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

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In previous publications we have criticized the usual application of information theory to quantal situations and proposed a new version of information-theoretic quantum statistics. This paper is the first in a two-part series in which our new approach is applied to the fundamental problem of thermodynamic equilibrium. Part I deals in particular with informational definitions of equilibrium and the identification of thermodynamic analogs in our modified quantum statistics formalism.

1. A NEW FORMAT FOR INFORMATION-THEORETIC QUANTUM STATISTICS

In two recent articles, we have criticized the orthodox information-theoretic foundations of quantum statistics[1] and indicated how to develop a correct informational approach to quantal situations.[2] The present paper and its sequel describe the application of our new version of information-theoretic quantum statistical mechanics to the fundamental problem of thermal equilibrium. Although we anticipate no final results at variance with empirically established formulas of statistical theormodynamics, we do expect to present new derivations which are not subject to the serious theoretical objections we have raised against former treatments.

In the customary union of quantum mechanics and information theory, the density operator ρ is given an *ignorance interpretation*, according to which the eigenvalue spectrum of ρ is a subjective probability distribution defined over the associated eigenvectors, one of which is assumed to be the state

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vector describing the true but unknown quantum state. The information-theoretic entropy, or missing information function, is defined by

$$I = -k \operatorname{Tr} \rho \ln \rho \tag{1}$$

where k is an arbitrary constant. The best-guess density operator $\hat{\rho}$ is then taken to be the one that maximizes (1) subject to whatever constraints define the physical situation. In the aforementioned articles, we scrutinized this approach and found it to be incompatible with the foundations of quantum mechanics. We then suggested the following new format for the application of information theory to quantum mechanical situations.

According to general quantum theory, there exist many preparations of state that are describable by no state vector whatever; thus the most that can be asserted a priori about an unknown quantum state is that it is surely represented by some density operator ρ. The domain $\mathscr{D}$ of density operators consists of all Hermitian, nonnegative-definite, trace-unity operators on Hilbert space $\mathscr{H}$ of the system. If $\mathscr{L}$ denotes the space of Hermitian operators defined on $\mathscr{H}$, then $\mathscr{D}$ is a convex subset of $\mathscr{L}$. As in past work, we use the term *quorum* to denote a linearly independent set $\{Q_j\}$, where each Q_j is an element of $\mathscr{L}$. Thus every operator of $\mathscr{L}$ and a fortiori every ρ in $\mathscr{D}$ may be expressed as a linear combination of quorum elements:

$$\rho\{q_j\} = \sum_j q_j Q_j \tag{2}$$

We call the coefficients $\{q_j\}$ *quorum parameters* and usually regard them as coordinates in an auxiliary space $\mathscr{L}'$. Points $\{q_j\}$ corresponding to density operators lie in a convex domain $\mathscr{D}'$ within $\mathscr{L}'$.

Let $w\{q_j\}$ be a subjective probability distribution defined over $\mathscr{D}'$. If the true quantum state $\rho\{q_j\}$ is unknown, then information theory can provide the distribution $w\{q_j\}$ that best characterizes our incomplete knowledge. Since $\mathscr{D}'$ is a continuum, the *missing information* functional[3] is defined by

$$I \equiv -\kappa \int_{\mathscr{D}'} \prod_j dq_j \, w\{q_j\} \ln(w\{q_j\}/p\{q_j\}) \tag{3}$$

where κ is an arbitrary positive constant and $p\{q_j\}$ is the prior probability distribution. Hobson[4] has proved from several very reasonable informational postulates that $-I$ is the *unique* measure of the information gain associated with the replacement of a prior distribution $p\{q_j\}$ by a posterior distribution $w\{q_j\}$. When $w\{q_j\}$ is unconstrained except by normalization, the nonpositive functional I attains its maximum value (zero) when $w\{q_j\} = p\{q_j\}$; thus $p\{q_j\}$ is the subjective probability density over $\mathscr{D}'$ that describes total ignorance concerning the true state ρ of the system.

