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On the Time Arrow and the Theory of Irreversible Processes

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Abstract. In the existing theories of irreversible processes, the time arrow and the irreversibility are introduced by means of various specific assumptions. In a elementary discussion, it is shown that time arrow and irreversibility can be introduced by a general 'probability Ansatz', i.e. a relation between two sets of probabilities at two instants of time. This Ansatz leads directly to the Master equation. In the quantum theory, this Ansatz may be founded on the random-phase hypothesis which leads to the Pauli equation. Special attention is paid to the time reversal properties of the theories of irreversible processes with respect to the time symmetry of the underlying microscopic theories.

I. Introduction

The statistical mechanical interpretation of the macroscopic irreversibility of the approach of a gas towards thermodynamic equilibrium is well known.

In the underlying *classical* microscopic theory, the basic LIOUVILLE equation is invariant upon the reversal of time and describes only reversible processes. In order to get a macroscopic view of the gas, the use of probability or statistical concepts is necessary; it enables one to formulate a theory of irreversible processes. This irreversibility pertains only to the probabilities in the macroscopic picture, and of course does not contradict the reversibility of molecular dynamics in the microscopic picture. Consider the GIBBS statistical ensemble method, for instance. Instead of the 'fine grained[1])' distribution function $D\ (q_1 \ldots, q_N \ldots, p_N, t)$ in the γ-space that satisfies the LIOUVILLE equation, one works with the «coarse grained»[1]) $\overline{D}$ which is the average D over phase cells of non-vanishing finite dimensions $\Delta\alpha_1 \ldots \Delta q_N \Delta p_1 \ldots \Delta p_N$ representing the limits of feasibility of practical observations. It is by using this $\overline{D}$, which no longer satisfies the LIOUVILLE equation, that the H-theorem is established. In oder, however, to have a quantitative theory that will describe the macroscopically irreversible processes towards equilibrium, it is usual to introduce a specific Ansatz in one form of another. The older theory was that of BOLTZMANN, developed in the μ-space. In recent years, there have been proposed other theories, notably those of BOGOLIUBOV and of KIRKWOOD. The basic assumptions in these classical theories are different, both in their forms and their physical meaning. In these macroscopic views, it seems hence of interest to see how closely is the use of probability concepts connected with the appearance of a time arrow and irreversibility.

In the underlying microscopic *quantum* theory, the fact that probabilities are introduced in a fundamental way through the uncertainty principle does not prevent on one hand the SCHROEDINGER equation to be invariant under the (WIGNER) time reversal. On the other hand KLEIN [2]) has shown that irreversibility may already be obtained with the quantum 'fine grained' distribution function *without* introducing a coarse-grained function, although a more satisfactory form of the H theorem does make use of the last one. Therefore also in quantum theory it appears of interest to investigate what kind of connection exists between the probability concepts and the appearance of a time arrow and irreversibility. It is the purpose of the present note to undertake this task in an elementary manner. Both in the classical and the quantum theory, we shall see the close relationship between the time arrow, irreversibility, and a general 'probability Ansatz', of a much less specific form than those introduced in the theories mentioned above. Incidentally, we shall discuss the occurrence of two equations representing irreversible processes, one towards the future and the other 'towards the past', the existence of which is a consequence of the symmetry in time of the basic theories—classical dynamics or quantum mechanics.

II. Probability Ansatz and irreversibility

Before reviewing the basic assumptions in the physical theories we shall show that a theory containing a time arrow and describing irreversible processes can be founded on a 'probability Ansatz' of a very general form. By 'probability Ansatz' here, we mean a relation connecting two sets of probabilities at two instants of time.

Let $w_k^0 = w_k(t^0)$ be a set of probabilities at time t^0, and $w_k = w_k(t)$ be their values at time t. We require of the w_k^0 and w_k the following properties

$$w_k^0 \geqq 0\,, \qquad \sum_k w_k^0 = 1\,; \qquad w_k \geqq 0\,, \qquad \sum_k w_k = 1\,. \tag{1}$$

Let us assume that there existe a 'transition probability' A_{ik} from k at t^0 to i at t, and let us make the probability Ansatz

$$w_i(t) = \sum_k A_{ik}\, w_k(t^0)\,. \tag{2}$$

The A_{ik} must then satisfy the following requirements

$$\sum_k A_{ik} = 1\,, \qquad \sum_i A_{ik} = 1 \tag{3}$$

and

$$0 \leqq A_{ik} \leqq 1\,. \tag{3a}$$

Three inferences can now be drawn from this probability Ansatz.

