ΦΥΣΙΚΗ.— **The Concept of Entropy in Quantum Statistical Information Systems,** *by C. Syros* *. Ἀνεκοινώθη ὑπὸ τοῦ Ἀκαδημαϊκοῦ κ. Π. Θεοχάρη.

1. INTRODUCTION

Information Theory was born in the fourties as the science of handling and transmission of information data. Since then important developments have been achieved in various directions of the theory. An area which will probably be very important in future for Information Theory is the set of problems on the quantum level related to the production of the information data and the influences to which they are subjected during the above mentioned processes of handling and transmission.

Of course, the idea of quantizing the output of an information source is not new in the Information Theory [1] but the rigorous application of the principles of quantum theory throughout the areas of Information Theory where this is purposeful and physically feasible is still an open problem. Also the mathematical tools have not yet been worked out. For the sake of definiteness and to clarify the ideas let us mention the following examples where Quantum Physics is in fact an inseparable ingredient of the Information Theory processes:

(i) It is a generally accepted fact that the visual receptors can be activated by the absorption of a single quantum and thus they can be considered as single quantum counters. For example, at night time a receptor might catch the light quanta at the rate of about one per hour and when playing on the sunny summer beach of Patras the photon registration rate might reach hundreds of counts per second [2].

(ii) A photomultiplier has the possibility to produce an observable output if it is excited by a single photon.

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(iii) A Geiger - Müller tube detects usually single γ - quanta or single charged particles entering its active region.

(iv) The Josephson contacts constitute another important example of electronic devices in which quantum effects determine largely the output of the information source **[3]**, etc.

All these devices constitute sources which by means of known processes give rise to a more or less well defined output which may be the subject of the main interest of Information Theory in many instances. The words «more or less» above have been stressed. This is not accidental: while the usual information theoretical quantisation of the output of a random source is a useful mathematical technique, the quantum nature of a physical information source output is fundamentally crucial to the mathematical analysis and to the interpretation of the information about the phenomenon.

It is, therefore, clear that Information Theory on the long range will have to adapt at least a part of the required mathematical tools to the conditions imposed by the quantum behavior of the ultimate constituents of the information sources when they cannot be described by classical Statistical Mechanics.

To make this statement clear it is sufficient to realize that the fundamental equation of Information Theory:

$$I(x) = -\sum_{n} P_n(x) \ln P_n(x) \tag{1. 1}$$

will acquire a new dimension when the probability, $P_n(x)$, for the event x is subject to the principles of Quantum Mechanics.

Moreover, since $P_n(x)$ is directly related to the entropy of the system under consideration there will be needed sufficient clarification as to what sbould be the meaning of entropy of a quantum system composed of a small number of particles.

The present paper is organized in 6 sections. In section 2 the Uncertainty Principle is used to calculate the entropy of a system of given degrees of freedom. Section 3 gives the properties of the calculated entropy. The entropy production in a system interacting via a complex Hamiltonian is given in section 4. In section 5 the theory is further elaborated for the calculation of the internal and external entropy productions. Finally, in section 6 some remarks and conclusions are given.

2. UNCERTAINTY PRINCIPLE AND ENTROPY

Let us consider a system producing information by means of the F degrees of freedom of μ particles. By this we mean, for example, the information produced by the appearance of a number of particles in an elementary volume of the phase space.

It will be supposed that each of these particles possesses a certain number of degrees of freedom. We shall factorize, therefore, the total number of degrees of freedom, F, in the form:

$$F = 2\nu N \mu \tag{2.1}$$

In (2.1) ν is the dimension of the physical space, N the number of possible quantum mechanical degrees of freedom per dimension and particle.

In contemplating the application of the Uncertainty Principle for the calculation of the entropy we have to specify completely our understanding of the uncertainties of the relevant physical quantities.

First it is assumed that the Uncertainty Principle applies experimentally to directly observable quantities.

By this statement the fact is expressed that every time in experiment is measured the total momentum uncertainty. This uncertainty, Δp, can of course be made identical with any projection Δp_x, Δp_y, Δp_z, provided the appropriate axis rotation has been done, but even then Δp does not cease to be the total uncertainty of the linear momentum, the projections on the other axis being equal to zero. This can be made even clearer by considering the gedankenexperiment of fig. 2.1:
Assuming that the resolving power of the lens is the same in all directions, the observation point of the scattered photon at P will be found inside the sphere of radius $\Delta q \sim \lambda / \sin$ [3], ε where λ is the wave length of the photons scattered.

