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Thermodynamical Proof of the Gibbs Formula for Elementary Quantum Systems

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An elementary derivation is given of the formula for the thermal equilibrium states of quantum systems that can be described in finite-dimensional Hilbert spaces. The three assumptions made, Passivity, Structural Stability, and Consistency, have phenomenological interpretations. Except at zero temperature, Structural Stability follows already from Passivity and a weak form of Consistency.

KEY WORDS: Statistical mechanics; thermal equilibrium; Gibbs states.

1. INTRODUCTION

The basic formula of equilibrium statistical mechanics is

$$\rho = (1/Z)e^{-\beta H} \tag{1}$$

where β and Z are constants. It may of course be regarded as an axiom, but various justifications of it can be given. Such justifications are a standard feature of the textbook literature, indeed they go back to the creator of statistical mechanics, J. Willard Gibbs.[(1)] In recent years a number of attempts have been made to derive the nature of thermal equilibrium states from phenomenologically motivated postulates, using standards of rigor typical of modern mathematical physics. A characteristic feature of this literature[2] is the consideration of systems with infinitely many degrees of freedom. This is justified on the ground that thermodynamics deals with spatially homogeneous properties of physical objects, and that can be modelled only with mechanical systems that have infinitely many degrees of freedom. In this view, finite systems are only approximations from which the true models arise by limiting processes. While this attitude is philosophically cogent, and has even

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[2] For a review see, for instance, Ref. 2.

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mathematical advantages, there can be no doubt that the necessary mathematics is quite technical. For this reason alone, it would seem justified to give a rigorous derivation of the Gibbsian formula (1) from first principles, using only mathematics familiar to the average theoretical physicist.

This will be done in the following, starting from three principles, to be called Passivity, Structural Stability, and Consistency. The first of these, introduced in a recent interesting paper by Pusz and Woronowicz,[3] can be thought of as a form of the Second Law of Thermodynamics: No work can be obtained from an adiabatically isolated system in thermal equilibrium by varying external parameters. This defines the concept of a passive (statistical) state. By structural stability is meant, roughly speaking, that if the parameters of the system are slightly varied, then the altered system still has a passive state close to the passive state of the original one. The third principle has to do with the qualitative idea of equality of temperature, what is sometimes called the Zeroth Law of Thermodynamics. Consistency requires that one should be able to assign to every system a structurally stable passive state in such a manner that the state assigned to a composite system is the product of the states assigned to the components.

Of course these principles can be mathematically implemented only if one makes a precise definition of what is meant by a "system." To eliminate altogether the need for technicalities (unbounded operators, C^*-algebras, etc.) we restrict ourselves to quantum systems that can be described in a *finite*-dimensional Hilbert space. From a mathematical point of view, a "system" will be therefore a pair $(\mathscr{H}, H)$, where $\mathscr{H}$ is a finite-dimensional complex Hilbert space and H is a self-adjoint operator acting in $\mathscr{H}$. A state of such a system is specified, in the well-known manner, by a positive operator ρ of trace 1.

In the sections to follow we answer successively the questions: When is ρ passive? When is ρ structurally stable? When does ρ belong to a consistent family of states? The final answer is easily stated: Precisely when ρ is of the form (1) with $0 \leqslant \beta \leqslant \infty$.

2. PASSIVE STATES

Let $(\mathscr{H}, H)$ be any system, $\dim(\mathscr{H}) < \infty$, H a self-adjoint operator acting in $\mathscr{H}$. By a time-limited perturbation K of H we mean a function on the real line whose values are self-adjoint operators $K(t)$ acting in $\mathscr{H}$, subject to two conditions. First, K is of class $\mathscr{C}^1$ (has a continuous derivative with respect to t), and, second, $K(t) = H$ for all $t \leqslant 0$ and $t \geqslant 1$. If $K(t)$ is regarded as a time-dependent Hamiltonian, a state of the system evolves in time according to the differential equation

$$i\, d\rho(t)/dt = [K(t), \rho(t)] \tag{2}$$

where, as usual, $[A, B] = AB - BA$. The total work done by the perturbation on the system (to be precise, the expectation value of the total work) is

$$W(K, \rho_0) = \int_0^1 \operatorname{Tr} \rho(t) \frac{dK(t)}{dt}\, dt \tag{3}$$

where $\rho_0 = \rho(0)$. A state ρ_0 of the system $(\mathscr{H}, H)$ is called *passive* if $W(K, \rho_0) \geqslant 0$ for all time-limited perturbations K. This definition is due to Pusz and Woronowicz.[(3)]

