambda(B \cap \sigma_j^{**})| < \epsilon$ .  $\square$

### Proof of Theorem 2

For any  $\Omega > 1$ , any measurable set  $\sigma_j, f_i \in \mathcal{L}_p, 1 < p < \infty$ , and  $s_i \in \mathcal{L}_p$ , the following inequalities hold:

$$\begin{aligned} &\left| \int \xi_{\sigma_j} f_i d\lambda - (1/\Omega) \int f_i d\lambda \right| \\ &\leq \left| \int \xi_{\sigma_j} f_i d\lambda - \int \xi_{\sigma_j} s_i d\lambda \right| + \left| \int \xi_{\sigma_j} s_i d\lambda - (1/\Omega) \int f_i d\lambda \right| \\ &\leq \left| \int \xi_{\sigma_j} (f_i - s_i) d\lambda \right| + (1/\Omega) \left| \int (f_i - s_i) d\lambda \right| + \left| \int \xi_{\sigma_j} s_i d\lambda - \int (s_i/\Omega) d\lambda \right| \end{aligned} \tag{4}$$

$$\leq \|\xi_{\sigma_j}\|_p \|f_i - s_i\|_p + (1/\Omega) \|f_i - s_i\|_p \|\xi_{\nu}\|_p + \left| \int \xi_{\sigma_j} s_i d\lambda - \int (s_i/\Omega) d\lambda \right| \tag{5}$$

where  $\|\cdot\|_p$  is the  $\mathcal{L}_p$  norm and  $p' \equiv p/(p - 1)$ . Equation (5) is a consequence of Hölder's inequality.<sup>(13)</sup> If  $p = 1$ , then it follows from Eq. (4) that

$$\left| \int \xi_{\sigma_j} f_i d\lambda - (1/\Omega) \int f_i d\lambda \right| \leq \|f_i - s_i\|_1 + (1/\Omega) \|f_i - s_i\|_1 + \left| \int \xi_{\sigma_j} s_i d\lambda - (1/\Omega) \int s_i d\lambda \right| \tag{6}$$

Now, given any  $1 \leq p < \infty$ , choose for each  $f_i$  a simple function such that  $\|f_i - s_i\|_p < \epsilon/3(\|\xi_V\|_{p'} + 1)$ . This is possible because the simple functions are dense in  $\mathcal{L}_p(V)$ .<sup>(13)</sup> Thus, both Eqs. (5) and (6) imply that

$$\left| \int \xi_{\sigma_j} f_i d\lambda - (1/\Omega) \int f_i d\lambda \right| \leq 2\epsilon/3 + \left| \int \xi_{\sigma_j} s_i d\lambda - (1/\Omega) \int s_i d\lambda \right| \tag{7}$$

Writing  $s_i = \sum_{k=1}^n \mathcal{O}_{ki} \xi_{A_{ki}}$ , where  $|\mathcal{O}_{ki}| < \infty$  and  $A_{ki} \subset V$  and  $A_{ki}$  is measurable, Eq. (7) becomes

$$\begin{aligned} \left| \int \xi_{\sigma_j} f_i d\lambda - (1/\Omega) \int f_i d\lambda \right| &\leq 2\epsilon/3 + \left| \int \sum_{k=1}^{n(i)} \mathcal{O}_{ki} (\xi_{\sigma_j \cap A_{ki}} - \xi_{A_{ki}}/\Omega) d\lambda \right| \\ &= 2\epsilon/3 + \left| \sum_{k=1}^{n(i)} \mathcal{O}_{ki} (\lambda(\sigma_j \cap A_{ki}) - \lambda(A_{ki})/\Omega) \right| \\ &\leq 2\epsilon/3 + \sum_{k=1}^{n(i)} |\mathcal{O}_{ki}| \left| \lambda(\sigma_j \cap A_{ki}) - \lambda(A_{ki})/\Omega \right| \end{aligned}$$