The fundamental rule that we have proposed for information-theoretic quantum statistics may now be expressed as follows. Maximize (3)—not (1)—subject to whatever constraints define the physical situation; then use the result $\hat{w}\{q_j\}$ to form the best-guess density operator by averaging over $\mathscr{D}'$:

$$\hat{\rho} = \int_{\mathscr{D}'} \prod_j dq_j \, \hat{w}\{q_j\} \, \rho\{q_j\} \tag{4}$$

Our present objective is to apply this rule to the problem of thermal equilibrium. For a thorough analysis of the philosophical foundations of this new approach, the reader is again referred to our earlier articles.[1,2]

In this paper (Part I) we discuss informational definitions of equilibrium and show how to identify the standard parameters of equilibrium thermodynamics within our modified quantum statistics formalism. The sequel (Part II) will consider the problem of selecting the prior distribution $p\{q_j\}$ and then complete the derivation of the best-guess $\hat{\rho}$ for thermodynamic equilibrium.

2. THE CASE OF WEAK EQUILIBRIUM

Consider a system whose Hamiltonian H depends on a single known external parameter V. Let the system be prepared in the manner that would be characterized in equilibrium thermodynamics by the extensive parameters (U, V), where U denotes internal energy. Such thermodynamic knowledge is translated into information-theoretic quantum statistics by imposing upon the subjective probability distribution $w\{q_j\}$ the following constraint:

$$\langle \bar{H} \rangle = \int_{\mathscr{D}'} \prod_j dq_j \, w\{q_j\} \, \bar{H}\{q_j\} = U \tag{5}$$

where

$$\bar{H}\{q_j\} \equiv \mathrm{Tr}[\rho\{q_j\} \, H(V)] \tag{6}$$

We call the problem of maximizing the I of Eq. (3) subject to constraint (5) the *weak equilibrium* case to distinguish it from a situation to be treated in the next section, where more than just (5) is considered known in advance. In orthodox quantum statistics based upon the ignorance misinterpretation of ρ and the quantally incorrect missing information function (1), the counterpart to constraint (6) is simply

$$\mathrm{Tr}(\rho H) = U \tag{7}$$

Maximization of (1) subject to (7) leads in a familiar derivation[5] to the canonical density operator

$$\hat{\rho} = \frac{\exp[-H(V)/kT(U, V)]}{\mathrm{Tr}\exp[-H(V)/kT(U, V)]} \tag{8}$$

as the best information-theoretic description of a system whose thermodynamic state is (U, V). The temperature function $T(U, V)$ is uniquely determined by (7).

The practical utility of the canonical density operator (8) can hardly be challenged. Experience amply demonstrates its empirical potency. Although we have repudiated the orthodox bases of quantum statistics, we cannot dismiss the scientific achievements of that discipline, which follow from myriad well-known applications of (8). Providing a new derivation of the canonical density operator must therefore be a major goal of the present study.

The maximization of (3) subject to the constraint (5) and to the normalization constraint on $w\{q_j\}$ is an elementary problem in the calculus of variations which bears strong mathematical resemblance to standard manipulations in ordinary statistical physics. The result is

$$\hat{w}\{q_j\} = \frac{p\{q_j\} \exp\{-\beta(U, V) \operatorname{Tr}[\rho\{q_j\} H(V)]\}}{R(U, V)} \tag{9}$$

where R and β are uniquely determined by the constraints. Expressed as a function of $\beta(U, V)$ and V, R has the form

$$R(U, V) = \int_{\mathscr{D}'} \prod_j dq_j \, p\{q_j\} \exp(-\beta \bar{H}\{q_j\}) \tag{10}$$

where $\bar{H}\{q_j\}$, a function of V, was defined in (6).

The best-guess density operator in the weak equilibrium situation is therefore

$$\hat{\rho} = \frac{\int_{\mathscr{D}'} \prod_j dq_j \, p\{q_j\}[\exp(-\beta \bar{H}\{q_j\})] \, \rho\{q_j\}}{\int_{\mathscr{D}'} \prod_j dq_j \, p\{q_j\} \exp(-\beta \bar{H}\{q_j\})} \tag{11}$$

