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Rigorous Information-Theoretic Derivation of Quantum-Statistical Thermodynamics. II[1]

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Part I of the present work outlined the rigorous application of information theory to a quantum mechanical system in a thermodynamic equilibrium state. The general formula developed there for the best-guess density operator $\hat{\rho}$ was indeterminate because it involved in an essential way an unspecified prior probability distribution over the continuum $\mathscr{D}_{\mathrm{H}}$ of strong equilibrium density operators. In Part II mathematical evaluation of $\hat{\rho}$ is completed after an epistemological analysis which leads first to the discretization of $\mathscr{D}_{\mathrm{H}}$ and then to the adoption of a suitable indifference axiom to delimit the set of admissible prior distributions. Finally, quantal formulas for information-theoretic and thermodynamic entropies are contrasted, and the entire work is summarized.

4. DISCRETIZATION[3]

For philosophical reasons, such as parsimony, elegance, and tractability, the fundamental physical theories have always been constructed within a framework of continuum mathematics. Thus space and time are normally regarded as continuous, as are classical phase space and the Hilbert space of quantum mechanics. Of particular interest here, the Hermitian operator space $\mathscr{L}$ and its density operator domain $\mathscr{D}$ are also both continuous. In all of these cases it is epistemologically interesting to realize that the associated *data are never continuous*. For example, the list of possible instants that can be read from any actual clock, no matter how refined, is equivalent to a denumerable set of

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[3] All notation, including the numbering of sections and equations, is continued from Part I.[1] Specific equations in Part I are occasionally cited.

rational numbers rather than the entire real line. A similar remark applies to spatial measurements.

In quantum mechanics, we have a probabilistic theory that predicts values for objective probabilities that may be any number in the continuum between zero and unity. Yet the epistemic meaning of quantal probability entails an essential discreteness. Quantum theoretical probability is linked to empirical experience through the notion of ensemble, and the objective probability of a given event is defined operationally as the relative frequency of its occurrence in the ensemble. Therefore in any actual experiment designed to measure a quantal probability, the list of possible results would not be a continuum; for, in any such measurement, there would be a finite number X of elements in the ensemble (runs of the experiment). Let x denote the number of occurrences of the event of interest. The objective probability w for that event would by definition be

$$w = x/X \tag{47}$$

Since the numbers x and X in (47) are both nonnegative integers, the most complete list of possible values for w that would ever be *measured* is the set

$$\mathscr{W}_X = \{0,\ 1/X,\ 2/X, \ldots,\ (X-1)/X,\ 1\} \tag{48}$$

Obviously the $X + 1$ elements of $\mathscr{W}_X$ do not comprise a continuum; nevertheless, when X is sufficiently large, experimental physicists routinely employ (47) as the basic empirical rule for testing the probabilistic predictions of quantum mechanics. Just as every clock face or ruler has a least count, every scattering experiment has a finite number of runs. Time, space, and probability alike are theoretically continuous but datally discrete.

Now, in information-theoretic quantum statistics, we have a similar situation. Theoretically the unknown density operator might be any point in the continuous domain $\mathscr{D}$. However, if we consider the nature of experimental studies that would be required to determine ρ empirically, we find that the list of density operators that could be found by analysis of data is in fact a discrete subset of $\mathscr{D}$.

To illustrate this claim, it suffices to take a strong equilibrium case in which the coordinates $\{z_k\}$ are for some reason already known. (An example would be a system with totally nondegenerate H and hence a unique set of projectors $\{|\psi_n\rangle\langle\psi_n|\}$.) The domain $\mathscr{D}_H\{z_k\}$ of possible density operators will then consist of all density operators of the form (45) with $\{z_k\}$ fixed at the given values:

$$\mathscr{D}_H\{z_k\} = \left\{\rho \mid \rho = \sum_n w_n(|\psi_n\rangle\langle\psi_n|;\{z_k\}),\ \{w_n\} \in \mathscr{N}\right\} \tag{49}$$

The set $\mathscr{D}_H\{z_k\}$ is theoretically continuous. But let us imagine the sort of experiment that would be needed to determine which element of $\mathscr{D}_H\{z_k\}$ is the true ρ for a specified preparation, i.e., the sort of experiment that would determine the $\{w_n\}$. Physically w_n is an objective probability whose measure is the relative frequency of "yes" answers to the "question" represented by the projection operator $(|\,\psi_n\rangle\langle\psi_n\,|;\{z_k\})$. It follows immediately that the list of empirically ascertainable values for each w_n is just the set $\mathscr{W}_X$ defined by (48), and that the actual list of density operators in $\mathscr{D}_H\{z_k\}$ that might be determined by experiment is therefore just the discrete subset

$$\mathscr{D}_H{}^X\{z_k\} \equiv \left\{\rho \mid \rho(\{x_n\},\{z_k\}) = \sum_n \frac{x_n}{X}(|\,\psi_n\rangle\langle\psi_n\,|;\{z_k\}),\ \{x_n\}\in\mathscr{N}_X\right\} \tag{50}$$

where

$$\mathscr{N}_X \equiv \left\{\{x_n\} \mid x_n \geqslant 0,\ x_n \text{ an integer}, \sum_n x_n = X\right\} \tag{51}$$

