ARTICLES

Irreversible evolution of isolated quantum systems and a discreteness of time

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The statistical operators of those isolated nonrelativistic quantum systems that are presumed to exhibit intrinsically irreversible evolutionary behavior are shown to be capable of undergoing only discontinuous changes that occur at successive instants of time that are suggestive of possible temporal discreteness and that result in "mixed-state" conditions of the systems. Presuming such discrete temporal structure, a temporally asymmetric difference equation is derived for these statistical operators that suffices to imply their irreversible discontinuous evolution and from which both predictability and retrodictability of their temporal behavior are possible, but the latter cannot be extended indefinitely into the past.

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INTRODUCTION

From antiquity to the present, considerable attention from an enormous number of viewpoints has been devoted to time [1–5]. During the past century and a half, in particular, it has been devoted increasingly to the *irreversibility* which presumably [6] is characteristic of naturally occurring physical and chemical processes and to the *time directedness* [7] which is implied thereby. The attention to be given here is to expose a relationship existing between the two: how the irreversible behavior which may be exhibited by isolated quantum systems is involved in characterizing the times with which they are associated [8] and, conversely, how the times so designated are involved in characterizing the presumed [6] irreversible behavior of the systems. Our ultimate concern is the effects that their irreversibility may have on the equation of motion of their statistical operators.

Many aspects of irreversibility will not be addressed by the theory which is to be described here. However, it does establish a basic association of intrinsically irreversible evolutionary changes of isolated quantum systems with a discreteness of time. Furthermore, by yielding a temporally asymmetric equation of motion for their statistical operators, it also provides a direct and desirable conciliation of their irreversibility with their dynamics. These results of the theory motivate the exposition of the present paper. There are also others.

In the section that follows, we consider the time dependence of statistical operators of an isolated nonrelativistic quantum system. Two essentially kinematic basic assumptions are made regarding the temporal transformers which determine their evolutionary behavior; they are (i) the major premise of Huygens's principle due to Hadamard [9] and (ii) an axiom of noninvertibility of temporal transformers [6]. It then follows that all evolutionary changes in the resulting statistical operators must occur discontinuously at characteristic times compounded of consecutive discrete intervals of finite, nonzero, and indivisible duration [10] rather than of continua of durationless instants [11].

The intrinsic irreversible behavior of the resulting statistical operators, free of any additional constraints or external influences, is verified and illustrated in the next section. Two of the examples involve properties which consist solely of functions of the statistical operators. With passing time of finite duration, their expectation values can change only monotonically; in the usual quantum-mechanical description, they would never change. One of them shows that, contrary to conventional anticipation, a changing statistical operator originally in a "pure-state" condition cannot maintain such a condition but must evolve to form statistical "mixtures"; the other fulfills the well-known decreasing behavior of the $\mathcal{H}$ function of Boltzmann [12]. It is further shown that the mean-square fluctuation of the expectation value of an arbitrary time-independent observable about its temporally asymptotic value must vanish as time increases indefinitely; it would not do so in conventional quantum-mechanical terms [13].

In the succeeding section, a basic dynamical assumption is made regarding the temporal transformers; it is (iii) a conjecture of temporal-structure independence of laws of evolutionary dynamics. The result is a discrete temporally asymmetric equation of motion for statistical operators that reflects their discontinuous evolution. Formal solutions of the equation consist of Laplace averages of solutions of von Neumann's original temporally continuous equation [14]. Despite the noninvertibility of the resulting temporal transformers, the discrete equation of motion is readily "reversed." As a result, prior statistical operators can be calculated from a knowledge of later ones, with an accompanying retrodictability [15–17]. The latter, however, cannot be extended indefinitely into the past. In particular, retrodiction from a statistical operator in an evolving "pure-state" condition to yield any prior proper statistical operator proves to be impossible.

The time intervals which are characteristic in irreversible evolutionary processes are considered in the next section. A lower bound similar to a time-energy uncertainty relation is obtained for them in terms of the dispersion in the energy, the changes in a property used to determine them, and the precision of the latter. As a result, any reliable direct determination of them does not appear too promising, although the possibility of doing so from the changing properties of a two-state system is examined.

A brief summary is given in the final section concerning some of the results of the theory, together with pertinent comments. In particular, we note the supplemental role that idealized measurement processes have in promoting the irreversibility of the isolated systems considered here [6]. Similarly, the supportive bearing that the reversal of time, particle-antiparticle interchange, and spatial inversion (TCP) theorem of relativistic quantum field theory [18] may have on the present theory is considered. In a highly speculative vein, the possibility is mentioned of the limited retrodictability of the present theory being applicable to justify the currently held view of the finite age of the universe. Several appendixes contain various mathematical details of the theory which is developed here.

NONINVERTIBLE TEMPORAL TRANSFORMERS

A quantum system of interest here is an isolated member of a Gibbsian ensemble of identical nonrelativistic systems; it has a finite number of degrees of freedom and is confined to a region of space of finite extent. The measured values of its properties are to be identified with the expectation values of corresponding observables of the system. The operands of the latter are elements of a relevant Hilbert space [19]. A particularly important observable is the statistical operator of the system, which conforms to all the symmetry requirements of the system and contains all the information about the ensemble needed to determine the various expectation values. How this observable changes with the passage of time is our central concern.

To deal with this, we let $\rho(0)$ be an arbitrary statistical operator at some initial instant of time, designated as 0, which evolves [20] to yield a statistical operator $\boldsymbol{\rho}(t)$ at a later finite instant of time t [21]. To express this, we suppose that there exists a linear identity-preserving temporal transformer $\mathbf{T}\,[t;\cdots]$ of the system's statistical operators such that, for $t \geq 0$,

$$\mathbf{T}[t;\boldsymbol{\rho}(0)]=\boldsymbol{\rho}(t)\ , \tag{1}$$

$$\boldsymbol{\rho}^{\dagger}(t)=\boldsymbol{\rho}(t)\ , \tag{2}$$

$$0 \leq \boldsymbol{\rho}(t)\ , \tag{3}$$

and [22]

$$\mathrm{Tr}\boldsymbol{\rho}^2(t) \leq \mathrm{Tr}\boldsymbol{\rho}(t)=1\ . \tag{4}$$

As shown in Appendix A, the most general temporal transformer then must have the following form [23]:

$$\mathbf{T}[t;\cdots]=\sum_n \lambda_n \mathbf{S}_n(t)[\cdots]\mathbf{S}_n^{\dagger}(t)\ , \tag{5}$$

where

$$\sum_n \lambda_n=1,\quad \lambda_n^*=\lambda_n \geq 0,\quad \text{all } n\ , \tag{6}$$

$$\sum_n \lambda_n \mathbf{S}_n(t)\mathbf{S}_n^{\dagger}(t)=\sum_n \lambda_n \mathbf{S}_n^{\dagger}(t)\mathbf{S}_n(t)=\mathbf{I}\ , \tag{7}$$

and

$$\mathbf{S}_n(0)=\mathbf{S}_n^{\dagger}(0)=\mathbf{I},\quad \text{all } n\ . \tag{8}$$

We now introduce two basic assumptions.

