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Quantum Thermodynamics [1] is a unified quantum theory that includes within a single uncontradictory nonstatistical structure—the whole of Quantum Mechanics and Classical Equilibrium Thermodynamics, as well as a general description of nonequilibrium states, their entropy, and their irreversible motion towards stable equilibrium. Quantum Thermodynamics postulates that a system has access to a much broader set of states than contemplated in Quantum Mechanics. Specifically, for a system that is strictly uncorrelated from any other system, namely, a system for which Quantum Mechanics contemplates only states that are described by a state vector $|\Psi\rangle$, Quantum Thermodynamics postulates that in addition to the quantum mechanical states there exist many other states that cannot be described by a vector $|\Psi\rangle$ but must be described by a self-adjoint, unit-trace, nonnegative-definite linear operator ρ that we call the state operator.

In contrast with the density operators used in Statistical Mechanics to characterize either a heterogeneous ensemble of identical uncorrelated systems that are generally distributed over a range of different states, or a homogeneous ensemble of identical systems that are correlated with some other system such as a heat bath or a reservoir, we emphasize that the state operators in Quantum Thermodynamics are used to characterize a homogeneous ensemble of identical uncorrelated systems each of which is exactly in the same state as all the others. In other words, state operators ρ in Quantum Thermodynamics describe the uncorrelated states of a system, in the same sense as the state vectors $|\psi\rangle$ in Quantum Mechanics describe the uncorrelated states of a system. Clearly, all the states of Quantum Mechanics form a subset of the states contemplated in Quantum Thermodynamics, namely, the subset of idempotent states operators ρ such that $\rho^2 = \rho = |\psi\rangle < \psi|$.

Postulating the augmentation just cited of the set of conceivable states of an uncorrelated system allows a unification of mechanics and thermodynamics at the fundamental microscopic level [2]. Entropy emerges as a state property much in the same way in which energy is understood to be a state property. Energy is represented by the state functional TrHp where H is the Hamiltonian of the system. Entropy is represented by the state functional -kTrplnp where k is the Boltzmann constant [2]. Among all the different states p with a given value $\langle E \rangle$ of the energy, i.e., such that TrHp = $\langle E \rangle$, the value of the entropy spans from zero for the idempotent quantum mechanical states to a maximum value for the classical thermodynamical state p = $\exp(-\beta H)/Tr\exp(-\beta H)$, where β is uniquely determined by $\langle E \rangle$. State operators with values of the entropy between zero and the maximum value represent states that, in general, are nonequilibrium and are not contemplated either in Quantum Mechanics or in Classical Thermodynamics.

Because the nonidempotent state operators represent nonmechanical states, the description of their time evolution cannot be derived from the laws of mechanics. Specifically, it cannot be derived from the unitary evolution generated by the Schroedinger equation $d|\psi\rangle/dt = -iH|\psi\rangle/\hbar$. Quantum Thermodynamics postulates that the time evolution of the state operator ρ is given in general by the solution of a general equation of motion [1] which for a

single material constituent has the form

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\frac{\mathrm{i}}{\hbar} \left[H, \rho \right] - \frac{1}{\tau} F(\rho) , \qquad (1)$$

where the operator $F(\rho)$ is given explicitly in [1] and can be visualized geometrically [3] as the projection of the gradient of the entropy functional -kTrplnp onto the hyperplane generated by the normalization functional Trp, the energy functional TrHp and, for a field with number operator N (with [N,H] = 0), the number-of-particle functional TrNp.

The coefficient τ in Equation 1 cannot be inferred other than from experiments on the relaxation of nonequilibrium states. Mathematically, all the general results that we summarize below unfold identically whether τ is a universal constant, a constant that depends on the system, or any positive functional of ρ . At present, we have not found a way to estimate τ on the basis of available experimental data. However, we have discussed specific implications of Equation 1 which should in principle be experimentally verifiable [4].

The operator $F(\rho)$ has many interesting features. It reduces to the null operator whenever $\rho^2=\rho$, namely, for each quantum mechanical state. Equation 1 maintains idempotent any initially idempotent state operator and, therefore, all the unitary evolutions of mechanical states generated by the Schroedinger equation are also solutions of Equation 1. Thus, we conclude that Quantum Thermodynamics contains the whole of Quantum Mechanics. But it is more general, because for the nonmechanical states, i.e., for $\rho^2\neq\rho$, $F(\rho)$ does indeed contribute to the time evolution. The two terms in Equation 1 compete with each other in the sense that $-i[H,\rho]/\hbar$ tends to "pull" ρ in a direction tangent to the local constant entropy hypersurface whereas $-F(\rho)/\tau$ tends to "pull" ρ in the local direction of steepest entropy ascent while maintaining it on a constant energy and constant number of particles hyperplane.