The fact that the theoretically continuous list of possible strong equilibrium states $\mathscr{D}_H\{z_k\}$ has a *discrete* datal counterpart $\mathscr{D}_H{}^X\{z_k\}$ may be naturally interpreted in information theory as a condition on the prior probability distribution $p(\{w_n\},\{z_k\})$. Thus we set

$$p(\{w_n\},\{z_k\}) = \sum_{\mathscr{N}_X} \delta(\{w_n\},\{x_n/X\})\, P(\{x_n\},\{z_k\}) \tag{52}$$

where the δ-function assigns zero prior probability to all members of $\mathscr{D}_H\{z_k\}$ except those also in $\mathscr{D}_H{}^X\{z_k\}$ and $P(\{x_n\},\{z_k\})$ is the prior probability distribution for the unknown ρ to have eigenvectors determined by $\{z_k\}$ and eigenvalues $\{x_n/X\}$, $\{x_n\}$ being an element of the *discrete* set $\mathscr{N}_X$.

5. LAPLACIAN INDIFFERENCE AND THE DISCRETE SET $\mathscr{D}_H{}^X\{z_k\}$

Having taken into account the empirical countability of the possible values of objective probability, we now have the form (52) for the prior probability distribution needed in the strong-equilibrium best-guess calculation; but $P(\{x_n\},\{z_k\})$ remains to be specified. In seeking an explicit postulate for the function $P(\{x_n\},\{z_k\})$, we must consider both a priori philosophical criteria as well as a posteriori physical consequences.

From an epistemological standpoint, we would hope to be able to select $P(\{x_n\},\{z_k\})$ in a manner that seems inherently plausible, natural, and parsimonious. In past axiomatizations of quantum statistics, the prior probability has been specified by such metaphysical chestnuts as the random phase hypothesis or the postulate of equal probability for orthogonal pure states. We certainly want to base our choice of $P(\{x_n\}, \{z_k\})$ on more cogent and satisfying philosophical grounds than are offered by such blatantly ad hoc quantum statistical traditions.

The a posteriori constraint upon the choice of $P(\{x_n\}, \{z_k\})$ relates to a point discussed earlier. It is well verified experimentally that the canonical density operator (8) is an excellent quantal description of thermal equilibrium. Accordingly, we shall require that $P(\{x_n\}, \{z_k\})$ be chosen so that it leads to the canonical density operator as the strong equilibrium best guess.

The function $P(\{x_n\}, \{z_k\})$ has been defined as the a priori joint probability that the unknown ρ has eigenvalues corresponding to the element $\{x_n\}$ of the discrete set $\mathscr{N}_X$ and probability density that it has eigenvectors corresponding to the point $\{z_k\}$ of the continuum $\mathscr{Y}_H$. To focus attention on the $\{x_n\}$ dependence of P, let us assume as in the last section that $\{z_k\}$ is known. Our problem then is to adduce sound theoretical reasons for choosing some particular expression for the probability $P_{\{z_k\}}(x_n\})$, defined by

$$P_{\{z_k\}}(\{x_n\}) \equiv P(\{x_n\}, \{z_k\}) / \sum_{\mathscr{N}_X} P(\{x_n\}, \{z_k\}) \tag{53}$$

This is of course the a priori probability distribution associated with the set $\mathscr{D}_H{}^X\{z_k\}$.

Now the set $\mathscr{D}_H{}^X\{z_k\}$ is discrete, and it therefore seems appropriate, in view of established practice in discrete probability theory, to invoke the Laplacian indifference rule as a theoretical guideline for selecting $P_{\{z_k\}}(\{x_n\})$. However, it is not immediately evident how this should be done; for there are at least two physically reasonable ways in which to be "indifferent" to the choice of a density operator in $\mathscr{D}_H{}^X\{z_k\}$. We shall call these two possibilities *state indifference* and *data indifference*.

An *axiom of state indifference* would make the theoretically simple assertion that, given no information, equal probability should be attributed to each element of the set $\mathscr{D}_H{}^X\{z_k\}$; i.e.,

$$P_{\{z_k\}}(\{x_n\}) = 1 \Big/ \sum_{\mathscr{N}_X} (1) = P^{s}\{x_n\} \tag{54}$$

To formulate an axiom of data indifference, we continue to emphasize the empirical considerations that originally motivated discretization. To systematize discussion of an empirical state determination method, let Π denote the reproducible operational procedure for preparing the system. What is unknown is which density operator ρ in $\mathscr{D}_H{}^X\{z_k\}$ correctly characterizes Π. Let us suppose that Π is performed repeatedly and followed each time by measurement of one of the observables $\{(|\psi_n\rangle\langle\psi_n|; \{z_k\})| \, n = 1, 2,..., N\}$, where N is the dimensionality of the Hilbert space. Let each question

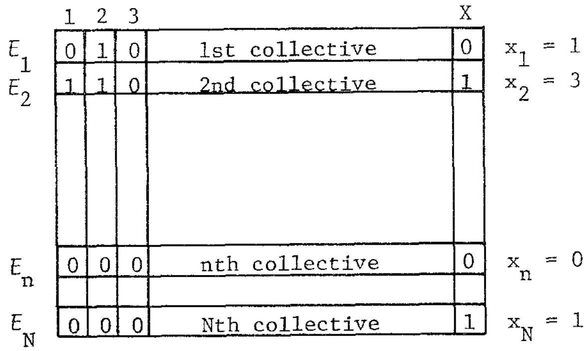

Fig. 1. Data matrix for determination of ρ in $\mathscr{D}_H{}^X[z_k]$. A few sample entries are filled in; illustrative x values are computed as though all other entries were zero.