To identify in the present theory statistical analogs to basic thermodynamic parameters, we employ the usual approach introduced by Gibbs[6] but applicable as well to other forms[7] of statistical mechanics. Along a quasistatic path defined by a continuous sequence of (U, V) points, the differential of the quantity $R(U, V)$ is given by

$$\begin{aligned} dR &= \left[\int_{\mathscr{D}'} \prod_j dq_j \, p\{q_j\}(-\bar{H}\{q_j\}) \exp(-\beta \bar{H}\{q_j\})\right] d\beta(U, V) \\ &\quad + \left[\int_{\mathscr{D}'} \prod_j dq_j \, p\{q_j\}\left(-\beta \frac{\partial \bar{H}\{q_j\}}{\partial V}\right) \exp(-\beta \bar{H}\{q_j\})\right] dV \\ &= -R \langle \bar{H} \rangle \, d\beta(U, V) + \beta R \left\langle -\overline{\frac{\partial H}{\partial V}} \right\rangle dV \end{aligned} \tag{12}$$

The expectation value $\langle \bar{H} \rangle$ of the quantal mean $\bar{H}$ of H has already been identified with U. The expectation value $\langle -\overline{\partial H/\partial V} \rangle$ may be written out as

$$P \equiv \langle -\overline{\partial H/\partial V} \rangle = \langle \mathrm{Tr}[\hat{\rho}(-\partial H(V)/\partial V] \rangle \tag{13}$$

which indicates that $\langle -\overline{\partial H/\partial V} \rangle$ is the thermodynamic analog of the intensive parameter P associated with the external extensive parameter V. If V were volume, $-\partial H(V)/\partial V$ would be the quantal pressure operator, and thermodynamic pressure P would thus be identified statistically as the expectation value of the quantal mean of $-\partial H(V)/\partial V$.

With these identifications, (12) takes the form

$$dR/R = -U\,d\beta + \beta P\,dV \tag{14}$$

Consider next a quantity D defined by

$$D \equiv \ln R + U\beta \tag{15}$$

Differentiating (15) and substituting (14), we obtain

$$dD/\beta = P\,dV + dU \tag{16}$$

Comparison of (16) with the $T\,dS$ equation of thermodynamics then gives

$$dD/\beta = T\,dS \tag{17}$$

from which we make these correspondences between β and D and thermodynamic temperature T and entropy S:

$$1/\beta = cT \tag{18}$$

$$cD = S - S_0 \tag{19}$$

The proportionality constant c determines the units of measurement for T and S, and S_0 is a constant of integration.

It is now easy to establish a connection between thermodynamic entropy S and the constrained maximum value $\hat{I}$ of information-theoretic entropy. Substituting (9) into (3), we obtain

$$\hat{I} = \kappa D \tag{20}$$

where D is defined by (15). It then follows from (19) that

$$\hat{I} = (\kappa/c)(S - S_0) \tag{21}$$

Thus $\hat{I}$ and S could be made numerically equal up to an additive constant by adopting as a convention in quantum statistics the following harmless redefinition of missing information to replace (3):

$$I \equiv -c \int_{\mathscr{D}'} \prod_j dq_j \, w\{q_j\} \ln(w\{q_j\}/p\{q_j\}) \tag{22}$$

A thermodynamic argument to determine S_0 can be based on the third law in the form

$$\lim_{T \to 0} S = 0 \tag{23}$$

An expression for S as a function of T and V is obtained by combining (15), (18), and (19):

$$S = c \ln R + (U/T) + S_0 \tag{24}$$

where

$$R(T, V) = \int_{\mathscr{D}'} \prod_j dq_j \, p\{q_j\} \exp(-\bar{H}\{q_j\}/cT) \tag{25}$$

and

$$U(T, V) = \int_{\mathscr{D}'} \prod_j dq_j \, p\{q_j\} \, \bar{H}\{q_j\} \frac{\exp(-\bar{H}\{q_j\}/cT)}{R(T, V)} \tag{26}$$

However, we are unable to apply (23) to (24) and thus find S_0, because the integrals (25) and (26) involve the unknown prior distribution $p\{q_j\}$ in an essential way.