(i) The major premise of Huygens's principle due to Hadamard [9]. In the present context, a statistical operator $\boldsymbol{\rho}(t)$, which has evolved from an arbitrary initial statistical operator $\boldsymbol{\rho}(0)$, may be regarded equally well as having evolved from an intermediate statistical operator $\boldsymbol{\rho}(t')$, $t \geq t' \geq 0$, where $\boldsymbol{\rho}(t')$ has evolved from $\boldsymbol{\rho}(0)$. Expressed mathematically, we suppose that

$$\mathbf{T}[t;\boldsymbol{\rho}(0)]=\mathbf{T}[t-t';\mathbf{T}[t';\boldsymbol{\rho}(0)]],\quad t \geq t' \geq 0\ . \tag{9}$$

(ii) An axiom of noninvertibility of temporal transformers. In the present context, a statistical operator $\boldsymbol{\rho}(t)$, which has evolved from an arbitrary initial statistical operator, $\boldsymbol{\rho}(0)$, $t \geq 0$, cannot have its temporal behavior formally inverted to yield the original one. Expressed mathematically, we suppose that

$$\mathbf{T}[-t;\mathbf{T}[t;\boldsymbol{\rho}(0)]] \neq \mathbf{T}[0;\boldsymbol{\rho}(0)],\quad t>0\ . \tag{10}$$

Since the left-hand side may be interpreted as representing a statistical operator that has presumably undergone an evolutionary process which has been followed by its detailed reversal without the action of any external agent, the axiom is equivalent to an assumption of intrinsic irreversibility [6] of the temporal evolution of isolated quantum systems.

To obtain the consequences of these assumptions, we get from Eqs. (5) and (9),

$$\sum_n \lambda_n \mathbf{S}_n(t)\boldsymbol{\rho}(0)\mathbf{S}_n^{\dagger}(t) =\sum_{n,m} \lambda_m \lambda_n \mathbf{S}_m(t-t')\mathbf{S}_n(t')\boldsymbol{\rho}(0)\mathbf{S}_n^{\dagger}(t')\mathbf{S}_m^{\dagger}(t-t')\ , \quad t \geq t' \geq 0\ . \tag{11}$$

Since the left-hand side of this equation is independent of t', so is the right-hand side. Then since the initial statistical operator is arbitrary [but conforms to Eqs. (2)–(4)], we must have the time independence expressed by

$$\delta_{t'}\{\mathbf{S}_m(t-t')\mathbf{S}_n(t')\boldsymbol{\rho}(0)\mathbf{S}_n^{\dagger}(t')\mathbf{S}_m^{\dagger}(t-t')\}=\mathbf{0}\ , \quad \text{all } m,n,\ t \geq t' \geq 0\ . \tag{12}$$

If the transformation operators were to be continuous functions of nonconstant t', it would follow that

$$\mathbf{S}_m(t-t')\mathbf{S}_n(t')\boldsymbol{\rho}(0)\mathbf{S}_n^\dagger(t')\mathbf{S}_m^\dagger(t-t')=\mathbf{A}_{mn}(t)\ ,\quad \text{all } m,n,\ t\ge t'\ge 0\ . \tag{13}$$

Then, by Eq. (8) and with $t'\to 0,t$, it would further follow that

$$\mathbf{S}_m(t)\boldsymbol{\rho}(0)\mathbf{S}_m^\dagger(t)=\mathbf{A}_{mn}(t)=\mathbf{S}_n(t)\boldsymbol{\rho}(0)\mathbf{S}_n^\dagger(t)\ ,\quad \text{all } m,n,\ t\ge 0\ . \tag{14}$$

As a result, we would obtain from Eq. (5),

$$\mathbf{T}[t;\cdots]=\sum_n \lambda_n \mathbf{S}_n(t)[\cdots]\mathbf{S}_n^\dagger(t) =\mathbf{S}(t)[\cdots]\mathbf{S}^\dagger(t),\quad t\ge 0\ , \tag{15}$$

where

$$\mathbf{S}(t)=\mathbf{S}_m(t),\quad \text{all } m,\ t\ge 0\ , \tag{16}$$

and, by Eq. (7),

$$\mathbf{S}(t)\mathbf{S}^\dagger(t)=\mathbf{I},\quad t\ge 0\ . \tag{17}$$

Since

$$\mathbf{S}^\dagger(t)=\mathbf{S}^{-1}(t)=\mathbf{S}(-t)\ , \tag{18}$$

the resulting temporal transformers would evidently be invertible [24] and would thus be incompatible with assumption (ii), Eq. (10).

Accordingly, we must conclude that an isolated quantum system of which the temporal evolution is intrinsically irreversible [6] not only must have noninvertible temporal transformers of the form of Eq. (5), but they must also not be continuous nonconstant functions of time [25]. The statistical operators must change only discontinuously as they evolve, which behavior can be expressed by

$$\boldsymbol{\rho}(t)=\boldsymbol{\rho}(0)+\sum_{n=1}^{\infty}[\boldsymbol{\rho}(t_n)-\boldsymbol{\rho}(t_{n-1})]\Theta(t-t_n)\ ,\quad t_n>t_{n-1},\ t_0=0\ , \tag{19}$$

with

$$\boldsymbol{\rho}(t_n)=\mathbf{T}[t_n-t_{n-1};\boldsymbol{\rho}(t_{n-1})],\quad n\ge 1\ , \tag{20}$$

where Θ is the Heaviside unit function of its argument. Since these statistical operators have values only corresponding to those at the instants $\{t_n\}$, Eqs. (19) and (20) indicate a discreteness of time that correlates with the changes that occur in the system [8] as a consequence of their irreversibility—or, possibly, the converse [26]. Accordingly, the time involved is expressible as

$$t=\sum_{n=1}^{\infty}(t_n-t_{n-1})\Theta(t-t_n) \equiv \sum_{n=1}^{\infty}\tau_n\Theta(t-t_n),\quad \tau_n>0,\ \text{all } n\ . \tag{21}$$

NONINVERTIBILITY AND IRREVERSIBILITY

To verify that irreversible behavior is indeed exhibited by an isolated quantum system which manifests noninvertibility of its temporal transformers, we examine three of its properties. It is to be emphasized that the demonstrated irreversibility requires neither the exploitation of any detailed dynamics pertaining to the system nor the incorporation of any external influences to act on it.