$(|\,\psi_n\rangle\langle\psi_n\,|;\{z_k\})$ be asked X times; in other words, there are to be X runs of the experiment $\mathscr{E}_n$ consisting of preparation Π followed by measurement of the observable $(|\,\psi_n\rangle\langle\psi_n\,|;\{z_k\})$. The resulting numerical data may then be recorded (cf. Fig. 1) in the form of a matrix whose N rows are each labeled by an $\mathscr{E}_n$ and whose columns are numbered 1 through X to correspond to the X runs of $\mathscr{E}_n$. Each entry in the data matrix will be either zero ("no") or unity ("yes"). If X is sufficiently large, each row of the matrix becomes a statistical *collective* of data associated with an *ensemble* of identically prepared systems, as contemplated in the axioms of quantum mechanics. Let x_n denote the number of times unity occurs in row $\mathscr{E}_n$. If X is in fact large enough and quantum mechanics is a valid theory, then it will be true that $\sum_n x_n = X$; i.e., $\{x_n\} \in \mathscr{N}_X$, and the density operator may be computed by substituting the $\{x_n\}$ and X into the formula

$$\rho = \sum_n (x_n/X)(|\,\psi_n\rangle\langle\psi_n\,|;\{z_k\}) \tag{55}$$

Now, information-theoretic quantum statistics becomes necessary only when such a state determination procedure is infeasible in practice, i.e., when all or most of the information in our hypothetical data matrix is unavailable. Thus it seems reasonable from an empirical standpoint to identify total ignorance as to which ρ in $\mathscr{D}_H{}^X\{z_k\}$ is the correct one with total ignorance as to the entries in the data matrix. An *axiom of data indifference* would assert that, given no information, equal probability should be attributed to every possible data matrix. Possible data sets consist of all conceivable entries in the matrix for which the associated $\{x_n\}$ belong to $\mathscr{N}_X$. The number of such data sets describable by a given $\{x_n\}$ may easily be converted to a standard combinatorial problem. There are X entry slots in each row, and x_n is the number of times unity appears in the row $\mathscr{E}_n$. Hence the number $C\{x_n\}$ of ways to have x_1 units in row $\mathscr{E}_1$, x_2 units in row $\mathscr{E}_2$, etc., so that the sum of the $\{x_n\}$ is X, is given by

$$C\{x_n\} = X!\Big/\prod_n x_n! \tag{56}$$

Superficially this resembles the old statistical formula for the Boltzmann "complexion count." It should be evident, however, that the philosophical premises underlying our derivation of (56) and hence our interpretation of that formula are incompatible with the archaic and quantally absurd concept of complexion.

The quantity $C\{x_n\}$ is the number of different data matrices that would determine the same density operator (55). Thus, if the axiom of data indifference is adopted, it follows that the a priori probability $P_{\{z_k\}}(\{x_n\})$ is given by

$$P_{\{z_k\}}(\{x_n\}) = C\{x_n\}\Big/\sum_{\mathscr{N}_X} C\{x_n\} \equiv P^d\{x_n\} \tag{57}$$

Comparison of (54) and (57) reveals at once that the axioms of state indifference and data indifference lead to unequal prior probability distributions over the set $\mathscr{D}_H{}^X\{z_k\}$. Unfortunately, no metaphysical or aesthetic criterion seems to favor state indifference over data indifference, or vice versa. State indifference—reminiscent of Gibbsian considerations in phase space—effects a certain theoretical beauty; but data indifference seems closer somehow to the true empirical situation in statistical physics. Hence the decision as to which, if either, of these axioms to adopt in the present reformulation of quantum statistics will have to be made on a posteriori grounds.

To obtain the strong equilibrium best guess $\hat{\rho}$, we combine (52) and (53) to get an expression for the prior probability density:

$$p(\{w_n\}, \{z_k\}) = \Big[\sum_{\mathscr{N}_X} \delta\left(\{w_n\}, \left\{\frac{x_n}{X}\right\}\right) P_{\{z_k\}}(\{x_n\})\Big]\Big[\sum_{\mathscr{N}_X} P(\{x_n\}, \{z_k\})\Big] \tag{58}$$

Either (54) or (57) is to be substituted for $P_{\{z_k\}}(\{x_n\})$ in (58), depending on which indifference axiom is adopted. In each case the quantity $P_{\{z_k\}}(\{x_n\})$ is independent of $\{z_k\}$, an important property easily deduced by inspection of (54), (57), and their derivations. The prior distribution (58) therefore assumes the multiplicative form

$$p(\{w_n\}, \{z_k\}) = p_w\{w_n\}\, p_z\{z_k\} \tag{59}$$

where

$$p_w\{w_n\} = \sum_{\mathscr{N}_X} \delta\left(\{w_n\}, \left\{\frac{x_n}{X}\right\}\right) P\{x_n\} \tag{60}$$