Ideally, we should now be near the conclusion of our program of erecting quantum statistics upon a philosophically sound foundation. We have avoided the quantally untenable hypotheses which tarnish the standard approach, and have for the first time correctly applied information theory to a quantum system whose mechanical state is unknown but whose thermodynamic state is known to be (U, V). If the resulting information-theoretic quantum statistics is valid, then our weak equilibrium best-guess (11) must lead to the same physical predictions as the empirically successful canonical density operator (8). A necessary and sufficient condition that these two density operators make the same expectation value estimates of the quantal mean values of every observable is that they be equal; i.e.,

$$\frac{\int_{\mathscr{D}'} \prod_j dq_j \, p\{q_j\} \{\exp[-\mathrm{Tr}(\rho\{q_j\} H)/cT]\} \, \rho\{q_j\}}{\int_{\mathscr{D}'} \prod_j dq_j \, p\{q_j\} \exp[-\mathrm{Tr}(\rho\{q_j\} H)/cT]} = \frac{\exp(-H/kT)}{\mathrm{Tr} \exp(-H/kT)} \tag{27}$$

Therefore, if Eq. (27) could be proved, our analysis would be complete, except for some minor generalizations to several external parameters, several constraints, etc. Unfortunately, there are at least two barriers to proving the desired theorem. One is essentially philosophical: The prior distribution $p\{q_j\}$, needed in this continuum problem because of the inadequacy of the Laplacian rule of indifference, remains unknown. The other obstacle is mathematical: Even if $p\{q_j\}$ were known, we could not perform the required integrals because we have no useful analytical description of the domain $\mathscr{D}'$ and its boundary. It is to be hoped that a solution of the mathematical problem will be discovered in future research.

In Part II of the present investigation we reconsider the prior probability question, but in the context of a stronger informational definition of equilibrium, to which we now turn.

3. THE CASE OF STRONG EQUILIBRIUM

In the preceding section, the term *weak equilibrium* was used to denote an information-theoretic situation in which all that is known are the values of thermodynamic parameters (U, V). To call such a state of knowledge "equilibrium" is standard practice in statistical mechanics; yet from a mechanical viewpoint it seems strange that a description of human ignorance could claim to capture the essence of the physical concept of thermodynamic equilibrium. After all, to say that a system is in thermal equilibrium is to say, with Planck, that the energy of the system cannot be transferred to lift a weight without also affecting external systems in some permanent way. It is difficult to believe that such a proposition could be equivalent to an information-theoretic assertion that *only* (U, V) happen to be known. Indeed it seems easy enough to imagine systems *not* in thermal equilibrium for which (U, V) are nonetheless the only known parameters. In such cases we may reasonably be skeptical about the unproved proposition (27) that would make canonical equilibrium the "best guess."

It would be a mistake, however, to construe criticism of this type as an attack upon the information-theoretic approach. Information theory only claims to make the best guess $\hat{\rho}$ compatible with whatever is known. Thus it is entirely possible that given merely (U, V), the theory may guess a $\hat{\rho}$ that will turn out to have additional properties characteristic of the physical meaning of equilibrium. In fact this is precisely what does happen in the orthodox version of quantum statistics. When the missing information functional (1) is maximized in the weak equilibrium situation, the resulting canonical $\hat{\rho}$ in (8) is observed a posteriori to be itself a time-independent form, which implies that all quantal mean values computed from it are likewise time independent. Consequently, it can be affirmed that given (U, V) only, the best guess would indeed be that the system is in a state of very complete mechanical equilibrium.

Now, in the present development of information-theoretic foundations for quantum statistics, we face a somewhat different logical situation. Having disavowed (1), replaced it by (3), and obtained best guess (11) for $\hat{\rho}$, we find that $\hat{\rho}$ is indeterminate because $p\{q_j\}$ is unspecified. Thus our "weak equilibrium" result does not exhibit any properties that justify even a posteriori the usage of the term "equilibrium" to describe a state of knowledge in which only (U, V) happen to be known.