On the other hand the uncertainty of the momentum is calculated from the relation $p = h/\lambda$, where the wave length λ corresponds to the total momentum but not to a particular component. The result is, of course,

$$\Delta p \cdot \Delta q \geqslant h . \tag{2. 2}$$

The hypothesis of the statistical fluctuations leading the formation of dissipative structures as those proposed by Prigogine [6] is used in connection with the Uncertainty Principle to calculate the entropy of a

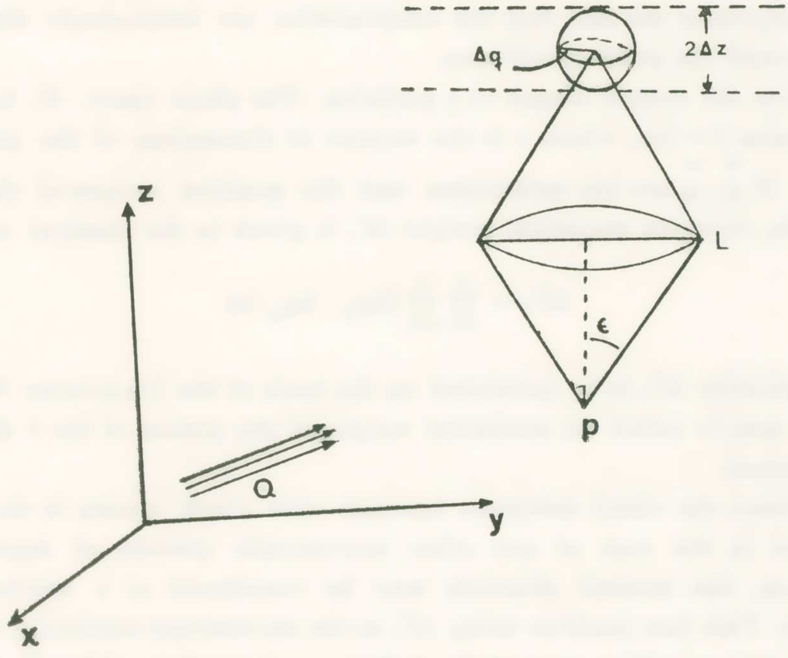

Fig. 2. 1. The resolving power of the lens, L, is Δq and equals the radius of the uncertainty region. The shape of this region depends among other parameters on the resolving power of L along the z-axis.

quantum mechanical system of particles. The first assumption made here is that the physical mechanism according to which ordered motion energy is generated in a particle system consists of the cooperative addition of the statistical fluctuations in position and momentum coordinates of a sufficiently large number of particles.

The second assumption is that the uncertainties Δp, Δq in the coordinates of the various degrees of freedom of a particle appear after each collision as a consequence of the Uncertainty Principle independently of whether the system is being observed or not. This is in accordance with the fact that to a given eigenvalue of, e.g., the momentum operator is associated a root mean square deviation which is calculated with the help of the density matrix of the system. The uncertainties are independent of p, q. The third assumption is that the uncertainties, as mentioned above, appearing in the relation $\Delta p \cdot \Delta q \geqslant h$ correspond to the absolute value of the vectors to which they refer. This expresses the fact that the uncertainties are isotropically distributed around the point of collision.

Let the system consist of s particles. The phase space, R^f, has the dimension $f = 2\nu s$, where ν is the number of dimensions of the physical space. If $\vec{p}_i$, $\vec{q}_i$ are the momentum and the position vectors of the i-th particle, then the statistical weight $\Delta\Gamma_f$ is given in the classical case by

$$\Delta\Gamma_f = \prod_{i=1}^{s} \prod_{j=1}^{\nu} (\Delta p_{ij} \cdot \Delta q_{ij} / h) . \tag{2. 3}$$

The quantity $\Delta\Gamma_f$ to be calculated on the basis of the Uncertainy Principle is usually called the statistical weight of the system of the f degrees of freedom.

Since the visual receptors interact with single quanta in the same way as in the case of any other macroscopic systems of degrees of freedom, the present situation may be considered as a macroscopic system. This fact justifies using $\Delta\Gamma_f$ as the macroscopic statistical weight of the corresponding state of the f degrees of freedom, although Δp, Δq obey the Uncertainty Principle.

In the quantum mechanical case the space R^Q has the dimension $Q = 2\nu sN$, where 2N is the number of quantum mechanical degrees of freedom corresponding to each dimension of the space (for classical point particles 2, for quantum mechanical particles 2N). The statistical weight, $\Delta\Gamma_Q$, in the present case will be defined in polar coordinates by

$$\Delta\Gamma_Q = \prod_{i=1}^{sN} \left\{ \left(\frac{p_i^{\nu-1} \cdot q^{\nu-1}}{h} \cdot \prod_{j=1}^{\nu-1} (\sin\vartheta_j \sin\varphi_j)^{\nu-j-1} \Delta\vartheta_j \Delta\varphi_j \cdot \Delta p_i \Delta q_i / h \right) \right\} \tag{2. 4}$$