and

$$p_z\{z_k\} = \sum_{\mathscr{N}_X} P(\{x_n\}, \{z_k\}) \tag{61}$$

The new symbol $P\{x_n\}$ in (60) represents either the state indifference probability $P^s\{x_n\}$ defined in (54) or the data indifference probability $P^d\{x_n\}$ defined in (57). Substituting (60) into (46) and integrating over $\mathscr{N}$, we obtain an expression for the strong-equilibrium best guess which incorporates the indifference axioms of interest:

$$\hat{\rho} = \sum_l \left[\int_{\mathscr{Y}_H} p_z\{z_k\}(|\,\psi_l\rangle\langle\psi_l\,|; \{z_k\}) \prod_k dz_k\right] \hat{w}_l \tag{62}$$

where

$$\hat{w}_l \equiv Q_l/XQ \tag{63}$$

$$Q_l \equiv \sum_{\mathscr{N}_X} x_l P\{x_n\} \prod_n \exp(-\beta x_n E_n/X) \tag{64}$$

and

$$Q \equiv \sum_{\mathscr{N}_X} P\{x_n\} \prod_n \exp(-\beta x_n E_n/X) \tag{65}$$

6. CALCULATION OF $\hat{w}_l$ BY THE SADDLE POINT METHOD

The quantity $\hat{w}_l$ has a mathematical form similar to well-known expressions occurring in the Darwin–Fowler[2–4] approach to statistical physics. This suggests that $\hat{w}_l$ can probably be evaluated by the saddle point method. We attack this problem in turn for the cases of state indifference and data indifference.

6.1. State-Indifference Calculation of $\hat{w}_l$

Let $M(z)$, a function of complex variable z, be defined as follows:

$$M(z) \equiv \sum_{\{x_n\}} z^{\sum_n x_n} \prod_n \exp\left(-\frac{\beta x_n E_n}{X}\right) \tag{66}$$

where $\sum_{\{x_n\}}$ signifies independent, unrestricted summation of each integral index x_n from 0 to ∞. Hence $M(z)$ may also be written in the form

$$M(z) = \prod_n \sum_{x=0}^{\infty} [z \exp(-\beta E_n/X)]^x \tag{67}$$

Summing the geometric series in (67), we then obtain

$$M(z) = \prod_n [1 - z\exp(-\beta E_n/X)]^{-1} \tag{68}$$

Finally we differentiate (68) to get the expression

$$\frac{\partial M}{\partial E_l} = -\frac{\beta M(z)}{X}\left[z^{-1}\left(\exp\frac{\beta E_l}{X}\right) - 1\right]^{-1} \tag{69}$$

Now consider the following contour integral along a closed path about the origin in the z plane:

$$\oint \frac{M(z)}{z^{X+1}}\,dz = \sum_{\{x_n\}} \prod_n \exp\left(-\frac{\beta x_n E_n}{X}\right) \oint \frac{dz}{z^{X+1-\Sigma_n x_n}} \tag{70}$$

where (66) has been substituted for $M(z)$. Since $X + 1 - \sum_n x_n$ is always an integer, $z = 0$ is never a branch point and we have by the calculus of residues that

$$\oint \frac{dz}{z^{X+1-\Sigma x_n}} = \begin{cases} 0, & \{x_n\} \notin \mathcal{N}_X \\ 2\pi i, & \{x_n\} \in \mathcal{N}_X \end{cases} \tag{71}$$

Hence

$$\oint \frac{M(z)\,dz}{z^{X+1}} = 2\pi i \sum_{\mathcal{N}_X} \prod_n \exp - \frac{\beta x_n E_n}{X} \tag{72}$$

A similar derivation leads quickly to the expression

$$\oint \frac{\partial M(z)}{\partial E_l}\frac{dz}{z^{X+1}} = 2\pi i\left(-\frac{\beta}{X}\sum_{\mathcal{N}_X} x_l \prod_n \exp - \frac{\beta x_n E_n}{X}\right) \tag{73}$$

where $\partial M(z)/\partial E_l$ is derived directly from (66) rather than (69).

To obtain the state-indifference version of $\hat{w}_l$, we substitute (54) into (63):

$$\hat{w}_l = \left(\sum_{\mathcal{N}_X} x_l \prod_n \exp - \frac{\beta x_n E_n}{X}\right)\Big/\left(X \sum_{\mathcal{N}_X} \prod \exp - \frac{\beta x_n E_n}{X}\right) \tag{74}$$

By comparing (72), (73), and (74), we are led immediately to the expression

$$\hat{w}_l = \left(\oint \frac{\partial M}{\partial E_l}\frac{dz}{z^{X+1}}\right)\Big/\left(-\beta \oint \frac{M dz}{z^{X+1}}\right) \tag{75}$$

When (69) is substituted, (75) assumes the simpler form

$$\hat{w}_l = \left\{\oint \frac{M\,dz}{z^{X+1}}\left[z^{-1}\left(\exp\frac{\beta E_l}{X}\right) - 1\right]^{-1}\right\}\Big/\left(X \oint \frac{M\,dz}{z^{X+1}}\right) \tag{76}$$

Equation (76), with $M(z)$ given by (68), is mathematically identical to an expression encountered as an intermediate step in the Darwin–Fowler treatment of a Bose assembly, and its evaluation by the saddle point method proceeds as follows. The function $M(z)/z^X$ has one saddle point ζ within the circle $|z| < 1$, and ζ is real and positive. If the contour about $z = 0$ passes through ζ along the path of steepest descent, the major contributions to the integrals in (76) are from values of the integrands in the neighborhood of ζ. This approximation becomes more and more accurate as X increases, and in our analysis X is necessarily large, since it is the number of elements in a quantal ensemble used to define objective probabilities. Therefore an excellent approximation to (76) is given by

$$\hat{w}_l^{\mathscr{s}} = X^{-1}[\zeta^{-1}\exp(\beta E_l/X) - 1]^{-1} \tag{77}$$

where the superscript $\mathscr{s}$ indicates that (77) is based on the axiom of state indifference.

