Quantum Thermodynamics. A New Equation of Motion for a General Quantum System (*).

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Summary. — A novel nonlinear equation of motion is proposed for a general quantum system consisting of more than one distinguishable elementary constituent of matter. In the domain of idempotent quantum-mechanical state operators, it is satisfied by all unitary evolutions generated by the Schrödinger equation. But, in the broader domain of nonidempotent state operators not contemplated by conventional quantum mechanics, it generates a generally nonunitary evolution, it keeps the energy invariant and causes the entropy to increase with time until the system reaches a state of equilibrium or a limit cycle.

PACS. 03.65. – Quantum theory; quantum mechanics.

1. – Introduction.

This paper is a continuation of work published in this journal [1]. Its purpose is to present a novel nonlinear equation of motion for a general isolated quantum system consisting of two or more distinguishable elementary constituents of matter. The equation includes the description of irreversible conservative motion from any initial state to a thermodynamic equilibrium state.

(*) This work is based on part of a doctoral dissertation submitted by the first author to the Massachusetts Institute of Technology.
[1] G. P. BERETTA, E. P. GYFTOPOULOS, J. L. PARK and G. N. HATSOPOULOS: *Nuovo Cimento B*, **82**, 169 (1984).

The sciences of mechanics and thermodynamics developed quite independently of each other. They are both concerned with the description of properties and changes in properties of matter, but all their implications are not identical. For example, energy is a property of matter that has unified our understanding of physical phenomena. It appears prominently in both mechanics and thermodynamics and its conservation is a keystone of both microscopic and macroscopic phenomena. By contrast, entropy is not relevant to mechanics, while it holds a supreme position in thermodynamics.

The two sciences have enjoyed great successes both in regularizing innumerable physical observations and in generating far reaching and verifiable predictions, but in the hierarchy of physical theories they are usually placed on different levels. Mechanics is regarded as providing a complete and fundamental description of physical reality, whereas thermodynamics is considered as a statistical approximation to the complicated mechanical behaviour of large systems.

For longer than a century, generations of physicists have delved into the statistical interpretation of thermodynamics, but the results of this intensive inquiry remain inconclusive. For example, JANCEL ([2]) states: « Nevertheless, we cannot say that the problems raised by the foundations of statistical mechanics have thus far received a definitive solution; quite the contrary, the numerous points which remain to be explained or defined more precisely can give birth to interesting projects ».

An alternative that has received limited attention is that perhaps thermodynamics is not a statistical theory. HATSOPOULOS and GYFTOPOULOS ([3]) pursued this alternative. They proposed a unified quantum theory which, within a single structure, encompasses both mechanics and thermodynamics and which presumes that, in the hierarchy of physical principles, the second law of thermodynamics deserves a position on the same level as the great conservation laws and the fundamental postulates of quantum mechanics. Their unified theory applies to all individual states, equilibrium and nonequilibrium, of all physical systems, composite and simple, large and small, macroscopic and microscopic.

A fundamental hypothesis of the theory is that every single strictly isolated (*i.e.* uncorrelated and noninteracting) system can exist not only in an individual state described by a quantum-mechanical one-dimensional orthogonal projection operator P ([4]), but also in an individual state described by a nonidempotent

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([2]) R. JANCEL: *Foundations of Classical and Quantum Statistical Mechanics* (Pergamon Press, Oxford, 1969).

([3]) G. N. HATSOPOULOS and E. P. GYFTOPOULOS: *Found. Phys.*, **6**, 15, 127, 439, 561 (1976).

([4]) If $|\psi\rangle$ is an eigenvector of the idempotent quantum-mechanical state operator P ($P^2 = P$), such that $P|\psi\rangle = |\psi\rangle$ and $\langle\psi|\psi\rangle = 1$, then $P = |\psi\rangle\langle\psi|$ and $|\psi\rangle$ is the quantum-mechanical state vector

state operator ϱ. The operator ϱ has the same defining mathematical properties as a statistical or density operator of traditional (von Neumann) quantum-statistical mechanics, but here it represents an individual state of a single isolated system and not the index of statistics from a generally heterogeneous ensemble of identical systems distributed over a range of different idempotent states. This hypothesis is the key to the present work as well.

For what concerns the time evolution of the postulated broader class of individual quantum states, HATSOPOULOS and GYFTOPOULOS conclude that, for a system with Hamiltonian operator H, the von Neumann equation of motion

$$(1) \qquad\qquad \frac{\mathrm{d}\varrho}{\mathrm{d}t} = -\frac{i}{\hbar}[H, \varrho]$$

is valid for unitary processes, but is inadequate for a unified theory of mechanics and thermodynamics because it describes neither nonunitary reversible processes nor irreversible processes in which a system approaches thermodynamic equilibrium. For a variety of reasons, statistical, phenomenological, thermodynamic, information-theoretic, or quantum-theoretic, other investigators have concluded that eq. (1) is incomplete even in the framework of von Neumann quantum-statistical mechanics [5], and several mathematical generalizations of the equation have been considered [6].

Recently, the first author [7] proposed an equation of motion which satisfies the requirements of quantum thermodynamics and describes conservative irreversible processes even for a single isolated particle. In ref. [1] we presented the form of the equation for a single isolated constituent of matter [8]. Here we present the form of the equation for a general system consisting of more than one distinguishable elementary constituent.

[5] See, e.g., R. JANCEL: *Foundations of Classical and Quantum Statistical Mechanics* (Pergamon Press, Oxford, 1969); J. MEHRA and E. C. G. SUDARSHAN: *Nuovo Cimento B*, **11**, 215 (1972); R. S. INGARDEN and A. KOSSAKOWSKI: *Ann. Phys.*, **89**, 451 (1975); J. L. PARK and W. BAND: *Found. Phys.*, **8**, 239 (1978); A. WEHRL: *Rev. Mod. Phys.*, **50**, 221 (1978), and references therein.

[6] See, e.g., W. H. LOUISELL: *Quantum Statistical Properties of Radiation* (Wiley, New York, N. Y., 1973); E. B. DAVIES: *Commun. Math. Phys.*, **39**, 91 (1974); P. PEARLE: *Phys. Rev. D*, **13**, 857 (1976); I. BIALYNICKI-BIRULA and J. MYCIELSKI: *Ann. Phys.* (*N. Y.*), **100**, 62 (1976); G. LINDBLAD: *Commun. Math. Phys.*, **48**, 119 (1976); V.GORINI, A. KOSSAKOWSKI and E. C. G. SUDARSHAN: *J. Math. Phys.* (*N. Y.*), **17**, 821 (1976); V. GORINI, A. FRIGERIO, M. VERRI, A. KOSSAKOWSKI and E. C. G. SUDARSHAN: *Rep. Math. Phys.*, **13**, 149 (1978); R. F. SIMMONS jr. and J. L. PARK: *Found. Phys.*, **11**, 297 (1981); N. GISIN and C. PIRON: *Lett. Math. Phys.*, **5**, 379 (1981); P. CALDIROLA and L. A. LUGIATO: *Physica A*, **116**, 248 (1982), and references therein.

[7] G. P. BERETTA: Sc.D. Thesis, M.I.T. (1981), unpublished.

[8] See also G. P. BERETTA: in *Frontiers of Nonequilibrium Statistical Physics*, edited by G. T. MOORE and M. O. SCULLY (Plenum Press, New York, N. Y., 1985), in press.