We are inclined therefore to refine somewhat our initial information-theoretic characterization of thermal equilibrium. To pursue this, let us acknowledge first that a thermal equilibrium situation is indeed at least a weak equilibrium situation; i.e., the values (U, V) are, as before, assumed to be known. However, a thermal equilibrium situation is more than this; it is a dynamical condition in which quantal mean values have ceased evolving, and reflect a state of "relaxation" or "disorder" or "stagnation." Accordingly, we shall adopt as a part of the statistical definition of thermal equilibrium the assertion that the density operator ρ commutes with the Hamiltonian H:

$$[\rho, H] = 0 \tag{28}$$

It is well known that (28) implies constancy in time for the quantal mean values of all (except intrinsically time-dependent) observables. Conversely, if all quantal mean values are constants of the motion, then the unknown quantum state ρ must satisfy (28). It may well be argued that the total quantum mechanical equilibrium contemplated here is too strong a statistical analog for thermodynamic equilibrium, since practical observations that would serve as tests for thermodynamic equilibrium could involve only a small subset of quantal observables. Nevertheless, we adopt the condition (28) for its elegance and tractability, and note its conceptual similarity to Gibbs' universally accepted definition of an equiblibrium density-in-phase as one that is intrinsically time independent.

We shall henceforth designate as a *strong equilibrium* case a quantum statistical analysis in which both the values (U, V) and the validity of (28) are assumed known. If a system is characterized thermodynamically as being in thermal equilibrium state (U, V), it seems to us, for the reasons noted above, that the proper quantum statistical treatment of that system should be based upon the case of strong rather than weak equilibrium. Thus the objective of information-theoretic statistical thermodynamics should be to derive the canonical density operator (8) as the best guess, given not just (U, V), but also the fact that the system is in thermodynamic equilibrium.

To consider in detail the case of strong equilibrium, the new constraint (28) must first be converted to a useful form. By an elementary theorem it follows from (28) that ρ and H share a common complete orthonormal set of eigenvectors. Thus ρ has a spectral expansion of the form

$$\rho = \sum_n w_n \mid \psi_n\rangle\langle\psi_n \mid \tag{29}$$

where the $\{\mid \psi_n\rangle\}$ satisfy

$$H \mid \psi_n\rangle = E_n \mid \psi_n\rangle \tag{30}$$

If H has an ω-fold degenerate eigenvalue, there will be ω values of the index n for which E_n is the same number, and the associated $\{\mid \psi_n\rangle\}$ will not be uniquely determined by (30). The constraint (28) therefore restricts the list of possible density operators to a set $\mathscr{D}_H$ defined as follows:

$$\mathscr{D}_H = \{\rho(\{w_n\}, \{\mid \psi_n\rangle\}) \mid \rho = \sum_n w_n \mid \psi_n\rangle\langle\psi_n \mid ; \quad w_n \geqslant 0, \quad \sum_n w_n = 1; \; \{\mid \psi_n\rangle\} \text{ a complete orthonormal set of } H\text{-eigenvectors}\} \tag{31}$$

Since all the complete orthonormal sets of H-eigenvectors are continuously related by unitary transformations in Hilbert space, and the possible $\{w_n\}$ obviously comprise a continuous set, we conclude that $\mathscr{D}_H$ is a continuous subset of $\mathscr{D}$. In the auxiliary space of quorum parameters $\{q_j\}$, there corresponds to $\mathscr{D}_H$ a subregion $\mathscr{D}_H'$ of $\mathscr{D}'$.

To obtain a quorum parametrization well suited to the strong equilibrium case, we recall that the significance of the points $\{q_j\}$ lies in the fact that they correspond uniquely to density operators, so that knowing $\{q_j\}$ is tantamount to knowing ρ. Another set of mathematical objects that will uniquely determine ρ is indicated in the spectral expansion— the eigenvalues $\{w_n\}$ and the orthogonal projectors $\{\mid \psi_n\rangle\langle\psi_n \mid\}$. It follows that there must be a one-to-one mapping between the ordinary quorum parameters $\{q_j\}$ and the double set $\{w_n\}$, $\{\mid \psi_n\rangle\langle\psi_n \mid\}$. For an N-dimensional Hilbert space, there are N^2 elements in $\{q_j\}$ and N elements in $\{w_n\}$. Thus if we adopt the $\{w_n\}$ themselves as coordinates for the space $\mathscr{L}'$, we shall need an additional $N^2 - N$ new coordinates $\{y_m\}$ in order to have a complete coordinate transformation:

$$q_j = q_j(\{w_n\}, \{y_m\}); \qquad w_n = w_n(\{q_j\}), \quad y_m = y_m(\{q_j\}) \tag{32}$$

