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

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In this and the following paper, a new approach for the justification of ensembles in statistical mechanics is given. The essential physical idea is that a measurement is an average of values arising from disjoint regions in three-space. This idea is given a mathematical basis in terms of a class of operators called "local operators," and the first paper is devoted primarily to the development of the properties of local operators. In particular, a complete characterization of the bounded local operators on $\mathscr{L}_2$ spaces of finite measure is given. Two results of importance for statistical mechanics are also derived. First, it is shown that the observables of quantum mechanics are local operators. Second, it is shown that the expectation value of an observable for a pure state can be written formally as an ensemble average. In the following paper, these results are used to develop a new approach for the justification of statistical ensembles.

KEY WORDS: Local operators; ensemble average; microcanonical ensemble; foundations of statistical mechanics.

1. INTRODUCTION

A central problem in the foundation of statistical mechanics is the justification of the use of statistical averages or ensembles. The use of such averages was introduced by Gibbs at the end of the nineteenth century,[1] although the averages were conceived

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by him as merely a formal device for understanding macroscopic systems. Gibbs' ideas have worked so well, however, that they are now accepted as essential to the theory of statistical mechanics.

Gibbs' idea of statistical averaging is a simple one. Namely, if the mechanical "state" of a system is unknown, a value for an observable of the system may be calculated by averaging over all those states which might conceivably represent the unknown state of the system. Such an average over possible states is called a representative ensemble average, where the term "representative" is meant to convey that each state in the average actually represents a system which is identical in its preparation to the system of interest. Tolman[2] and others[3,4] have made it plausible that the average should be an equally weighted one for closed systems—the ultimate justification for such an assumption being that predictions based on it are verified experimentally. Thus, the physical picture of an ensemble is a collection of independent systems which are prepared in the same fashion. The ensemble average is performed by making measurements on each system and averaging the results.

Although the introduction of ensembles by Gibbs was made well before the advent of quantum mechanics, it seemed to foreshadow some of the more profound aspects of the quantum theory. For example, in the Copenhagen interpretation of quantum mechanics,[5] it is assumed that the state of any physical system is a vector ψ in a Hilbert space. The state ψ, however, gives information only about the distribution of measured values taken from experiments on a collection of independent systems all in the state ψ. Such a collection is called a pure state ensemble and corresponds closely to the ensemble of Gibbs'. Of course, Gibbs did not envision that dispersion might arise from the mechanical state itself.

The notion of a pure state in quantum mechanics has a natural generalization called by von Neumann a mixed state.[6] The idea, in fact, is exactly that of Gibbs but with deeper implications. Von Neumann considered preparations for which the state ψ of the system was unknown. Under these conditions, it is not possible to prepare the pure state ensemble which is the meaningful object in quantum mechanics. Von Neumann, however, argued that it is possible to prepare an ensemble in which it is required only that each system have the same preparation as the system of interest. When the distribution of measured values for such an ensemble is obtained, these constitute the "state" of the incompletely prepared system in exactly the same way that a pure state ensemble contains the information relevant to a pure state ψ.[7] Since the distribution of measured values for such a mixed state ensemble can be represented by a density operator, it is concluded that the "state" of a physical system is actually given by a density operator.

In this way, von Neumann's mixed state seems to vindicate the Gibbs' idea. Unfortunately, it does so in a very unsatisfactory way, because the density operator is a purely observational property: it must be determined experimentally in the same sense that a pure state ψ must be determined. In other words, the conclusion is that a density operator, i.e., a representative ensemble average, correctly describes a physical system but that there is no theoretical way of determining the density operator. This indeterminacy of the density operator has been stressed by Tolman[2] and more recently by Fano.[7]

There is another disadvantage to this method of looking at ensembles. The formalism is set up to deal with measurements that are made on an ensemble of systems. Since this is the case for small systems—for example, individual particles in an "ensemble" formed by a beam of noninteracting particles—the density-operator formalism is extremely useful. The formalism can clarify interesting properties of large systems, however, only when the density operator is known. For example, an important question for macroscopic systems is why macroscopically identical systems maintain their macroscopic identity over time. The density-operator formalism can answer only that over time the density operator corresponds to a "sharp" distribution of values. But this can be checked only when the density operator is known, and the size of large systems makes this prohibitive.[2,7,8]

There is, however, an alternative approach for justifying the use of ensembles in statistical mechanics which uses an idea familiar in both quantum and classical mechanics. This approach assumes the existence of a vector ψ (or, in the case of classical mechanics, a collection of coordinates and momenta) which describes the state of the system completely even if the vector ψ is unknown. Of course, when ψ is unknown, it has no operational or predictive value. However, if a system has been prepared in some way, it certainly can be said that its state ψ is one of those states compatible with that preparation. Thus, even though ψ is unknown, it is possible to examine all the states compatible with the preparation of the system to see if they have any common properties—for example, similar distributions of measured values. In fact, this is exactly the tactic used in ergodic theory[9] and will be adopted here.

1.1. Ergodic Theory

Quantum ergodic theory is a natural extension of the ideas of the classical theory and originated in the work of von Neumann.[10] Von Neumann proved two kind of ergodic theorems, a so-called fined-grained and a coarse-grained theorem. The first of these is of little use since it applies only to pure state preparations of macroscopic systems[9]; the coarse-grained version has recently fallen into ill-repute because of a certain averaging process involved in the proof.[9,11] The central ideas of von Neumann, however, are clear, and recent attempts have been made to repair his work.[11]

Ergodic theory considers an equilibrium preparation of a closed system and seeks to examine the nature of the distribution of each pure state ψ consistent with the preparation. This is done by assuming that the actual distribution is a time average of the quantum mechanical distribution. Since a pure state distribution can be determined completely by the expectation values of the moments of observables, it suffices to examine the distribution by considering expectation values. Thus, the expectation value of an operator A at time t, $(\psi(t), A\psi(t))$, is replaced by its time-average value

$$\overline{(\psi(t), A\psi(t))} = (1/t_0) \int_t^{t+t_0} (\psi(t'), A\psi(t'))\, dt'$$

In order to justify the use of the microcanonical density operator, ergodic theory attempts to show that $\overline{(\psi(t), A\psi(t))}$ equals the microcanonical average of A for all times and all initial states that agree with the equilibrium preparation. The techniques that are used, however, show only that this holds for almost all initial states and almost all initial times.[11] Moreover, to prove even this, it must be assumed that states agreeing with the preparation occur in nature with equal likelihood.[11] But this, it is clear, is equivalent to *assuming* the microcanonical form for the density operator in von Neumann's formalism, and so this method creates no new insight into the problem.[9]

1.2. Introductory Notions

Since quantum ergodic theory sheds little light on the use of ensembles in statistical mechanics, an entirely different approach to the problem is presented in this paper. In fact, the methods developed here are more general than those of ergodic theory and can be applied to preparations corresponding to systems both in and out of equilibrium.

The basic technique of this method is the same as that of ergodic theory. Thus, for a given type of preparation for a system, the quantum mechanical distributions of all states ψ consistent with the preparation are examined. It is not necessary to introduce time averages into this approach and so the distribution of a pure state will be examined solely by looking at expectation values.

It should be stressed at the outset that the question to which this work is directed concerns the specification of the "state" of a large system. The exact question is, "For what preparations can a density operator, i.e., a representative ensemble average, be used to calculate expectation values for all systems agreeing with the preparation?" In other words, an attempt is made to understand the observation that identically prepared macroscopic systems behave identically over time if the preparation is specific enough. The important question of the details of the temporal behavior, e.g., approach to equilibrium or macroscopic conservation laws, is not discussed since its answer seems to be disjoint from the present considerations.