Given a time-limited perturbation K, we associate with it a function U defined on the real axis as follows. $U(t)$ is the solution of the differential equation

$$i\, dU(t)/dt = e^{itH} K(t) e^{-itH} U(t) - HU(t) \tag{4}$$

which satisfies $U(0) = 1$. Now U is of class $\mathscr{C}^2$, $U(t)$ is unitary for all t, $U(t) = 1$ for $t \leqslant 0$, $U(t) = U_1$ is constant for $t \geqslant 1$. When K is expressed in terms of U,

$$K(t) = H + ie^{-itH} \frac{dU(t)}{dt} U^*(t) e^{itH} \tag{5}$$

it is seen that from the listed properties of U it follows that K is a time-limited perturbation of H. An elementary calculation shows that the solution of (2) subject to $\rho(0) = \rho_0$ is given by

$$\rho(t) = e^{-itH} U(t) \rho_0 U^*(t) e^{itH} \tag{6}$$

One consequence of this is the identity $\operatorname{Tr}[\rho(1)K(1)] = \operatorname{Tr}(\rho_0 U_1{}^* H U_1)$, so that integration by parts in (3) yields

$$W(K, \rho_0) = \operatorname{Tr}(\rho_0 U_1{}^* H U_1) - \operatorname{Tr}(\rho_0 H) \tag{7}$$

This shows that W depends on the function K only through U_1, which must of course be regarded as a functional of K.

Theorem 1.[3] A state ρ_0 for the system $(\mathscr{H}, H)$ is passive if and only if $\operatorname{Tr}(\rho_0 U_1{}^* H U_1) \geqslant \operatorname{Tr}(\rho_0 H)$ for all unitary operators U_1 acting in $\mathscr{H}$.

Proof. It is obvious from (7) that the condition is sufficient for passivity. To show its necessity, let ρ_0 be a passive state and U_1 any unitary operator. Let $U(t)$ be obtained from U_1 by retaining its eigenvectors and replacing each of its eigenvalues, say $e^{i\theta}$, by $e^{if(t)\theta}$, where f is a function of class $\mathscr{C}^2$ such that $f(t) = 0$ for $t \leqslant 0$, $f(t) = 1$ for $t \geqslant 1$. Then define K by (5). This implies that (7) holds, whence the required inequality. QED

[3] This is just Theorem 2.1 of Ref. 3, expressed in the language of elementary quantum mechanics.

Given two self-adjoint operators A and B acting in the finite-dimensional Hilbert space $\mathscr{H}$, when is it true that the function $U \to \mathrm{Tr}(AU^*BU)$, defined over the set of unitary U, assumes its minimum at $U = 1$?

Theorem 2. Let $\dim(\mathscr{H}) < \infty$, A and B self-adjoint. Then $U \to \mathrm{Tr}(AU^*BU)$ is a minimum with respect to unitary U at $U = 1$ if and only if $\mathscr{H}$ contains an orthonormal basis of common eigenvectors for A and B and the eigenvalues α_j of A and β_j of B satisfy $(\alpha_j - \alpha_k)(\beta_j - \beta_k) \leqslant 0$ for all j and k.

Proof. Let A and B have common eigenvectors, and U be an arbitrary unitary operator acting in $\mathscr{H}$. Let the matrix of U with respect to the eigenvector basis be (u_{jk}). Then

$$\mathrm{Tr}(AU^*BU) = \sum_j \sum_k \alpha_j \beta_k |u_{jk}|^2 \tag{8}$$

The matrix $(|u_{jk}|^2)$ is doubly stochastic (nonnegative entries, row and column sums equal 1). Doubly stochastic square matrices of a given size from a convex set whose extremal elements are the permutation matrices.[4] Therefore

$$\mathrm{Tr}(AU^*BU) = \sum_\pi c_\pi \sum_j \alpha_j \beta_{\pi(j)} \tag{9}$$

for suitable $c_\pi \geqslant 0$, $\sum_\pi c_\pi = 1$, where π runs over the permutations of $1, 2,..., n = \dim(\mathscr{H})$. If we assume that $\alpha_j < \alpha_k$ implies $\beta_j \geqslant \beta_k$, then[5]