The first property, by Eqs. (5), (20), and (21), is

$$\mathrm{Tr}\boldsymbol{\rho}^2(t_n)=\sum_{j,k}\lambda_j\lambda_k\mathrm{Tr}\{\mathbf{S}_j^\dagger(\tau_n)\mathbf{S}_k(\tau_n)\boldsymbol{\rho}(t_{n-1}) \times\mathbf{S}_k^\dagger(\tau_n)\mathbf{S}_j(\tau_n)\boldsymbol{\rho}(t_{n-1})\}\ . \tag{22}$$

As a result of straightforward manipulation, it can then be readily verified that

$$\mathrm{Tr}\boldsymbol{\rho}^2(t_{n-1})-\mathrm{Tr}\boldsymbol{\rho}^2(t_n) =\tfrac{1}{2}\sum_{j,k}\lambda_j\lambda_k\mathrm{Tr}\{[\mathbf{S}_j^\dagger(\tau_n)\mathbf{S}_k(\tau_n),\boldsymbol{\rho}(t_{n-1})] \times[\boldsymbol{\rho}(t_{n-1}),\mathbf{S}_k^\dagger(\tau_n)\mathbf{S}_j(\tau_n)]\}\ge 0\ . \tag{23}$$

As shown in Appendix B, the equality cannot be realized at any finite time. Hence $\mathrm{Tr}\boldsymbol{\rho}^2(t_n)$ must be a monotonic decreasing function in any finite time interval, viz.

$$\mathrm{Tr}\boldsymbol{\rho}^2(t_n)<\mathrm{Tr}\boldsymbol{\rho}^2(t_{n-1}),\quad t_n<\infty\ . \tag{24}$$

This is in marked contrast to the constancy it would maintain in terms of the usual quantum-mechanical description. Furthermore, an asymptotic statistical operator

$$\boldsymbol{\rho}(\infty)\equiv\lim_{t_n\to\infty}\boldsymbol{\rho}(t_n) \tag{25}$$

must exist. This is also contrary to the behavior that results from conventional quantum theory, but is usually expected from irreversibility [27,28].

Equation (24) has an important consequence: if it changes at all, any statistical operator initially consisting of a projection, corresponding to a "pure-state" condition of the system, cannot continue in such a condition as time passes, but must evolve to form "mixtures" [29]. This follows from Eq. (24) since, then,

$$\mathrm{Tr}\boldsymbol{\rho}^2(t_n)<\mathrm{Tr}\boldsymbol{\rho}^2(0)=\mathrm{Tr}\boldsymbol{\rho}(0)=\mathrm{Tr}\boldsymbol{\rho}(t_n)\ ,\quad \text{all } t_n<0\ . \tag{26}$$

As a consequence, the usual quantum-mechanical time-dependent equation of Schrödinger [30] will not have a fundamental role in the present theory. (It will have an important one, nevertheless, as we shall see later.)

As another property, we consider the long-term mean-square fluctuation of the time-dependent expectation value of an arbitrary time-independent observable $\boldsymbol{\alpha}$ about its long-term average value, which we express by [23]

$$\Phi(\alpha;t_n)\equiv\sum_{k=0}^{\infty}w_k[\mathrm{Tr}\{\boldsymbol{\rho}(t_{n+k})\boldsymbol{\alpha}\}-\mathrm{Tr}\{\boldsymbol{\rho}(\infty)\boldsymbol{\alpha}\}]^2\ , \tag{27}$$

where

$$\sum_{k=0}^{\infty}w_k=1,\quad 0\le w_k^*=w_k\le 1\ . \tag{28}$$

Since the series of Eq. (27) is bounded from above by its maximum term, whatever the distribution may be, Eq. (25) immediately yields

$$0 \le \lim_{n\to\infty} \Phi(\alpha;t_n) \le \lim_{n\to\infty} \max[\mathrm{Tr}\{\boldsymbol{\rho}(t_{n+k})\boldsymbol{\alpha}\} - \mathrm{Tr}\{\boldsymbol{\rho}(\infty)\boldsymbol{\alpha}\}]^2 = 0 \ . \quad (29)$$

Thus expectation values of those time-independent observables that do not even exhibit monotonic temporal changes must ultimately achieve genuine asymptotic values, in marked contrast to the ceaseless fluctuations expected of them from the usual description of isolated quantum systems [13,27,28].

Finally, we consider the $\mathcal{H}$ function of Boltzmann [12,23],

$$\mathcal{H}(t_n) \equiv \mathrm{Tr}\boldsymbol{\rho}(t_n)\ln\boldsymbol{\rho}(t_n) = \sum_j \rho_j(t_n)\ln\rho_j(t_n) \ , \quad (30)$$

where $\{\rho_j(t_n)\}$ is the set of eigenvalues of $\boldsymbol{\rho}(t_n)$ which satisfies

$$\langle \psi_j | \boldsymbol{\rho}(t_n) | \psi_k \rangle = \rho_j(t_n)\delta_{jk} \ . \quad (31)$$

Upon introducing the eigenvalues $\{\rho_j(t_{n-1})\}$ of $\boldsymbol{\rho}(t_{n-1})$ which satisfy

$$\langle \phi_j | \boldsymbol{\rho}(t_{n-1}) | \phi_k \rangle = \rho_j(t_{n-1})\delta_{jk} \ , \quad (32)$$

we can obtain, after straightforward manipulation with the aid of Eqs. (5), (20), and (21),

$$\begin{aligned}\mathcal{H}(t_n) &= \sum_j \left\{ \sum_k \sum_m \lambda_m |\langle \psi_j | \mathbf{S}_m(\tau_n) | \phi_k \rangle|^2 \rho_k(t_{n-1}) \ln \sum_k \sum_m \lambda_m |\langle \psi_j | \mathbf{S}_m(\tau_n) | \phi_k \rangle|^2 \rho_k(t_{n-1}) \right\} \\ &\le \sum_j \left\{ \sum_k \sum_m \lambda_m |\langle \psi_j | \mathbf{S}_m(\tau_n) | \phi_k \rangle|^2 \rho_k(t_{n-1}) \ln \sum_k \sum_m \lambda_m |\langle \psi_j | \mathbf{S}_m(\tau_n) | \phi_k \rangle|^2 \right\} \\ &\quad + \sum_j \left\{ \sum_k \sum_m \lambda_m |\langle \psi_j | \mathbf{S}_m(\tau_n) | \phi_k \rangle|^2 \rho_k(t_{n-1}) \ln\rho_k(t_{n-1}) \right\} \ , \end{aligned} \quad (33)$$