The space R^Q is generated via the prescription for the definition of the Wigner functions. To proceed, the distribution function of the particle system in the space of the uncertainties is needed. In contrast to the classical case, in the quantum case the distribution function, $\varrho_s(\vec{p}_1, \dots \vec{q}_{sN}; \alpha_1, \dots \alpha_{sN})$ will depend not only on $\{\vec{p}_i, \vec{q}_i\}$ but also on the fluctuations $\{\Delta p_i \cdot \Delta q_i = h + \alpha_i\}$. This fact emerges naturally from the relation:

$$f_s^w(\vec{p}_1, \vec{q}_1 \dots \vec{p}_s, \vec{q}_s) = (8\pi^3)^{-s} \int dk_1 \dots dk_s \cdot \exp\left[-i \sum_{n=1}^{s} \vec{k}_n \vec{p}_n\right] \cdot$$
$$\cdot \mathrm{Sp}\left[\hat{\varrho}\, \Psi^+\left(\vec{q}_1 - \frac{h}{2}\vec{k}_1\right) \dots \Psi^+\left(\vec{q}_s - \frac{h}{2}\vec{k}_s\right) \cdot\right.$$
$$\left.\cdot\, \Psi\left(\vec{q}_1 + \frac{h}{2}\vec{k}_1\right) \dots \Psi\left(\vec{q}_s + \frac{h}{2}\vec{k}_s\right)\right],$$

where $\left\{\frac{h}{2}\vec{k}_n\right\}$ can be visualised as the uncertainties in question, if by a slight change of the above definition the k-integration is eliminated.

The distribution function will in general be defined on $\widetilde{R}^{\Omega} \otimes \widetilde{R}^{\Omega/2\nu}$, where $\widetilde{R}^{\Omega/2\nu}$ is the space of the action uncertainties, $\widetilde{\alpha}_i = \Delta p_i \cdot \Delta q_i / h$. Obviously, $\widetilde{\alpha}_i \geqslant 0$ for all i. For the present only the $\widetilde{\alpha}_i$-dependent part of the distribution function is of interest to us.

Let $g(\vec{p}_1, \dots \vec{p}_s)$ represent the probability for the event that from a sub-set $\widetilde{A} \subseteq \widetilde{R}^{\Omega/2\nu}$ of the fluctuations a macroscopically observable cooperative phenomenon emerges. Since the fluctuations are stochastic and $\varrho_s(\vec{p}_1, \dots q_{sN}; \widetilde{\alpha}_1, \dots \widetilde{\alpha}_{sN})$ is independent of the polar angles, g will be assumed constant on $\widehat{A}$.

Next the relation $\varrho_s \cdot g \cdot \Delta\Gamma_\Omega \simeq 1$ is used from which it follows that [**4**]

$$\varrho_s = \frac{\left[g \cdot \prod_{i=1}^{sN} (p_i^{\nu-1}\, q_i^{\nu-1} / h^{\nu-1} \cdot d\Omega_i\right]^{-1}}{\prod_{i=1}^{s} (\Delta p_i \cdot \Delta q_i / h)}. \tag{2. 5}$$

In (2. 5) the factor g accounts for the fact that a much larger element, $\Delta\Gamma_\Omega$, of the space R^Ω is required in order that the cooperative fluctuations be included in this space element.

The Uncertainty Principle is written down for each pair of degree of freedom. According to the definition of the Uncertainty, $\widetilde{\alpha}_i$, the equality

$$\Delta p_i \cdot \Delta q_i = h + \widetilde{\alpha}_i \tag{2.6}$$

results from the Uncertainty Principle.

3. SOME PROPERTIES OF THE ENTROPY

Taking the product of all the equalities with respect to i the expression is obtained

$$\prod_{i=1}^{sN} (\Delta p_i \cdot \Delta q_i / h) = \prod_{i=1}^{sN} (1 + \alpha_i) ; \quad \alpha_i = \widetilde{\alpha}_i / h . \tag{3.1}$$

Therefore, $\{\alpha_i\}$ is for the present physically more relevant than $\{\Delta p_i, \Delta q_i\}$ and ϱ_s is normalised to the unity on $R^{\Omega/2\nu} = \widetilde{R}^{\Omega/2\nu}/h$, where h is Planck's constant.

From (2.5) and (3.1) it follows, after normalisation in the cell $\alpha_i \leqslant A_i$, that

$$\varrho_s = \left\{ \prod_{i=1}^{sN} [\ln (1 + A_i)] (1 + \alpha_i) \right\}^{-1} . \tag{3.2}$$

Since ϱ_s is approximately equal to the distribution function of the uncertainties $\{\alpha_i\}$ according to (2.5), the density distribution, $S(\alpha_1, \ldots \alpha_{sN})$, of the entropy in $A^{\Omega/2\nu}$ can be expressed as usual through the relation

$$S(\alpha_1, \ldots \alpha_{sN}) = - \varrho_s \ln \varrho_s =$$

$$= - \sum_{i-1}^{sN} \ln [(1 + \alpha_i) \ln (1 + A_i)] \left\{ \prod_{i=1}^{sN} (1 + \alpha_i) \ln (1 + A_i) \right\}^{-1} . \tag{3.3}$$