(i) *The probability Ansatz defines an arrow of time*

Let us assume that the inverse matrix A^{-1} of A in (2) exists*) and let us try to calculate the w_k^0 from the w_i by inverting (2):

$$w_k(t^0) = \sum_i A_{ki}^{-1}\, w_i(t)\,. \tag{4}$$

From $A^{-1} A = 1$ and (3), it follows that A_{ik}^{-1} also have the proporties (3). But from these and (3a), it also follows that

$$0 \leqq A_{ik}^{-1} \leqq 1$$

is *not* satisfied (except for $A_{ik} = A_{ik}^{-1} = \delta_{ik}$, which however is a case of no physical interest). Thus in (4) A_{ik}^{-1} does not describe a 'transition probability' and in this sense the relation (2) giving w_i in terms of w_k^0 cannot be inverted to give w^0 in terms of the w[3]).

Following an initial idea of STUECKELBERG[4]) and with the aid of an inequality relation due to GIBBS, from (1)–(3), PAULI[5]) proved in a very simple manner the following relation

$$-\sum_k w_k \log w_k \geqq -\sum_k w_k^0 \log w_k^0 \tag{5}$$

which again shows the presence of a definite order, or arrow, in the two instants t^0 and t.

The above result depends only on the form of the probability relation (2), quite irrespective of the specific physical meaning of the probabilities w. For example, we may think of the w_k as the probability that a random variable x has the value x_k. But in the theory of gases, the w_k may be

*) If A^{-1} *does not exists*, the probability Ansatz (2) defines certainly an arrow of time.

identified with the average $\bar{D}$ over the phase cell $\prod_i \Delta x_i \, \Delta p_i$ at a point in the γ-phase space of the system. In this case the relation (5) then acquires a very important meaning: on identifying the entropy S with the expression $-\Sigma_k w_k \log w_k$, we obtain the law of increasing entropy in the direction of time from t^0 to t.

$$S(t) \geqq S(t^0) . \tag{6}$$

ii) *The probability Ansatz leads to the Master equation describing the evolution of the w_k's*

From (2) and (3), on calling $t - t^0 = \Delta t$, we obtain

$$w_i - w_i^0 = \sum_k (A_{ik} \, w_k^0 - A_{ki} \, w_i^0) . \tag{7}$$

On writing

$$A_{ik} = a_{ik} \Delta t , \qquad \Delta t > 0 \tag{8}$$

where a_{ik} are the transition probabilities per unit time, (7) becomes (dropping the index ^{0})

$$\frac{\Delta w_i}{\Delta t} = \sum_k (a_{ik} \, w_k - a_{ki} \, w_i) \tag{9}$$

which states that w_i is increased by the transitions from all states k to the state i, and is descreased by the transitions from the state i to all other states k. (7) or (9), is known as the Master equation. Both are not invariant upon the reversal of time.

One may note that (7) is of the same form as the Master equation for a Markovian chain[6]). For a stochastic variable capable of taking on a set of discrete values x_k, the conditional probability $P(x_k, n) \equiv P(x_j \mid x_k, n)$ that x, having the value x_j at time $t = t^0$, has the value x_k at time $t = t^0 + n\Delta t$ (Δt being the interval between two successive observations of x), is given by the equation

$$P(x_i, n + 1) - P(x_i, n) = \sum_k [P(x_k, n) \; Q(x_k, x_i) - P(x_i, n) \; Q(x_i, x_k)] \tag{10}$$

where $Q(x_k, x_i) \equiv P(x_k \mid x_i, l)$ is the transition probability from x_k to x_i in the time interval Δt. The reason for the similarity between (10) and (7) is of course the similarity between the Ansatz (2) and the SMOLUCHOWSKI law for stochastic processes.