the inequality resulting from a general convexity inequality [31]. Since, by Eq. (7),

$$\sum_j \sum_m \lambda_m |\langle \psi_j | \mathbf{S}_m(\tau_n) | \phi_k \rangle|^2 = \sum_k \sum_m \lambda_m |\langle \psi_j | \mathbf{S}_m(\tau_n) | \phi_k \rangle|^2 = 1 \ , \quad (34)$$

we obtain

$$\mathcal{H}(t_n) \le \sum_k \rho_k(t_{n-1})\ln\rho_k(t_{n-1}) \equiv \mathcal{H}(t_{n-1}) \ , \quad (35)$$

in agreement with the celebrated $\mathcal{H}$ theorem of Boltzmann [12], originally obtained on the basis of classical-mechanical considerations [32]. However, because of Eq. (24), we evidently must have the monotonic behavior

$$\mathcal{H}(t_n) < \mathcal{H}(t_{n-1}), \quad t_n < \infty \ , \quad (36)$$

which is sometimes referred to as the generalized $\mathcal{H}$ theorem [33].

From the foregoing examples, it is clear that the evolution of statistical operators expressed by Eqs. (5) and (19)–(21) is manifestly irreversible, but in a stronger sense than is usually understood. Especially in the case of the $\mathcal{H}$ function, one ordinarily expects that statistical fluctuations can occur on occasion in macroscopic systems to reverse the pertinent monotonic behavior, although the fluctuations are presumed not to be very likely [32,33]. No such reversal is possible for the expectation values considered here.

TEMPORALLY ASYMMETRIC EQUATION OF MOTION

So far, the temporal transformers we have considered have conformed to essentially kinematical constraints which have been imposed on them. We now examine the effect of imposing a basic dynamical restriction.

(iii) A conjecture of temporal-structure independence of laws of evolutionary dynamics. In the present context, when expressed in integral-equation form, the dynamical laws which determine the evolutionary changes that produce a statistical operator $\boldsymbol{\rho}(t)$, from an arbitrary initial statistical operator $\boldsymbol{\rho}(0)$, $t \ge 0$, are independent of whether time is continuous or discrete in structure. In mathematical terms, we suppose that [34]

$$\mathbf{T}[t;\boldsymbol{\rho}(0)] - \mathbf{T}[0;\boldsymbol{\rho}(0)] = \int_0^t dt' \mathbf{K}[t';\boldsymbol{\rho}(0)] \ , \quad t \ge 0 \ , \quad (37)$$

where the kernel $\mathbf{K}[t';\boldsymbol{\rho}(0)]$ is an operator which is assumed to be independent of the structure of time and is yet to be determined; the integral is a Stieltjes integral [35], the evaluation and ensuing consequences of which do depend on the structure of time.

Because conventional quantum theory treats time as continuous in nature, we can determine $\mathbf{K}[t;\boldsymbol{\rho}(0)]$ since Eq. (37) must then reduce to the equation of motion of von Neumann [14] for the statistical operator, viz. [34,36]

$$\frac{\partial \boldsymbol{\rho}(t)}{\partial t} = -i[\mathbf{H},\boldsymbol{\rho}(t)] \ , \quad (38)$$

where **H** is the time-independent Hermitian Hamiltonian of the system of interest [36]. In temporally continuous circumstances we obtain

$$\frac{\partial \rho(t)}{\partial t} = \lim_{t^* \to t} \{\mathbf{T}[t^*;\rho(0)] - \mathbf{T}[t;\rho(0)]\}/\{t^* - t\}$$
$$= \lim_{t^* \to t} \left\{ \int_t^{t^*} dt' \mathbf{K}[t';\rho(0)] \right\} / \{t^* - t\}$$
$$= \mathbf{K}[t;\rho(0)] , \tag{39}$$

so that

$$\mathbf{K}[t;\rho(0)] = -i[\mathbf{H},\rho(t)] , \tag{40}$$

where ρ is presumably a continuous function of its argument.

Hence, after appropriate transcription, Eq. (37) becomes

$$\rho(t) - \rho(0) = -i \left[\mathbf{H}, \int_0^t dt' \rho(t') \right] . \tag{41}$$

From this, we see that the irreversible evolutionary behavior that may be anticipated for statistical operators is to be ascribed directly to the discreteness of time, Eq. (21), rather than to any intrinsic discontinuous behavior of the operators themselves. When, as suggested by Eqs. (19) and (20), a step-function behavior is also assumed for ρ, contrary to the continuous behavior required of it, the resulting statistical operator proves to be invertible and, hence, cannot exhibit the irreversible behavior required of it by assumption (ii); the details are given in Appendix C. We thus obtain with the aid of Eq. (21),

$$\rho(t) - \rho(0) = -i \left[\mathbf{H}, \sum_{n=1}^{\infty} \tau_n \rho(t_n) \Theta(t - t_n) \right]$$
$$= \sum_{n=1}^{\infty} \{ -i\tau_n [\mathbf{H},\rho(t_n)] \} \Theta(t - t_n) . \tag{42}$$

Now it is evident, despite an intrinsic continuity required of ρ, that the consequent $\rho(t)$ must have the step-function behavior expressed by Eqs. (19) and (20), whereupon it follows that

$$\rho(t_n) - \rho(t_{n-1}) = -i\tau_n [\mathbf{H},\rho(t_n)], \quad n \ge 1 . \tag{43}$$

This is the discrete temporally asymmetric equation of motion that we seek, which reflects the irreversible evolutionary behavior of isolated quantum systems.

Since

$$\lim_{t_n \to \infty} \mathrm{Tr}[\mathbf{H},\rho(t_n)][\rho(t_n),\mathbf{H}]$$
$$= \lim_{t_n \to \infty} \mathrm{Tr}[\rho(t_n) - \rho(t_{n-1})]^2/\tau_n^2$$
$$= 0 , \tag{44}$$

by Eqs. (21) and (25), it now follows that

$$[\mathbf{H},\rho(\infty)] = \mathbf{0} . \tag{45}$$

An immediate dynamical consequence of irreversibility is thus seen to be that the asymptotic statistical operator of an isolated quantum system $\rho(\infty)$ is a temporal invariant, as might have been anticipated. It is to be noted, however, that the resulting restriction on the asymptotic statistical operator is not sufficient to characterize statistical mechanical equilibrium, only necessary.