6.2. Data-Indifference Calculation of $\hat{w}_l$

Let $N(z)$, a function of complex variable z, be defined as follows:

$$N(z) \equiv \sum_{\{x_n\}} z^{\Sigma_n x_n} \prod_n \left[\frac{\exp(-\beta x_n E_n/X)}{x_n!}\right] \tag{78}$$

Rearrangement of sums and product in (78) yields

$$N(z) = \prod_n \sum_{x=0}^{\infty} \frac{[z\exp(-\beta E_n/X)]^x}{x!} \tag{79}$$

which, after the exponential series is summed, takes the form

$$N(z) = \prod_n \exp[z\exp(-\beta E_n/X)] \tag{80}$$

As in the previous case, a derivative of $N(z)$ will also be needed:

$$\frac{\partial N}{\partial E_l} = -\frac{\beta N(z)}{X} z \exp -\frac{\beta E_l}{X} \tag{81}$$

From (71) and (78), it follows that

$$\oint \frac{N(z)\,dz}{z^{X+1}} = 2\pi i \sum_{\mathscr{N}_X} \prod_n \frac{\exp(-\beta x_n E_n/X)}{x_n!} \tag{82}$$

and

$$\oint \frac{\partial N(z)}{\partial E_l} \frac{dz}{z^{X+1}} = 2\pi i \left(-\frac{\beta}{X} \sum_{\mathscr{N}_X} x_l \prod_n \frac{\exp(-\beta x_n E_n/X)}{x_n!}\right) \tag{83}$$

To obtain the data-indifference version of $\hat{w}_l$, we substitute (57) into (63):

$$\hat{w}_l = \Big(\sum_{\mathscr{N}_X} x_l \prod_n \frac{\exp(-\beta x_n E_n/X)}{x_n!}\Big)\Big/\Big(X \sum_{\mathscr{N}_X} \prod_n \frac{\exp(-\beta x_n E_n/X)}{x_n!}\Big) \quad (84)$$

By comparing (82), (83), and (84), we are led to write

$$\hat{w}_l = \Big(\oint \frac{\partial N}{\partial E_l} \frac{dz}{z^{X+1}}\Big)\Big/\Big(-\beta \oint \frac{N\,dz}{z^{X+1}}\Big) \quad (85)$$

an expression which may be simplified, by substitution of (81), to the form

$$\hat{w}_l = \Big[\oint \frac{N\,dz}{z^{X+1}} \Big(z \exp - \frac{\beta E_l}{X}\Big)\Big]\Big/\Big(X \oint \frac{N\,dz}{z^{X+1}}\Big) \quad (86)$$

Equation (86), with $N(z)$ given by (80), is mathematically identical to an expression which occurred as an intermediate step in the Darwin–Fowler treatment of a classical Boltzmann assembly. Its evaluation by the saddle point method is entirely analogous to the analysis described above under (76). The result is therefore

$$\hat{w}_l{}^d = X^{-1}\eta \exp(-\beta E_l/X) \quad (87)$$

where η is the saddle point of $N(z)/z^X$ and the superscript d indicates that (86) is based on the axiom of data indifference.

7. EVALUATION OF $\hat{\rho}$ AND THE FAILURE OF STATE INDIFFERENCE

By rearranging (62), we may express the strong-equilibrium best guess in the form

$$\hat{\rho} = \int_{\mathscr{U}_H} p_z\{z_k\}\, B\{z_k\} \prod_k dz_k \quad (88)$$

with

$$B\{z_k\} \equiv \sum_l \hat{w}_l(|\,\psi_l\rangle\langle\psi_l\,|; \{z_k\}) \quad (89)$$

where either $\hat{w}_l{}^s$ or $\hat{w}_l{}^d$ is to be substituted for $\hat{w}_l$, depending upon which indifference axiom is adopted. In both cases, however, inspection of (77) and (87) shows that $\hat{w}_l$ depends only upon the single energy eigenvalue E_l. Mathematically this implies that the operator $B\{z_k\}$ is a function of the operator H. To see this, we have only to recall that for any $\{z_k\}$, $\{(|\,\psi_l\rangle\langle\psi_l\,|; \{z_k\})\}$ is an orthogonal set of projectors with the index l keyed to the set $\{E_l\}$ such that the spectral expansion of H is given by

$$H = \sum_l E_l(|\,\psi_l\rangle\langle\psi_l\,|; \{z_k\}) \quad (90)$$

Comparison of (89) and (90) shows at once that $B\{z_k\}$ is a function of H if $\hat{w}_l$ is a function of E_l.