The motivation for the approach developed here is physical. Because measurements on a large system involve interactions with immense numbers of particles, it is reasonable to expect that the "statistical" aspects of statistical mechanics arise from the measuring process itself. That is, disjoint portions of a large system somehow contribute incoherently to measured values and so *an ensemble average is actually performed during a measurement.*

In order to develop a stronger feeling for this notion, consider a measurement of an intensive quantity $g(r)$, for example, the momentum density. Using the particle-number-operator formalism and interpreting $g(r)$ as the expectation value of a field-density operator, it is easy to see that the values of $g(r)$ in a three-space region σ depend only on the wave function in a small part of configuration space, N_σ. In fact, N_σ is just that part of configuration space for which one of the particles is in the region σ. This is illustrated in Fig. 1 for the case of two one-dimensional particles.

The fact that only a small portion of the wave function is needed to specify $g(r)$ in the region σ implies that localized measurements in three-space have a kind of localized analog in configuration space. In particular, a measurement in a region σ of three-space "detects" only that part of the wave function defined on the associated region N_σ in configuration space. Moreover, it is clear from Fig. 2 that there is only

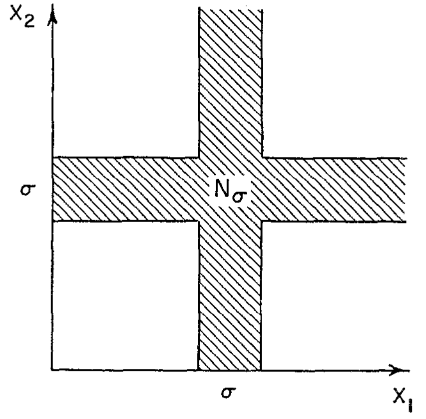

Fig. 1. Configuration space for two particles in one dimension. The cross-hatched region N_σ is that part of configuration space for which at least one particle is in the region σ.

slight overlap between configuration-space regions N_{σ_1} and N_{σ_2} which are associated with *disjoint* three-space regions σ_1 and σ_2. Thus, *measurements* at a fixed time in disjoint regions of three-space are in general *independent* of one another.

To see what implications this "independence of measurements" has for large systems, consider the spectrophotometric measurement of the density at a point r in a large system. The measurement is carried out in two steps. In the first step, a photon is directed into a small region Σ around r; in the second step, a detector determines whether or not the photon has been absorbed. The total measurement is a sum of similar processes involving many photons. Consider next that the region Σ has been

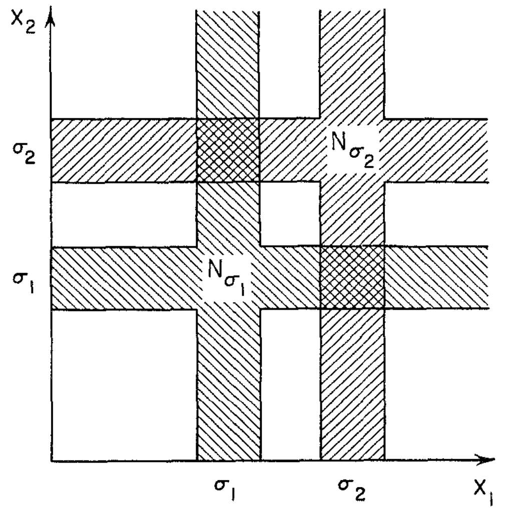

Fig. 2. The overlap of the configuration-space regions N_{σ_1} and N_{σ_2} is shown by the double cross-hatching. See text for explanation.

divided up into disjoint subregions σ and then form the corresponding regions in configuration space N_σ. Then, the photons that traverse through the region σ "measure" a density determined only by the wave function defined on the configuration-space region N_σ. But since the values of the wave function on different regions N_σ are independent of one another, the final measured value will be just an incoherent average of the values obtained from each region N_σ. This may be written as

$$d = \sum_\sigma P_\sigma d_\sigma$$

where d is the measured density at r, d_σ is the density obtained from the region N_σ, and P_σ is some weight factor depending on the division of Σ into subregions. Clearly, by choosing the division appropriately, P_σ will be the same for each subregion. Thus, the measured value can be thought of as an equally weighted average of values each of which arises from an independent portion of the wave function. It should be stressed that, to arrive at this notion, the particles in the three-space regions σ are *not* considered to be independent. In fact, it is the measured values which are independent and independence is obtained only by looking at the configuration space.

If this physical idea that measured values are a superposition of values obtained from different "local" regions in configuration space is correct, it is reasonable to expect that quantum mechanics has some sort of "local" property built into its structure. In fact, it turns out that this notion of localness can be given an exact mathematical formulation in terms of a class of operators, called local operators, which is defined below. The important result in this connection is that the *observables* in quantum mechanics are local operators. Using this property, it is shown that independent contributions to expectation values do indeed come from disjoint regions in configuration space.

The first paper in this series is devoted to the development of the mathematical properties of local operators. The most useful result obtained here is a theorem that demonstrates the existence for any local operator of a nontrivial extension which is also a local operator. Using this theorem, a complete characterization of the bounded local operators on $\mathscr{L}_2$ spaces of finite measure is given. Finally, a preliminary result of importance in statistical mechanics is obtained by showing that a *pure state* expectation value of a local operator can be written exactly in the form of an ensemble average. The second paper in this series considers the special case of large systems and attempts to connect the formal ensemble average developed in this paper to the physical ensemble average of Gibbs.

2. MATHEMATICAL PRELIMINARIES

Since it is attempted in this series of papers to examine the foundations of statistical mechanics using quantum mechanics, it is necessary to explore the mathematics of quantum mechanics in detail. Certain theorems developed in this section concerning quantum mechanical operators and the topology of configuration space are absolutely essential to the final results.

The notation used in this and the following paper is that of Hewitt and Stromberg[12] and is relatively standard. Thus, if E is a point set, E' is its complement; E^- its closure; E° its interior; and ∂E its boundary. The symbol $\bigcup$ means the set union, and $\bigcap$ the intersection. The symbols $\bigcup_k$, $\bigcap_j$, etc. represent the repeated union or intersection over a collection of indexed sets. The notation $\{\alpha_k\}_{k=1}^{\infty}$ (often written $\{\alpha_k\}$) means a collection of sets α_k indexed by the integers.

The customary mathematical setting for quantum mechanics is a Hilbert space. Following von Neumann,[6] the Hilbert space for an N-particle system without spin is taken to be $\mathscr{L}_2(R^{3N})$, the space of all Lebesgue, $3N$-dimensional, square-integrable, complex-valued functions defined on R^{3N}. Since only closed systems in bounded containers are considered, attention is restricted to the functions in $\mathscr{L}_2(V)$, where V is the open subset of R^{3N} for which the coordinates of the particles are inside the container.

In the following, the $3N$-dimensional Lebesgue measure of a set E is written $\lambda(E)$, while the notation for the corresponding Lebesgue integral of a function f is $\int f\,d\lambda$. The scalar product and norm in $\mathscr{L}_2(V)$ are defined by $(f, g) = \int f^*g\,d\lambda$ and $\|f\| = (f, f)^{1/2}$, respectively.

2.1. Local Operators

The operators on $\mathscr{L}_2$ that correspond to observables in quantum mechanics are the Hermitian operators. For these operators, the scalar product (f, Af) has the usual interpretation of an expectation value. There is, however, another class of the linear operators that includes many of the observables of quantum mechanics and whose members are appropriately called local operators.[2]

Definition. A linear operator A defined on $\mathscr{D}(A) \subset \mathscr{L}_2$ is called a local operator if, whenever $\psi_1, \psi_2 \in \mathscr{D}(A)$ and $\psi_1 = \psi_2$ almost everywhere[3] on an open set N, then $A\psi_1 = A\psi_2$ a.e. on N. Notice that, since A is linear and $\mathscr{D}(A)$ is a linear subspace, this definition is equivalent to the following: A is a local operator if, whenever $\psi \in \mathscr{D}(A)$ and $\psi = 0$ a.e. on an open set N, then $A\psi = 0$ a.e. on N.