It can easily be shown that $S(\alpha_1, \ldots \alpha_{sN})$ has an extremum. The sufficient and necessary conditions for this

$$\frac{\partial S}{\partial \alpha_1} = - \left(\frac{\partial W}{\partial \alpha_1} + \frac{\partial W}{\partial \alpha_1} \ln W \right) = 0, \quad \frac{\partial^2 S}{\partial \alpha_1^2} < 0, \tag{3.4}$$

where
$$W = \left\{ \prod_{i=1}^{sN} (1 + \alpha_i) \ln (1 + A_i) \right\}^{-1} ,$$

lead to the equation

$$\prod_{i=1}^{sN} (1+\bar{a}_i)\ln(1+A_i) = e. \tag{3. 5}$$

The quantities $\{\bar{a}_i / i = \leqslant sN\}$ determine the position of the extremum in $A^{Q/2\nu}$. This is indeed a maximum since the condition $\partial^2 S/\partial \alpha_1^2$ is satisfied as it is seen from $\left(\frac{\partial W}{\partial \alpha_1}\right)^2 > 0$ for all l. The entropy, $\bar{S}$, of the system is obtained by the integration in $A^{Q/2\nu}$ and multiplication by the number of dimensions, ν, of the physical space,

$$\bar{S} = \nu \int_0^{A_1} d\alpha_1 \ldots \int_0^{A_{sN}} d\alpha_{sN}\, S(\alpha_1, \ldots \alpha_{sN}). \tag{3. 6}$$

Assuming that $A_i = A$ for all $i \leqslant sN$, we get the expression

$$\bar{S} = \frac{Q}{2}\left[\frac{2\nu}{Q} + \frac{1}{2}\,\frac{\exp(2\nu/Q)}{1+\bar{a}} - \ln(1+\bar{a})\right]. \tag{3. 7}$$

The entropy, $\bar{S}$, as it is seen from (3. 7) is not an additive quantity, if the number of degrees of freedom, Q, is such that $2\nu Q^{-1} \neq 0$.

The entropy of the system has in general a minimum whose position and value are functions af $\bar{a}$. For $\bar{a} = 0$, it follows that

$$(\partial \bar{S} / \partial Q) = 0, \qquad (\partial^2 \bar{S} / \partial Q^2) > 0. \tag{3. 8}$$

From (3. 8) it follows that for one particle

$$Q = 2\nu; \qquad (s = 1) \tag{3. 9}$$

and consequently, $N = 1$ for $\bar{a} = 0$.

The physical interpretation of (3. 9) is that the maximum order in nature is observable for $Q = 2\nu$, because at $Q = 2\nu$ the entropy attains its minimum value.

For a classical point mass particle the space must be observable as three - dimensional,

$$Q = 2 \cdot 3 = 6. \tag{3. 10}$$

In relativistic quantum mechanics new degrees of freedom appear in addition to those of classical mechanics. The corresponding variables are, e. g., (q^0, q^1, q^2, q^3) and (p^0, p^1, p^2, p^3).

In other situations in which the particles' identities become also variable and, therefore, the particle acquires internal degrees of freedom the number of degrees of freedom increases, e. g., spin, magn. quantum number, space parity, helicity and isospin, charge, charge conjugation, strangeness. This gives in total 16 degrees of freedom per particle but it is not clear that these are all.

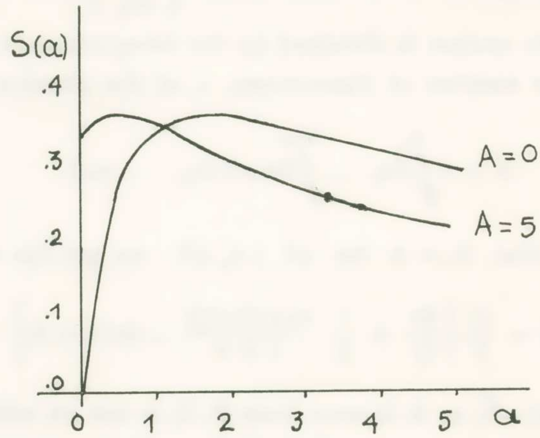

Fig. 2. 2. A plane cut of the entropy distribution density in the action uucertainty space, $A^{\Omega/\nu}$, as function of $\bar{a}$. The flat maximum implies high probability for fluctuations. The action a_i is measured in h units (Planck's constant). The larger the uncertainty $\bar{a}$ determining the maximum position the larger the expectation value of the fluctuating physical quantity.