iii) *The existence of the 'symmetric' probability Ansatz*

While (2) defines a time arrow and cannot be inverted into (4) without losing its probability meaning, it appears important to note that instead of (2) the following probability Ansatz

$$w_i(\tau) = \sum_k A_{ik} w_k(\tau^0) \tag{2a}$$

can be made, where

$$\tau^0 = t^0 ; \qquad \tau = \tau^0 + \Delta\tau = t^0 - \Delta t = -t + 2 t^0 \tag{11}$$

τ increases 'towards the past'. By writing as in (8)

$$A_{ik} = a_{ik} \Delta\tau , \qquad \Delta\tau > 0 \tag{8a}$$

one gets the Master equation

$$\frac{\Delta w_i}{\Delta\tau} = \sum_k (a_{ik} w_k - a_{ki} w_i) \tag{9a}$$

which is symmetric to (9) and, of course, incompatible with it.

III. Classical theories of irreversible processes

In the theory of BOLTZMANN developped in the μ-space, the basic hypothesis is the *Stosszahlansatz* according to which the *probable* number of collisions in the time interval Δt in the volume element Δr between molecules having velocities between v_i and $v_i + \Delta v_i$ and those between v_k and $v_k + \Delta v_k$ is

$$g_{ik} \bar{f}_k \bar{f}_i \, b \, db \, d\varphi \cdot \Delta r \, \Delta v_i \, \Delta v_k \, \Delta t \tag{12}$$

where $\bar{f}_k = \bar{f}\,(r, v_k, t)$, $\bar{f}_i = f(r, v_i, t)$, φ is the 'impact azimuth', b the impact parameter and $g_{ik} = |v_i - v_k|$. This leads to the BOLTZMANN equation

$$\frac{\partial \bar{f}}{\partial t} + v_i \frac{\partial \bar{f}}{\partial x_i} = \int dv_k \, d\varphi \, db \cdot b \, g_{ik} \, [\bar{f}'_k \bar{f}'_i - \bar{f}_k \bar{f}_i] \tag{13}$$

where $\bar{f}'_i = \bar{f}(r, v'_i, t)$, the v'_i being the velocities after collision.

That (12) is an Ansatz of a probability nature can be seen from the following considerations. In the first place, in order that (12) may represent the probable number of collisions, the elements Δt, Δr, Δv_i, Δv_k must not be arbitrarily (vanishingly) small, and the $\bar{f}_i$, $\bar{f}_k$ must consequently be taken to mean some kind of 'coarse-grained' functions, i.e., the average values of the 'fine-grained' f_i, f_k over the phase cells $\Delta r_i \, \Delta v_i$, $\Delta r_k \, \Delta v_k$ and the interval Δt. In the second place, the BOLTZMANN equation (13) is seen to be a special form of (9). In fact by making the specialization

$$w_i \to \bar{f}(r, v_i, t)$$

and

$$\sum_k a_{ki} \to \int dv_k \, d\varphi \, db \cdot b \, g_{ik} \, \bar{f}(r, v_k, t)$$

the integral on the right is seen to be the transition probability of $\bar{f}_i$ due to binary collisions with all particles k in state $\bar{f}_k$.

The BOLTZMANN equation (13) is seen to be non-invariant under reversal time: upon replacing t by $-t$ (13) becomes in fact a particular instance of (9a), physically meaningless (see section V, vii, below). Equation (13) is not a dynamical equation giving a microscopic description; because of the probability (Stosszahl) Ansatz (12), it deals with the probable values $\bar{f}_i$, $\bar{f}_k$ in the macroscopic view. It has a definite time arrow and describes irreversible processes in that direction of time. It is the failure to emphasize this probability nature that has led to such objections as that of the 'Umkehreinwand' of LOSCHMIDT and of the 'Wiederkehreinwand' of ZERMELO.