$$\sum_j \alpha_j \beta_{\pi(j)} \geqslant \sum_j \alpha_j \beta_j = \mathrm{Tr}(AB) \tag{10}$$

for all π, as was to be shown. Conversely, assume that the minimum occurs at $U = 1$. In the neighborhood of 1, U can be parametrized as a power series

$$U = 1 + 2M + 2M^2 + 2M^3 + \cdots \tag{11}$$

where $M^* = -M$ and $\|M\| < 1$. Thus

$$\mathrm{Tr}(AU^*BU) = \mathrm{Tr}(AB) + 2\,\mathrm{Tr}([A, B]M) + O(\|M\|^2) \tag{12}$$

whence it follows that $\mathrm{Tr}[A, B]M = 0$ for all skew-adjoint (and therefore all) M. This means $[A, B] = 0$, so that A and B can be simultaneously diagonalized. Let U_θ be the one-parameter family of unitary operators acting as the matrix

$$\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

in the subspace of the two joint eigenvectors of A and B corresponding to the eigenvalues α_j and α_k of A, β_j and β_k of B, and the identity in the orthogonal complement. Then

$$\mathrm{Tr}(AU_\theta{}^*BU_\theta) - \mathrm{Tr}(AB) = -(\alpha_j - \alpha_k)(\beta_j - \beta_k)\sin^2\theta \tag{13}$$

and this has a minimum at $\theta = 0$ only if $(\alpha_j - \alpha_k)(\beta_j - \beta_k) \leqslant 0$. QED

The first part of our analysis is complete: *A state ρ for the system $(\mathscr{H}, H)$ is passive if and only if ρ and H commute and their simultaneous corresponding eigenvalues, ϵ_j of H and λ_j of ρ, have the property that $\epsilon_j < \epsilon_k$ implies $\lambda_j \geqslant \lambda_k$.*

3. STRUCTURAL STABILITY

A passive state ρ_0 of the system $(\mathscr{H}, H_0)$ will be called *structurally stable* if, given any neighborhood $\mathscr{N}$ of ρ_0, no matter how small, there is some neighborhood $\mathscr{M}$ of H_0 such that for every $H \in \mathscr{M}$ there is at least one state $\rho \in \mathscr{N}$ which is passive for the system $(\mathscr{H}, H)$. Roughly speaking, a small change in the Hamiltonian allows a small change in the state without destroying its passivity. The relevance of a condition like this for determining the nature of a thermal equilibrium state was emphasized by Haag and coworkers.[6]

Theorem 3. A passive state ρ_0 for the system $(\mathscr{H}, H_0)$ is structurally stable if and only if there is a nonincreasing function f defined on the spectrum of H_0 such that $\rho_0 = f(H_0)$.

If $\epsilon_j{}^0$ and $\lambda_j{}^0$ are the respective eigenvalues of H_0 and ρ_0, passivity of ρ_0 demands that $\epsilon_j{}^0 < \epsilon_k{}^0$ implies $\lambda_j{}^0 \geqslant \lambda_k{}^0$. The stronger condition of structural stability demands that, in addition, $\epsilon_j{}^0 = \epsilon_k{}^0$ implies $\lambda_j{}^0 = \lambda_k{}^0$.

Proof of Theorem 3. Suppose that a function f with the stated properties exists. It can be extended to a continuous, nonincreasing, nonnegative function on the whole real line. Since $\mathrm{Tr}\, f(H_0) = 1$, clearly $f(x) > 0$ for sufficiently large, negative x. Let

$$F(H) = \frac{1}{\mathrm{Tr}\, f(H)} f(H) \tag{14}$$

be defined as a continuous function on the set of those self-adjoint operators H for which $\mathrm{Tr}\, f(H) > 0$. For every H in this set, $F(H)$ is a state, and $F(H_0) = \rho_0$. Let $\mathscr{N}$ be any neighborhood of ρ_0, and let $\mathscr{M}$ be the complete inverse image $F^{-1}(\mathscr{N})$ of this neighborhood under F. This $\mathscr{M}$ is an open set because F is continuous, and $H_0 \in \mathscr{M}$. Let $H \in \mathscr{M}$; then $F(H) = \rho \in \mathscr{N}$. Since f is nonincreasing $\epsilon_j < \epsilon_k$ implies $\lambda_j \geqslant \lambda_k$ for the eigenvalues of H and ρ, respectively. Therefore ρ is a passive state for the system $(\mathscr{H}, H)$. This shows that ρ_0 is structurally stable.