The new equation of motion conforms to the following essential and stringent requirements: *a*) It is satisfied by idempotent states evolving according to the Schrödinger equation of motion, and by a special class of nonidempotent states evolving according to the von Neumann equation; thus, it includes the unitary processes of conventional quantum mechanics. *b*) It keeps the energy functional $e(\varrho) = \mathrm{Tr}(H\varrho)$ invariant; thus it is consistent with the first law of thermo-dynamics. *c*) It causes the state functional $s(\varrho) = - k\,\mathrm{Tr}(\varrho \ln \varrho)$ to increase until the system reaches a state of equilibrium or a limit cycle, and implies that $s(\varrho)$ satisfies all the requirements of entropy of thermodynamics, where k is the Boltzmann constant; thus it conforms to the requirement that $s(\varrho)$ is the only expression [3] for the entropy consistent with the von Neumann equation. *d*) It reduces to several independent equations of motion for several noninteracting and uncorrelated constituents; thus it is compatible with the definition of an isolated system. *e*) Subject to the proof of a conjecture, it implies the existence of a unique stable equilibrium state for each set of values of the constants of the motion; thus it is consistent with the second law of thermodynamics [3].

The paper is organized as follows. Statements of the nondynamical postulates of quantum theory and the proposed equation of motion are given in sect. **2**, some important theorems in sect. **3** and conclusions in sect. **4**.

To avoid unnecessary repetitions, we use many results from ref. [1].

2. – Postulates.

The postulates of the proposed quantum theory are as follows.

2`1. *Postulate* 1: *Systems*. – To every physical system there corresponds a Hilbert space $\mathscr{H}$. In general, given M distinguishable elementary constituents of matter (single particles, single assemblies of indistinguishable particles and single fields), each associated with a Hilbert space $\mathscr{H}^L$, for $L = 1, 2, ..., M$, the Hilbert space $\mathscr{H}$ of the overall composite system is the direct product space

$$(2) \qquad \mathscr{H} = \bigotimes_{L=1}^{M} \mathscr{H}^L = \mathscr{H}^1 \otimes \mathscr{H}^2 \otimes ... \otimes \mathscr{H}^M = \mathscr{H}^J \otimes \mathscr{H}^{\bar{J}},$$

where $\mathscr{H}^{\bar{J}}$ denotes the space of all constituents except the J-th, so that

$$(3) \qquad \mathscr{H}^{\bar{J}} = \bigotimes_{\substack{L=1 \\ L \neq J}}^{M} \mathscr{H}^L = \mathscr{H}^1 \otimes \mathscr{H}^2 \otimes ... \otimes \mathscr{H}^{J-1} \otimes \mathscr{H}^{J+1} \otimes ... \otimes \mathscr{H}^M$$

for each $J = 1, 2, ..., M$.

For a single constituent of matter, this postulate reduces to postulate 1 of ref. ([1]).

Postulate 2: The correspondence principle; *Postulate* 3: State preparations, and *Postulate* 4: Observables, measurements, data and ensembles are identical to the respective postulates in ref. ([1]). As a result of postulate 4, we have that the mean value $e(\varrho)$ of the energy of the composite system in state ϱ is given by the value of the functional

$$(4) \qquad e(\varrho) = \mathrm{Tr}(H\varrho) \,.$$

Again, if elementary constituent J is a field (*i.e.* $\mathscr{H}^J$ is a Fock space) and the composite system is in state ϱ, the value $n_J(\varrho)$ of the number of particles in field J is given by the value of the functional

$$(5) \qquad n_J(\varrho) = \mathrm{Tr}\big[(N(J)\otimes I(\bar{J}))\varrho\big] \,,$$

where $N(J)$ is the particle number operator on $\mathscr{H}^J$ and $I(\bar{J})$ the identity on $\mathscr{H}^{\bar{J}}$.

Postulates 1 to 4, or some equivalent statements, represent the quantum foundations of the kinematics of any system. For the dynamics, we will adopt the equation of motion proposed by BERETTA ([7]). As discussed in ref. ([1]), the dynamics of a single isolated elementary constituent of matter is determined by a set of linearly independent generators of the motion, in addition to the Hamiltonian. We will see that these generators also determine the dynamics of the composite system.

2'2. *Postulate 5: Equation of motion for a general quantum system.* – For an isolated composite system of M distinguishable elementary constituents of matter, the state operator ϱ evolves according to the equation

$$(6) \qquad \frac{\mathrm{d}\varrho}{\mathrm{d}t} = -\frac{i}{\hbar}[H, \varrho] + \frac{\mathrm{D}\varrho}{\mathrm{D}t} \,,$$

where $[H, \varrho] = H\varrho - \varrho H$, $\mathrm{D}\varrho/\mathrm{D}t$ is a linear, self-adjoint operator on the Hilbert space of the system, defined as a nonlinear function of ϱ by

$$(7) \qquad \frac{\mathrm{D}\varrho}{\mathrm{D}t} = -\sum_{J=1}^{M} \frac{1}{\tau_J} D_J \otimes \varrho_{\bar{J}} \,,$$

$$(8) \qquad D_J = \tfrac{1}{2}\big(\sqrt{\varrho_J}\tilde{D}_J + (\sqrt{\varrho_J}\tilde{D}_J)^\dagger\big) \,,$$

τ_J is a positive time constant for constituent J,

$$(9) \qquad \varrho_J = \mathrm{Tr}_{\bar{J}}(\varrho) \,, \qquad \varrho_{\bar{J}} = \mathrm{Tr}_J(\varrho) \,.$$

$\text{Tr}_{\bar{J}}$ denotes the partial trace over $\mathscr{H}^{\bar{J}}$, Tr_J the partial trace over $\mathscr{H}^J$, $X^\dagger$ the adjoint of operator X,

$$(10) \quad \bar{D}_J = \frac{\begin{vmatrix} \sqrt{\varrho_J}(B \ln \varrho)^J & \sqrt{\varrho_J}(R_{0J})^J & \sqrt{\varrho_J}(R_{1J})^J & \dots & \sqrt{\varrho_J}(R_{z(J)J})^J \\ (R_{0J}, B \ln \varrho)^J & (R_{0J}, R_{0J})^J & (R_{0J}, R_{1J})^J & \dots & (R_{0J}, R_{z(J)J})^J \\ (R_{1J}, B \ln \varrho)^J & (R_{1J}, R_{0J})^J & (R_{1J}, R_{1J})^J & \dots & (R_{1J}, R_{z(J)J})^J \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (R_{z(J)J}, B\ln\varrho)^J & (R_{z(J)J}, R_{0J})^J & (R_{z(J)J}, R_{1J})^J & \dots & (R_{z(J)J}, R_{z(J)J})^J \end{vmatrix}}{\Gamma^J(\varrho; R_{0J}, R_{1J}, \dots, R_{z(J)J})},$$

$$(11) \quad \Gamma^J(\varrho; R_{0J}, R_{1J}, \dots, R_{z(J)J}) =$$

$$= \begin{vmatrix} (R_{0J}, R_{0J})^J & (R_{0J}, R_{1J})^J & \dots & (R_{0J}, R_{z(J)J})^J \\ (R_{1J}, R_{0J})^J & (R_{1J}, R_{1J})^J & \dots & (R_{1J}, R_{z(J)J})^J \\ \vdots & \vdots & \ddots & \vdots \\ (R_{z(J)J}, R_{0J})^J & (R_{z(J)J}, R_{1J})^J & \dots & (R_{z(J)J}, R_{z(J)J})^J \end{vmatrix},$$

$$(12) \quad (F)^J = \text{Tr}_{\bar{J}}[(I_J \otimes \varrho_{\bar{J}})F] = (F)^{J\dagger},$$

$$(13) \quad (F, G)^J = (G, F)^J = \tfrac{1}{2}\text{Tr}_J\left(|\varrho_J|\{(F)^J, (G)^J\}\right) =$$

$$= (\sqrt{\varrho_J}(F)^J|\sqrt{\varrho_J}(G)^J)^J = (\sqrt{\varrho_J}(G)^J|\sqrt{\varrho_J}(F)^J)^J,$$

$$(14) \quad (F_J|G_J)^J = (G_J|F_J)^J = \tfrac{1}{2}\text{Tr}_J(F_J^\dagger G_J + G_J^\dagger F_J),$$