Certainly, an operator whose effect is to multiply functions by some given function is a local linear operator. Also, it is clear that all orders of differential operators are local operators since the derivative of a function depends only on the values of the function in an arbitrarily small neighborhood of the point of evaluation. Hence, the Hamiltonian as well as the position and momentum operators are local linear operators. Integral operators are not, in general, local.

Before investigating the properties of local operators, it is important to make a remark about the domain of definition of quantum mechanical operators. It is well known, for example, that the differential operator is undefined for most elements of $\mathscr{L}_2$ and is defined properly only for those functions that have square-integrable

[2] This terminology should not be confused with that of "local observables" which has been used elsewhere.[18] Indeed, the only common feature of the two concepts seems to be the adjective "local."

[3] Hereafter written a.e.

derivatives. Indeed, it is necessary[6] that the domain $\mathscr{D}(A)$ of a linear operator be a linear subspace and have property that, if $f \in \mathscr{D}(A)$, then $Af \in \mathscr{L}_2$.

In case A is a local linear operator and $\mathscr{D}(A)$ is the domain of A, there is a natural way of extending A to a local linear operator $\tilde{A}$ which agrees with A on $\mathscr{D}(A)$.

Definition. Let Γ be the set of all $f \in \mathscr{L}_2$ such that $f = \sum_k \xi_{E_k} f_k$ except possibly on $(\bigcup_k E_k)' \cap V$, where *(i)* $\{E_k\}$ is a countable collection of pairwise disjoint open subsets of V, *(ii)* $\lambda((\bigcup_k E_k)' \cap V) = 0$, and *(iii)* $f_k \in \mathscr{D}(A)$.[4] Then, for $f \in \Gamma$, define

$$\tilde{A}f = \sum_k \xi_{E_k} A f_k \tag{1}$$

if the right-hand side converges. $\mathscr{D}(\tilde{A})$ is the set of all $f \in \Gamma$ on which $\tilde{A}$ is defined, and $\tilde{A}$ is called the natural extension of A.

The following theorem asserts that $\tilde{A}$ is a proper extension of A.

Theorem 1. If $\tilde{A}$ is the natural extension of a local linear operator A, then the following hold:

(i) If $f \in \mathscr{D}(A)$, then $f \in \mathscr{D}(\tilde{A})$ and $\tilde{A}f = Af$.

(ii) $\mathscr{D}(\tilde{A})$ is a domain for $\tilde{A}$ and $\tilde{A}$ is linear on $\mathscr{D}(\tilde{A})$.

(iii) $\tilde{A}$ is a local operator.

(iv) If $f = \sum_k \xi_{E_k} f_k$ and $f = \sum_k \xi_{F_k} g_k$ (in the sense of the definition of the natural extension), then $\sum_k \xi_{E_k} A f_k = \sum_k \xi_{F_k} A g_k$ a.e. That is, the extension is single-valued.

Proof. Part *(i)* is easy to prove since $\lambda(V' \cap V) = 0$. Thus, if $f \in \mathscr{D}(A)$, then $f = \xi_V f$ and $\tilde{A}f = \xi_V Af = Af$. Since $f \in \mathscr{D}(A)$, $\tilde{A}f = Af \in \mathscr{L}_2$.

To prove *(ii)*, let $f \in \mathscr{D}(\tilde{A})$. Then, $f = \sum_k \xi_{E_k} f_k$ except possibly on $(\bigcup_k E_k)' \cap V$. Thus, for any complex number α, $\alpha f = \sum_k \xi_{E_k} \alpha f_k$ except possibly on $(\bigcup_k E_k)' \cap V$ and $\alpha f_k \in \mathscr{D}(A)$, since $\mathscr{D}(A)$ is a linear subspace. Also,

$$\tilde{A}(\alpha f) = \sum_k \xi_{E_k} A(\alpha f_k) = \sum_k \xi_{E_k} \alpha A f_k = \alpha \sum_k \xi_{E_k} A f_k = \alpha \tilde{A} f$$

because A is linear. Since $\tilde{A}f \in \mathscr{L}_2$, so is $\alpha \tilde{A} f = \tilde{A}(\alpha f) \in \mathscr{L}_2$.

Now, let $f \in \mathscr{D}(\tilde{A})$ be defined as above and $g \in \mathscr{D}(\tilde{A})$, with $g = \sum_j \xi_{F_j} g_j$ except possibly on $(\bigcup_j F_j)' \cap V$. Define $C = (\bigcup_k E_k) \cap (\bigcup_j F_j)$ so that $C = \bigcup_k \bigcup_j (E_k \cap F_j)$. Then define $C_\nu = E_k \cap F_j$, where ν is the image of (k, j) in a one-to-one map between the sets $\{\nu\}$ and $\{(k, j)\}$. Thus, $C = \bigcup_\nu C_\nu$. It is clear that $C_\nu \bigcap C_{\nu'} = \varnothing$ unless $\nu = \nu'$ because $C_\nu \bigcap C_{\nu'} = (E_k \cap F_j) \cap (E_{k'} \cap F_{j'}) = \varnothing$ unless $k = k'$ and $j = j'$, i.e., unless $\nu = \nu'$. Also,

$$V \cap \left[\left(\bigcup_k E_k\right)' \cup \left(\bigcup_j F_j\right)'\right] = \left(V \cap \left(\bigcup_k E_k\right)'\right) \cup \left(V \cap \left(\bigcup_j F_j\right)'\right)$$

[4] The notation ξ_B will be consistently used for the characteristic function of a set B. That is, $\xi_B(x) = 1$ if $x \in B$ and $\xi_B(x) = 0$ if $x \notin B$.

so

$$\lambda(V \cap C') \leqslant \lambda\left(V \cap \left(\bigcup_k E_k\right)'\right) + \lambda\left(V \cap \left(\bigcup_j F_j\right)'\right) = 0$$

Therefore, the collection $\{C_\nu\}$ satisfies properties (*i*) and (*ii*) of the definition of the natural extension.

It is easy to show that $f + g = \sum_\nu \xi_{C_\nu}(f + g)_\nu$, except possibly on $V \cap C'$, where $(f + g)_\nu = f_k + g_j \in \mathscr{D}(A)$ and $\nu = (k, j)$. To see this, let $x \in C$. Then, $x \in C_\nu$ for one and only one $\nu = (k, j)$. Thus, $x \in E_k$ and $x \in F_j$. So,

$$\sum_\nu \xi_{C_\nu}(f + g)_\nu(x) = f_k(x) + g_j(x)$$

and

$$(f + g)(x) = \sum_r \xi_{E_r} f_r(x) + \sum_r \xi_{F_r} g_r(x) = f_k(x) + g_j(x)$$

Thus, $f + g \in \mathscr{D}(\tilde{A})$ if $\tilde{A}(f + g)$ is in $\mathscr{L}_2$. But a similar argument shows that $\tilde{A}(f + g) = \tilde{A}f + \tilde{A}g$ a.e. So, since $\tilde{A}f + \tilde{A}g \in \mathscr{L}_2$, $\tilde{A}(f + g) \in \mathscr{L}_2$. Thus, $\mathscr{D}(\tilde{A})$ is a domain and $\tilde{A}$ is linear on $\mathscr{D}(\tilde{A})$.