To prove the converse, let ρ_0 be a passive state for the system $(\mathscr{H}, H_0)$, but suppose no function f with the required properties exists. Then there are two eigenvalues $\epsilon_1{}^0$ and $\epsilon_2{}^0$ of H_0, corresponding to eigenvectors ψ_1 and ψ_2, such that $\epsilon_1{}^0 = \epsilon_2{}^0$, but the corresponding eigenvalues of ρ_0 are unequal, say $\lambda_1{}^0 < \lambda_2{}^0$. Let $\mathscr{N}$ be the open set in the space of states defined by the inequality

$$(\psi_1, \rho\psi_1) < (\psi_2, \rho\psi_1) \tag{15}$$

Evidently $\rho_0 \in \mathscr{N}$. Let $\mathscr{M}$ be any neighborhood of H_0. Choose an $H \in \mathscr{M}$ that has distinct eigenvalues and shares its eigenvectors with H_0 and ρ_0, and moreover its eigenvalues corresponding to ψ_1 and ψ_2 satisfy $\epsilon_1 < \epsilon_2$. Let ρ be any passive state for the system $(\mathscr{H}, H)$. Then its eigenvalues corresponding to ψ_1 and ψ_2 must satisfy $\lambda_1 \geqslant \lambda_2$. This shows that $\rho \notin \mathscr{N}$, and therefore ρ_0 is not structurally stable. QED

4. CONSISTENCY AND THERMAL EQUILIBRIUM STATES

The above analysis depends on properties of systems that can be formulated by considering each system in isolation by itself. That such an analysis cannot lead to the Gibbsian formula (1) for thermal equilibrium states is not surprising, since the essence of the thermal equilibrium phenomenon is the notion of temperature, and that is connected with the so-called Zeroth Law of Thermodynamics, involving as it does, systems in "thermal contact." To say that a particular system is in thermal equilibrium, by itself, is meaningless unless one imagines that all other systems have suitable states with which the given system can be compounded without any observable changes resulting. Strictly speaking, thermal contact will cause a slight adjustment of the state of the two systems brought together, but this is a small boundary effect that can be neglected. These informal remarks motivate the following definitions.

A consistent family R of structurally stable passive states (briefly, a consistent family) is a function defined on the class $\mathscr{S}$ of all systems $(\mathscr{H}, H)$ under consideration such that $\rho = R(\mathscr{H}, H)$ is a structurally stable, passive state for the system $(\mathscr{H}, H) \in \mathscr{S}$, and such that for any two systems $(\mathscr{H}, H)$ and $(\mathscr{H}', H')$ in $\mathscr{S}$ the identity

$$R(\mathscr{H} \otimes \mathscr{H}', H \otimes 1' + 1 \otimes H') = R(\mathscr{H}, H) \otimes R(\mathscr{H}', H') \tag{16}$$

holds. The system $(\mathscr{H} \otimes \mathscr{H}', H \otimes 1' + 1 \otimes H')$ represents the compound of the two given systems, "interaction neglected." This neglect is conceptually justified by insisting that all states in the range of R are structurally stable. The consistent family R is our mathematical model for the notion of equality of temperature. It is entirely qualitative, as is the temperature notion in thermodynamics.

A state ρ_0 for a system $(\mathscr{H}_0, H_0)$ will be called a *thermal equilibrium state* if a consistent family R exists such that $\rho_0 = R(\mathscr{H}_0, H_0)$.

The mathematically minded reader may be inclined perhaps to worry about the obscurity of $\mathscr{S}$, the class of "all" systems. To be precise here, one should take $\mathscr{S}$ to mean any indexed set of systems $\{(\mathscr{H}, H_\alpha): \alpha \in A\}$ where the index set A is really irrelevant as long as it is large enough. We only insist on two requirements. First, for any two systems belonging to $\mathscr{S}$, their compound (tensor product Hilbert space, Hamiltonians added) also belongs to $\mathscr{S}$. Second, given any spectrum, that is, a nonempty, finite set of real numbers with finite multiplicities, there is at least one system belonging to $\mathscr{S}$ whose Hamiltonian has the given spectrum. Otherwise the reader may fancy A to be as large as he pleases.