$|\varrho_J| = \sqrt{\varrho_J^\dagger \varrho_J}$ [9], $\{F_J, G_J\} = F_J G_J + G_J F_J$, F and G are self-adjoint operators on $\mathscr{H}$, F_J and G_J operators (in general non–self-adjoint) on $\mathscr{H}^J$, ϱ_J and $\varrho_{\bar{J}}$ (eq. (9)) the reduced state operators of constituent J and of the composite of constituents $1, 2, \dots, J-1, J+1, \dots, M$, respectively, $\Gamma^J(\varrho; R_{0J}, R_{1J}, \dots, R_{z(J)J})$ (eq. (11)) is the Gram determinant of operators $\sqrt{\varrho_J}(R_{0J})^J$, $\sqrt{\varrho_J}(R_{1J})^J$, ..., $\sqrt{\varrho_J}(R_{z(J)J})^J$ (in general, non–self-adjoint) with respect to the real scalar product defined by eq. (14) on the set of linear operators on $\mathscr{H}^J$, B the idempotent operator obtained from ϱ by substituting unity for each nonzero eigenvalue of ϱ, and operators R_{iJ}, for $i = 0, 1, \dots, z(J)$, are determined as follows.

For each elementary constituent J considered as isolated, the generators of the motion are defined in ref. [1]. They are the linearly independent self-adjoint operators $\{I(J), H(J), N_1(J), \dots, N_{n(J)}(J)\}$ on the Hilbert space $\mathscr{H}^J$ of the elementary constituent, where $I(J)$ is the identity, $H(J)$ the Hamiltonian and

[9] See footnote [10] in G. P. BERETTA, E. P. GYFTOPOULOS, J. L. PARK and G. N. HATSOPOULOS: *Nuovo Cimento B*, **82**, 168 (1984).

each $N_i(J)$, for $i = 1, ..., n(J)$, commutes with the Hamiltonian. Any linear combination with real coefficients of the linearly independent generators of the motion, which always include the identity and the Hamiltonian, is also a well-defined self-adjoint operator on $\mathscr{H}^J$, and has been shown to represent a constant of the motion [1] of the isolated constituent J. Thus the generators of the motion define both the causal evolution and the time invariants of each isolated elementary constituent J.

For each elementary constituent J considered as part of the isolated composite system of M distinguishable constituents, we define the set of linearly independent self-adjoint operators $\{I, H, N_{1J}, ..., N_{n(J)J}\}$ on the Hilbert space $\mathscr{H}$ of the composite system by the relations

(15) $$I = I(J) \otimes I(\bar{J}) \,,$$

(16) $$H = \sum_{L=1}^{M} H(L) \otimes I(\bar{L}) + V \,,$$

(17) $$N_{iJ} = N_i(J) \otimes I(\bar{J}) \qquad \text{for } i = 1, ..., n(J),$$

where V is the Hamiltonian operator that represents the interactions among the constituents of the composite. In essence, operators I and N_{iJ} are representations on the Hilbert space $\mathscr{H}$ of the non-Hamiltonian generators of the motion of elementary constituent J. But H is the Hamiltonian operator of the composite and accounts for all interactions between constituents. We call the set of operators I, H and N_{iJ}, for $i = 1, 2, ..., n(J)$ and $J = 1, 2, ..., M$, the generators of the motion of the composite system.

For each operator ϱ and each elementary constituent J, if the operators $\{\sqrt{\varrho_J}(I)^J, \sqrt{\varrho_J}(H)^J, \sqrt{\varrho_J}(N_{1J})^J, ..., \sqrt{\varrho_J}(N_{n(J)J})^J\}$ are linearly independent, then $z(J) = n(J) + 1$ and operators R_{iJ} are the generators of the motion $\{R_{0J} = I, R_{1J} = H, R_{2J} = N_{1J}, ..., R_{z(J)J}\}$. If the operators $\{\sqrt{\varrho_J}(I)^J, \sqrt{\varrho_J}(H)^J, \sqrt{\varrho_J}(N_{1J})^J, ..., \sqrt{\varrho_J}(N_{n(J)J})^J\}$ are linearly dependent, then $z(J) < n(J) + 1$ and the set $\{R_{iJ}\}$ is any smaller subset of generators of the motion of the composite such that operators $\{\sqrt{\varrho_J}(R_{0J})^J, \sqrt{\varrho_J}(R_{1J})^J, ..., \sqrt{\varrho_J}(R_{z(J)J})^J\}$ are linearly independent and span the set $\{\sqrt{\varrho_J}(I)^J, \sqrt{\varrho_J}(H)^J, \sqrt{\varrho_J}(N_{1J})^J, ..., \sqrt{\varrho_J}(N_{n(J)J})^J\}$. Using well-known properties of determinants, it can be readily verified that operator $\tilde{D}_J$ is invariant under transformation from one set $\{R_{iJ}\}$ to any other set $\{R'_{iJ}\}$ with the same defining properties. Moreover, it follows from the definition of operators R_{iJ} that the Gram determinant defined by eq. (11) is always strictly positive.

For a single constituent ($M = 1$), eq. (6) reduces to the form presented in ref. [1].

If some generators of the motion are unbounded, the self-adjoint operator $d\varrho/dt$ (eq. (6)) will be well defined only on a subset $\tilde{Q}$ of the linear, self-adjoint, unit-trace operators ϱ on $\mathscr{H}$. The technical problem to find necessary and sufficient conditions that define the set $\tilde{Q}$ remains to be solved. An operator-

valued function $\varrho(t)$ defined for $t \geqslant 0$ will be called a solution if and only if $\varrho(0)$ is in $\tilde{Q}$ and $\varrho(t)$ satisfies eq. (6) for every $t \geqslant 0$. We will see that solutions remain in $\tilde{Q}$ for every $t \geqslant 0$ because $\varrho(t)$ remains self-adjoint and unit trace (theorems 1 and 2). A solution $\varrho(t)$ will be called physical if and only if $\varrho(t)$ is also nonnegative definite, *i.e.* $|\varrho(t)| = \varrho(t)$ for every $t \geqslant 0$. We will denote by Q the subset of operators ϱ in $\tilde{Q}$ through which there passes a physical solution. Thus, by definition, every physical solution lies entirely in Q. Only the operators ϱ in Q will qualify as state operators. The technical problem to prove that, for every nonnegative definite $\varrho(0)$ in $\tilde{Q}$, the equation of motion admits of a unique physical solution remains to be solved [10]. To proceed, we will assume that physical solutions exist in addition to the trivial unitary solutions discussed in theorems 3 and 8.

Similar technical problems were identified in the analysis of the equation of motion for a single constituent [1]. There, in support of the assumption of existence of physical solutions, we derived a particular class of nontrivial, nonunitary, approximate solutions [10]. Moreover, in support of our conjectures on the general existence and uniqueness of physical solutions, we discussed the rudiments of an approach to the proofs of an existence and uniqueness theorem, and a nonnegativity conservation theorem. Those heuristic and circumstantial arguments have also some bearing on the technical issues regarding the general form of the equation of motion discussed here.

3. – Theorems.