Equation (43) can be recognized as a Laplace average of von Neumann's original equation [37], with the solution

$$\rho(t_n) = \int_0^\infty dx \, \{ e^{-ix\tau_n \mathbf{H}} \rho(t_{n-1}) e^{+ix\tau_n \mathbf{H}} \} , \quad n \ge 1 . \tag{46}$$

As a result, we can now give an explicit expression for the temporal transformers that describe the evolutionary behavior of an isolated quantum system. It is

$$\mathbf{T}[t; \cdots] = \mathbf{T}\left[\sum_{n=1}^{\infty} \tau_n \Theta(t - t_n); \cdots \right]$$
$$= \prod_{n=1}^{\infty} \mathbf{T}[\tau_n \Theta(t - t_n); \cdots]$$
$$= \prod_{n=1}^{\infty} \int_0^\infty dx_n \{ e^{-x_n} e^{-ix_n \tau_n \Theta(t - t_n)\mathbf{H}} [\cdots] e^{+ix_n \tau_n \Theta(t - t_n)\mathbf{H}} \} , \tag{47}$$

which is evidently a multiple Laplace average of a solution of von Neumann's equation [14]. To identify with Eq. (5), we need only represent

$$\sum_m \lambda_m \{ \cdots \} \to \int_0^\infty dx_n e^{-x_n} \{ \cdots \} \tag{48}$$

and

$$\mathbf{S}_m(\tau_n) \to e^{-ix_n \tau_n \Theta(t - t_n)\mathbf{H}} . \tag{49}$$

Because of the form of Eq. (47), it is clear that many properties of an irreversibly evolving isolated quantum system will be the same as those obtained with appropriate Laplace averages of reversibly evolving statistical operators [13,37–39]. As a result, the solutions of Schrödinger's time-dependent equation [30] or its von Neumann counterpart [14]—either exact or approximate—provide an important starting point in describing the actual irreversible behavior of an isolated quantum system.

The temporal asymmetry of Eq. (43) is reflected in the fact that changing the sign of τ_n in its solution, Eq. (46), without changing the sign of **H** (since it is presumably independent of τ_n), does not produce a statistical operator for an earlier instant of time from one to which it could have evolved at a later instant. There is, accordingly, no possibility of time-reversal invariance, i.e., reversibility, of the evolutionary processes characterized by these equations. Nevertheless, the equation of motion does enable a prior statistical operator to be determined readily from a subsequent one, viz.

$$\rho(t_{n-1})=\rho(t_n)+i\tau_n[\mathbf{H},\rho(t_n)], \quad n\geq 1 \ . \tag{50}$$

As a consequence, it is possible to calculate the past behavior of an isolated quantum system [15–17], viz. to retrodict its behavior, as well as to calculate its future behavior, viz. to predict its behavior, both from a knowledge of the system's initial statistical operator, its Hamiltonian, and the characteristic time intervals $\{\tau_n\}$. The resulting predictability-retrodictability duality that exists despite an irreversibility of the basic equation of motion has long been unexpected [40].

Nevertheless, the present retrodictability has an important limitation not shared by the predictability: it cannot be realistically extended indefinitely. To show this, we obtain, as a result of straightforward manipulations involving Eq. (50), that

$$\mathrm{Tr}\rho^2(t_{n-1})-\mathrm{Tr}\rho^2(t_n) =\tau_n^2\mathrm{Tr}[\mathbf{H},\rho(t_n)][\rho(t_n),\mathbf{H}]>0 \ , \quad \infty>n\geq 1 \ , \tag{51}$$

in accord with Eq. (24); the latter inequalities follow from Eqs. (21) and (45). We may, therefore, choose an origin of time t_0 to correspond to that instant for which

$$\mathrm{Tr}\rho^2(t_{-1})>1\geq \mathrm{Tr}\rho^2(t_0), \quad t_{-1}>t_0=0 \ . \tag{52}$$

But the lower bound inequality at t_{-1} constitutes a violation of Eq. (4) unless we understand it to mean that no proper statistical operators, viz. satisfy Eqs. (2)–(4), can have existed for $t_n<0$ which would have evolved to produce proper ones for $t_n\geq 0$. With this understanding, an isolated quantum system considered here which currently undergoes changes can only have a determinable history that is limited to a finite past.

The foregoing limitation is especially striking when a system of interest is in a changing condition corresponding to a "pure state" at some finite instant of time. With no loss of generality, we may designate that instant as the temporal origin, whereupon retrodiction from that instant to yield any proper statistical operator from which the original one may have evolved is impossible. As we observed earlier, an isolated quantum system in a nonstationary "pure-state" condition can evolve only to form "mixtures." We have now shown that an isolated quantum system in a nonstationary "mixture" condition cannot evolve to form "pure states." The latter can be produced only by processes which reflect the influence of external agents of some sort upon the otherwise isolated quantum system of interest.

DETERMINABILITY OF CHARACTERISTIC TIME INTERVALS

Qualitative features of the irreversible evolutionary behavior that an isolated quantum system is presumed to exhibit appear to be adequately accounted for by the theory we have described. The quantitative features of that behavior, however, are another matter. For the latter to be dealt with by the theory, knowledge of the characteristic time intervals $\{\tau_n\}$ is needed, a knowledge which is currently unavailable [26].

If time were to be intrinsically discrete in nature, its constituent time intervals could not be determined with precision by direct measurement. Any material clock which might be used to do so would itself be limited by inherent temporal discreteness: it could not measure reliably any duration smaller than the smallest of its own time intervals. To determine the latter, also reliably, another clock that could measure time intervals of even smaller duration would be needed. These, in turn, would require additional clocks capable of determining still smaller time intervals that, ultimately, would be required to be vanishingly small. As a result, time would have to be intrinsically continuous and the systems that could serve as clocks to measure it would have to evolve essentially continuously. Just such behavior is exhibited by systems that can be described in classical dynamical terms, as is shown in Appendix D. Determination of the time intervals $\{\tau_n\}$ pertinent to various isolated quantum systems is thus possible in principle, although there will be inherent limitations on their measurability [41–44].