If two systems have Hilbert spaces of the same dimension and the spectra of their Hamiltonians differ only by an additive constant, we should regard them as having identical properties (from the present point of view). We call them *equivalent*. If $(\mathscr{H}, H)$ and $(\mathscr{H}', H')$ are equivalent systems, a unitary operator $U: \mathscr{H} \to \mathscr{H}'$ exists, and a real number c, such that $H' = UHU^* + c1'$.

Theorem 4. Let $(\mathscr{H}, H)$ and $(\mathscr{H}', H')$ be equivalent systems, U the unitary operator as above. If ρ and ρ' are structurally stable, passive states for the respective systems such that the product state $\rho \otimes \rho'$ is a structurally stable, passive state for the compound system, then $\rho' = U\rho U^*$.

Proof. Let ϵ_j and λ_j be the corresponding eigenvalues of H and ρ, respectively, and $\epsilon_j' = \epsilon_j + c$ and λ_j' the corresponding eigenvalues of H' and ρ'. The eigenvalues of the compound Hamiltonian are the $\epsilon_j + \epsilon_k + c$, the corresponding eigenvalues of the product state the $\lambda_j\lambda_k'$. By assumption, $\epsilon_j + \epsilon_k \leqslant \epsilon_l + \epsilon_m$ implies $\lambda_j\lambda_k' \geqslant \lambda_l\lambda_m'$. ρ has at least one positive eigenvalue, say λ_1. Taking $k = l = 1$, we see that $\epsilon_j \leqslant \epsilon_m$ implies $\lambda_j\lambda_1' \geqslant \lambda_1\lambda_m'$, in particular $\lambda_j\lambda_1' \geqslant \lambda_1\lambda_j'$ for all j. Summing over j, one obtains $\lambda_1' \geqslant \lambda_1$. Now take $j = m = 1$; this shows that $\epsilon_k \leqslant \epsilon_l$ implies $\lambda_1\lambda_k' \geqslant \lambda_l\lambda_1'$, in particular $\lambda_1\lambda_k' \geqslant \lambda_k\lambda_1'$ for all k. Summing over k, one obtains $\lambda_1 \geqslant \lambda_1'$; thus $\lambda_1 = \lambda_1' > 0$. But then $\lambda_j' = \lambda_j$ follows for all j. QED

This theorem shows an important property of any consistent family R, namely that the spectrum of H (regarded modulo an additive constant) completely determines the spectrum of $\rho = R(\mathscr{H}, H)$; thus for equivalent systems the functions f that figure in Theorem 3 are all the same. The spectrum of a system $(\mathscr{H}, H)$ with $\dim(\mathscr{H}) = 2$ is determined (up to an irrelevant additive constant) by a single number $x \geqslant 0$, say $\epsilon_1 = 0$, $\epsilon_2 = x$. The spectrum $\{\lambda_1, \lambda_2\}$ of the state $\rho = R(\mathscr{H}, H)$ is then completely determined by x; we write

$$\lambda_2/\lambda_1 = \phi(x) \tag{17}$$

Evidently $0 \leqslant \phi(x) \leqslant 1$, $\phi(0) = 1$. But it is also easy to see that ϕ is *nonincreasing*. Indeed, consider the compound of two systems with two-dimensional Hilbert spaces, with energy spectra, say, $\{0, x\}$ and $\{0, x'\}$. The spectrum of the compound system is $\{0, x, x', x + x'\}$, while the spectrum of the state assigned to it by R has spectrum $\{\lambda_1\lambda_1', \lambda_2\lambda_1', \lambda_1\lambda_2', \lambda_2\lambda_2'\}$ in obvious notation. The condition of its passivity yields that $x < x'$ implies $\lambda_2\lambda_1' \geqslant \lambda_1\lambda_2'$, which means $\phi(x) \geqslant \phi(x')$.

We are now ready to prove the Gibbs formula (1).

Theorem 5. Suppose ρ_0 is a thermal equilibrium state for the system $(\mathscr{H}_0, H_0)$. Then there are three possibilities. (I) ρ_0 is a multiple of the projection operator corresponding to the smallest eigenvalue of H_0. (II) There is a positive number β such that ρ_0 is a multiple of $\exp(-\beta H_0)$. (III) ρ_0 is a multiple of the identity operator 1.