Some important consequences of the theory represented by postulates 1 to 5 are the following.

Theorem 1. Any solution $\varrho(t)$ of eq. (6) is self-adjoint.

Theorem 2. Any solution $\varrho(t)$ of eq. (6) is unit trace.
The proofs of these two theorems are analogous to the proofs of theorems 1 and 2 in ref. [1].

Theorem 3. If $\psi(t)$ is a solution of the Schrödinger equation

$$(18) \qquad\qquad \frac{\mathrm{d}\psi}{\mathrm{d}t} = -\frac{i}{\hbar} H\psi,$$

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[10] See also G. P. BERETTA: *Int. J. Theor. Phys.*, **24**, 119 (1985), where existence and uniqueness of solutions in both forward and backward time are proved rigorously for a single isolated two-level system.

then $\varrho(t) = P_{\psi(t)}$ is a physical solution of eq. (6), where $P_{\psi(t)}$ is the projector onto the one-dimensional subspace of $\mathscr{H}$ spanned by vector $\psi(t)$.

Proof. Substituting projector $P_{\psi(t)}$ into eq. (6), we find that all entries of the first column of determinant $\tilde{D}_J$ (eq. (10)), for $J = 1, ..., M$, vanish for every t because $B(t) = P_{\psi(t)}$ and $P_{\psi(t)} \ln P_{\psi(t)}$ is the null operator. With each operator $\tilde{D}_J$ equal to the null operator, eq. (6) reduces for every t to the von Neumann equation which is satisfied by $P_{\psi(t)}$. Thus theorem 3 is proved.

If uniqueness of physical solutions were proved, then theorem 3 would be strengthened so that « given a solution $\varrho(t)$ with $\varrho(0) = P_{\psi(0)}$, then $\varrho(t) = P_{\psi(t)}$ for all times t ». In other words, for idempotent states eq. (6) would reduce to the Schrödinger equation.

In what follows, we establish conditions under which a physical observable is a constant of the motion. We will see that all such constants are also invariants of the von Neumann equation, but that the converse is not true.

Definition 1. Preconstants of the motion.
A physical observable represented by a linear, self-adjoint operator A will be called a preconstant of the motion if and only if for all state operators ϱ

$$(19) \qquad \mathrm{Tr}\left(A\frac{\mathrm{D}\varrho}{\mathrm{D}t}\right) = 0 \,.$$

Theorem 4. A physical observable represented by a linear, self-adjoint operator A is a preconstant of the motion if there exist scalars λ_{IJ}, λ_{HJ} and λ_{iJ}, for $i = 1, ..., n(J)$ and $J = 1, ..., M$, such that operator A satisfies the set of M equations

$$(20) \qquad A = \lambda_{IJ} I + \lambda_{HJ} H + \sum_{i=1}^{n(J)} \lambda_{iJ} N_{iJ}, \qquad J = 1, ..., M\,.$$

Another less restrictive sufficient condition is that there exist real state functionals $\lambda_{IJ}(\varrho)$, $\lambda_{HJ}(\varrho)$ and $\lambda_{iJ}(\varrho)$, for $i = 1, ..., n(J)$ and $J = 1, ..., M$, such that for every ϱ operator A satisfies the set of M equations

$$(21) \qquad \varrho_J(A)^J = \varrho_J\left[\lambda_{IJ}(\varrho)I(J) + \lambda_{HJ}(\varrho)(H)^J + \sum_{i=1}^{n(J)} \lambda_{iJ}(\varrho) N_i(J)\right], \qquad J = 1, ..., M\,.$$

Proof. By virtue of definition 1 and eqs. (6)-(14), we find

$$(22) \qquad \mathrm{Tr}\left(A\frac{\mathrm{D}\varrho}{\mathrm{D}t}\right) =$$
$$= -\sum_{J=1}^{M} (\tilde{D}_J|\sqrt{\varrho_J}(A)^J)^J/\tau_J = -\sum_{J=1}^{M} m_J(\varrho)/\tau_J \Gamma^J(\varrho; R_{0J}, R_{1J}, ..., R_{z(J)J})\,,$$

where

$$(23) \quad m_J(\varrho) = \begin{vmatrix} (A, B \ln \varrho)^J & (A, R_{0J})^J & (A, R_{1J})^J & \dots & (A, R_{z(J)J})^J \\ (R_{0J}, B \ln \varrho)^J & (R_{0J}, R_{0J})^J & (R_{0J}, R_{1J})^J & \dots & (R_{0J}, R_{z(J)J})^J \\ (R_{1J}, B \ln \varrho)^J & (R_{1J}, R_{0J})^J & (R_{1J}, R_{1J})^J & \dots & (R_{1J}, R_{z(J)J})^J \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (R_{z(J)J}, B \ln \varrho)^J & (R_{z(J)J}, R_{0J})^J & (R_{z(J)J}, R_{1J})^J & \dots & (R_{z(J)J}, R_{z(J)J})^J \end{vmatrix}.$$

When either condition (20) or (21) is satisfied, then $m_J(\varrho)$ (eq. (23)) vanishes for every ϱ and J because operator $\sqrt{\varrho_J}(A)^J$ is a linear combination of operators $\sqrt{\varrho_J}(R_{iJ})^J$ and, therefore, the first row of determinant $m_J(\varrho)$ is a linear combination of the other rows. It follows that the right-hand side of eq. (22) vanishes and, thus, theorem 4 is proved.

Corollary 1. Each generator of the motion is a preconstant of the motion.

Indeed, each generator of the motion satisfies condition (20) with all the λ's equal to zero except one that equals unity.

Definition 2: Constants of the motion.

A physical observable represented by a linear, self-adjoint operator C will be called a constant of the motion of the system if and only if for all state operators ϱ

$$(24) \qquad \frac{dc(\varrho)}{dt} = \frac{d}{dt} \mathrm{Tr}\,(C\varrho) = \mathrm{Tr}\left(C\frac{d\varrho}{dt}\right) = 0 \,.$$

Corollary 2. A physical observable represented by a well-defined self-adjoint operator C is a constant of the motion if

$$(25) \qquad C = \sum_{k=1}^{q} \gamma_k C_k,$$

where C_k is a constant of the motion and γ_k a real scalar, for $k = 1, ..., q$.

This follows immediately from condition (24) and the linearity of the trace functional.

Theorem 5. A physical observable represented by operator C is a constant of the motion if and only if C commutes with the Hamiltonian operator H and is a preconstant of the motion.

Proof. By virtue of eq. (6), the rate of the change of mean value $c(\varrho)$ of observable C is given by the relation

$$(26) \qquad \mathrm{Tr}\left(C\frac{d\varrho}{dt}\right) = -\frac{i}{\hbar}\mathrm{Tr}\,([C, H]\varrho) + \mathrm{Tr}\left(C\frac{D\varrho}{Dt}\right).$$

For C to be a constant of the motion, the right-hand side of eq. (26) must vanish for every ϱ. This occurs if and only if each of the two terms vanishes independently because the first term is a linear and the second a nonlinear functional of ϱ. The first term vanishes for every ϱ if and only if $[C, H] = 0$. The second term vanishes if and only if C is a preconstant of the motion. Thus theorem 5 is proved.

Corollary 3. The Hamiltonian H is a constant of the motion.

Indeed, $[H, H] = 0$ and H satisfies conditions (20) with $\lambda_{HJ} = 1$ for every J, and all the other scalar constants equal to zero.

Corollary 3 shows that state property energy, $e(\varrho) = \mathrm{Tr}(H\varrho)$, is conserved. In addition, the change of this property in any adiabatic process is uniquely related to the amount of work involved in the process [³]. Hence we conclude that the proposed equation of motion implies the first law of thermodynamics.