The operator H is independent of the choice of $\{z_k\}$ in $\mathscr{Y}_H$, since H may be expressed in the form

$$H = \sum_E EP_E \tag{91}$$

where each eigenvalue E, regardless of its degeneracy, occurs but once in the summation and P_E denotes the projector onto the eigenspace belonging to E. The operator P_E is of course invariant to the choice of basis vectors for the E eigenspace, and hence independent of $\{z_k\}$.

Since H is independent of $\{z_k\}$, and $B\{z_k\}$ is a function of H, it follows that $B\{z_k\}$ is itself independent of $\{z_k\}$, a property which considerably simplifies (88). Removing B from the integrand in (88), we obtain

$$\hat{\rho} = B \int_{\mathscr{Y}_H} P_z\{z_k\} \prod_k dz_k \tag{92}$$

Since $p_z\{z_k\}$ is normalized over $\mathscr{Y}_H$, (92) reduces finally to

$$\hat{\rho} = B \tag{93}$$

In the state-indifference case, substitution of (77) into (89) yields

$$\begin{aligned} B^s(H) &= \sum_l X^{-1}[\zeta^{-1} \exp(\beta E_l/X) - 1]^{-1}(|\,\psi_l\rangle\langle\psi_l\,|; \{z_k\}) \\ &= X^{-1}[\zeta^{-1} \exp(\beta H/X) - 1]^{-1} \end{aligned} \tag{94}$$

Similarly, substitution of (87) into (89) yields for the data-indifference case

$$\begin{aligned} B^d(H) &= \sum_l X^{-1}\eta \exp(-\beta E_l/X)(|\,\psi_l\rangle\langle\psi_l\,|; \{z_k\}) \\ &= X^{-1}\eta \exp(-\beta H/X) \end{aligned} \tag{95}$$

The saddle points in (94) and (95) may be expressed as functions of X and of the quantities $\{\beta E_l/X\}$ by solving the equation arising in each case from the condition that B have trace unity. The solution $\zeta(X; \{\beta E_l/X\})$ cannot be given in closed form, but $\eta(X; \{\beta E_l/X\})$ is easily determined:

$$\eta\left(X; \left\{\frac{\beta E_l}{X}\right\}\right) = \frac{X}{\operatorname{Tr} \exp(-\beta H/X)} \tag{96}$$

Hence

$$B^d(H) = \frac{\exp(-\beta H/X)}{\operatorname{Tr} \exp(-\beta H/X)} \tag{97}$$

Now if we recall from Part I that $\beta = 1/cT$, c being a proportionality constant used to fix the temperature scale, and then compare (97) with the canonical density operator (8), we find that $B^d(H)$ takes the canonical form, provided we set

$$c = k/X \tag{98}$$

where k is Boltzmann's constant, which appears in (8). On the other hand, $B^s(H)$ approaches the canonical form only in a high-T approximation. Consequently we are motivated through hindsight to render a verdict in favor of the *axiom of data indifference*, since from it we can deduce the empirically valid canonical density operator as the strong-equilibrium best guess:

$$\hat{\rho} = \frac{\exp(-H/kT)}{\operatorname{Tr}\exp(-H/kT)} \tag{99}$$

By contrast, the best guess (91) based on state indifference is physically unacceptable.

8. THERMODYNAMIC AND INFORMATION-THEORETIC ENTROPIES

The so-called Gibbs–von Neumann entropy expression

$$I \propto \operatorname{Tr} \rho \ln \rho \tag{100}$$

was disavowed in Part I on the ground that it is not an appropriate measure of missing information in a quantally rigorous information-theoretic approach to statistical physics. Instead of (100) with its attendant ignorance interpretation of the density operator, we adopted the more general information-theoretic entropy function defined by an integral over the continuum of alternative quantum states. In the strong equilibrium case, this missing information function has the form

$$I = -\kappa \int_{\mathscr{N}} \prod_n dw_n \int_{\mathscr{Y}_H} \prod_k dz_k \, w(\{w_n\}, \{z_k\}) \ln \frac{w(\{w_n\}, \{z_k\})}{p(\{w_n\}, \{z_k\})} \tag{101}$$

Choosing $\kappa = c$, we obtain from (21) the connection between thermodynamic entropy S and the constrained maximum $\hat{I}$ of (101):

$$S = \hat{I} + S_0 \tag{102}$$

According to (24), (102) may be expressed as

$$S = c \ln R + (U/T) + S_0 \tag{103}$$

To derive R for the case of strong equilibrium, we replace $\mathscr{D}'$ by $\mathscr{D}_H'$ in (24), the integral definition of R, and substitute (43), (57), (69), and (60); hence

$$R = \int_{\mathscr{N}} \prod_n dw_n \int_{\mathscr{Y}_H} \prod_k dz_k \, p(\{w_n\}, \{z_k\}) \prod_n \exp(-w_n E_n/cT) \tag{104}$$

where

$$p(\{w_n\}, \{z_k\}) = p_z\{z_k\} \sum_{\mathscr{N}_X} \delta\left(\{w_n\}, \left\{\frac{x_n}{X}\right\}\right) \frac{\prod_n (1/x_n!)}{\sum_{\mathscr{N}_X} \prod_n (1/x_n!)} \tag{105}$$