In order to see how the temporal behavior of an isolated quantum system may be utilized to obtain some measure of the values of the $\{\tau_n\}$, we consider solutions of Eq. (43). Guided by the successes which have resulted from conventional quantum-mechanical theory in which time has been treated as continuous in nature, we will only consider situations where

$$\tau_m \ll t_n, \quad \text{all } m, \ t_n>0 \ . \tag{53}$$

In terms of a basis of energy eigenfunctions $\{|\psi_k\rangle\}$, which satisfy

$$\langle\psi_j|\mathbf{H}|\psi_k\rangle=E_k\delta_{jk} \ , \tag{54}$$

we obtain

$$\langle\psi_j|\rho(t_n)|\psi_k\rangle=\frac{\langle\psi_j|\rho(t_{n-1})|\psi_k\rangle}{1+i\tau_n(E_j-E_k)}=\frac{\langle\psi_j|\rho(0)|\psi_k\rangle}{\prod_{m=1}^{n}[(1+i\tau_m(E_j-E_k)]}$$
$$=\langle\psi_j|\rho(0)|\psi_k\rangle\exp\left\{-\sum_{m=1}^{n}\ln[1+i\tau_m(E_j-E_k)]\right\}, \quad t_n>0 \ . \tag{55}$$

We further restrict our attention to those systems for which

$$\tau_m^p |E_j - E_k|^p \ll 1, \quad \infty > m, \quad p > 0 , \tag{56}$$

i.e., the τ_m's are intrinsically small. We may then expand the logarithm in a power series and retain the real and imaginary terms of lowest order to get

$$\langle \psi_j|\rho(t_n)|\psi_k\rangle \doteq \langle \psi_j|\rho(0)|\psi_k\rangle \exp\{-it_n(E_j-E_k)\} \times \exp\{-\tfrac{1}{2}t_n\langle\tau\rangle_n(E_j-E_k)^2\} , \quad t_n > 0 , \tag{57}$$

where

$$t_n = \sum_{m=1}^{n} \tau_m \tag{58}$$

and

$$\langle\tau\rangle_n \equiv \sum_{m=1}^{n} \tau_m^2 \Big/ \sum_{m=1}^{n} \tau_m \geq \sum_{m=1}^{n} \tau_m/n \equiv \bar{\tau}_n . \tag{59}$$

$\langle\tau\rangle_n$ is an effective characteristic time interval and $\bar{\tau}_n$ is a mean characteristic time interval, both of which may have values that depend on the prevailing distribution of the τ_m's. This, however, is unknown so that it may be possible at most only to determine $\langle\tau\rangle_n$ from the observed evolutionary behavior of the system.

Before considering how, we note that Eq. (57) gives explicit expression to the irreversible behavior we have already described. For example, as $t_n \to \infty$, we see that

$$\lim_{t_n\to\infty} \langle \psi_j|\rho(t_n)|\psi_k\rangle = \langle \psi_j|\rho(0)|\psi_k\rangle \delta_{E_jE_k} , \tag{60}$$

so that Eq. (45) is fulfilled. We also see, as previously noted, how the solutions of von Neumann's original equation of motion—the first two factors of the right-hand side of Eq. (57)–can serve as a starting point in describing the aforementioned irreversible behavior.

Perhaps the simplest and least ambiguous quantitative test of the present theory can come from an application of Eq. (57) to a real two-state system in which the actual lack of isolation from its surroundings can be properly taken into account. Then, if $\boldsymbol{\alpha}$ is an appropriate time-independent observable, its time-dependent expectation value would be

$$\langle\alpha(t_n)\rangle \equiv \mathrm{Tr}\boldsymbol{\rho}(t_n)\boldsymbol{\alpha} \doteq \sum_{k=1}^{2} \langle\psi_k|\boldsymbol{\rho}(0)|\psi_k\rangle\langle\psi_k|\boldsymbol{\alpha}|\psi_k\rangle + 2\,\mathrm{Re}[\langle\psi_1|\boldsymbol{\rho}(0)|\psi_2\rangle\langle\psi_2|\boldsymbol{\alpha}|\psi_1\rangle\exp\{-it_n(E_1-E_2)\}]\exp\{-\tfrac{1}{2}t_n\langle\tau\rangle_n(E_1-E_2)^2\} , \quad t_n>0 . \tag{61}$$

Presuming that $\langle\tau\rangle_n$ is independent of n, i.e., t_n, the two-state system should exhibit a damped oscillatory decay of the expectation value $\langle\alpha(t_n)\rangle$ to a temporally asymptotic value $\langle\alpha(\infty)\rangle$. The oscillating frequency and the decay constant are so related that their determined values would permit $\langle\tau\rangle_n$ to be obtained. All depends, of course, on being able to surmount the lack of isolation of the real system from its surroundings.

As a final matter, we consider a lower bound for the $\langle\tau\rangle_n$ that can serve to expose the limitations on their determinability, whatever their duration may be. Let $\boldsymbol{\alpha}$ be an arbitrary time-independent observable. Then, by Eq. (43) and the properties of the trace, the change in its expectation value is

$$\langle\alpha(t_n)\rangle - \langle\alpha(t_{n-1})\rangle \equiv \mathrm{Tr}\boldsymbol{\rho}(t_n)\boldsymbol{\alpha} - \mathrm{Tr}\boldsymbol{\rho}(t_{n-1})\boldsymbol{\alpha} = -i\tau_n \mathrm{Tr}[(\boldsymbol{\alpha}-\lambda\mathbf{I}),\boldsymbol{\rho}(t_n),(\mathbf{H}-\mu\mathbf{I})] , \tag{62}$$

where

$$[\mathbf{A},\mathbf{B},\mathbf{C}] = \mathbf{ABC}-\mathbf{CBA} \tag{63}$$

and λ and μ are arbitrary parameters. After straightforward manipulation involving the Cauchy-Schwarz-Buniakowsky inequality [45] we can obtain

$$|\langle\alpha(t_n)\rangle - \langle\alpha(t_{n-1})\rangle| \leq 2\tau_n \Delta^{1/2}(\alpha;t_n)\Delta^{1/2}(H) , \tag{64}$$

where

$$\Delta(\alpha;t_n) \equiv \mathrm{Tr}\boldsymbol{\rho}(t_n)(\boldsymbol{\alpha}-\langle\alpha(t_n)\rangle)^2 \tag{65}$$

and

$$\Delta(H) \equiv \mathrm{Tr}\boldsymbol{\rho}(t_n)(\mathbf{H}-\langle H\rangle)^2, \quad n>0 \tag{66}$$

are the dispersions in the indicated properties, the latter one in the energy being a temporal invariant. Now, for the expectation-value change to be determined with adequate precision, we must require that

$$|\langle\alpha(t_n)\rangle - \langle\alpha(t_{n-1})\rangle| \gg \Delta^{1/2}(\alpha;t_n) . \tag{67}$$

Hence we obtain

$$\tau_n\Delta^{1/2}(H) \geq \frac{|\langle\alpha(t_n)\rangle - \langle\alpha(t_{n-1})\rangle|}{2\Delta^{1/2}(\alpha;t_n)} \gg \frac{1}{2}, \quad n>0 . \tag{68}$$

This relation bears a resemblence to what is sometimes referred to as a time-energy uncertainty relation [46], but it is not one [47,48]. Although the precision with which the energy of a system can be measured is not restricted by the time interval generally involved in such a measurement [48], the restriction here is justified since it involves the time intervals which are intrinsic to the changes that occur in the system [8], i.e., the changing system is acting formally as its own clock [48]. It involves, in addition, certain of the changes in the expectation values of some appropriate time-independent observable that occur and their precision [46]. It would appear that when these changes are to be determined even with moderate precision, τ_n's of extremely short duration will require the system to be in a condition that exhibits a large uncertainty in its energy. As a result, the reliable determination of such characteristic time intervals does not appear too promising.