The term $-i[H,\rho]/\hbar$ maintains invariant the entropy functional by maintaining invariant each of the eigenvalues of the state operator ρ . If H is time-dependent, then this term describes an adiabatic exchange of energy between the system and some other external systems during which the two systems remain uncorrelated. The adiabatic rate of energy change, $Tr(dH/dt)\rho$, depends on the rate of change of the Hamiltonian operator H. Even if H is time-dependent, the term $-F(\rho)/\tau$ does not contribute to changing the value of the energy functional $TrH\rho$, but for most nonidempotent states it increases the value of the entropy functional $-Tr\rho\ln\rho$. Interestingly, the rate of entropy increase is independent of the rate of change dH/dt of the Hamiltonian operator and, therefore, adiabatic energy exchanges can be made to approach reversibility, i.e., vanishing entropy production, in the limit of very fast changes of the Hamiltonian.

The magnitude of the rate of entropy increase is a nonlinear function of $\boldsymbol{\rho}$ which goes to zero smoothly at many states, including the idempotent states, the equilibrium states, and the limit cycles. It is therefore interesting to note that if a state is very close to, say, an idempotent state, then the term $-F(\rho)/\tau$ may be so small compared to the term -i[H, \rho]/h that its effect may be negligible for a long time, during which the evolution may seem dominated by the unitary term -i[H,p]/fi. According to Equation 1, however, all the idempotent states, the limit cycles, and the less-than-maximum-entropy equilibrium states are unstable in the sense of Lyapunov, i.e., arbitrarily close to each one of them there is a trajectory that after some finite time (perhaps very long) carries the state to a finite distance. The only equilibrium states that are in the sense of Lyapunov are the maximum entropy states $\rho = \exp(-\beta H)/\text{Trexp}(-\beta H)$, i.e., equilibrium the states $\circ \mathbf{f}$ classical thermodynamics.

From the results just summarized it follows that if we postulate that the uncorrelated states of a system are described by state operators ρ that are not

necessarily idempotent and evolve in time according to Equation 1, then we obtain a quantum theory that when restricted to the idempotent state operators reduces to the whole of Quantum Mechanics, and when restricted to the maximum entropy state operators, which turn out to be the only stable equilibrium states -- a conclusion that is equivalent to the second law of thermodynamics [2], reduces to the whole of Equilibrium Thermodynamics.

Moreover, the theory implies general conclusions on the nature of the nonequilibrium states and their irreversible, energy conserving but entropy increasing, motion towards stable equilibrium. A general state operator ρ can always be written as

$$\rho = B \exp(-\sum_{i} f_{i} X_{i})$$
 (2)

where the self-adjoint linear operators X_1 , X_2 , ..., X_j , ... form a fixed set spanning the real space of all self-adjoint linear operators, the coefficients f_1 , f_2 , ..., f_j , ... are real numbers, and B is an idempotent, self-adjoint linear operator. In terms of this expression, the entropy functional

$$S = -kTr\rho ln\rho = k\sum_{j} f_{j} Tr X_{j} \rho = k\sum_{j} f_{j} \langle X_{j} \rangle$$
(3)

so that

$$kf_{j} = \frac{\partial S}{\partial x_{j}} \left| \left\langle x_{i \neq j} \right\rangle \right|, \tag{4}$$

and the coefficient \mathbf{f}_i can be interpreted as a generalized affinity associated with the observable represented by operator \mathbf{X}_i .

The particular structure of the dissipative term ${}^-\!F(\rho)/\tau$ in the equation of motion of Quantum Thermodynamics is such that its contribution to the rate of change $dTrX_{j}\rho/dt$ of the mean value of observable X_{j} can be written as $-\text{TrX}_{i}F(\rho)/\tau = \sum_{i}f_{i}L_{ii}(\rho)$, thus implying the existence of linear interrelations between the dissipative contribution to the rate of change of $\langle X_i \rangle$ and the generalized affinities f_i . The coefficients $L_{ii}(\rho)$ may be interpreted as generalized conductivities. The explicit structure of the functionals $L_{ij}(\rho)$ is such that $L_{ii}(\rho) = L_{ij}(\rho)$ and the symmetric matrix $[L_{ij}(\rho)]$ is nonnegative definite. Thus, we conclude that the particular structure of the dissipative term in Equation 1, when coupled with the general expression for nonequilibrium states given by Equation 2 implies a general result that we may identify with an extension of Onsager's reciprocity principle to all nonequilibrium states. We emphasize that this result follows directly with no further assumptions from the specific structure of the operator $-F(\rho)/\tau$, which implies the existence of an endogenous irreversible dynamical tendency of nonequilibrium states to follow the local direction of steepest entropy ascent. The complete dynamical behavior results from the competition between the endogenous irreversible tendency towards the direction of steepest entropy ascent, contributed by the term $-F(\rho)/\tau$ in the equation of motion, and the reversible Hamiltonian tendency towards a unitary evolution, contributed by the term $-i[H,\rho]/\hbar$.