Under physical conditions in which only the first 8 degrees of freedom appear, the number of dimensions of the physical space must equal four

$$\Omega = 2 \cdot 4 = 8. \tag{3. 11}$$

The assumption that the value $\bar{a} = 0$ has been considered, is supported by the fact that the probability density distribution introduced by Einstein

$$P(\alpha_1, \ldots \alpha_{sN}) \simeq \exp\left[S(\alpha_1, \ldots \alpha_{sN})\right] \tag{3. 12}$$

exhibits the sharpest maximum at $\bar{a}_i = 0$ for all $i \leqslant sN$.

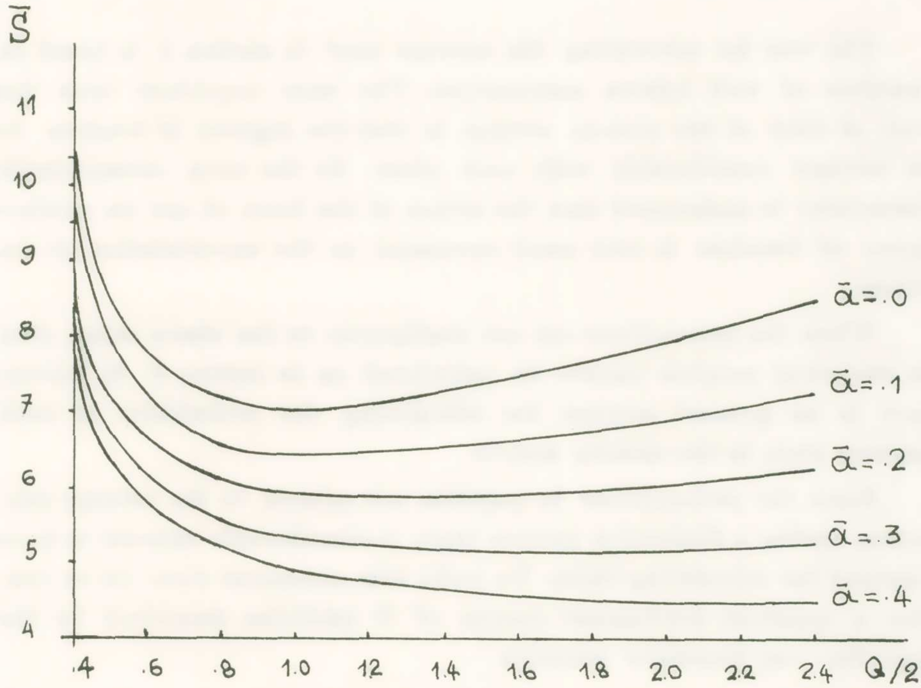

Fig. 2.3. The entropy for $\bar{a} = 0$ exhibits an absolute minimum if the number of degrees of freedom equals 2ν. For larger uncertainties, $\bar{a}$, the entropy minimum diminishes and its position shifts toward larger numbers of degrees of freedom. ν is the dimension of the physical space.

It follows from (3.7) that for Q→ large number, the entropy becomes additive. Macroscopically $\bar{S}$ is clearly additive taking the form

$$\bar{S} = \frac{1}{2}\nu sN, \tag{3.13}$$

where νsN is the total number of quantum mechanical degrees of freedom. By relating the entropy to the temperature the relation

$$\Delta E = \frac{1}{2}\nu sNkT \tag{3.14}$$

is obtained.

In another treatment the entropy appears as the imaginary part of the expectation value of a non-hermitian Hamiltonian.

4. ENTROPY PRODUCTION IN DISSIPATIVE SYSTEMS

The way for calculating the entropy used in section 2 is based on a number of well known assumptions. The most important from the point of view of the present section is that the degrees of freedom do not interact considerably with each other. By the term «considerable interaction» is understood that the action of the force of one on another degree of freedom is very small compared to the uncertainties of the actions.

When the interactions are not negligeable in the above sense, then the statistical weights cannot be calculated as in section 2. Moreover, there is no general method for calculating the probability of each quantum state in the density matrix.

Since the probabilities in question are related to the entropy production during a dissipative process there is considerable interest to have a method for calculating them. To make this statement clear let us consider a quantum mechanical system of N particles described by the Liouville - von Neumann equation

$$i\dot{\varrho} = H\varrho - \varrho H, \qquad h = 1. \tag{4.1}$$

H is the Hamiltonian of the system and $\varrho(x_1, \ldots x_N, t)$ the density matrix.

Let us suppose that the Hamiltonian has the form

$$H = H - u(t_0 - t)\,H_1 + iu(t - t_0)\,H_1 - iu(t_1 - t_0)\,H_1;\; t_1 > t_0, \tag{4.2}$$

where $u(t)$ is the unit step function. From this definition of H for time $t < t_0$ the Hamiltonian is hermitian, $H = H^+$. For $t > t_0$ the Hamiltonian ceases to have the property of hermiticity since the part H_1 of it becomes imaginary and $H^+ \neq H$, $t > t_0$ and $t < t_1$.