For a composite system, it is clear that not every preconstant of the motion is necessarily a constant of the motion. For example, each non-Hamiltonian generator of the motion of the composite system is a preconstant of the motion (corollary 1), but is not necessarily a constant of the motion because it does not necessarily commute with the Hamiltonian. By contrast, for a system consisting of a single constituent of matter, it can be readily verified that every preconstant of the motion is also a constant of the motion because the operator corresponding to such an observable commutes with the Hamiltonian operator [¹].

Corollary 4. All constants of the motion are also constants of the motion according to the von Neumann equation because they all commute with H (see corollary 1 in ref. [¹]).

In general, however, not all constants of the motion according to the von Neumann equation are constants of the motion according to eq. (6) because not all of them are preconstants of the motion. For example, the square of the Hamiltonian operator, H^2, does not represent a constant of the motion as it should because energy fluctuations are not conserved when an isolated system evolves from a nonequilibrium state towards an equilibrium state.

It is noteworthy that, whereas the invariance properties of the von Neumann equation under the usual symmetry groups are fully and uniquely determined by the invariance properties of the Hamiltonian operator H, the invariance properties of eq. (6) are determined not only by the symmetry properties of the Hamiltonian but also by the non-Hamiltonian generators and the nonlinear structure of the equation. The invariance properties of eq. (6) under the usual symmetry groups remain to be carefully investigated.

The next theorem is important because it is shown later that the functional $s(\varrho) = - k \, \mathrm{Tr}(\varrho \ln \varrho)$ represents the thermodynamic entropy of the composite system in any state ϱ.

Theorem 6. State property $s(\varrho) = - k \operatorname{Tr}(\varrho \ln \varrho)$ is a nondecreasing function of time.

Proof: Using eq. (6), eqs. (7)-(14) and theorem 2, we find [11]

$$(27a) \qquad \frac{ds(\varrho)}{dt} = - k \operatorname{Tr}\left(\frac{d\varrho}{dt} B \ln \varrho\right) - k \operatorname{Tr}\left(\frac{d\varrho}{dt}\right),$$

$$(27b) \qquad \frac{ds(\varrho)}{dt} = \sum_{J=1}^{M} \frac{k}{\tau_J} \cdot$$

$$\cdot \frac{\begin{vmatrix} (B \ln \varrho, B \ln \varrho)^J & (B \ln \varrho, R_{0J})^J & (B \ln \varrho, R_{1J})^J & \cdots & (B \ln \varrho, R_{z(J)J})^J \\ (R_{0J}, B \ln \varrho)^J & (R_{0J}, R_{0J})^J & (R_{0J}, R_{1J})^J & \cdots & (R_{0J}, R_{z(J)J})^J \\ (R_{1J}, B \ln \varrho)^J & (R_{1J}, R_{0J})^J & (R_{1J}, R_{1J})^J & \cdots & (R_{1J}, R_{z(J)J})^J \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (R_{z(J)J}, B \ln \varrho)^J & (R_{z(J)J}, R_{0J})^J & (R_{z(J)J}, R_{1J})^J & \cdots & (R_{z(J)J}, R_{z(J)J})^J \end{vmatrix}}{\Gamma^V(\varrho; R_{0J}, R_{1J}, \ldots, R_{z(J)J})},$$

$$(27c) \qquad \frac{ds(\varrho)}{dt} = \sum_{J=1}^{M} \frac{k}{\tau_J} \frac{\Gamma^V(\varrho; B \ln \varrho, R_{0J}, R_{1J}, \ldots, R_{z(J)J})}{\Gamma^V(\varrho; R_{0J}, R_{1J}, \ldots, R_{z(J)J})},$$

$$(27d) \qquad \frac{ds(\varrho)}{dt} = \sum_{J=1}^{M} \frac{k}{\tau_J} (\tilde{D}^J | \tilde{D}_J)_J,$$

where the last of relations (27) follows from the fact that $(\tilde{D}_J | \sqrt{\varrho_J}\,(R_{iJ})^J)^J = 0$ for every i and J and, therefore, $(\tilde{D}_J | \sqrt{\varrho_J}\,(B \ln \varrho)^J)^J = (\tilde{D}_J | \tilde{D}_J)^J$. The right-hand side of eq. (27c) is nonnegative because each Gram determinant $\Gamma^V(\varrho; B \ln \varrho, R_{0J}, R_{1J}, \ldots, R_{z(J)J})$ is nonnegative and, by definition, $\Gamma^V(\varrho; R_{0J}, R_{1J}, \ldots, R_{z(J)J})$ is strictly positive. Similarly, the scalar product $(\tilde{D}_J | \tilde{D}_J)^J$ in eq. (27d) is nonnegative. Thus $ds(\varrho)/dt$ is nonnegative and theorem 6 is proved.

The equation of motion implies two alternative classifications of states, the first is into dissipative and nondissipative states, and the second into nonequilibrium, nonstable equilibrium and stable equilibrium states. Each class entails physically interesting characteristics which we discuss below.

Definition 3: nondissipative states.

A state operator ϱ is said to be nondissipative if and only if for that state $ds(\varrho)/dt = 0$. Otherwise, the state operator will be called dissipative.

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[11] By the definition of operator B given in postulate 5, $\varrho = B\varrho = \varrho B$ and $B^2 = B$. It follows that i) $\dot{\varrho} = \dot{\varrho}B + \varrho\dot{B}$, ii) $\dot{B} = \dot{B}B + B\dot{B}$ and, therefore, iii) $B\dot{B}B = 0$. Hence, $d\operatorname{Tr}(\varrho \ln \varrho)/dt = \operatorname{Tr}(\dot{\varrho} \ln \varrho) + \operatorname{Tr}(\dot{\varrho}) = \operatorname{Tr}(\dot{\varrho}B \ln \varrho) + \operatorname{Tr}(\varrho\dot{B} \ln \varrho) + \operatorname{Tr}(\dot{\varrho})$. But $\operatorname{Tr}(\varrho\dot{B} \ln \varrho) = \operatorname{Tr}(\varrho B\dot{B} \ln \varrho) = \operatorname{Tr}(B\dot{B}\varrho \ln \varrho) = \operatorname{Tr}(B\dot{B}B\varrho \ln \varrho) = 0$ and thus eq. (27a) is proved.

Corollary 5. The operator $D\varrho/Dt$ (eq. (7)) is the null operator if and only if ϱ is nondissipative.

Indeed, relations (27) imply that $ds(\varrho)/dt = 0$ if and only if $\tilde{D}_J = 0$ for each J. Thus, if ϱ is nondissipative, $D\varrho/Dt = 0$. Conversely, if $D\varrho/Dt = 0$, $d\varrho/dt$ is given by eq. (1) and then it is well known that $ds(\varrho)/dt = 0$ and, hence, ϱ is nondissipative.