To prove part (*iii*), that $\tilde{A}$ is a local operator, the equivalent definition of a local operator given above is used. Thus, let $g \in \mathscr{D}(\tilde{A})$ and $g = 0$ a.e. on an open set $N \subset V$. It is shown that $\tilde{A}g = 0$ a.e. on N. By hypothesis, $g = \sum_k \xi_{F_k} g_k$ and $\tilde{A}g = \sum_k \xi_{F_k} A g_k$. Also, $N = (N \cap (\bigcup_k F_k)') \cup (N \cap (\bigcup_k F_k))$. In case $x \in N \cap (\bigcup_k F_k)'$, then $x \in (\bigcup_k F_k)' \cap V$ and so $\tilde{A}g = 0$ by definition. If, on the other hand, $x \in N \cap \bigcup_k F_k = \bigcup_k (F_k \cap N)$, then let $Q = \{x \in \bigcup_k F_k \cap N: (\tilde{A}g)(x) \neq 0\}$. Clearly, $Q = \bigcup_k Q_k$, where $Q_k = \{x \in F_k \cap N: (\tilde{A}g)(x) \neq 0\}$. Now, on the set $F_k \cap N \subset F_k$, $g = g_k$. But $F_k \cap N \subset N$ and so $g_k = 0$ a.e. on $F_k \cap N$ by hypothesis. Since A is a local operator and $N \cap F_k$ is open, $A g_k = A(0) = 0$ on $N \cap F_k$ except on a set σ_k which has zero measure. Thus, since $\tilde{A}g = A g_k$ on $F_k \cap N$, $\tilde{A}g = 0$ on $F_k \cap N$ except on σ_k. This means that $Q_k = \sigma_k$ and $\lambda(Q_k) = 0$. But $\lambda(Q) = \sum_k \lambda(Q_k) = 0$, so $\tilde{A}g = 0$ on N except on Q, which has zero measure.

It is now easy to prove part (*iv*), that the extension is unique. Let $f \in \mathscr{D}(\tilde{A})$ and $f = \sum_k \xi_{E_k} f_k$ and also $f = \sum_k \xi_{F_k} g_k$, except possibly on $(\bigcup_k E_k)' \cap V$ and $(\bigcup_k F_k)' \cap V$. Define $f_1 = \sum_k \xi_{E_k} f_k$ and $f_2 = \sum_k \xi_{F_k} g_k$. Now, on the open set $D = (\bigcup_k E_k) \cap (\bigcup_j F_j)$, $f_1 = f = f_2$ everywhere; so, by part (*iii*), $\tilde{A}f_1 = \tilde{A}f = \tilde{A}f_2$ a.e. on D. It is easy to see that $\lambda(D' \cap V) = 0$, so $\tilde{A}f_1 = \tilde{A}f = \tilde{A}f_2$ a.e. □[5]

If A is a local operator and $\tilde{A}$ is its natural extension, then it is not difficult to show that $\tilde{\tilde{A}} = \tilde{A}$. To see that this is true, it must be shown that $\tilde{\tilde{A}}$ and $\tilde{A}$ have the same domain and that on this domain $\tilde{\tilde{A}}f = \tilde{A}f$. Since $\mathscr{D}(\tilde{A}) \subset \mathscr{D}(\tilde{\tilde{A}})$ and $\tilde{A}$ and $\tilde{\tilde{A}}$ agree on $\mathscr{D}(\tilde{A})$ by Theorem 1, it suffices to show that $\mathscr{D}(\tilde{\tilde{A}}) \subset \mathscr{D}(\tilde{A})$.

Lemma 1. If A is a local linear operator, then $\tilde{\tilde{A}} = \tilde{A}$.

[5] The symbol □ denotes the end of the proof.

Proof. The above remarks show that it suffices to have $\mathscr{D}(\tilde{A}) \subset \mathscr{D}(\tilde{A})$. To show this, let $f \in \mathscr{D}(\tilde{A})$. Then, $f = \sum_k \xi_{C_k} f_k$, except possibly on $(\bigcup_k C_k)' \cap V$, which has zero measure, and where $f_k \in \mathscr{D}(\tilde{A})$. Also, $\tilde{A}f = \sum_k \xi_{C_k} \tilde{A} f_k$ and $\tilde{A}f \in \mathscr{L}_2$. Since $f_k \in \mathscr{D}(\tilde{A})$, it follows that $f_k = \sum_r \xi_{F_{kr}} g_{kr}$, except possibly on $(\bigcup_r F_{kr})' \cap V$, and $\tilde{A} f_k = \sum_r \xi_{F_{kr}} A g_{kr}$, where $g_{kr} \in \mathscr{D}(A)$ and $\tilde{A} f_k \in \mathscr{L}_2$.

Form the countable collection of open sets $\{D_\nu\} = \{C_k \cap F_{kr}\}$. It is easy to see that $D_\nu \cap D_{\nu'} = \varnothing$ unless $\nu = \nu'$, so that the collection $\{D_\nu\}$ is disjoint and open and $D_\nu \subset V$ for all ν.

To see that $\lambda((\bigcup_\nu D_\nu)' \cap V) = 0$, notice that if suffices to show that $\lambda(\bigcup_\nu D_\nu) = V$. Now, $\bigcup_\nu D_\nu = \bigcup_k \bigcup_r C_k \cap F_{kr} = \bigcup_k C_k \cap B_k$, where $B_k = \bigcup_r F_{kr}$. Also, each set in $\{C_k \cap B_k\}$ is measurable and its members are pairwise disjoint, so $\lambda(\bigcup_k C_k \cap B_k) = \sum_k \lambda(C_k \cap B_k)$. By hypothesis, $\lambda(B_k' \cap V) = 0$ and $C_k \subset V$. Therefore, $\lambda(B_k' \cap C_k) = 0$, which means that $\lambda(B_k \cap C_k) = \lambda(C_k)$. From these computations, it follows that

$$\lambda\left(\bigcup_\nu D_\nu\right) = \sum_k \lambda(C_k \cap B_k) = \sum_k \lambda(C_k) = \lambda\left(\bigcup_k C_k\right) = \lambda(V)$$

Thus, $\lambda((\bigcup_\nu D_\nu)' \cap V) = 0$.

Let $\{g_{kr}\}$ be the functions in the definition of f_k, and, using the correspondence $\nu \Leftrightarrow (k, r)$, write $g_{kr} = g_\nu$. Then, as in the proof of Theorem 1, part (*ii*), it is easy to show that $\sum_\nu \xi_{D_\nu} g_\nu = f$, except possibly on $(\bigcup_\nu D_\nu)' \cap V$.

Therefore, $f = \sum_\nu \xi_{D_\nu} g_\nu$ a.e., where $g_\nu \in \mathscr{D}(A)$, and $\{D_\nu\}$ satisfies the conditions required by the natural extension. Thus, if $\sum_\nu \xi_{D_\nu} A g_\nu \in \mathscr{L}_2$, then $f \in \mathscr{D}(\tilde{A})$. Since $\tilde{A}f \in \mathscr{L}_2$, it suffices to show that $\tilde{A}f = \sum_\nu \xi_{D_\nu} A g_\nu$ a.e. But again, this follows easily by the method of Theorem 1, part (*ii*), so that $f \in \mathscr{D}(\tilde{A})$ and $\mathscr{D}(\tilde{A}) \subset \mathscr{D}(\tilde{A})$, which was to be proved. □

It is clear that the effect of the operator $\tilde{A}$ is essentially the same as A. In fact, if $\mathscr{D}(A)$ is made up of functions with certain analytical properties, then $\mathscr{D}(\tilde{A})$ is the set of functions that have countably piecewise the same analytical properties. For example, if $A = d/dx$ and $\mathscr{D}(d/dx) = C^1$, then $\mathscr{D}(\tilde{d}/dx)$ is the set of countably piecewise C^1 functions. The theorems above show that the extension of an operator to piecewise domains with each "piece" giving an independent contribution is possible for any local operator.

Because of the "local" character of an extended local operator A, it is possible to commute A with the characteristic functions of certain open sets.