Proof. By definition, there is a consistent family R such that $\rho_0 = R(\mathscr{H}_0, H_0)$. Let ϕ be the function constructed from R as above. Let $(\mathscr{H}, H)$ be an arbitrary system in the class $\mathscr{S}$; ϵ_j the eigenvalues of H; and λ_j the corresponding eigenvalues of $\rho = R(\mathscr{H}, H)$. Let $(\mathscr{H}_x, H_x)$ be a system with $\dim(H_x) = 2$ and the eigenvalues of H_x be 0 and x, where x is an arbitrarily chosen nonnegative number. The eigenvalues of $\rho_x = R(\mathscr{H}_x, H_x)$ are then in the ratio 1 to $\phi(x)$. The eigenvalues of the Hamiltonian for the compound of these two systems are the numbers ϵ_j and $\epsilon_j + x$. The state $\rho \otimes \rho_x$ assigned to it by R must be passive and structurally stable. Therefore $\epsilon_j + x \leqslant \epsilon_k$ implies $\lambda_j\phi(x) \geqslant \lambda_k$, while $\epsilon_j + x \geqslant \epsilon_k$ implies $\lambda_j\phi(x) \leqslant \lambda_k$. Choose $x = \epsilon_k - \epsilon_j$; it follows that

$$\lambda_k = \lambda_j\phi(\epsilon_k - \epsilon_j) \tag{18}$$

This is true for all k and j such that $\epsilon_k \geqslant \epsilon_j$. Now let $x, y \geqslant 0$ be arbitrary, and choose $(\mathscr{H}, H)$ so that $\epsilon_1 - \epsilon_2 = x$, $\epsilon_2 - \epsilon_3 = y$. Then from (18) we obtain

$$\phi(x)\phi(y) = \phi(x + y) \tag{19}$$

valid for all $x, y \geqslant 0$. There are now three possibilities.[4]

(I) $\phi(x) = 0$ for all $x > 0$. In this case, for any system $(\mathscr{H}, H)$ in $\mathscr{S}$ whose Hamiltonian has the eigenvalues $\epsilon_1 = \epsilon_2 = \cdots = \epsilon_k < \epsilon_{k+1} \leqslant \epsilon_{k+2} \leqslant \cdots \leqslant \epsilon_n$, the state $\rho = R(\mathscr{H}, H)$ has the eigenvalues $\lambda_1 = \lambda_2 = \cdots = \lambda_k = k^{-1}$, $\lambda_{k+1} = \cdots = \lambda_n = 0$. Physically, this is the case of zero temperature.

(II) ϕ is a nontrivial exponential function. Since it is nonincreasing it must have the form $\exp(-\beta x)$ with some $\beta > 0$. In this case $\lambda_k = Z^{-1}\exp(-\beta\epsilon_k)$ for all k and for all systems $(\mathscr{H}, H)$ in $\mathscr{S}$. Physically, this is the case of positive temperature.

[4] This follows from a theorem of Darboux.[7]

(III) $\phi(x) = 1$ for all $x \geqslant 0$. In this case $\lambda_1 = \lambda_2 = \cdots = \lambda_n = n^{-1}$, where $n = \dim(\mathscr{H})$, for all systems $(\mathscr{H}, H)$ in $\mathscr{S}$. Physically, this is the case of infinite temperature.

The proof is complete.

5. COMPLETE PASSIVITY

From the point of view of physics it is satisfactory that the nature or those statistical states that are intended models of thermal equilibrium can be derived rigorously from three natural postulates, rather than assumed as an axiom of statistical mechanics to be justified only *a posteriori* by its empirical success. It is the more remarkable that considerably less than our three postulates suffice—with one small reservation—for the derivation of the Gibbs formula. Except in the zero-temperature case, structural stability can be abandoned as a postulate. It can be proved as a theorem from the hypotheses of passivity and consistency. But even consistency can be replaced by a much weaker requirement, essentially the weakest possible one that makes sense. For a given system $(\mathscr{H}, H)$ it is enough to consider the class $\mathscr{S}_0$ of systems generated by it under the operation of forming compounds, and all that is required for a passive state ρ is to belong to a consistent family of states over the class $\mathscr{S}_0$. Systems belonging to this class are simply compounds made up out of a finite (but arbitrarily large) number of copies of $(\mathscr{H}, H)$. The required property is called *complete passivity*;[3] formally stated, ρ is a completely passive state for the system $(\mathscr{H}, H)$ if for all positive integers ν the state $\rho \otimes \rho \otimes \cdots \otimes \rho$ (ν factors) is a passive state for the system obtained by compounding ν copies of $(\mathscr{H}, H)$.