It is clear from the definition that for $t > t_0$ the eigenvalues of H are complex and the energy is obviously not conserved. The gain or loss of interaction energy by means of collisions with other degrees of freedom of the system has as a consequence * the production of positive or

* See Prigogine, ref. 5, p. 24.

negative entropy. As an illustration, Prigogine mentions the «Bénard problem» in classical hydrodynamics: when a horizontal fluid layer is heated uniformly from below the so called adverse temperature gradient is created. For small values of the temperature gradient the fluid remains at rest. As soon as a critical value is reached there is an abrupt inset of macroscopic motion (thermal convection flow).

Before the inset of the macroscopic motion the whole energy was in the form of thermal motion. This corresponded to a definite entropy of the system. After the beginning of the thermal convection a part of the energy was in the form of ordered macroscopic motion. If this energy is E_h, then the negative entropy production is $\Delta S = -E_h / T$, where T is some appropriate temperature.

We shall now try to give an approximate description of the entropy production on the basis of Quantum Mechanics.

Let us suppose that the thermal convection sets in at the time $t = t_0$. The system is described by the equation

$$i\dot{\varrho} = H\varrho - \varrho H^+ ; \qquad H^+ \neq H . \tag{4. 3}$$

It has been shown [7] that if H is hermitian then the system is in a steady state because the expectation value of any dynamical quantity is constant. However, when entropy is produced this cannot be the case anymore. On the other hand, production of entropy is connected with energy flow from or to the system. This can be described by means of a non-hermitian Hamiltonian.

To show this fact let us write the density matrix in the form $(t = t_0 = 0)$

$$\varrho(x ; x', 0) = R^{-1} \sum_{nn'} \psi_n^* (x) \psi_{n'}(x') , \tag{4. 4}$$

where R is a normalization constant and $\{\psi_n | n \in I\}$ is a solution of the Schrödinger equation

$$i\dot{\psi}_n = H\psi_n \tag{4. 5}$$

for the many-body problem.

The summation is taken over the elements of the index set, I, in the indicated manner.

Next we develop $\varrho(x; x', t)$ in a Taylor series

$$\varrho(x; x', t) = \sum_{\nu=0}^{\infty} \varrho^{(\nu)}(x; x', 0) \frac{t^\nu}{\nu!} . \tag{4.6}$$

This series converges for all $t < \infty$, because the derivatives $\varrho^{(\nu)}$ are all bounded from above. This is a consequence of (4. 3) and the boundedness of H. It is easily verified that

$$\varrho^{(\nu)}|_{t=0} = \sum_{\lambda=0}^{\nu} (-)^\lambda \binom{\nu}{\lambda} E_{n'}^{\lambda} \cdot E_n^{\nu-\lambda} \cdot \varrho|_{t=0} . \tag{4.7}$$

From (4. 6) and (4. 7) it follows that

$$\varrho(x; x', t) = R^{-1} \sum_{nn'} \psi_n^{\nu}(x) \, \psi_{n'}(x') \, e^{-i(\varepsilon_n - \varepsilon_{n'})t} \cdot e^{(\tilde{\varepsilon}_n + \tilde{\varepsilon}_{n'})t} , \tag{4.8}$$

where

$$\varepsilon_n = \operatorname{Re} E_n , \quad \tilde{\varepsilon}_n = \operatorname{Im} E_n . \tag{4.9}$$

Equation (4. 8) gives the density matrix of which the diagonal elements are time dependent in contradistinction to the case of the hermitian Hamiltonian. Nevertheless, the expectation values of all real dynamical functions are real.

Obviously, the expectation values are time dependent, a property expressing the fact that the system is not in equilibrium and hence entropy production ocurrs.

Were the imaginary parts $\{\tilde{\varepsilon}_n \mid n \in I\}$ of the energy eigenvalues all equal to zero, then no entropy production would be possible. It is to be expected, therefore, that $\tilde{\varepsilon}_n$ should be directly related to the entropy associated to the particular state of the system described by the many-body wave function $\psi_n(x)$.

Of course, the set $\{\tilde{\varepsilon}_n \mid n \in I\}$ may contain both positive or negative parts and consequently $\varrho(x; x', t)$ would tend to infinity in some cases if $t \to \infty$. This is, however, not possible in actual systems which produce entropy. Due to energy conservation in energy closed system the subsystem gaining energy and the subsystem losing energy will eventually come to an equilibrium such that their temperatures T_1 and T_2 will attain the same value, T.

The time

$$\tau = t_1 - t_0 \tag{4.10}$$

in which equilibrium will establish itself is related to the common temperature, T.