In the more recent theory of BOGOLIUBOV[7]), the time arrow, and consequently the irreversibility, are introduced by the 'initial' of 'asymptotic' condition for the weakening of the correlation effect among particles with the increase in interparticle distances:

$$\operatorname*{Lim}_{t\to\infty} S_{-t}^{(s)}\left[F_s(q_1\ldots q_s, p_2\ldots p_s;\ S_t^{(1)} F_1(t)) - \prod_i^s S_t^{(1)} F_1(q_i, p_i, t)\right] = 0 \tag{14}$$

where $S_{-t}^{(s)}$ is the operator of a canonical transformation generated by the Hamiltonian H_s of the s-particle subsystem of the N-particle system, tracing the system s backward in time for an interval t. The limit $t \to \infty$ means that t be long compared with the duration *of* a collision. The functions F_s, $s = 1, \ldots N$, satisfy the system of equations known as the BORN-GREEN-BOGOLIUBOV-KIRKWOOD-YVON hierarchy which is equivalent to the LIOUVILLE equation and hence invariant upon time reversal. The Ansatz (14) now introduces the time arrow and the theory is no longer invariant upon time reversal. In fact, to the first order in gas density, the equation for $F_1(q, p, t)$ reduces, upon some approximations*), to the BOLTZMANN equation (13). That the time arrow is introduced by (14) can be seen from the calculations of BOGOLIUBOV in obtaining the 'generalized BOLTZMANN equation' for F_1, but this has recently been brought out more explicitly by COHEN and BERLIN[8]). These authors have shown that if one reverses the direction of time in (14), i.e., assumes the correlation to vanish *in the future* instead of *in the past*, then the equation for F_1 would have become a 'BOLTZMANN equation' that describes irreversible processes towards equilibrium in the past. Such an Ansatz correspond to (2a). Thus we may say that the Ansatz (14) is a kind of generalized 'Stosszahlansatz' of a probability nature, i.e. equivalent to a special case of (2).

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*) Mainly very low density of particles and substitution of one *step* function for the short or long range forces.

In the theory of KIRKWOOD [9]), the passage from the LIOUVILLE equation to the BOLTZMANN equation is effected by an averaging of f_i over finite phase cells, a 'time-smoothing', and a product Ansatz for the two-particle correlation function, playing a role similar to (14). The time arrow and irreversibility of the resulting BOLTZMANN equation are again the consequences of the probability Ansatz of the type (2) for the macroscopic description.

IV. Quantum theory of irreversible processes

Let us consider now the problem of irreversibility and time arrow from the quantum theory point of view. Let $\psi(q, t^0) = \psi^0$ be the state of a system at an arbitrary instant of time that we shall call t^0. Let $\psi = \psi(q, t)$ be the state at a later instant $t = t^0 + \Delta t$. Let the Hamiltonian of the system be $H = H_0 + H_1$ where H_1 describes some perturbation interaction, responsable for establishement of equilibrium via transitions between eigenstates of H_0. Let ψ^0 and ψ be expanded in the complete set of stationary states $\varphi_k(q)$ of H_0 with eigenvalues E_k:

$$\begin{cases} \psi(q, t^0) = \sum\limits_k \psi_k(t^0)\, \varphi_k(q) \exp\left(-\dfrac{i\, E_k\, t^0}{\hbar}\right), \\ \psi(q, t) \;= \sum\limits_k \psi_k(t)\, \varphi_k(q) \exp\left(-\dfrac{i\, E_k\, t}{\hbar}\right). \end{cases}$$

The amplitudes $\psi_k(t^0)$ and $\psi_k(t)$ are connected by the unitary operator U

$$\psi_i(t) = \sum_k U_{ik}\, \psi_k(t^0)\,. \tag{15}$$

Then

$$\psi_i(t)\, \psi_i^*(t) = \sum_k U_{ik}\, U_{ik}^*\, \psi_k(t^0)\, \psi_k^*(t^0) + \sum_{k \neq l} U_{ik}\, U_{il}^*\, \psi_k(t^0)\, \psi_l^*(t^0)\,. \tag{16}$$

The

$$|\, U_{ik}(t^0, t)\,|^2 = A_{ik}(t^0, t) = A_{ik}(\Delta t) \tag{17}$$

are the transition probabilities in the time interval Δt. The unitary of U garantees the relations

$$\sum\nolimits_i |\psi_i(t)^2| = \sum\nolimits_i |\psi_i(t^0)\,|^2 = 1\,.$$

Consider now an ensemble of N similar systems and form the density matrix

$$\varrho_{ij} = \frac{1}{N} \sum_{\alpha}^{N} \psi_i^{(\alpha)}\, \psi_j^{(\alpha)*} = \overline{\psi_i\, \psi_j^*} \tag{18}$$

where the bar indicates the average over the systems of the ensemble. Now, as a consequence of the axioms of quantum mechanics, the wave function of a state always contains an undeterminable phase factor. Let this phase factor be absorbed in the amplitudes ψ_k^0 and ψ_k in (15). On averaging (16) over the systems of the ensemble, one usually *assumes* that[10])

$$\varrho_{ij}(t^0) = \overline{\psi_i(t^0)\, \psi_j^*(t^0)} = 0 \quad \text{for} \quad i \neq j\,. \tag{19}$$