When (105) is substituted into (104) and the integration is performed, R assumes the form

$$R = \left(\sum_{\mathscr{N}_X} \prod_n \frac{\exp(-x_n E_n/XcT)}{x_n!}\right) \Big/ \left(\sum_{\mathscr{N}_X} \prod_n \frac{1}{x_n!}\right) \tag{106}$$

which, according to (56) and (82), may be rewritten as

$$R = \left(\frac{1}{2\pi i} \oint \frac{N(z)}{z^{X+1}} \, dz\right) \Big/ \left(\frac{1}{X!} \sum_{\mathscr{N}_X} C\{x_n\}\right) \tag{107}$$

For large X we may approximate the integral in (107) by recalling that η is the saddle point of $N(z)/z^X$; thus

$$R = X! \, N(\eta)/\eta^X C \tag{108}$$

where

$$C \equiv \sum_{\mathscr{N}_X} C\{x_n\} \tag{109}$$

and where $N(\eta)$ is given by (80) as

$$N(\eta) = \prod_n \exp[\eta \exp(-E_n/XcT)] \tag{110}$$

Therefore

$$\ln R = \ln X! + \sum_n \eta \exp(-E_n/XcT) - X \ln \eta - \ln C \tag{111}$$

which, upon substitution of (96) and (98), becomes

$$\ln R = \ln X! + X - X \ln X + X \ln \operatorname{Tr} \exp(-H/kT) - \ln C \tag{112}$$

For large X, the first three terms of (112) cancel by Stirling's approximation, and when the surviving terms are substituted into (103), the following expression is obtained for thermodynamic entropy:

$$S = k \ln \operatorname{Tr} \exp(-H/kT) + (U/T) + S_0 - (k/X) \ln C \tag{113}$$

We are now in a position to understand why the von Neumann functional (100) may successfully be taken as a measure of thermodynamic entropy despite its general inappropriateness as a measure of missing information in quantum mechanics. As is well known, if $\hat{\rho}$ is the canonical density operator, then

$$-k \operatorname{Tr} \hat{\rho} \ln \hat{\rho} = k \ln \operatorname{Tr} \exp(-H/kT) + (U/T) \tag{114}$$

Comparing (113) and (114), we therefore have

$$S = -k \operatorname{Tr} \hat{\rho} \ln \hat{\rho} + S_0 - (k/X) \ln C \tag{115}$$

If, as is customary, we assume that the ground state of H is nondegenerate and then determine S_0 by invoking the third law in the form (23), we are led by a straightforward computation to select

$$S_0 = (k/X) \ln C \tag{116}$$

so that finally the usual quantum statistical expression for thermodynamic entropy emerges:

$$S = -k \operatorname{Tr} \hat{\rho} \ln \hat{\rho} \tag{117}$$

9. SUMMARY AND CONCLUSIONS

Having produced a new derivation of the canonical density operator and of the established statistical analogs to such thermodynamic parameters as temperature and entropy, the present study has achieved its major goals. However, because some of the mathematical techniques we employed are quite standard in various versions of statistical physics, it may appear in a cursory review of our equations that we have merely concocted a somewhat eccentric blend of old results rather than creating new foundations for quantum statistics. To dispel such an illusion, one must carefully reflect upon the meanings of the equations and upon the philosophical underpinnings of our approach. In this regard it is instructive to emphasize again what was not assumed as well as what was.

Our general viewpoint has been to accept appreciatively the modern definition of statistical physics as a discipline which unites theoretical physics and information theory into a potent schema for making educated inferences concerning physical situations in which exact mechanical analysis is not feasible. We argued, nevertheless, that the orthodox applications of information theory to quantum mechanical situations have not been grounded in a rational quantum theoretical background but have instead been based upon numerous misconceptions, which have been scrutinized elsewhere.[5,6] The principal consequence of these misconceptions for information-theoretic quantum statistics was an incorrect starting point, an unjustifiably restrictive —indeed *inexhaustive*—list of quantum states over which the subjective probability distribution of information theory has heretofore been defined. The problem we attacked may therefore be characterized as follows: Quantum statistics ought to be the result of an information-theoretic analysis of quantum mechanics; but no such analysis has ever been performed correctly, for indeed none has ever even been initiated correctly.

We began by recognizing that the true logical spectrum of quantum states is theoretically a continuum embracing both pure states and mixtures. Being a continuum, that spectrum engendered well-known ambiguities for probabilistic or information-theoretic reasoning, a dilemma that can be resolved only by an axiom specifying an a priori probability distribution over the logical spectrum.

The problem of thermal equilibrium was formulated in two ways, dubbed weak and strong. The case of weak equilibrium, defined by constraints normally adopted in orthodox quantum statistics, remains incompletely solved due to our lack of a rational axiom of prior distribution over the entire domain $\mathscr{D}$ of density operators. The case of strong equilibrium, defined by the weak equilibrium constraints plus a stringent but reasonable dynamical condition, proved more amenable to detailed investigation primarily because the associated set $\mathscr{D}_H$ of possible density operators exhibited certain properties notably simpler than those of $\mathscr{D}$.