An additional indication of inherent difficulty arises when one examines the time t_n for which the off-diagonal elements of Eq. (57) become extremely small. For energy differences that are comparable with or greater than $\Delta^{1/2}(H)$, which certainly includes a good portion of those possible, we see from Eq. (68) that

$$\tfrac{1}{2}t_n\langle\tau\rangle_n(E_j-E_k)^2 \geq \tfrac{1}{2}t_n\langle\tau\rangle_n\Delta(H) \gg \tfrac{1}{4}(t_n\langle\tau\rangle_n/\tau_n^2) \ . \tag{69}$$

Assuming that $\langle\tau\rangle_n$ and τ_n are comparable, we further see that

$$\exp\{-\tfrac{1}{2}t_n\langle\tau\rangle_n(E_j-E_k)^2\} \ll \exp\{-\tfrac{1}{4}(t_n/\tau_n)\} \ , \tag{70}$$

which, by Eq. (53), will be extremely small. In fact, even if t_n is just a moderate multiple of τ_n, negligible values would result for the pertinent matrix elements of the statistical operator. Except for those pairs of energy eigenstates that differ only slightly in energy, the latter would then be "almost diagonal in energy" and would appear to evolve seemingly reversibly—with evident difficulty in reliably determining the τ_n's in such circumstances.

SUMMARY AND COMMENTS

Of the many aspects of irreversibility that the theory described here does not address [49], we shall take note–only briefly—of the role played by idealized measurement processes [50]. These impose abrupt, discontinuous changes in the conditions of a system being measured and so bear some similarity to the basic evolutionary behavior accorded it by the present theory. Indeed, the irreversibility of the idealized measurement process [51] and that of the present evolutionary behavior are essential features common to both. The changes accompanying the measurements, however, involve the action of external agents upon the system [52] and so contrast markedly with those experienced by the isolated systems considered here. In the present context, idealized measurement processes can serve only to augment the intrinsic irreversibility we have found for them.

The three physical assumptions on which the present theory is based merit some comment.

(i) The first assumption, the Huygens-Hadamard principle premise, seems entirely reasonable in the sense that it expresses a feature of determinism that a proper physical theory should have [9].

(ii) The second assumption, essentially an assumption of evolutionary irreversibility, is a reasonable asymptotic extrapolation of observed behavior [6].

(iii) The third assumption, that dynamical laws of evolutionary behavior expressed in integral-equation terms rather than in differential-equation terms are independent of the structure of time, is clearly a conjecture, but seems to be a reasonable way to bridge the temporally continuous with the temporally discrete.

Of the three assumptions, the second might appear to be the primary one, since invertible transformers which exhibit reversible behavior can easily satisfy the constraints of the other two. But that assumption alone can be satisfied by the transformers which can be associated with idealized measurement processes, so that all three assumptions we have made seem to be not only sufficient but necessary to produce the results we have obtained [53].

A few of the results which have been obtained here also merit some comment.

(i) Although the discreteness in time expressed in Eq. (21) and used to derive Eq. (43) proves to be both necessary and sufficient for the irreversible behavior of the isolated systems considered here, there is no reason at present to believe that such discreteness is an intrinsic characteristic of time itself, independent of the actual quantum system involved [6]. Accordingly, to give rise to their temporally discrete behavior, a distinct possibility must be considered that evolving systems may change on a more fundamental level than the one with which we have dealt. Perhaps a temporally discrete hidden-variables theory might accomplish this [54].

(ii) The temporally asymmetric equation of motion, Eq. (43), relates the statistical operators at successive instants of time. By changing the sign of all time instants occurring explicitly and implicitly in that equation, one obtains its temporal reverse. Should the Hamiltonian here be regarded as invariant to such changes, the resulting equation will be of the same form but will involve a characteristic time interval with changed sign and an interchange of the anterior and posterior roles of the statistical operators. As a result of the latter, the temporally reversed equation cannot be arranged to depict the same evolutionary behavior as the original equation of motion. Since the latter equation presumably determines all the observable changes which are possible, those determined by the temporally reversed equation would appear not to be observable. If time were to be regarded as intrinsically nonpositive, later times would be more negative than earlier times, contrary to the usual convention we have employed [21]. Thereupon, the roles of the anterior and posterior statistical operators would again be interchanged and the original equation and its temporal reverse would then be compatible, although with a fixed temporal convention neither is. Perhaps the most striking example of the latter incompatibility is the one in which an initial statistical operator can evolve from a "pure-state" condition to form "mixtures" but cannot have evolved from them.

(iii) An obvious limitation of the present theory would seem to lie in its nonrelativistic formulation. However, should the systems considered here have relativistic Hamiltonians and have statistical operators that satisfy discretized equations of motion which are invariant to proper Lorentz transformations of the system, the theory would then have a reasonable relativistic basis [55]. Thereupon, a consequence of some importance emerges.

Under the foregoing circumstances, which seem reasonable to assume for isolated quantum systems, it also seems reasonable to suppose that the necessary conditions that a quantum field theory must fulfill to satisfy the TCP theorem [18,56] will also be fulfilled by a proper relativistic version of the present theory. Then the evolutionary behavior of an isolated quantum system should be invariant to the simultaneous set of transformations: (T) reversal of time, (C) particle-antiparticle interchange, and (P) spatial inversion [57–59]. A lack of invariance to any one of them implies a lack of invariance to the combination of the remaining two. Since the present theory, clearly, concludes that T invariance will not be observed, no invariance to the combined CP transformation also must be expected. This lack of invariance as is known, has been predicted [60] and has been observed [61–63]. Although it provides a measure of support for the temporal asymmetry of the present theory, a proper relativistic version of it is required for unequivocal support. Nevertheless, the lack of the time-reversal invariance that results from the present nonrelativistic theory cannot be dismissed entirely in its absence [64].