Theorem 7. A given state operator ϱ is nondissipative if and only if there exist real scalars λ_{IJ}, λ_{HJ} and λ_{iJ}, for $i = 1, ..., n(J)$, and $J = 1, ..., M$, such that operator ϱ satisfies the M equations

$$(28) \qquad \varrho_J(B \ln \varrho)^J = \varrho_J\left[\lambda_{IJ}I(J) + \lambda_{HJ}(H)^J + \sum_{i=1}^{n(J)} \lambda_{iJ}N_i(J)\right], \quad J = 1, ..., M.$$

Proof. Using definition 3, relation (27c) and the fact that Gram determinants are nonnegative, we find that $ds(\varrho)/dt = 0$ for the given state operator ϱ if and only if for each J

$$(29) \qquad \Gamma^v(\varrho; B \ln \varrho, R_{0J}, R_{1J}, ..., R_{z(J)J}) = 0.$$

The Gram determinant Γ^v vanishes if and only if operators $\sqrt{\varrho_J}(B \ln \varrho)^J$, $\sqrt{\varrho_J}(R_{0J})^J$, $\sqrt{\varrho_J}(R_{1J})^J, ..., \sqrt{\varrho_J}(R_{z(J)J})^J$ are linearly dependent. Using the definition of operators R_{iJ} (postulate 5) and relations (12), (15) and (17), we find that for every ϱ and each J

$$(30) \qquad (I)^J = I(J),$$

$$(31) \qquad (N_{iJ})^J = N_i(J)$$

and that the requirement of linear dependence is given by condition (28). Thus, theorem 7 is proved.

Corollary 6. A given state operator ϱ is nondissipative if there exists a preconstant of the motion A such that, for each J,

$$(32) \qquad \varrho_J(B \ln \varrho)^J = \varrho_J(A)^J.$$

Indeed, for the given state operator ϱ, substituting $\varrho_J(B \ln \varrho)^J$ by $\varrho_J(A)^J$ in eq. (27), we find that $\Gamma^v(\varrho; B \ln \varrho, R_{0J}, R_{1J}, ..., R_{z(J)J}) = m_J(\varrho)$ (eq. (23)) for each J. Thus eq. (27) becomes $ds(\varrho)/dt = -k \operatorname{Tr}(A(D\varrho/Dt))$. But the right-hand side of the last relation is equal to zero because A is a preconstant of the motion (condition (19)).

Definition 4: Nondissipative solutions or limit cycles.

A physical solution $\varrho(t)$ is said to be nondissipative or, equivalently, to be a limit cycle if and only if $ds(\varrho(t))/dt = 0$ for every t.

Definition 5: Strongly nondissipative states.

A state operator ϱ is said to be strongly nondissipative if and only if it belongs to a nondissipative solution.

Corollary 7. A physical solution $\varrho(t)$ is nondissipative if and only if $\varrho(t)$ satisfies conditions (28) for every t, *i.e.* $\varrho(t)$ is nondissipative for every t.

However, a physical solution passing through a nondissipative state is not necessarily nondissipative because the fact that condition (28) is satisfied at one time does not necessarily imply that it is satisfied at all times. In other words, a nondissipative state is not necessarily also strongly nondissipative. By contrast, for a system composed of a single constituent of matter every physical solution passing through a nondissipative state is nondissipative [1], *i.e.* every nondissipative state is also strongly nondissipative.

Corollary 8. Every nondissipative solution satisfies the von Neumann equation.

Indeed, a nondissipative solution $\varrho(t)$ of eq. (6) is also a solution of eq. (1) because $D\varrho(t)/Dt = 0$ for every t (corollary 3).

Corollary 8 implies that conventional Hamiltonian dynamics is included in the proposed dynamics as a special case. Said differently, conventional quantum dynamics describes only the unitary limit cycles of quantum thermodynamics. A special class of nondissipative solutions is discussed in theorem 8.

Theorem 8. For M noninteracting elementary constituents, *i.e.* for $V = 0$ in eq. (16), a solution $\varrho_n(t)$ of the von Neumann equation is also a nondissipative physical solution of eq. (6) if and only if $\varrho_n(0)$ is nondissipative.

Proof. Being a solution of eq. (1), $\varrho_n(t) = U(t)\varrho_n(0)U^{-1}(t)$, where the unitary transformation $U(t) = \exp[-itH/\hbar] = \exp[-itH(1)/\hbar] \otimes ... \otimes \exp[-itH(M)/\hbar]$ because $V = 0$. If $\varrho_n(0)$ is nondissipative, then we find that condition (28) is satisfied by $\varrho_n(0)$ and $\varrho_n(t)$ for every t for the same scalars λ_{IJ}, λ_{HJ} and λ_{iJ}: It follows that $\varrho_n(t)$ is nondissipative for every t, $D\varrho_n(t)/Dt = 0$ for every t (corollary 5) and, therefore, $\varrho_n(t)$ satisfies eq. (6). Conversely, if $\varrho_n(t)$ is a solution of both eqs. (1) and (6), then $D\varrho_n(t)/Dt = 0$ for every t and, therefore, $\varrho_n(t)$ is nondissipative for every t (corollary 5). Thus theorem 8 is proved.

If uniqueness of physical solutions were proved, then theorem 8 would be strengthened so that « if initially in a nondissipative state, a physical solution for M noninteracting constituents evolves only through such states. » In other words, for such initial states, eq. (6) would reduce to the von Neumann equation.

Theorem 9. A state operator ϱ represents an equilibrium state (definition 3 in ref. [1]) if ϱ commutes with the Hamiltonian operator H and is nondissipative.

The proof of this theorem is analogous to that of theorem 9 in ref. [1].

Definition 6: Complete set of constants of the motion.

A set of $q+2$ linear, self-adjoint, linearly independent operators $\{I, H, K_1, ..., K_q\}$ is said to represent a complete set of constants of the motion if and only if every constant of the motion C of the system can be expressed as

$$(33) \qquad C = c_I I + c_H H + \sum_{j=1}^{q} c_j K_j,$$

where c_I, c_H and c_j, for $j = 1, 2, ..., q$, are real scalars.

The linearly independent constants of the motion I and H (theorem 2 and corollary 3) are always members of the complete set. Clearly, each of the remaining members $K_1, ..., K_q$ commutes with H (theorem 5) and can be selected in a variety of ways. For a given system, however, the number q is fixed by the completeness and linear independence conditions.

Theorem 10. For given finite mean values of the operators in a complete set of constants of the motion $\{I, H, K_1, ..., K_q\}$, there exists one and only one state operator ϱ_0 for which $s(\varrho_0) = -k \operatorname{Tr}(\varrho_0 \ln \varrho_0)$ is greater than $s(\varrho)$ of any other state operator corresponding to the same mean values. The state operator ϱ_0 is given by the relation

$$(34) \qquad \varrho_0 = \exp\left[-\beta H + \sum_{j=1}^{q} \varkappa_j K_j\right] \Big/ \operatorname{Tr}\left[\exp\left[-\beta H + \sum_{j=1}^{q} \varkappa_j K_j\right]\right],$$

where the coefficients β and $\varkappa_j$, for $j = 1, 2, ..., q$, are determined by the given mean values.

The theorem is proved in the literature ([12]). Relation (34) is a generalization of the known thermodynamic equilibrium distributions. If $\mathscr{H}$ is infinite-dimensional and some generators of the motion are unbounded, we will impose on the generators of the motion the additional condition that, for each given set of finite mean values of the constants of the motion, the state operator ϱ_0 (relation (34)) be well defined.

By virtue of theorems 7 and 9, it is clear that ϱ_0 is an equilibrium state. For given mean values of the constants of the motion, the system may admit other equilibrium states in addition to ϱ_0. In what follows, we examine the stability of the equilibrium states in the special sense that, as we explained in ref. ([1]), captures the essence of the second law of thermodynamics.

Definition 7: Subset Ω.

We denote by Ω the set of all the linear, self-adjoint, unit trace, nonnegative-definite operators ϱ on $\mathscr{H}$ that correspond to given finite mean values of a

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([12]) A. KATZ: *Principles of Statistical Mechanics* (W. H. Freeman, San Francisco, Cal., 1967), p. 45.

complete set of constants of the motion H and K_i, i.e. such that $\mathrm{Tr}\,(H\varrho) =$ $= e < \infty$ and $\mathrm{Tr}\,(K_i\varrho) = k_i < \infty$, where e and k_i are fixed given constants, for $i = 1, ..., q$.