In the case of strong equilibrium we discovered important clues that may lead eventually to the development of a general axiom concerning the prior distribution over $\mathscr{D}$. In particular, it was demonstrated in the present paper that $\mathscr{D}_H$ is *theoretically continuous* but *datally discrete*. It seems likely that a similar analysis of the empirical meaning of the more general quorum theory for determining points of $\mathscr{D}$ would lead to the same conclusion. After effecting a partial discretization of $\mathscr{D}_H$ on empirical grounds, we found ourselves for the first time able to enunciate theoretically appealing axioms regarding the a priori distribution over $\mathscr{D}_H$, axioms based on the ancient indifference rule of Laplace.

The difficult choice to be made was between alternative axioms called state indifference and data indifference. Hindsight now informs us that the latter is the proper choice, since it alone leads to experimentally verified predictions. Philosophically, state indifference had seemed attractive, probably because of its superficial resemblance to the old idea that equal volumes in classical phase space are a priori equally probable. However, if we emphasize the informational aspect of statistical physics and contemplate in particular the nature of physical information, then data indifference begins to seem inherently the more plausible. In this connection, our hypothetical data matrix discussed in Section 5 is a useful metaphor. Along with discretization, it seems likely that the concept of data indifference could be generalized beyond the case of strong equilibrium to provide a universal axiom giving the a priori probability distribution over the entire domain $\mathscr{D}$.

In the present work we were content to finish just the strong equilibrium case. This was accomplished by borrowing some mathematical methods popularized in the early days of quantum statistics by Darwin and Fowler, but it would be philosophically incorrect to say that we have merely reproduced their statistical method. The quantum statistics of Darwin and Fowler treated the quantal ensemble as an noninteracting assembly of systems each of which possesses some definite if unknown pure state vector chosen from a complete orthogonal master list of eigenvectors; and every such configuration, or complexion, of vector assignments to the systems was regarded as a priori equally probable. Obviously this point of view is utterly contradictory to the quantal foundations[5,6] upon which we have based our analysis. Nevertheless, since our partially discretized, strong equilibrium case did involve mathematical forms that are also characteristic of the Darwin–Fowler model, we naturally exploited this similarity. We do not yet know if related mathematical techniques will be helpful in more general cases, such as weak equilibrium, that may be developed within our new framework.

Finally, a few remarks concerning the concept of entropy seem in order. It is generally well accepted that information-theoretic entropy—missing information—and thermodynamic entropy should be regarded as distinct concepts originating in different disciplines. Nevertheless, in orthodox quantum statistics this important distinction is effectively forgotten when an ignorance interpretation is given to the density operator and the formula

$$S = -k \operatorname{Tr} \rho \ln \rho \tag{118}$$

becomes erroneously for every ρ both the missing information and a generalization of thermodynamic entropy. In our theory, on the other hand, the two entropy constructs never merge. The information-theoretic entropy, or missing information functional, I does not depend on any single quantum state ρ but only on a subjective probability distribution defined over all density operators. The thermodynamic entropy S has been identified for thermal equilibrium only and found to be given by the usual formula (117); but even at equilibrium, S and $\hat{I}$ are unequal, the statistical analog for S being not $\hat{I}$ but $\hat{I} + (k/X) \ln C$ [cf. (102), (116)]. This thoroughgoing nonequivalence of equilibrium thermodynamic and information-theoretic entropies raises an interesting question—which one is the appropriate generalization of thermodynamic entropy to nonequilibrium cases?

If the informational aspect of entropy is considered primary, then it would seem natural to adopt a formula like

$$S = I + (k/X) \ln C \tag{119}$$

as the general (not just equilibrium) statistical analog to thermodynamic entropy. Through I, such a nonclassical S would be dependent upon both prior and posterior probability distributions, and thereby perhaps offer, for example, an elegant means for treating nonequilibrium systems having "memory." If, by contrast, the function-of-state aspect of entropy is regarded as fundamental, then the trace formula (118) would seem to offer the most satisfying extension of thermodynamic entropy to nonequilibrium cases. In this series of papers[1,5,6] and in our continuing research, we have been motivated by the belief that entropy should be defined as a functional of the state of the system as described by the density operator, whether that state is an equilibrium one or not, and that information theory is to be used to assist us to make the best guess at entropy when the state is not completely determined by available data. We do not at present believe that the missing information functional should in general be linked closely with entropy, even though in special cases, such as thermal equilibrium (weak or strong), the contrained maximum $\hat{I}$ is indeed strongly associated with thermodynamic entropy. We regard this association as confirmation that missing information was correctly assessed to describe the actual physical situation, not as evidence that generalization (119) may be valid. Nevertheless, we do not propose here any final judgment as to whether (118) or something like (119) offers the more suitable generalization; but it is our firm conclusion that, outside equilibrium, (118) and (119) are not equivalent, and that (118) cannot be both entropy and missing information, since it is definitely not a measure of the latter.

REFERENCES

1. J. L. Park and W. Band, *Found. Phys.* **7**, 233 (1977).
2. R. H. Fowler, *Statistical Mechanics* (Cambridge Univ. Press, 1936).
3. H. Margenau and G. Murphy, *The Mathematics of Physics and Chemistry* (D. Van Nostrand, New York, 1943), pp. 436–449.
4. E. Schrödinger, *Statistical Thermodynamics* (Cambridge Univ. Press, 1946).
5. J. L. Park and W. Band, *Found. Phys.* **6**, 157 (1976).
6. W. Band and J. L. Park, *Found. Phys.* **6**, 249 (1976).