This assumption, known as *the random-a priori-phase hypothesis* (R.P.H.), is not only plausible on account of the random distribution of the (unknowable) phases of the $\psi_k^{(\alpha)}(t^0)$ but even seems unavoidable, for otherwise, instead of

$$\varrho_{ii}(t) = \sum_k A_{ik}(\Delta t) \cdot \varrho_{kk}(t^0) \tag{20}$$

which results from (16), (18) and (19), one would have obtained for the probability density $\varrho_{ii}(t)$ an expression which would depend on the fundamentally undeterminable phases differences of $\psi_j^{(\alpha)}(t^0)$ and $\psi_i^{(\alpha)}(t^0)$ and such a result would have been outside the realm of quantum mechanics[11]).

The relation (20) is seen to be of the same form as the probability Ansatz (2). In the classical theory, the Ansatz (2) on the probabilities depends on the necessity of the adoption of the macroscopic view by introducing phase cells of finite (i.e., non-vanishing) size. In the quantum theory, the finite size of the phase cells is already a consequence of the uncertainty principle. The R.P.H. may therefore be regarded as the quantum equivalent of the Ansatz (2).

From (20), in the same way as (5) is established from (2)–(4), we readily obtain the law of increasing entropy

$$S(t) \geqq S(t^0)$$

if

$$S(t) \equiv S_f(t) \equiv -\sum_k \varrho_{kk}(t) \log \varrho_{kk}(t) \tag{21}$$

is the 'fine-grained' entropy, as defined by KLEIN[2])*).

For small Δt (but large compared with the microscopic periodic times of the individual systems), U_{ki} can be calculated according to the pertur-

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*) It is known (TOLMAN, ref. 1, the footnote p. 461) that a complete statistical treatment of the problem uses a «coarse-grained» entropy, $S_c = -\sum_k w_K \log w_K$, with $w_K = 1/n \sum_{i=1}^{n} \varrho_{k_i k_i}$ averaged over a group of n states between which macroscopic measurement cannot distinguish. The transition from S_f to S_c is then obtained through an argument which is essentially the same as that already used in the classical theory (see section III) and which, for this reason, is no longer relevant to the present section. See also PAULI and FIERZ's paper[12]).

bation theory of DIRAC and A_{ik} may be shown to be equal to $a_{ik}\Delta t$. From (20), with (17), we obtain, as in (9)

$$\frac{\Delta \varrho_{ii}}{\Delta t} = \sum_k (a_{ik}\,\varrho_{kk} - a_{ki}\,\varrho_{ii}) \tag{22}$$

which is known as the Master, or the PAULI equation[13]).

Thus by making the R.P.H. (19) at any arbitrary instant t^0 of time, one can calculate, or predict, the ϱ_{ii} at a *later* instant or time by (20) or (22). Either of these equations, however, does *not* permit one to calculate the $\varrho_{ii}(t^0)$ from the $\varrho_{ii}(t)$. We have seen that the relation (4) obtained by inverting (2) has no probability meaning. Here in quantum mechanics, the reason for this can be made more explicit. In order to calculate the $\varrho_{ii}(t^0)$ from an observation of $\varrho_{kk}(t)$, at the time t, *one must make the R.P.H. at the instant* t, as is obvious simply by inverting t and t^0 in the argument leading to (20).