Theorem 2. Let B be an open subset of V satisfying $\lambda(B' \cap B^-) = \lambda(\partial B) = 0$ and let A be an extended local operator. Then, for any $f \in \mathscr{D}(A)$, it follows that $\xi_B f \in \mathscr{D}(A)$ and $A(\xi_B f) = \xi_B A f$ a.e.

Proof. The set B satisfies $V = B \cup (\partial B) \cup (B^-)'$ with $(B^-)'$ open and

$$\lambda((B \cup (B^-)')' \cap V) = \lambda(\partial B) = 0$$

So, by Theorem 1 and Lemma 1, if $f \in \mathscr{D}(A)$, then $\xi_B f \equiv \xi_B f + \xi_{(B^-)'} 0 \in \mathscr{D}(A)$, whenever $A(\xi_B f) = \xi_B A f + \xi_{(B^-)'} A(0) = \xi_B A f$ is in $\mathscr{L}_2$. But clearly $\| \xi_B A f \| \leqslant \| A f \|$, so $A(\xi_B f) = \xi_B A f$ and $\xi_B f \in \mathscr{D}(A)$. □

Since the notion of localness for operators is the key to the development of these papers, it is necessary to have some knowledge of the topological structure of configuration space. Specifically, it is important to see to what extent the configuration space can be approximated by unions of disjoint open cubes. The theorem of Vitali contains all of the information that will be needed.

Definition. A Vitali cover for any set $S \subset R^{3N}$ is a collection Λ of closed cubes with the property that, if $x \in S$ and $\epsilon > 0$, there exists an $\alpha \in \Lambda$ with $x \in \alpha$ and $\lambda(\alpha) < \epsilon$.

A version of Vitali's theorem is:

Theorem. (*Vitali*). For an arbitrary set $S \subset R^{3N}$ and Λ, a Vitali cover of S, there exists a countable disjoint collection $\{J_n\}$ of elements of Λ such that $\lambda(S \cap (\bigcup_n J_n)') = 0$. In addition, if $\lambda(S) < \infty$, then, for any $\epsilon > 0$, there is a *finite* disjoint collection $\{I_n\}_{n=1}^{N}$, and $\lambda(S \cap (\bigcup_n I_n)') \leqslant \epsilon$.

The proof to this theorem can be found in most textbooks on analysis.[12,13] The corollaries to this theorem that are needed here are stated and proved below.

Lemma 2. If S is an open set, then there exists a Vitali cover Λ such that each member of Λ is contained entirely in S.

Proof. Since S is open, for each $x \in S$, there exists an open neighborhood of x contained entirely in S. Within this neighborhood, it is easy to construct a closed cube centered at x and contained entirely within the neighborhood. Call this cube C_x. Let

$$J_x = \{\alpha\colon \quad \alpha \subset C_x \quad \text{and } \alpha \text{ is a closed cube centered at } x\}.$$

Let $\Lambda = \bigcup_{x \in S} J_x$. Clearly, Λ is the desired Vitali cover. □

Corollary 1. Let S be an open set and Λ be the Vitali cover of Lemma 2. Then,

(*i*) The countable collection $\{J_n\}$ which exists by Vitali's theorem is infinite.

(*ii*) $\lambda(S \cap (\bigcup_n J_n^0)') = 0$, where J_n^0 is the interior of J_n, and $J_n^0 \cap J_m^0 = \varnothing$ for $m \neq n$.

Proof. To prove (*i*), assume that $\{J_n\}$ is finite. Then, since each J_n is closed, $(\bigcup_n J_n)'$ is open and $S \cap (\bigcup_n J_n)'$ is open. But $\lambda(S \cap (\bigcup_n J_n)') = 0$, so $S \cap (\bigcap_n J_n)' = \varnothing$. Therefore, $\bigcup_n J_n = S$, which contradicts that fact that $\bigcup_n J_n$ is not open. Thus, $\{J_n\}$ is countably infinite.

The proof of (*ii*) follows from the obvious identity $\lambda(\bigcup_n J_n) = \lambda(\bigcup_n J_n^0)$, the fact that $\lambda(S \cap (\bigcup_n J_n)') = 0$, and the inclusion $J_m^0 \subset J_m$. □

Corollary 2. Let S be a bounded open set and Λ be the Vitali cover of Lemma 2. If $\{I_n\}$ is a *finite* subcollection of Λ with the properties implied by Vitali's theorem, then the collection of open cubes $\{I_n^0\}$ has the following properties:

(*i*) $I_n^0 \cap I_m^0 = \varnothing$ if $m \neq n$, $\bigcup_n I_n^0$ is open, and $\bigcup_n I_n^0 \subset S$.

(*ii*) $0 \leqslant \lambda(S) - \lambda(\bigcup_n I_n^0) \leqslant \epsilon$.

(*iii*) $\lambda(\partial(\bigcup_n I_n^0)) = 0$.

Proof. Part (*i*) is clear, since $I_n \cap I_m = \varnothing$ for $m \neq n$, I_n^0 is open, and $I_n \subset S$ for all n.

The proof of (*ii*) and (*iii*) follows readily from the fact that $\lambda(\partial I_n^0) = 0$. □

2.2. A Characterization of Bounded Local Operators

The linear operators on a Hilbert space are conveniently divided into the bounded and unbounded operators. A bounded operator satisfies the condition $\| Ax \| \leqslant \alpha \| x \|$, for some fixed and finite real number α and all $x \in \mathscr{D}(A)$.(14) While it is not true that all local linear operators are bounded—for example, the differential operator is unbounded—the class of all bounded local operators has a simple characterization. In fact, the set of all bounded local operators is exactly the set of all operators that multiply functions by an essentially bounded function—loosely, the multiplicative operators. Theorem 3 gives the precise connection.

It is necessary first to prove two lemmas.

Lemma 3. Let $\mathscr{L}_2(V)$ be the usual Hilbert space on a subset $V \subset R^{3N}$ and let $\lambda(V) < \infty$. If g is a measurable function and $\| gf \| < \infty$ for all $f \in \mathscr{L}_2$, then g is bounded a.e.

Proof. By hypothesis, $\| gf \|^2 = \int | gf |^2 \, d\lambda = \int || g |^2 f^2 | \, d\lambda < \infty$ for all $f \in \mathscr{L}_2$, i.e., for all integrable f with $\int | f |^2 \, d\lambda < \infty$. But it is easy to see that $\mathscr{L}_1 = \{ f^2 : f \in \mathscr{L}_2 \}$. Thus, the hypothesis means that $\int || g |^2 h | \, d\lambda < \infty$ for all $h \in \mathscr{L}_1$. But, by Theorem 20.15 of reference 12, $| g |^2$ is bounded a.e. and so g is also. □[6]

Lemma 4. Let $f_n \in \mathscr{L}_2$ and $\{f_n\}$ be a Cauchy sequence in the $\mathscr{L}_2$ norm. If $\{f_n\}$ converges pointwise to a function $f \in \mathscr{L}_2$, then $f_n \to f$ in the $\mathscr{L}_2$ norm.

Proof. The proof of this lemma is contained in the proof of Theorem 13.10 of reference 12.

Theorem 3. Let A be an operator whose domain is $\mathscr{L}_2(V)$. Then A is a bounded linear local operator if and only if

(*i*) $Af = (A\xi_V)f$.

(*ii*) $\|(A\xi_V)f\| < \infty$ for all $f \in \mathscr{L}_2$.

Proof. The proof of the forward implication is easy. Since $\mathscr{D}(A) = \mathscr{L}_2(V)$, $A\xi_V \in \mathscr{L}_2$, and so $A\xi_V$ is defined a.e. on V. Thus, if $f = g$ a.e. on N, an open set,

[6] This short proof was kindly suggested to me by Professor R. Bonic.