A criterion for complete passivity follows from the passivity criterion of Section 2. A state ρ for $(\mathscr{H}, H)$ is completely passive if and only if ρ commutes with H, and for nonnegative integers a_j and b_j

$$\sum a_j = \sum b_j \tag{20}$$

and

$$\sum a_j \epsilon_j < \sum b_j \epsilon_j \tag{21}$$

imply

$$\prod \lambda_j^{a_j} \geqslant \prod \lambda_j^{b_j} \tag{22}$$

where the ϵ_j and λ_j are the corresponding eigenvalues of H and ρ, respectively, and 0^0 is interpreted as 1 in (22).

To handle the zero-temperature case correctly, we need a definition. A state ρ_0 for the system $(\mathscr{H}, H)$ is called a *ground state* if $\mathrm{Tr}(\rho_0 H) \leqslant \mathrm{Tr}(\rho H)$

for all states ρ. If $\mathscr{H}$ is written as a direct sum $\mathscr{H}' \oplus \mathscr{H}''$ with respect to which H has the form

$$\begin{pmatrix} \epsilon_0 1' & 0 \\ 0 & H'' \end{pmatrix}$$

with all eigenvalues of H'' strictly larger than ϵ_0, then a ground state has the form

$$\rho_0 = \begin{pmatrix} \rho_0' & 0 \\ 0 & 0 \end{pmatrix}$$

Note that ρ_0' need not have equal eigenvalues, and if it does not, then ρ_0 is not structurally stable.

Theorem 6. A ground state is completely passive. A completely passive state that is not a ground state is structurally stable.

Proof. Let ρ be a ground state for $(\mathscr{H}, H)$; ϵ_j the eigenvalues of H; λ_j those of ρ; and ϵ_0 the smallest eigenvalue of H. By definition, $\lambda_j = 0$ when $\epsilon_j > \epsilon_0$. Conditions (20) and (21) can be satisfied only if $b_j > 0$, $\epsilon_j > \epsilon_0$, for at least one j. But then the right-hand side of (22) vanishes, so that (22) is trivially satisfied. This proves the first part of the theorem. Suppose now that ρ is a completely passive state but not a ground state. In view of Theorem 3 it must be shown that $\epsilon_j = \epsilon_k$ implies $\lambda_j = \lambda_k$. Let then $j \neq k$, $\epsilon_j = \epsilon_k$. Suppose $\epsilon_l < \epsilon_j = \epsilon_k$. Then, for any positive integer ν, $(\nu - 1)\epsilon_j + \epsilon_l < \nu\epsilon_k$, so that from (22), $\lambda_j^{\nu-1}\lambda_l \geqslant \lambda_k^{\nu}$. This shows $\lambda_k \leqslant \lambda_j$ and, since j and k can be interchanged, $\lambda_k = \lambda_j$. If $\epsilon_j = \epsilon_k$ is the smallest eigenvalue of H, there is necessarily another eigenvalue $\epsilon_l > \epsilon_j = \epsilon_k$ with the corresponding eigenvalue λ_l of ρ positive, since ρ is not a ground state. In this case $\nu\epsilon_k < (\nu-1)\epsilon_j + \epsilon_l$ yields $\lambda_k^{\nu} \geqslant \lambda_j^{\nu-1}\lambda_l$, whence $\lambda_j \leqslant \lambda_k$ and therefore, as before, $\lambda_j = \lambda_k$.

Theorem 7. A completely passive state is either a ground state or a thermal equilibrium state.[5]

Proof. Let ρ be a completely passive state for the system $(\mathscr{H}, H)$; λ_j the eigenvalues of ρ; ϵ_j the corresponding eigenvalues of H; and assume ρ is not a ground state. The eigenvalue λ_0 of ρ corresponding to the smallest eigenvalue ϵ_0 of H is positive, and there is at least one other positive eigenvalue λ_k of ρ corresponding to $\epsilon_k > \epsilon_0$ (since otherwise ρ would be a ground state). If H has only two distinct eigenvalues, then the formula $\rho = f(H)$ demanded by Theorems 6 and 3 can always be written in the form (1) with a uniquely determined $\beta \geqslant 0$ and $Z > 0$, so that the conclusion of the theorem holds in this case. We assume henceforth that H has at least three distinct eigenvalues. Let ϵ_j be a third eigenvalue of H, and assume $\epsilon_0 < \epsilon_j < \epsilon_k$. Then

[5] This is Theorem 1.4 of Pusz and Woronowitz,[3] restricted to the systems considered here.