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Nonlinear Dynamics and Chaos, Geometric Quantization, and Wigner Function

Y.S. Kim, and W.W. Zachary



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PREFACE

This volume consists of the papers presented at the First International Conference on the Physics of Phase Space, 20 - 23 May 1986, at the University of Maryland, College Park, Maryland, U.S.A.

The main motivation for holding this Conference was to bring together a diverse collection of researchers working in the general area of phase space to present their current research and exchange new ideas concerning various approaches to current problems in pure and applied physics. Indeed, the Conference covered many different fields. The papers presented at the Conference may be divided into the following general areas:

- A. Classical Nonlinear Dynamics and Chaos
- B. Ouantum Chaos
- C. Wigner Distributions
- D. Other Semiclassical Theories (WKB Methods, Maslov Theory, etc.)
- E. Symplectic Geometry and Quantization
- F. Relativity, Quantum Mechanics, and Thermodynamics

Almost sixty years have passed since the present form of quantum mechanics was formulated. Yet, the study of classical mechanics remains one of the major lines of research in physics, and interest in this field has been growing steadily in recent years. The transition from classical to quantum mechanics remains an interesting subject, and the number of investigations in this area has been growing very rapidly. The concept of phase space plays the decisive role in this area of physics, for example in nonlinear dynamics and chaos, geometric quantization, and the Wigner distribution function.

The Wigner function is one of the tools with which one can study the boundary between classical and quantum physics, and the number of publications on this subject has been increasing in recent years. In addition, other semiclassical approaches such as generalized WKB methods have recently become very important. The theory of geometric quantization comprises another procedure for studying the transition from classical to quantum physics. Current studies of nonlinear dynamics and chaos involve both classical mechanics and quantum physics, and investigation of the boundary between them. The purpose of this Conference was to emphasize the interconnection between these different fields.

In nonlinear dynamics and chaos, the Hamiltonian formulation on phase space is very important, particularly in the analysis of conservative systems. For example, in the relatively new subject of quantum chaos, direct use is made of phase space formulations in that usually this phenomenon is studied in systems for which classical

chaos is known to exist. Thus, this class of problem is one in which the transition between classical and quantum mechanics plays a fundamental role.

The subject of chaos, in both its classical and quantum aspects, is now being investigated by an increasing number of researchers. Quantum chaos is now just beginning to be investigated, and its definitive character has yet to be determined.

Geometric quantization has its roots in the representation theory of Lie groups, which yields procedures for studying quantization – the derivation of quantum theories from corresponding classical ones. It is based upon differential geometry and makes essential use of the mathematical theory of vector bundles. For this reason, until recent times, this approach had not had much impact on the research techniques employed by physicists. However, a recent development has been that many physicists, particularly those in general relativity and elementary particle theory, are also using and developing geometric quantization techniques.

Another major recent development in the physics of phase space has been, and still is, the application of the Wigner function to both pure and applied physics. The Wigner function was introduced by Wigner in 1932 in connection with his effort to understand the effect of quantum correlation in statistical mechanics. The Wigner function depends on both the position and momentum variables, and is defined on phase space. While this function has many properties similar to those of the classical distribution function and quantum probability distribution, it is clearly distinct from these distribution functions. For this reason, continuous efforts are being made to see what fundamental role the Wigner function plays in the interpretation of quantum mechanics. The Wigner function also generates some interesting mathematical physics.

The present volume reflects these current trends. The Conference provided a forum for researchers in these fields to exchange their views.

The Organizing Committee consisted of Y.S. Kim and W.W. Zachary. This Conference was supported in part by the Office of Naval Research, the National Science Foundation, the International Union of Pure and Applied Physics, the Naval Research Laboratory, and the University of Maryland. The Conference was one of the topical conferences of the American Physical Society. The Organizing Committee is indebted to Professors H. Araki, H. Doebner, J.R. Klauder, C.S. Liu, P. Mohr, M. Shlesinger, and E.P. Wigner for their support and encouragement.

December 1986

Y.S. Kim, University of Maryland W.W. Zachary, Naval Research Laboratory

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