But fundamentally, the necessity of the R.P.H. at time t for calculating $\varrho_{ii}(t^0)$ from $\varrho_{kk}(t)$ is a consequence of the connection between the R.P.H. and *the measurement of the 'fine-grained entropy* S_f*'*: in fact the R.P.H. at a given time, let say t^0, may be thought as the necessary result of the measurement at that thime t_0 of *the 'fine-grained' entropy* S_f *as given by* (21). This may be seen in two ways as follows:

In the first place, in order that $S_f(t^0) = \sum_k \varrho_{kk}(t^0)\,[-\log \varrho_{kk}(t^0)]$ is to be interpreted as an expectation value of a physical quantity at the time t_0, it is necessary that $\varrho_{ik}(t_0) = 0$ for $i \neq k$. For, then only, $S_f(t^0)$ may be written as $S_f(t^0) = Tr\,[\boldsymbol{\varrho} \cdot (-\log \boldsymbol{\varrho})]\,(t^0)$.

In the second place, in order to find $S_f(t^0)$ from *observations* at the time t^0, it is necessary to *measure* $\log \varrho_{kk}(t^0)$ or $\varrho_{kk}(t^0)$. And this imply the measurement of the complete set of observables E (which completly defines the eigenstates $\langle q \mid E_k, t^0\rangle = \varphi_k(q)\, e^{-(i E_k t^0)/\hbar}$) on each system (α) of the ensemble. Immediately after this measurement, the system (α) is in the state $\mid E^{(\alpha)}(t^0)\rangle$, and the density matrix is then given by [we find it convenient to use here DIRAC's notation instead of the conventional one]:

$$\varrho_{mn}(t^0) \equiv \langle E_m \,|\varrho(t^0)|\, E_n\rangle = \frac{1}{N}\sum_{(\alpha)} \langle E_m \mid E^{(\alpha)}\rangle\,(t^0)\,\langle E^{(\alpha)} \mid E_n\rangle\,(t^0)\,,$$

$$= \frac{1}{N}\sum_{\alpha} \delta_m^{(\alpha)}(t^0) \cdot \delta_n^{(\alpha)}(t^0)$$

which is always diagonal. As time goes on, transitions due to H_1 occur according to (15), and non-diagonal terms appear, so that at a later time $t > t^0$ one has on one hand

$$Tr\,[\boldsymbol{\varrho}(t)\,\mathbf{log}\,\boldsymbol{\varrho}(t)] = Tr\,[\boldsymbol{\varrho}(t^0)\,\mathbf{log}\,\boldsymbol{\varrho}(t^0)]$$

but, on the other hand

$$S_f(t) \equiv -\sum_k \varrho_{kk}(t) \log \varrho_{kk}(t) \geqq -\sum_k \varrho_{kk}(t^0) \log \varrho_{kk}(t^0) \equiv S_f(t^0)$$

for, obviously, $S_f(t) \neq Tr\,[\boldsymbol{\varrho}(t)\,\mathbf{log}\,\boldsymbol{\varrho}(t)]$ if $\boldsymbol{\varrho}(t)$ is not diagonal.

In order to *measure* S_f at the time t, one has to *measure* again the complete set of observables E at that time t, to get

$$\varrho_{mn}(t) = \frac{1}{N} \sum_{(\alpha)} \langle E_m / E^{(\alpha)} \rangle\,(t)\,\langle E^{(\alpha)} / E_n \rangle\,(t) = \frac{1}{N} \sum_{(\alpha)} \delta_m^{(\alpha)}(t)\,\delta_n^{(\alpha)}(t)$$

which is again diagonal! In the sense given above, the R.P.H. at time t is equivalent to the measurement of the 'fine-grained' entropy S_f at the time t. This emphasizes the prominant rôle of *the measurement for introducing irreversibility in quantum theory*[14]).

In order to compute $\varrho_{ii}(t^0)$ from $\varrho_{kk}(t)$, one use the inverse of (15) and rewrites (16) in the form

$$|\psi_i(t)|^2 = \sum_k A_{ik}\,|\psi(t^0)|^2 + \sum_m C_{im}\,|\psi_m(t)|^2 + \sum_{m \neq n} D_{imn}\,\psi_m(t)\,\psi_n^*(t) \qquad (23)$$

where

$$D_{imn} = \sum_{l \neq j} U_{il}\,U_{ml}^*\,U_{ij}^*\,U_{nj}\,, \qquad C_{im} = D_{imm}\,.$$