Now, select a partition  $\{\sigma_j\}_{j=1}^\Omega$  such that, for all refinements and each  $j, k$ , and  $i$ ,

$$\left| \lambda(\sigma_j \cap A_{ki}) - \lambda(A_{ki})/\Omega \right| \leq \epsilon/3 \left[ 1 + \max_i \left( \sum_{k=1}^{n(i)} |\mathcal{O}_{ki}| \right) \right] \tag{8}$$

Thus,

$$\left| \int \xi_{\sigma_j} f_i d\lambda - (1/\Omega) \int f_i d\lambda \right| \leq 2\epsilon/3 + \epsilon \sum_{k=1}^{n(i)} |\mathcal{O}_{ki}|/3 \left( 1 + \max_i \sum_{k=1}^{n(i)} |\mathcal{O}_{ki}| \right) < \epsilon$$

It is possible to pick such a partition, since one can be picked for  $A_{11}$ —say  $\{\sigma_j^*\}_{j=1}^\Omega$ —by Theorem 1. Also, a refinement of  $\{\sigma_j^*\}_{j=1}^\Omega$ —say  $\{\sigma_j^{**}\}_{j=1}^\Omega$ —can be chosen by Theorem 1 so that Eq. (8) holds for  $A_{12}$ . But since  $\{\sigma_j^{**}\}_{j=1}^\Omega$  refines  $\{\sigma_j^*\}_{j=1}^\Omega$ , Eq. (8) still holds for  $A_{11}$ . By repeating this process for all the sets  $\{A_{ki}\}_{k=1, i=1}^{n(i)m}$ , it is clear that the proper microcanonical partition can be obtained.  $\square$

### ACKNOWLEDGMENTS

The author would like to acknowledge Professor Terrell Hill, whose patience and permissiveness allowed this work to be carried out. A generous fellowship to the



author from the Battelle Memorial Institute is also gratefully acknowledged. Finally, a word of thanks must be given to Professors Paul Civin and I. E. Farquhar and Dr. Ronald Fox for reading the manuscript and to Professors Robert Hermann and Robert Bonic for advice during the initial stages of this work.

## REFERENCES

1. J. E. Keizer, *J. Stat. Phys.* 2:213 (1970).
2. A. Messiah, *Quantum Mechanics*, Vol. II (John Wiley and Sons, New York, 1958), Chapter 14.
3. I. E. Segal and R. A. Kunze, *Integrals and Operators* (McGraw-Hill Book Co., New York, 1968), Chapter VII.
4. A. Messiah, *Quantum Mechanics*, Vol. II (John Wiley and Sons, New York, 1958), Chapter 13.
5. A. Messiah, *Quantum Mechanics*, Vol. I (John Wiley and Sons, New York, 1958), p. 328.
6. R. Hermann, *Linear Algebra and Quantum Mechanics*, unpublished notes, 1967.
7. P. Roman, *Advanced Quantum Mechanics* (Addison-Wesley Publishing Co., Reading, Massachusetts, 1965), p. 45.
8. G. W. Mackey, *Mathematical Foundations of Quantum Mechanics*, (W. A. Benjamin, New York, 1963), p. 81.
9. A. Messiah, *Quantum Mechanics*, Vol. I (John Wiley and Sons, New York, 1958), p. 75.
10. G. Emch, in *Lectures in Theoretical Physics, Boulder, 1965*, Vol. 8a, (University of Colorado Press, Boulder, Colorado (1966).
11. I. E. Farquhar, *Ergodic Theory in Statistical Mechanics* (Interscience Publishers, London, 1964), p. 149.
12. T. L. Hill, *Introduction to Statistical Thermodynamics* (Addison-Wesley Publishing Co., Reading, Massachusetts, 1960), p. 28.
13. R. M. Lewis, *Arch. Ratl. Mech. Anal.* 5:355 (1960).
14. I. E. Farquhar, *Ergodic Theory in Statistical Mechanics* (Interscience Publishers, London, 1964)