$Af = (A\xi_V)f = (A\xi_V)g = Ag$ wherever $A\xi_V$ is defined on N and wherever $f = g$ on N. That is, a.e. on N. Thus, A is local and the linearity is clear. Since $\|(A\xi_V)f\| < \infty$ for all $f \in \mathscr{L}_2$, Lemma 3 shows that $A\xi_V$ is bounded a.e. Let $E \subset V$ be the set on which $A\xi_V$ is bounded. Because $\lambda(E' \cap V) = 0$,

$$\|(A\xi_V)f\|^2 = \int |A\xi_V|^2 |f|^2 \, d\lambda = \int_E |A\xi_V|^2 |f|^2 \, d\lambda$$
$$\leqslant \sup_{x \in E} |(A\xi_V)(x)|^2 \int_E |f|^2 \, d\lambda = Q^2 \int |f|^2 \, d\lambda = Q^2 \|f\|^2$$

Thus, $\| Af\| \leqslant Q \|f\|$ for all $f \in \mathscr{L}_2$. That is, A is bounded.

To show the converse—namely that boundedness, linearity, and localness imply (*i*) and (*ii*)—is slightly more complicated. The proof goes in three steps.

Step 1. Consider first the case for which $f = \xi_D$ for some open set $D \subset V$ with $\lambda(\partial D) = 0$. Now, since $\mathscr{D}(A) = \mathscr{L}_2(V)$, Lemma 1 implies both that $A = \tilde{A}$ and $\xi_V \in \mathscr{D}(A)$. Because D is open, $\lambda(\partial D) = 0$, and $\xi_D = \xi_D \xi_V$, Theorem 2 shows that $A\xi_D = \xi_D A\xi_V$ a.e.

Step 2. Consider next the case $f = \xi_B$ for some measurable set $B \subset V$. The idea is to approximate B by open sets with boundaries of measure zero. The following construction will provide a sequence of open sets $\{\sigma_n\}_{n=1}^{\infty}$ which satisfy $\lambda(\partial\sigma_n) = 0$ and which converge to ξ_B in the $\mathscr{L}_2$ norm.

To construct the sequence $\{\sigma_n\}_{n=1}^{\infty}$, proceed as follows. First, find a sequence of open sets U_n which satisfy $B \subset U_n$ and $\lambda(U_n \cap B') < 1/2^{n+1}$. This is possible since $\lambda(B) = \inf\{\lambda(U)\colon U \text{ is open and } B \subset U\}$. Then, for each U_n, construct a Vitali cover of closed cubes contained entirely within U_n—as described in Lemma 2. Select from this the finite collection $\{J_{nm}\}_{m=1}^{\alpha_n}$ with the property that $\lambda(U_n \cap (\bigcup_m J_{nm})) \leqslant 1/2^{n+1}$. As noted above in Corollary 2, the set $\sigma_n = \bigcup_m J_{nm}^o$ has the following properties: (1) $\lambda(\partial\sigma_n) = 0$, (2) σ_n is open, (3) $\lambda(U_n \cap \sigma_n') < 1/2^{n+1}$, and (4) $\sigma_n \subset U_n$.

It is easy to see that $\xi_{\sigma_n} \to \xi_B$ in the $\mathscr{L}_2$ norm. Thus,

$$\| \xi_{\sigma_n} - \xi_B \|^2 = \int (\xi_{\sigma_n} - \xi_B)^2 \, d\lambda$$

But

$$(\xi_{\sigma_n} - \xi_B)^2 (x) = 1 \quad \text{if} \quad x \in \sigma_n \cap B' \quad \text{or} \quad B \cap \sigma_n'$$
$$= 0 \quad \text{otherwise}$$

Thus,

$$(\xi_{\sigma_n} - \xi_B)^2 = \xi_{(\sigma_n \cap B') \cup (B \cap \sigma_n')}$$

So

$$\| \xi_{\sigma_n} - \xi_B \|^2 \leqslant \lambda(\sigma_n \cap B') + \lambda(B \cap \sigma_n') \leqslant \lambda(U_n \cap B') + \lambda(U_n \cap \sigma_n') < 1/2^n$$

Thus, $\lim_n \xi_{\sigma_n} = \xi_B$ in the $\mathscr{L}_2$ norm. Since A is bounded,

$$\lim_n A\xi_{\sigma_n} = \lim_n \xi_{\sigma_n}(A\xi_V) = A\xi_B$$

in the $\mathscr{L}_2$ norm. To finish the proof of Step 2, it suffices to show that $\lim_n \xi_{\sigma_n} A\xi_V = \xi_B A\xi_V$ in the $\mathscr{L}_2$ norm because $\mathscr{L}_2$ limits are unique a.e. To this end, write

$$\|(A\xi_V)(\xi_B - \xi_{\sigma_n})\|^2 = \int_{(B\cap\sigma_n')\cup(\sigma_n\cap B')} | A\xi_V |^2 \, d\lambda \leqslant \int_{(U_n\cap\sigma_n')\cup(U_n\cap B')} | A\xi_V |^2 \, d\lambda$$

as the work above shows. Since $|(A\xi_V)|^2 \in \mathscr{L}_1$ and $\lambda((U_n \cap \sigma_n') \cup (U_n \cap B')) < 1/2^n$, the last integral can be made arbitrarily small for n large enough.[7]

Step 3. Let f be an arbitrary function in $\mathscr{L}_2$. Note first that, if s is a simple function, i.e., $s = \sum_{n=1}^N \alpha_n \xi_{B_n}$ with B_n measurable, then, since A is linear, $As = (A\xi_V)s$.

Since $f \in \mathscr{L}_2$, there exists a sequence of simple functions $\{s_n\}$ such that $\lim_n s_n = f$ everywhere and also $\lim_n s_n = f$ in the $\mathscr{L}_2$ norm. Since A is bounded, $As_n = (A\xi_V)s_n \to Af$ in the $\mathscr{L}_2$ norm. Also, $(A\xi_V)s_n \to (A\xi_V)f$ everywhere. Moreover, the sequence $\{(A\xi_V)s_n\}$ is Cauchy in the $\mathscr{L}_2$ norm, so that it follows from Lemma 4 that $(A\xi_V)s_n \to (A\xi_V)f$ in the $\mathscr{L}_2$ norm. Hence, by the uniqueness of $\mathscr{L}_2$ limits a.e., $Af = (A\xi_V)f$.

Since A is bounded, $\| Af \| = \|(A\xi_V)f\| \leqslant \alpha \|f\| < \infty$ for all $f \in \mathscr{L}_2$. □

Thus, a bounded local operator A (defined everywhere on $\mathscr{L}_2$) is completely characterized by its action on ξ_V and is precisely the multiplicative operator $A\xi_V$. In fact, there is a trivial one-to-one map between the set of all bounded local operators and the subset of $\mathscr{L}_2$ containing the functions bounded a.e. that is $\mathscr{L}_\infty$. This characterization shows that localness is a very restrictive property when combined with boundedness and that the interesting local operators are the unbounded ones.

3. LOCAL OPERATORS IN QUANTUM MECHANICS

The notion of local operators was developed to see if the local properties of the measurement processes discussed in the introduction are inherent in quantum mechanics. Since the observables in quantum mechanics are linear operators, it is expected that the local nature of measurements should reside in their structure. In fact, in the so-called coordinate representation of quantum mechanics, i.e., $\mathscr{L}_2(V)$ observables are functions of the differential operators and the coordinates.[(5)] It is a simple matter to show that differential operators are local operators, and Theorem 3 shows that multiplicative operators are local. Moreover it can be shown that "analytic functions" of local operators are local, and so, if attention is restricted to such operators, all quantum mechanical observables are local.