On making the R.P.H. at time t, namely

$$\varrho_{mn}(t) = \overline{\psi_m(t)\,\psi_n^*(t)} = 0$$

one gets a matrix equation

$$\boldsymbol{\varrho}'(t^0) = \boldsymbol{A}^{-1}\,(\mathbf{1} - \boldsymbol{C})\,\boldsymbol{\varrho}(t) \qquad (24)$$

which is seen to be different from the inverse of (20), namely $\boldsymbol{\varrho}(t^0) = \boldsymbol{A}^{-1}\,\boldsymbol{\varrho}(t)$. This last relation has no probability meaning, just as (4). On the other hand, the entropy

$$S'(t^0) = -\sum \varrho'_{kk}(t^0) \log \varrho'_{kk}(t^0)$$

calculated at time t^0 from the R.P.H. at time t will satisfy the relation $S'(t^0) \geqslant S(t)$, but is different from $S(t^0)$ (see fig. 1).

While (20), or (22), has a definite time arrow and is meaningful only in the direction in which the entropy increases, it should be possible, by virtue of the invariance of the SCHROEDINGER equation upon the WIGNER time reversal (time reversal and complex conjugation of the equation), to formulate the symmetrical theory with the time arrow in the opposite direction to that in (20). This is done in (24), but can be put in a more symmetric form, similar to (2a) and (9a).

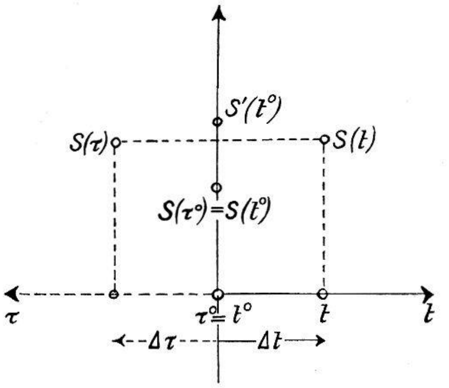

Fig. 1
Entropy probable values $S(t)$ and $S(\tau)$, given the measured value $S(t^0) = S(\tau^0)$, and entropy probable value $S'(t^0)$, given the measured value $S(t)$.

Let us start again from any arbitrary instant which we shall call $t^0 = \tau^0$, and let be $\tau = \tau^0 + \Delta\tau = t^0 - \Delta t = 2\,t^0 - t$ an earlier instant, τ *increasing towards the past*. From the invariance of the SCHROEDINGER equation, we have, similarly to (15) and (16):

$$\psi_i(\tau) = \sum_k U^*_{ik}\,\psi_k(\tau^0) \tag{15a}$$

and

$$\psi_i(\tau)\,\psi^*_i(\tau) = \sum_k U^*_{ik}\,U_{ik}\,\psi_k(\tau^0)\,\psi_k(\tau^0) + \sum_{k\neq l} U^*_{ik}\,U_{il}\,\psi_k(\tau^0)\,\psi_l(\tau^0)\,. \tag{16a}$$

On making the R.P.H. (19), we get as in (20)

$$\varrho_{ii}(\tau) = \sum_k B_{ik}\,\varrho_{kk}(t^0) \tag{20a}$$

where the $B_{ik}(\Delta\tau) = |\,U_{ik}(\Delta t)\,|^2$ are the same function of $\Delta\tau$ as the $A_{ik}(\Delta t)$ are of Δt in (17).

In the same way as in (21), we get this time (see fig. 1)

$$S(\tau) \geqq S(\tau^0)\,. \tag{21a}$$

For 'small' $\Delta\tau$, we have

$$B_{ik} = a_{ik}\,\Delta\tau\,, \qquad \Delta\tau > 0$$

and

$$\frac{\Delta\varrho_{ii}}{\Delta\tau} = \sum_k (a_{ik}\,\varrho_{kk} - a_{ki}\,\varrho_{ii}) \tag{22a}$$

which is of the same form in τ as (22) is in t. (20a) and (22a) are special cases of the general relations (2a) and (9a). It should be emphasized that (20a), or (22a), is valid only for the calculation, or 'postdiction', of the state at an *earlier* instant from the present (arbitrary) instant at which the R.P.H. is made. As (2a) and (9a), (20a) and (22a) become meaningless if the direction of time is reversed.