To each point in $\mathscr{L}'$ with coordinates $(\{w_n\}, \{y_m\})$ there corresponds a unique Hermitian operator with eigenvalues $\{w_n\}$ and eigenvectors determined by a mapping from the $\{y_m\}$ to a set of orthogonal projections: $\{y_m\} \rightarrow$

$\{| \psi_n\rangle\langle\psi_n |\}$. Among the conceivable values of the coordinates $\{w_n\}$, there is a set $\mathscr{N}$ defined as follows:

$$\mathscr{N} \equiv \left\{\{w_n\} \mid w_n \geqslant 0, \quad \sum_{n=1}^{N} w_n = 1\right\} \tag{33}$$

In terms of the coordinates $(\{w_n\}, \{y_m\})$, the region $\mathscr{D}'$ is defined by

$$\mathscr{D}' \equiv \{(\{w_n\}, \{y_m\}) \mid \{w_n\} \in \mathscr{N}\} \tag{34}$$

Among the possible values of the coordinates $\{y_m\}$, there is a set $\mathscr{Y}_H$ containing all sets $\{y_m\}$ that correspond to H-eigenvectors:

$$\mathscr{Y}_H \equiv \{\{y_m\} \mid \{y_m\} \to \{| \psi_n\rangle\langle\psi_n |\}, \quad H \mid \psi_n\rangle = E_n \mid \psi_n\rangle\} \tag{35}$$

The subregion $\mathscr{D}_H'$ of interest in the strong equilibrium case may now be defined by

$$\mathscr{D}_H' = \{(\{w_n\}, \{y_m\}) \mid \{w_n\} \in \mathscr{N}, \quad \{y_m\} \in \mathscr{Y}_H\} \tag{36}$$

In general, the set $\mathscr{Y}_H$ will be of lesser dimensionality than the set of all points $\{y_m\}$. If H is totally nondegenerate, the set $\mathscr{Y}_H$ contains only the one element that corresponds to the unique set of projectors $\{| \psi_n\rangle\langle\psi_n |\}$. At the opposite extreme, if H were totally degenerate, it would commute with the identity, and $\mathscr{Y}_H$ would contain every point $\{y_m\}$, since any set $\{| \psi_n\rangle\langle\psi_n |\}$ could serve as projectors in the spectral expansion of H. In intermediate cases, where H has distinct but degenerate eigenvalues, $\mathscr{Y}_H$ has a dimensionality between these extremes. It will be convenient to regard $\mathscr{Y}_H$ as a surface in the $\{y_m\}$ space described by parametric equations

$$y_m = y_m(\{z_k\}) \tag{37}$$

where the number of elements in $\{z_k\}$ is the dimensionality of $\mathscr{Y}_H$.

Mathematically, the maximization of I under the constraints of strong equilibrium differs only slightly from the weak equilibrium problem. To accommodate the new constraint (28), subjective probability zero must now be assigned to each ρ not contained in $\mathscr{D}_H$. We seek accordingly a subjective probability distribution defined only over $\mathscr{D}_H'$ In terms of the coordinates just defined, we immediately obtain as the distribution over $\mathscr{D}_H'$ that maximizes I

$$\hat{w}(\{w_n\}, \{z_k\}) = \frac{p(\{w_n\}, \{z_k\}) \exp[-\beta \overline{H}(\{w_n\}, \{z_k\})]}{R} \tag{38}$$

where, as before, (R, β) are uniquely determined as functions of (U, V). [Compare with Eqs. (9) and (6).] The best-guess density operator in the strong equilibrium case is therefore

$$\hat{\rho} = \left\{\int_{\mathscr{D}_H'} \prod_n dw_n \prod_k dz_k p(\{w_n\}, \{z_k\})\{\exp[-\beta \overline{H}(\{w_n\}, \{z_k\})]\} \rho(\{w_n\}, \{z_k\})\right\}$$
$$\times \left\{\int_{\mathscr{D}_H'} \prod_n dw_n \prod_k dz_k\, p(\{w_n\}, \{z_k\}) \exp[-\beta \overline{H}(\{w_n\}, \{z_k\})]\right\}^{-1} \tag{39}$$

All of the analysis leading to identification of statistical analogs for thermodynamic parameters may be taken over directly from the weak equilibrium case. It is not yet clear, however, that replacement of weak by strong equilibrium has been a fruitful exercise; superficially, (39) looks as intractable as the weak equilibrium result (11). In particular, the prior distribution remains unspecified.