$\epsilon_0 + \epsilon_j < 2\epsilon_k$ shows $\lambda_0\lambda_j \geqslant \lambda_k^2 > 0$, whence $\lambda_j > 0$. Next, assume $\epsilon_j > \epsilon_k$. Then $\epsilon_j + (\nu - 1)\epsilon_0 < \nu\epsilon_k$ for sufficiently large ν, and this shows $\lambda_j\lambda_0^{\nu-1} \geqslant \lambda_k^{\nu} > 0$, whence $\lambda_j > 0$. Thus all eigenvalues of ρ are positive; ρ is a strictly positive operator.

Let us consider three distinct eigenvalues $\epsilon_1 < \epsilon_2 < \epsilon_3$ of H, assumed positive without essential loss of generality. Let δ be an arbitrarily small positive number and let a_1, a_2, a_3, and A be positive integers such that the rational numbers a_2/A, a_3/A, and a_1/A are approximations to ϵ_1, ϵ_2, and ϵ_3, respectively, within δ, and such that

$$\left(\epsilon_1 - \frac{a_2}{A}\right)(\epsilon_3 - \epsilon_2) + \left(\epsilon_2 - \frac{a_3}{A}\right)(\epsilon_1 - \epsilon_3) + \left(\epsilon_3 - \frac{a_1}{A}\right)(\epsilon_2 - \epsilon_1) > 0 \quad (23)$$

Let $b_1 = a_3$, $b_2 = a_1$, and $b_3 = a_2$, so that (23) may be rewritten

$$\sum_{1\leqslant j\leqslant 3} a_j\epsilon_j < \sum_{1\leqslant j\leqslant 3} b_j\epsilon_j \quad (24)$$

The complete passivity criterion (22) shows

$$\lambda_1^{\epsilon_3+r_3}\lambda_2^{\epsilon_1+r_1}\lambda_3^{\epsilon_2+r_2} \geqslant \lambda_1^{\epsilon_2+r_2}\lambda_2^{\epsilon_3+r_3}\lambda_3^{\epsilon_1+r_1} \quad (25)$$

where $r_1 = \epsilon_1 - a_2/A$, $r_2 = \epsilon_2 - a_3/A$, and $r_3 = \epsilon_3 - a_1/A$. Since the $|r_j| \leqslant \delta$ and δ is arbitrarily small,

$$\lambda_1^{\epsilon_3}\lambda_2^{\epsilon_1}\lambda_3^{\epsilon_2} \geqslant \lambda_1^{\epsilon_2}\lambda_2^{\epsilon_3}\lambda_3^{\epsilon_1} \quad (26)$$

If instead of (23), the opposite inequality had been assumed, the opposite of (26) would have resulted. This shows that

$$\lambda_1^{\epsilon_3}\lambda_2^{\epsilon_1}\lambda_3^{\epsilon_2} = \lambda_1^{\epsilon_2}\lambda_2^{\epsilon_3}\lambda_3^{\epsilon_1} \quad (27)$$

Since all $\lambda_j > 0$, this can also be written

$$\left(\frac{\lambda_1}{\lambda_2}\right)^{1/(\epsilon_2-\epsilon_1)} = \left(\frac{\lambda_2}{\lambda_3}\right)^{1/(\epsilon_3-\epsilon_2)} \quad (28)$$

This shows that for distinct eigenvalues $\epsilon_j < \epsilon_k$ of H and corresponding eigenvalues $\lambda_j \geqslant \lambda_k > 0$ of ρ the number

$$\left(\frac{\lambda_j}{\lambda_k}\right)^{1/(\epsilon_k-\epsilon_j)} \geqslant 1 \quad (29)$$

is independent of j and k. Denote it e^{β}, $\beta \geqslant 0$. The resulting equation shows that

$$\lambda_j e^{\beta\epsilon_j} = \lambda_k e^{\beta\epsilon_k} \quad (30)$$

Thus $\lambda_j e^{\beta\epsilon_j}$ is independent of j. This constant is called Z^{-1}, and the Gibbs formula

$$\lambda_j = (1/Z)e^{-\beta\epsilon_j} \quad (31)$$

is established. QED

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