To make this clear let ϱ_1 and ϱ_2 be the density matrices of the two sub-systems of the system. If H_1 and H_2 are the Hamiltonians of the sub-system, then the common temperature T is given by

$$T = \frac{2}{kN_1} \mathrm{Tr}\,(\varrho_1 H_1) = \frac{2}{kN_2} \mathrm{Tr}\,(\varrho_2 H_2)\,, \tag{4.11}$$

where k is the Boltzmann constant and N_i, $i = 1, 2$, is the number of degrees of freedom of the i-th sub-system. Since ϱ_1, ϱ_2 are time dependent, (4.11) is a condition from which the relaxation time, τ, can be determined. After equilibrium is established the Hamiltonians become again hermitian and the traces of the corresponding density matrices become again time independent.

It should finally be pointed out in this connection that it is in principle possible to get, instead of one, more relaxation times $\{\tau_\lambda \,|\, \lambda = 1, 2, \dots \Lambda\}$. This is the case if more than one equilibria exist. Also it is possible that (4.11) has no root at all.

Now we are ready to calculate the produced entropies in the subsystems. According to (4.2) and (4.11) the imaginary parts

$$\widetilde{E}_1 = \mathrm{Im}\,\mathrm{Tr}\,(\varrho_1 H_1) \quad \text{and} \quad \widetilde{E}_2 = \mathrm{Im}\,\mathrm{Tr}\,(\varrho_2 H_2) \tag{4.12}$$

represent the missing parts of the real eigenvalues of the Hamiltonians. Since the motion towards equilibrium is a macroscopic motion the above energies $\widetilde{E}_1$, $\widetilde{E}_2$ are missing from the thermal motion.

According to Prigogine * we should have for the entropies

$$\Delta S_i = \widetilde{E}_i \,/\, T = \frac{kN_i}{2} \, \frac{\mathrm{Im}\,\mathrm{Tr}\,(\varrho_i H_i)}{\mathrm{Re}\,\mathrm{Tr}\,(\varrho_i H_i)}\,; \quad i = 1, 2. \tag{4.13}$$

The total entropy production is, therefore, given by

$$\begin{aligned} \Delta S = \Delta S_1 + \Delta S_2 &= \frac{kN_1}{2} \, \frac{\mathrm{Im}\,\mathrm{Tr}\,[(\varrho_1 H_1) + (\varrho_2 H_2)]}{\mathrm{Re}\,\mathrm{Tr}\,(\varrho_1 H_1)} = \\ &= \frac{kN_2}{2} \, \frac{\mathrm{Im}\,\mathrm{Tr}\,[(\varrho_1 H_1) + (\varrho_2 H_2)]}{\mathrm{Re}\,\mathrm{Tr}\,(\varrho_2 H_2)}\,. \end{aligned} \tag{4.14}$$

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* See ref. 5, p. 24.

Using the above results we can write the complex energy of the total system in the form

$$E = |E| \cdot \exp\left[i \tan^{-1}\left(\frac{2}{kN_1} \Delta S\right)\right]. \tag{4.15}$$

5. CENTER OF MASS MOTION AND ENTROPY PRODUCTION

In the foregoing section a first description was given of the way the sub-system can produce or lose entropy. In the present section some more details are to be elaborated. As it was repeatedly stated negative entropy is produced if random motion energy goes over to ordered macroscopic motion. By conveniently choosing the spatial extension of the sub-system to be described by Quantum Statistical Mechanics it is not difficult to identify the macroscopic motion with the center of mass motion of the sub-system under consideration. To this end let us consider again (4. 5) and suppose that it describes a sub-system with s degrees of freedom.

Next we introduce the center of mass coordinates and (4. 5) takes on the form [**3**]

$$i \dot{\Psi} = (H_{ma} + H_{mi} + H_I) \Psi. \tag{5.1}$$

In (5. 1) the Hamiltonians are all hermitian and the indices ma, mi, I signify the macroscopic, the microscopic and the interaction Hamiltonians, where by the center of mass motion is to be understood as a wave macroscopically observable like in scattering experiments.

We next factorise the wave function such that

$$\begin{gathered} \Psi(x_1, \ldots x_{s-3};\ X_1, X_2, X_3;\ t) \\ \psi(x_1, \ldots x_{s-3};\ t)\ \varphi(X_1, X_2, X_3;\ t). \end{gathered} \tag{5.2}$$

We again split H_I in two parts

$$H_I = (1 - e^{i\varphi}) H_I + e^{i\varphi} H_I. \tag{5.3}$$

The phase φ has been introduced in view of (4. 15). The necessity for the complex splitting is clear from what has been said in section 4. If the interaction splitting were real, the sub-system would not evolve because the density matrix to be constructed in this case would have time independent trace.