Clearly, every physical solution $\varrho(t)$ with $\varrho(0)$ in Ω lies entirely in Ω.

Theorem 11. For given finite mean values of a complete set of constants of the motion, the equilibrium state ϱ_0 corresponding to the maximum value $s(\varrho_0)$ of $s(\varrho)$ (theorem 10) is stable (definition 6 in ref. ([1])).

The proof of this theorem is the same as given in ref. ([1]).

Conjecture. For given finite mean values of a complete set of constants of the motion, all equilibrium states other than ϱ_0 of theorem 10 are unstable (definition 7 in ref. ([1])).

Arguments in support of this conjecture are given in ref. ([1]). They can be readily extended to the conjecture for a composite system.

For each combination of finite mean values of a complete set of constants of the motion, the conjecture and theorem 11 imply that a composite system admits one and only one stable equilibrium state. This is a generalization of the statement of the second law of thermodynamics used by HATSOPOULOS and GYFTOPOULOS ([3]) in their unified theory. Hence we conclude that the proposed equation of motion implies the second law of thermodynamics.

From consideration of the second law and unitary processes obeying eq. (1), it has been proved ([3]) that $- k\,\mathrm{Tr}\,(\varrho \ln \varrho)$ is the only state functional that satisfies all the requirements that must imposed on the entropy of a system. Because all arguments of the proof are valid here, we conclude that $s(\varrho) = = - k\,\mathrm{Tr}\,(\varrho \ln \varrho)$ represents the entropy also when the dynamics of a system is described by eq. (6).

In what follows, we study the effects of interactions and correlation between two subsystems of a composite isolated system. Thus we establish conditions under which each subsystem can be analysed independently of the other. The extension of the results to more than two subsystems is straightforward.

Definition 8: Subsystems.

Given a system of M distinguishable constituents, we define subsystems A and B by partitioning the set of constituents $1, 2, ..., M$ into two disjoint subsets of M_A and M_B constituents, respectively ($M_A + M_B = M$).

With subsystems A and B are associated Hilbert spaces $\mathscr{H}^A$ and $\mathscr{H}^B$ (postulate 1) such that

$$(35) \qquad \mathscr{H}^A \otimes \mathscr{H}^B = \mathscr{H}$$

and with every state ϱ of the composite are associated the reduced state operators

$$(36) \qquad \varrho_A = \mathrm{Tr}_B(\varrho) \quad \text{and} \quad \varrho_B = \mathrm{Tr}_A(\varrho)\,.$$

Subscripts A and B will denote operators on $\mathscr{H}^A$ and $\mathscr{H}^B$, respectively.

Definition 9: Noninteracting subsystems.

Subsystems A and B will be said to be noninteracting if and only if the interaction Hamiltonian operator V and, therefore, the overall Hamiltonian operator H (eq. (16)) can be written as

(37) $$V = V_A \otimes I_B + I_A \otimes V_B ,$$

(38) $$H = H_A \otimes I_B + I_A \otimes H_B .$$

In words, two subsystems A and B are noninteracting if and only if the interaction Hamiltonian between the constituents of A and those of B is equal to the null operator.

Theorem 12. If two subsystems A and B are noninteracting, then both operators $H_A \otimes I_B$ and $I_A \otimes H_B$ represent constants of the motion of the composite system, and have constant mean values equal to $\mathrm{Tr}_A(H_A \varrho_A)$ and $\mathrm{Tr}_B(H_B \varrho_B)$, respectively.

Proof. By virtue of eq. (38), $[H, (H_A \otimes I_B)] = [H, (I_A \otimes H_B)] = 0$. Moreover, it can be readily verified that for every state operator ϱ

(39a) $$(H_A \otimes I_B)^J = - I_J \, \mathrm{Tr}_B(\varrho_B H_B) + (H)^J \qquad \text{if } J \in A ,$$

(39b) $$(H_A \otimes I_B)^J = I_J \, \mathrm{Tr}_A(\varrho_A H_A) \qquad \text{if } J \in B ,$$

and

(40a) $$(I_A \otimes H_B)^J = I_J \, \mathrm{Tr}_B(\varrho_B H_B) \qquad \text{if } J \in A ,$$

(40b) $$(I_A \otimes H_B)^J = - I_J \, \mathrm{Tr}_A(\varrho_A H_A) + (H)^J \qquad \text{if } J \in B .$$

Thus each of the operators $H_A \otimes I_B$ and $I_A \otimes H_B$ commutes with the Hamiltonian operator H and satisfies condition (21) and, therefore, represents a constant of the motion. Moreover,

$$\mathrm{Tr}[(H_A \otimes I_B)\varrho] = \mathrm{Tr}_A(H_A \varrho_A) \quad \text{and} \quad \mathrm{Tr}[(I_A \otimes H_B)\varrho] = \mathrm{Tr}_B(H_B \varrho_B) .$$

Thus theorem 12 is proved.

For noninteracting subsystems, theorem 12 asserts that an energy can be assigned to each subsystem and that such an energy is conserved.

Theorem 13. If the two subsystems A and B are noninteracting, then the reduced state operators ϱ_A and ϱ_B satisfy the equations of motion

(41a) $$\frac{d\varrho_A}{dt} = - \frac{i}{\hbar} [H_A, \varrho_A] - \sum_{\substack{J=1 \\ J \in A}}^{M} \frac{1}{\tau_J} D_J \otimes (\varrho_A)_J ,$$

(41b) $$\frac{d\varrho_B}{dt} = - \frac{i}{\hbar} [H_B, \varrho_B] - \sum_{\substack{J=1 \\ J \in B}}^{M} \frac{1}{\tau_J} D_J \otimes (\varrho_B)_J ,$$

where operator D_J, for $J = 1, 2, \ldots, M$, is defined by eqs. (8)-(14), $(\varrho_A)_{\bar{J}} = \mathrm{Tr}_J(\varrho_A)$ and $(\varrho_B)_{\bar{J}} = \mathrm{Tr}_J(\varrho_B)$. For J in subset A (subset B), each operator D_J in eqs. (41) is identical to the corresponding operator defined by eqs. (8)-(14) for an overall system composed of only the elementary constituents in subset A (subset B) except for the logarithmic entries which are expressed in terms of operator $(B \ln \varrho)^J$ rather than operator $(B_A \ln \varrho_A)^J$ for A and operator $(B_B \ln \varrho_B)^J$ for B.

Proof. Equations (41a) and (41b) follow immediately from eq. (6), condition (38), and the fact that $d\varrho_A/dt = \mathrm{Tr}_B(d\varrho/dt)$ and $d\varrho_B/dt = \mathrm{Tr}_A(d\varrho/dt)$. Thus, theorem 13 is proved.

In general, operator $(B \ln \varrho)^J$ differs from both operators $(B_A \ln \varrho_A)^J$ and $(B_B \ln \varrho_B)^J$ and, therefore, the time evolution of the reduced state operator ϱ_A (ϱ_B) depends not only on ϱ_A (ϱ_B) but also on ϱ. The lack of interactions between the two subsystems guarantees that the energy of each subsystem is conserved (theorem 12), but does not imply that each subsystem evolves independently of the other.

Definition 10: Independent states of subsystems.