Before verifying these comments, it should be mentioned that in representations of Hilbert space other than the coordinate one the entire notion of localness may disappear. For example, in an energy representation in which the basis set is discrete, there is no analog of the open sets in configuration space. In other words, "localness" is not a natural concept in a discrete representation. Furthermore, even in a continuous momentum representation in which open sets naturally occur, operators corresponding

[7] For example, see Theorem 12.34, reference 12.

to multiplication by functions of the coordinates become nonlocal integral operators.[15] Thus, observables seem to have a local character only in the representation related to physical three-space. This anomoly is expected, however, since local operators are supposed to be the manifestation of the local character of measurements in three-space.

The following collection of theorems show that observables defined on $\mathscr{L}_2$ are local operators.

Theorem 4. The differential operator, defined on functions according to the usual limiting process, is a local operator.

Proof. Call D the differential operator and let N be an open set; assume that f is in $\mathscr{D}(D)$ and that $f = 0$ a.e. on N. It will be shown that $D(f) = 0$ a.e. on N.

Let $x \in N$ be a point at which $D(f)$ is defined and $f(x) = 0$, that is, x is almost any point in N. Now, assume that $D(f)(x) = t \neq 0$, and let $\sigma \subset N$ be any open neighborhood of x. Thus,

$$\left| \frac{f(y) - f(x)}{y - x} - t \right| = | t |$$

for almost all $y \in \sigma$. That is,

$$\lim_{y \to x} \frac{f(y) - f(x)}{y - x} \equiv Df(x) \neq t$$

Thus, $D(f)(x) = 0$ for almost all $x \in N$, and so D is local. □

Theorem 5. Polynomials of local operators are local operators.

Proof. Let $P = \sum_{m=1}^{n} A_m$, where $A_m = B_{m1} B_{m2} \cdots B_{mk}$ and each B_{mj} is a local operator. If $\psi \in \mathscr{D}(P)$ and $\psi = 0$ a.e. on N, then $\psi \in \mathscr{D}(B_{mj})$ for all m and j and $B_{mk}\psi = 0$ a.e. on N. Thus, $B_{mk-1}(B_{mk}\psi) = 0$ a.e. on N. Hence, for all m, $A_m\psi = 0$ a.e. on N, and so $P\psi = 0$ a.e. on N. □

It is possible to extend Theorem 5 to infinite series in polynomials of local operators, in two ways. The two methods depend on the definition of the "limit" of a sequence of operators. The first way is in terms of norm convergence.[16,17]

Let $\{A_n\}$ be a sequence of operators with domains $\mathscr{D}(A_n)$. Then, $\mathscr{D} = \bigcap_n \mathscr{D}(A_n)$ is a linear subspace since each of $\mathscr{D}(A_n)$ is. The limit of the sequence of operators $A \equiv \lim_n A_n$ is defined for $\psi \in \mathscr{D}$ by $A\psi \equiv \lim_n(A_n\psi)$ (in the $\mathscr{L}_2$ sense) if the right-hand side is in $\mathscr{L}_2$. The domain of A is $\mathscr{D}(A) = \{\psi \in \mathscr{D}$: the limit exists$\}$. Clearly, $\mathscr{D}(A)$ is a linear subspace and A is linear on $\mathscr{D}(A)$ since each A_n is linear.

The second method of defining the limit of a sequence of operators is in terms of pointwise convergence. Define $A \equiv \lim_n A_n$ for $\psi \in \mathscr{D}$ as $(A\psi)(x) = \lim_n(A_n\psi)(x)$ (in the pointwise sense) if the right-hand side is in $\mathscr{L}_2$. Clearly, A is linear on the linear subspace $\mathscr{D}(A) = \{\psi \in \mathscr{D}$: the limit exists$\}$.

Theorems 6a and 6b below show that, whichever method is used to define the limit, the limit operator is local if each operator in the sequence is.

Theorem 6a. Let $\{A_n\}$ be a sequence of local operators with domains $\mathscr{D}(A_n)$. If A is defined as the $\mathscr{L}_2$-type limit of these operators, then A is a local operator.

Proof. Let $f \in \mathscr{D}(A)$ and let $f = 0$ a.e. on an open set N. Then, since $f \in \mathscr{D}(A_n)$ for all n, $A_n f = 0$ a.e. on N and $\xi_N A_n f = 0$ a.e. Therefore,

$$\| \xi_N Af \| = \| \xi_N Af - \xi_N A_n f \| \leqslant \| Af - A_n f \| < \epsilon$$

for arbitrary $\epsilon > 0$ and n large enough. Thus, $\xi_N Af = 0$ a.e. and so $Af = 0$ a.e. on N. □

Theorem 6b. Let $\{A_n\}$ be a sequence of local operators with domains $\mathscr{D}(A_n)$. If A is defined as the pointwise-type limit of these operators, then A is local.

Proof. Let $f \in \mathscr{D}(A)$ and let $f = 0$ a.e. on an open set N. Thus, since $f \in \mathscr{D}(A_n)$ and A_n is local, $A_n f = 0$ on $N_n \subset N$, with $\lambda(N_n' \cap N) = 0$. Hence, $A_n f = 0$ on $M = \bigcap_n N_n$ and $\lambda(N \bigcap M') \leqslant \sum_n \lambda(N \cap N_n') = 0$. Thus, for all n, $A_n f = 0$ on M, which is almost all of N. So, if $x \in M$, then $\lim_n (A_n f)(x) = 0 = (Af)(x)$. □

The theorem that "analytic functions" of local operators are local is now easy.

Theorem 6c. Let A be defined by an analytic function in local operators in terms of either an $\mathscr{L}_2$-type limit or a pointwise-type limit. Then A is a local operator.

Proof. By hypothesis, $A = \lim_n A_n$ in either the $\mathscr{L}_2$ or pointwise sense, where $A_n = \sum_{m=1}^{n} P_m$ and P_m is a product of powers of local operators. Thus, A_n is a polynomial in local operators, and so, by Theorem 5, A_n is a local operator. This means that the hypothesis of either Theorem 6a or 6b are met, so A is a local operator. □

4. LOCAL OPERATORS AND FORMAL ENSEMBLES

Having developed the properties of local operators and having shown their connection to observables, it is possible to examine the extent to which measured values can be written as ensemble averages as conjectured in the introduction. This is done by looking at expectation values of local operators. It is shown in this section that expectation values can be written in a natural way as ensemble averages over certain "states."

The discussion which follows will be limited to closed systems which are contained in a bounded, connected, open region of three-space called V_3. The configuration space of such a system is the $3N$-dimensional real space R^{3N} and wave functions for the system vanish identically outside the open set $V = \{q \in R^{3N}: r_1 \in V_3, \ldots, r_N \in V_3\}$, where the notation $q = (r_1, r_2, \ldots, r_N)$ is used. The set V_3 is assumed to satisfy $\lambda(\partial V) = 0$, i.e., certain sets with pathological boundaries of nonzero measure are excluded.

In the work below, special partitions of the configuration space into disjoint subsets are used.

Definition. A finite collection $\sigma = \{\alpha_i\}_{i=1}^{\Omega}$ is called a *partition* of V if the sets σ_j are pairwise disjoint, open subsets of V with the property that

$$\lambda\left(\left(\bigcup_i \sigma_i\right)' \cap V\right) = 0$$

The following technical lemmas about these partitions will be needed. In the first lemma, the more general case $\Omega = \infty$ is treated, since this case is required elsewhere.

Lemma 5. Let $\{\sigma_i\}_{i=1}^{\infty}$ be a collection of pairwise disjoint, open subsets of V with the property $\lambda((\bigcup_i \sigma_i)' \cap V) = 0$ and $\lambda(\partial V) = 0$. Then

(*i*) $\lambda(\bigcup_i \partial\sigma_i) = 0$.

(*ii*) $\lambda(\partial\sigma_j) = 0$ for all j.