From (5. 1) - (5. 3) we get the equations

$$H_{ma}\,\varphi + (1 - e^{i\varphi})\,H_I^{ma}\,\varphi = E_{ma}\,\varphi \tag{5. 4}$$

and

$$H_{mi}\,\psi + e^{i\varphi}\,H_I^{mi}\,\psi = E_{mi}\,\psi\,, \tag{5. 5}$$

where

$$H_I^{ma} = (\psi,\; H_I\,\psi)\,, \tag{5. 6}$$

$$H_I^{mi} = (\varphi,\; H_I\,\varphi) \tag{5. 7}$$

and

$$E = E_{ma} + E_{mi} \tag{5. 8}$$

is the total energy of the sub-system and is defined as the above sum.

In (5. 4) and (5. 5) the interaction Hamiltonians are not hermitian and the equations describe the internal production of entropy.

From the solution of (5. 4) and (5. 5) two sets of wave functions can be obtained $\{\psi_n \mid n \in I_{mi}\}$ and $\{\varphi_m \mid m = \in I_{ma}\}$. The wave functions ψ_n and φ_m are so combined in the density matrix that the condition is satisfied.

$$\mathrm{Re}\,E_{nm} = \mathrm{Re}\,E_n + \mathrm{Re}\,E_m\,. \tag{5. 9}$$

Since the entropy of the system cannot decrease the sum of the imaginary parts as functions of n and m may be constant or not.

If the sub-system is not closed, then the Hamiltonian, H_{ma}, in (5. 4) has to have an imaginary part H_{ma}^{ext} for the description of the external production of entropy. The internal entropy production is given according to (4. 14).

$$\Delta S_{int} = \frac{2}{kS_{mi}} \cdot \frac{\mathrm{Im}\,\mathrm{Tr}\,\varrho_{mi}\,(H_{mi} + H_I^{mi})}{\mathrm{Re}\,\mathrm{Tr}\,\varrho_{mi}\,(H_{mi} + H_I^{mi})}\,. \tag{5. 10}$$

The external entropy production, ΔS_{ext}, can then be written in the form

$$\Delta S_{ext} = \frac{2}{kS_{ma}}\;\frac{\mathrm{Im}\,\mathrm{Tr}\,\varrho_{ma}\,H_{ma}^{ext}}{\mathrm{Re}\,\mathrm{Tr}\,\varrho_{mi}\,(H_{mi} + H_I^{mi})}\,, \tag{5. 11}$$

where S_{ma} is the number of degrees of freedom of the macroscopic motion and $S_{mi} + S_{ma} = S$.

6. REMARKS AND CONCLUSIONS

We have analyzed the concept of the entropy in the case of quantum mechanical information systems. It has been shown that in systems with few degrees of freedom the concept of entropy can be well defined of the basis of the Uncertainty Principle. This is in fact physically possible and meaningful because degrees of freedom with zero uncertainty in the variable of action have very small probability and the entropy becomes equal to zero. Similar is the probability behavior also in very large uncertainty values, where the entropy vanishes again.

This result is very important from the information theoretical point of view, because it shows that information theory can yield reliable conclusions even in the case of information systems of very small number of degrees of freedom obeying Quantum Mechanics.

This conclusion is underlined by the fact that the information is so closely related to the entropy as to obey the same equation (1. 1) as the entropy does. On the other hand, the fact that the concept of entropy and the Uncertainty Principle are so closely related implies the possibility to give an expression of the entropy on the basis of the density matrix obeying the Liouville equation.

The use of Quantum Mechanics enables one to show that the influence of external forces can lead like in the Bénard problem to the production of entropy coupled with the motion of the center of mass of the sub-system.

Finally, it has been found that the imaginary part of the energy plays a very important part both in the evolution of the systems and in the determination of the entropy, thus establishing a firm link between Quantum Mechanics and Thermodynamics.

ΠΕΡΙΛΗΨΙΣ

Ἡ ἀρχὴ τῆς ἀβεβαιότητος ἐχρησιμοποιήθη πρὸς ὑπολογισμὸν τῆς ἐντροπίας ἑνὸς συστήματος κβαντομηχανικῶν βαθμῶν ἐλευθερίας. Ἐκ τῶν εὑρεθέντων ἀποτελεσμάτων προκύπτει, ὅτι διὰ μικρὸν ἀριθμὸν βαθμῶν ἐλευθερίας ἡ ἐντροπία δὲν ἀποτελεῖ προσθετικὸν μέγεθος. Ἐπίσης ὅταν ὁ ἀριθμὸς βαθμῶν ἐλευθερίας ἰσοῦται πρὸς τὸν ἀριθμὸν διαστάσεων τοῦ φυσικοῦ χώρου, τότε ἡ ἐντροπία λαμβάνει ἐλαχίστην τιμήν. Ἀκολούθως ἐξετάζονται αἱ συνθῆκαι παραγωγῆς καὶ καταναλώσεως ἐντροπίας εἰς κβαντομηχανικὰ συστήματα περιγραφόμενα ὑπὸ μὴ ἑρμιτιανῶν ὀπιρατόρων Hamilton εἰς τὸ πλαίσιον τῆς ἐξισώσεως Liouville von Neumann.

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