V. Summary and Remarks

The above results (21) and (21a) which state that, starting from any arbitrary instant of time one will find a greater (at least equal) entropy in either the future or the past, must be carefully interpretated. We shall summarize the theory and its interpretation in the following propositions:

(i) *Starting from a probability observation* at any arbitrary instant of time, we may ask for the *probable* behavior of a system either at a *later*, or at an *earlier* time. At these two questions, the answers given by (20) to (22) and (20a)–(22a) respectively, are symmetrical. This symmetry in the *possibility* of making either choice in the direction of time and in the *resulting equations* is inherent in the symmetry in time of the basic theories namely, classical dynamics and quantum mechanics.

(ii) *This irreversibility pertains only to the probabilities* concerning this state of the system. Equation (20), or (4), gives a definite prediction of the *probable* result of an observation on the system. There is no conflict between the prediction of a probable increase in entropy and any fluctuation in an actual observation.

(iii) The two choices of the time arrow are, however, mutually exclusive in the sense that (20) is valid only for the prediction of the system at a later time, while (20a) is valid only for making a 'postdiction' – i.e. a statement about an earlier time, on the basis of the information at the (arbitrary) present instant.

(iv) Let us assume that a measurement of the 'fine-grained' entropy is made at an arbitrary instant, say $t = t^0$. Equations (20), (21) predict a greater (at least equal) entropy at any later instant $t > t_0$, let us say t_1. Let us assume that a second measurement of the fine-grained entropy is made on the system at t_1. Its *probable* value is given by (20) or (21) and the same equations predict the *probable* value of S_f at a time $t > t_1$, let say t_2. Equation (21) tells us that $S(t^0) \leqslant S(t_1) \leqslant S(t_2)$. This procedure can be continued to later times. By making the intervals $t_1 - t_0$. $t_2 - t_1 \ldots$ 'small' (but not arbitrary small), we may picture the entropy 'curve' from the instant $t = t^0$ as a sequence of points, which begins at $t = t^0$ and increases at later times, as indicated by the solid curve in Figure 2. But if an inquiry is made about the values of $S(\tau)$ at *earlier* instants, we have to use Equation (20 a) and (21 a) and we shall obtain an exactly symmetrical, but independent and separate, branch for the entropy 'curve', as indicated by the dotted curve in Figure 2.

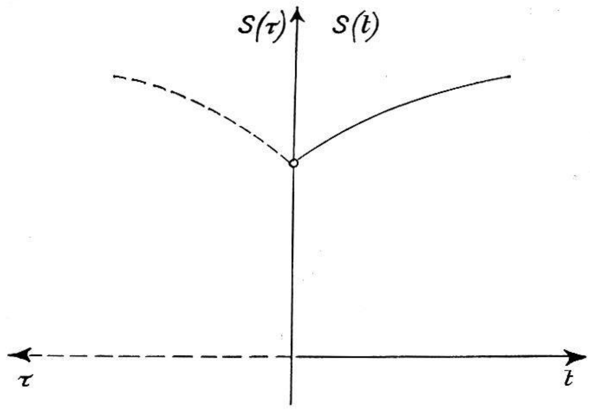

Fig. 2
Symmetrical 'entropy curres'

(v) From (ii) and (iv), it follows that *(22) and (22a) are mutually exclusive of each other* and that they do *not* imply

$$\frac{\Delta \varrho_{ii}}{\Delta t} = \frac{\Delta \varrho_i}{\Delta \tau} = 0$$

or equilibrium for the system.

(vi) If (20 a)–(22 a) 'postdict' that a system approaches an equilibrium state in the past in an irreversible manner, it is not to be interpreted to mean that a certain state of the system at present has *arisen from* an equilibrium state in the long, long past. To describe the evolution *from the past to the present,* one must use equations (20)–(22) which, however, do *not* describe a change from an equilibrium to a non-equilibrium state, but always describe an irreversible and monotonic approach to the equilibrium state.

(vii) While the two directions of time are on equal footing according to the basic theory (see (i) above), the 'postdiction' about an increase in entropy towards the *past* cannot be verified by comparison with observation, in the same way as a prediction about the future can be verified by observation. In fact, it is difficult to give any operational meaning to the 'postdicted' probabilities for the past. Thus, at least on the basis of our built-in biological time arrow, only (20)-22), describing irreversible evolutions towards equilibrium in the future in the ordinary sense, are of practical significance.

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