Proof. To prove (*i*), it is necessary to establish the following inclusion, which is easily verified:

$$\bigcup_i \partial\sigma_i \subset \left(\bigcup_i \sigma_i\right)' \tag{2}$$

The following identity and inclusion

$$\begin{aligned}\left(\bigcup_i \sigma_i\right)' \cap V^- &= \left(\left(\bigcup_i \sigma_i\right)' \cap V\right) \cup \left(\left(\bigcup_i \sigma_i\right)' \cap \partial V\right)\\ &\subset \left(\left(\bigcup_i \sigma_i\right)' \cap V\right) \cup \partial V\end{aligned} \tag{3}$$

follow from $V \cap \partial V = \varnothing$ and $V \cup \partial V = V^-$, and from (2) and (3) it follows that

$$\lambda\left(\left(\bigcup_i \partial\sigma_i\right) \cap V^-\right) \leqslant \lambda\left(\left(\bigcup_i \sigma_i\right)' \cap V^-\right) \leqslant \lambda\left(\left(\bigcup_i \sigma_i\right)' \cap V\right) + \lambda(\partial V) = 0$$

Thus, $\lambda((\bigcup_i \partial\sigma_i) \cap V^-) = 0$. But $\partial\sigma_i \subset V^-$. Hence, $\bigcup_j \partial\sigma_j \subset V^-$, which proves (*i*), that is,

$$\lambda\left(\bigcup_j \partial\sigma_j\right) = 0$$

Part (*ii*) is now a trivial consequence of (*i*). □

Lemma 6. If $\{\sigma_j\}_{j=1}^{\Omega}$ is a partition of V and if $B = \bigcup_j \sigma_j$, then (*i*) $\xi_B = \xi_V$ a.e. and (*ii*) $\xi_V = \sum_j \xi_{\sigma_j}$ a.e.

Proof. Part (*i*) follows from $(\bigcup_j \sigma_j) \cup ((\bigcup_j \sigma_j)' \cap V) = V$. Thus, $\xi_B = \xi_V$ except on $(\bigcup_j \sigma_j)' \cap V$, which has zero measure. To prove (*ii*), notice that $\sum_j \xi_{\sigma_j} = \xi_B$ because the σ_j are pairwise disjoint. Therefore, $\xi_V = \sum_j \xi_{\sigma_j}$ a.e. follows from (*i*). □

In order to make the transition from quantum mechanics to statistical mechanics, it is necessary to examine the expectation values of quantum mechanical operators. These, of course, are expressions of the form $(\psi, A\psi)$, where A is an operator representing some observable and ψ is the state of the system. The following theorem, which appears as a technical result applying to any extended local operator, is the crucial step in the transition.

Theorem 7. If A is an extended local linear operator and $\{\sigma_j\}_{j=1}^{\Omega}$ is a partition of V, then

$$(\psi, A\psi) = \sum_{j=1}^{\Omega} (\psi_j , A\psi_j), \qquad \text{where} \quad \psi_j \equiv \xi_{\sigma_j}\psi$$

Proof.

$$(\psi, A\psi) = \int \psi^* A\psi \, d\lambda = \int \xi_V \psi^* A\psi \, d\lambda = \int \left(\sum_{j=1}^{\Omega} \xi_{\sigma_j}\right) \psi^* A\psi \, d\lambda$$
$$= \sum_{j=1}^{\Omega} \int \xi_{\sigma_j}\psi^* A\psi \, d\lambda$$

which follows from Lemma 6. Now, A is an extended local operator and $\lambda(\partial\sigma_j) = 0$ by Lemma 5 above, so Theorem 2 implies that $\xi_{\sigma_j} A\psi = A\xi_{\sigma_j}\psi$ a.e. Therefore, since $\xi_{\sigma_j}^2 = \xi_{\sigma_j}$,

$$(\psi, A\psi) = \sum_{j=1}^{\Omega} \int \xi_{\sigma_j}\psi^* \xi_{\sigma_j} A\psi \, d\lambda = \sum_{j=1}^{\Omega} \int \xi_{\sigma_j}\psi^* A\xi_{\sigma_j}\psi \, d\lambda$$
$$= \sum_{j=1}^{\Omega} \int (\xi_{\sigma_j}\psi)^* A(\xi_{\sigma_j}\psi) \, d\lambda = \sum_{j=1}^{\Omega} (\psi_j , A\psi_j) \quad \square$$

Consider one of the functions $\psi_j = \xi_{\sigma_j}\psi$ which occur in Theorem 7. Its contribution to the expectation value is $(\psi_j , A\psi_j)$. Defining $P_j = \| \psi_j \|^2$, the decomposition can be rewritten as

$$(\psi, A\psi) = \sum_{j=1}^{\Omega} (\varphi_j , A\varphi_j) \, P_j \tag{4}$$

where $\varphi_j \equiv \psi_j / \| \psi_j \|$ and, clearly, $\sum_j P_j = 1$ and $0 \leqslant P_j \leqslant 1$. Thus, the expectation value of an extended local operator can be written as a weighted sum of expectation values. Because of the form of Eq. (4), this decomposition is called an *ensemble decomposition* of the pure state.

From Theorem 7, it is clear that the wave functions φ_j in Eq. (4) arise from disjoint regions in configuration space and are the analogs of the "portions of the wave function" giving independent contributions to measured values discussed in the introduction. Thus, the ensemble decomposition satisfies the essence of the idea that measured values are actually ensemble averages with local regions of space providing independent contributions. It should also be noted that the functions φ_j can be chosen in an uncountable number of different ways and that, for at least one of these choices, $P_j = 1/\Omega$ for all j. This choice corresponds to a kind of equal weighting of different portions of configuration space and will be useful when the connection to statistical mechanics is made.

It is also important to note that the operator A must be an extended local operator for the above theorem to hold. Indeed, it is the localness of the operator which allows disjoint pieces of the wave function to give independent contributions to the expectation value. It should be noted again, too, that while quantum operators are local, they are not, in general, extended. Thus, in quantum mechanics, the operator of the right-hand side of Eq. (4) is actually $\tilde{A}$.

The decomposition of Eq. (4) is certainly not unique. Moreover, the decomposition is essentially a formal result because the functions φ_j vanish in a much larger region of configuration space than the function ψ. Thus, the ensemble of functions $\{\varphi_j\}$ is not a physical ensemble although the two are formally similar. In fact, each φ_j is in $\mathscr{L}_2$ and in the domain of $\tilde{A}$.

Up to this point, the notion of a macroscopic system has been introduced only to ensure that the system is in a bounded container and has boundary-independent properties. The results above depend only on the topology of configuration space, the analytic behavior of the inner product, and the notion of localness for operators. Thus, all results obtained above—in particular, the ensemble decomposition—apply to any system.

In the second paper in this series, attention will be restricted to macroscopic systems. For such systems, special kinds of partitions are introduced which ultimately lead to a connection between Gibbsian ensembles and the formal ensembles developed here.

5. SUMMARY

This paper and its companion paper are concerned with the problem of justifying the use of ensembles in quantum statistical mechanics. In this paper, it is argued that the statistical aspects of large systems have their origin in the "local" character of measuring processes. This is in contrast to the long-established notion of ergodic theory that ensembles result from time averages of dynamical variables.

In order to formalize the physical idea of "localness," a type of operator, called a local operator, was introduced. It was shown that such an operator can be extended to another local operator which has the useful property that it commutes with the characteristic function of certain open sets. Using these developments, a complete characterization of the bounded local operators was given.

The relationship between local operators and measurements was made by showing that the observables in quantum mechanics are local operators. Finally, a preliminary connection to statistical mechanics was made by considering expectation values. It was shown that expectation values for local operators can be written exactly as formal ensemble averages. Moreover, these formal averages reflect the physical idea that measurements actually involve an average of measured values arising from disjoint local regions in three-space.

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