Nevertheless there is a major simplification inherent in the fact the integrals in (39) are only over $\mathscr{D}_H'$. Consider the quantity

$$\overline{H}(\{w_n\}, \{z_k\}) = \mathrm{Tr}[\rho(\{w_n\}, \{z_k\})\, H] \tag{40}$$

The density operator $\rho(\{w_n\}, \{z_k\})$ has eigenvalues $\{w_n\}$ and associated projectors $\{|\psi_n\rangle\langle\psi_n|\}$ determined by the $\{z_k\}$, which locate points in $\mathscr{Y}_H$. It is convenient to adopt a systematic convention, already implicit above, for the index n. Let the eigenvalues of H be arranged in an increasing monotone sequence $\{E_n\}$ which repeats each numerical E value as many times as its degree of degeneracy. Then, whenever a point $\{y_m\}$ lies in $\mathscr{Y}_H$ and thus determines a set of projectors $\{|\psi_n\rangle\langle\psi_n|\}$ onto H-eigenvectors, the index n of $|\psi_n\rangle$ is assigned so as to be the same as that of the corresponding eigenvalue E_n. Note that the multiple entries in the sequence $\{E_n\}$ assure a distinct index for each ψ_n in a degenerate eigenspace. The eigenvalues $\{w_n\}$ are similarly indexed with reference to the master list $\{E_n\}$.

With these indicial conventions, it is easy to see that (40) is actually independent of $\{z_k\}$. Consider the equation

$$Tr[\rho(\{w_n\}, \{z_k\})\, H] = \sum_n w_n\langle\psi_n, H\psi_n\rangle \tag{41}$$

For each value of n, different points $\{z_k\}$ of $\mathscr{Y}_H$ do yield different vectors to called ψ_n, but *all of them belong to the eigenspace of the same energy E_n*. Thus we have

$$\sum_n w_n\langle\psi_n, H\psi_n\rangle = \sum_n w_n E_n \tag{42}$$

and hence

$$\bar{H}(\{w_n\}, \{z_k\}) = \sum_n w_n E_n = \bar{H}\{w_n\} \tag{43}$$

an expression independent of $\{z_k\}$.

Now let us suppose for the sake of argument that the unknown prior distribution could be factored as follows:

$$p(\{w_n\}, \{z_k\}) = p_w\{w_n\}\, p_z\{z_k\} \tag{44}$$

In probability theory, Eq. (44) asserts of course that the eigenvalue spectrum of ρ is uncorrelated with its eigenvector set. We defer to the next part of this work any attempt to justify this proposed stochastic independence.

If (44) were accepted, the best-guess formula (39) would then reduce to a simpler form. Let $(|\,\psi_n\rangle\langle\psi_n\,|; \{z_k\})$ denote the nth projector $|\,\psi_n\rangle\langle\psi_n\,|$ of the set of projectors corresponding to the $\mathscr{Y}_H$ point $\{z_k\}$, so that

$$\rho(\{w_n\}, \{z_k\}) = \sum_l w_l(|\,\psi_l\rangle\langle\psi_l\,|\,; \{z_k\}) \tag{45}$$

Combining (31), (39), and (43)–(45), we obtain finally the following expression for the strong equilibrium best guess:

$$\hat{\rho} = \sum_l \left[\int_{\mathscr{Y}_H} p_z\{z_k\}(|\,\psi_l\rangle\langle\psi_l\,|\,; \{z_k\}) \prod_k dz_k\right] \times \frac{\int_{\mathscr{N}} w_l p_w\{w_n\} \prod_n \exp(-\beta w_n E_n)\, dw_n}{\int_{\mathscr{N}} p_w\{w_n\} \prod_n \exp(-\beta w_n E_n)\, dw_n} \tag{46}$$

In Part II we show how these integrals can be converted to discrete sums and evaluated by the saddle point method.

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