Given a system in state ϱ, two subsystems A and B are said to be in independent states ϱ_A and ϱ_B, respectively, if and only if

$$(42) \qquad\qquad \varrho_A \otimes \varrho_B = \varrho \;.$$

For independent states, we can readily verify that

$$(43) \qquad B \ln \varrho = B_A \ln \varrho_A \otimes I_B + I_A \otimes B_B \ln \varrho_B \;,$$

$$(44a) \qquad (B \ln \varrho)^J = (B_A \ln \varrho_A)^J + I_J \, \mathrm{Tr}_{\bar{B}}(\varrho_B \ln \varrho_B) \qquad \text{if } J \in A \;,$$

$$(44b) \qquad (B \ln \varrho)^J = (B_B \ln \varrho_B)^J + I_J \, \mathrm{Tr}_A(\varrho_A \ln \varrho_A) \qquad \text{if } J \in B \;.$$

Theorem 14. If initially in independent states, two noninteracting subsystems A and B evolve only through such states. Specifically, the equations of motion for the state ϱ of the system and the reduced states ϱ_A and ϱ_B are

$$(45) \qquad\qquad \frac{d\varrho}{dt} = \frac{d\varrho_A}{dt} \otimes \varrho_B + \varrho_A \otimes \frac{d\varrho_B}{dt} \;,$$

$$(46a) \qquad\qquad \frac{d\varrho_A}{dt} = -\frac{i}{\hbar}[H_A, \varrho_A] + \frac{D\varrho_A}{Dt} \;,$$

$$(46b) \qquad\qquad \frac{d\varrho_B}{dt} = -\frac{i}{\hbar}[H_B, \varrho_B] + \frac{D\varrho_B}{Dt} \;,$$

where the operator $D\varrho_A/Dt$ $(D\varrho_B/Dt)$ is given by the right-hand side of eq. (7) for a system consisting of only the elementary constituents of A (B).

Proof. Using eqs. (42)-(44) into eqs. (41), we can readily verify that $D\varrho_A/Dt$ and $D\varrho_B/Dt$ depend only on ϱ_A and ϱ_B, respectively. Thus, theorem 14 is proved.

Theorems 12 and 14 imply that two subsystems of a composite system can be analysed independently if and only if they are noninteracting and, initially, in independent (uncorrelated) states, *i.e.* if and only if each of the two subsystems conforms to the definition of a strictly isolated system ([13]).

Definition 11: Correlation functional.

Given a system partitioned into two subsystems A and B, the correlation functional between A and B will be defined by

$$(47a) \qquad \sigma_{AB}(\varrho) = \text{Tr}(\varrho \ln \varrho) - \text{Tr}_A(\varrho_A \ln \varrho_A) - \text{Tr}_B(\varrho_B \ln \varrho_B) =$$

$$(47b) \qquad = \text{Tr}\,[\varrho(\ln \varrho - B_A \ln \varrho_A \otimes I_B - I_A \otimes B_B \ln \varrho_B)].$$

By the well-known subadditivity property of the functional $\text{Tr}(\varrho \ln \varrho)$ ([14]), functional $\sigma_{AB}(\varrho)$ is nonnegative definite. Moreover, $\sigma_{AB}(\varrho) = 0$ if and only if the two subsystems are in independent states (condition (42)). In this sense, the terms independent and uncorrelated are interchangeable.

Theorem 15. The rate of change of the correlation functional is given by

$$(48) \qquad \frac{d\sigma_{AB}(\varrho)}{dt} = \dot\sigma_{AB}|_H - \dot\sigma_{AB}|_D\,,$$

where

$$(49) \qquad \dot\sigma_{AB}|_H = \frac{i}{\hbar}\,\text{Tr}\,\left(H[\varrho,\,B_A \ln \varrho_A \otimes I_B + I_A \otimes B_B \ln \varrho_B]\right),$$

$$(50) \qquad \dot\sigma_{AB}|_D = \sum_{\substack{J=1 \\ J\in A}}^{M} \frac{1}{\tau_J}(\tilde{D}_J|\sqrt{\varrho_J}(B\ln\varrho - B_A \ln \varrho_A \otimes I_B)^J)^J +$$

$$+ \sum_{\substack{J=1 \\ J\in B}}^{M} \frac{1}{\tau_J}(\tilde{D}_J|\sqrt{\varrho_J}(B\ln\varrho - I_A \otimes B_B \ln \varrho_B)^J)^J.$$

Proof. Equations (48)-(50) can be obtained by differentiating eq. (47), using ref. ([11]), relations $d\varrho_A/dt = \text{Tr}_B(d\varrho/dt)$ and $d\varrho_B/dt = \text{Tr}_A(d\varrho/dt)$, eq. (6), and relations (7)-(14). Equations (49) and (50) represent the contributions to $d\sigma_{AB}(\varrho)/dt$ arising from the Hamiltonian term $(-i[H,\varrho]/\hbar)$ and the dissipative term $(D\varrho/Dt)$ in eq. (6), respectively. Thus, theorem 15 is proved.

([13]) A system is said to be strictly isolated if and only if it interacts with no other system, and is at some time and, hence, at all times in an independent state when viewed as a subsystem of any conceivable composite system containing it.
([14]) H. ARAKI and E. LIEB: *Commun. Math. Phys.*, **18**, 160 (1970). See also A. WEHRL: *Rev. Mod. Phys.*, **50**, 242 (1978).

Based on our understanding of the properties of the equation of motion, we conjecture that $\dot{\sigma}_{AB}|_D$ is always nonnegative, *i.e.* that the dissipative term in the equation of motion can destroy but cannot create correlations between subsystems.

4. – Conclusions.

The proposed quantum theory appears to be in accord with both mechanics and thermodynamics. In particular, it includes the consequences of the first and second laws of thermodynamics as manifestations of inherent dynamical features of the elementary constituents of matter. Hence, those two laws need not be stated explicitly because the foundations of the theory include their implications. All the results have been achieved without information-theoretic or statistical reasoning, and without restrictions to and distinctions between microscopic and macroscopic descriptions.

The proposed theory, that we call quantum thermodynamics, maintains the fundamental conceptual structure of quantum physics, but extends the nonstatistical description of individual states from the zero entropy domain covered by quantum mechanics to an unexplored broader domain of nonzero entropy states, and contemplates a nonstatistical deterministic description of their irreversible causal evolution.

Our present knowledge of the mathematical properties of the new equation is far from complete. Several technical mathematical issues related to unbounded operators on infinite-dimensional Hilbert space and to the general question of existence and uniqueness of physical solutions remain to be resolved.

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● RIASSUNTO

Si propone una nuova equazione non lineare di evoluzione per un sistema quantistico generale costituito da più costituenti materiali elementari distinguibili. Nel dominio degli operatori di stato idempotenti della meccanica quantistica, l'equazione è soddisfatta da tutte le evoluzioni unitarie generate dall'equazione di Schrödinger. Ma, nel dominio più ampio degli operatori di stato non idempotenti, non contemplati dalla meccanica quantistica convenzionale, l'equazione genera un'evoluzione generalmente non unitaria, mantiene costante il valor medio dell'energia e causa aumenti di entropia finché il sistema non raggiunge uno stato di equilibrio oppure un ciclo limite.

Квантовая термодинамика. Новое уравнение движения для общей квантовой системы.

Резюме (*). — Предлагается новое нелинейное уравнение движения для общей квантовой системе, состоящей из более чем одной элементарной составляющей вещества. В области идемпотентных квантовомеханических операторов состояний удовлетворяются все унитарные эволюции, генерированные уравнением Шредингера. В более широкой области неидемпотентных операторов состояний, не рассматриваемой в обычной квантовой механике, возникает неунитарная эволюция, при этом энергия является инвариантной, а энтропия увеличивается со временем, пока система достигает состояния равновесия или предельного цикла.

(*) *Переведено редакцией.*