(iv) Finally, it follows from Eq. (52) that the behavior of any isolated quantum system which is currently undergoing changes cannot be retrodicted beyond a finite time in the past. Whether such a system has existed before that time or not is a moot question, but, if so, it could not then have had a proper statistical operator from which the current one could have evolved. Accordingly, it might even be said that the system had no realistic existence before that time. Supposing that this feature also will be exhibited by an appropriate relativistic version of the present theory, we would have to conclude that any portion of the universe which can be adequately described as an isolated quantum system would have a current behavior that is capable of being retrodicted only to a finite past. Were this to apply to the entire universe, it would appear to be in accord with the present views regarding its finite age [65]. At present, however, any such cosmological conclusion is highly speculative.

In conclusion, we must keep in mind that it is unknown if real physical systems actually exhibit the discontinuous irreversible evolutionary behavior and the associated temporal discreteness obtained here. If they do, we surely have another way to account for irreversibility that differs from the present one of regarding it to be nonintrinsic and, instead, only the result of our practical inability to make complete analyses of the pertinent processes in terms of current temporally reversible physical laws [7]. Of course, if they do, we shall have to examine the limitations that may then be imposed on these laws. If only for that reason, it is clearly desirable—if not mandatory—that some sort of experimental evidence be obtained that can discriminate between the two possibilities. It is to be hoped that such will not be long in coming.

APPENDIX A

Taking into account its role in transforming both Hilbert-space bases and their adjoints, we first express a general identity-preserving temporal transformer as [23]

$$\mathbf{T}[t;\cdots]=\sum_{j,k} a_{jk}\,\mathbf{A}_j(t)[\cdots]\,\mathbf{A}_k^\dagger(t)\,, \tag{A1}$$

where the $\{a_{jk}\}$ are time-independent coefficients and the $\{\mathbf{A}_j(t)\}$ are linearly independent transformation operators that are bounded such that

$$\mathbf{T}[t;\mathbf{I}]=\mathbf{I}\,. \tag{A2}$$

Equation (2) requires that the $\{a_{jk}\}$ comprise an Hermitian matrix which can be diagonalized, so that

$$\mathbf{T}[t;\cdots]=\sum_j b_j\mathbf{B}_j(t)[\cdots]\mathbf{B}_j^\dagger(t)\,, \tag{A3}$$

where the $\{b_j\}$ are real numbers, also independent of time. The $\{\mathbf{B}_j(t)\}$ are, again, linearly independent transformation operators that are bounded. Because of Eq. (3), we must have

$$b_j\geq 0,\quad \text{all } j\,; \tag{A4}$$

because of Eq. (A2), we must have

$$\sum_j b_j\mathbf{B}_j(t)\mathbf{B}_j^\dagger(t)=\mathbf{I}\,; \tag{A5}$$

because of Eq. (4), for arbitrary initial statistical operators, we must also have

$$\sum_j b_j\mathbf{B}_j^\dagger(t)\mathbf{B}_j(t)=\mathbf{I}\,. \tag{A6}$$

Now, since

$$\rho(0)=\sum_j b_j\mathbf{B}_j(0)\rho(0)\mathbf{B}_j^\dagger(0)\,, \tag{A7}$$

it follows that

$$\sum_j b_j\mathrm{Tr}\{[\mathbf{B}_j(0),\rho(0)][\rho(0),\mathbf{B}_j^\dagger(0)]\}=0\,, \tag{A8}$$

so that

$$[\mathbf{B}_j(0),\rho(0)]=\mathbf{0},\quad \text{all } j\,. \tag{A9}$$

Since $\rho(0)$ is an arbitrary statistical operator, it further follows that

$$\mathbf{B}_j(0)=c_j\mathbf{I},\quad \text{all } j\,. \tag{A10}$$

Hence by Eqs. (A5) and (A6),

$$\sum_j b_j|c_j|^2=1\,. \tag{A11}$$

As a result of Eq. (A4) we may introduce

$$\lambda_j\equiv b_j|c_j|^2\geq 0,\quad \text{all } j \tag{A12}$$

and

$$\mathbf{S}_j(t)\equiv\mathbf{B}_j(t)/c_j,\quad \text{all } j\,, \tag{A13}$$

whereupon it follows that

$$\mathbf{T}[t;\cdots]=\sum_j\lambda_j\mathbf{S}_j(t)[\cdots]\mathbf{S}_j^\dagger(t)\,, \tag{A14}$$

as expressed in Eq. (5). Equations (6)–(8) then follow from Eqs. (A10)–(A13).

APPENDIX B

The equality in Eq. (23) occurs if and only if the commutators there vanish, viz.

$$[\mathbf{S}_j^\dagger(\tau_n)\mathbf{S}_k(\tau_n),\boldsymbol{\rho}(t_{n-1})]=\mathbf{0} . \tag{B1}$$

As a consequence of Eqs. (5), (7), (20), and (21), and some straightforward manipulation, it then follows that

$$\mathbf{S}_k(\tau_n)\boldsymbol{\rho}^m(t_{n-1})=\boldsymbol{\rho}^m(t_n)\mathbf{S}_k(\tau_n), \quad m=1,2,\ldots . \tag{B2}$$

It further follows from Eq. (7) that

$$\mathrm{Tr}\boldsymbol{\rho}^m(t_{n-1})=\mathrm{Tr}\boldsymbol{\rho}^m(t_n), \quad m=1,2,\ldots . \tag{B3}$$

As a result, we must then have

$$\mathrm{Tr}f\{\boldsymbol{\rho}(t_{n-1})\}=\mathrm{Tr}f\{\boldsymbol{\rho}(t_n)\} , \tag{B4}$$

where $f\{x\}$, $0\le x\le 1$, is any arbitrary well-behaved function, e.g., admitting of a Taylor-series expansion in x. Expressed in terms of the eigenvalues of the statistical operators $\{\rho_k(t_n)\}$ and $\{\rho_k(t_{n-1})\}$, we can then have [23]

$$\sum_k f\{\rho_k(t_{n-1})\}=\sum_k f\{\rho_k(t_n)\} . \tag{B5}$$

With no undue loss of generality, we may suppose that the statistical operators have matrix representations which are of finite rank. It then follows, since $f\{x\}$ is arbitrary, that the eigenvalues $\{\rho_k(t_{n-1})\}$ and $\{\rho_k(t_n)\}$ are the same. Thereupon, being Hermitian, the two statistical operators would have to be unitarily equivalent which, by Eq. (5), they cannot be. Accordingly, the equality of Eq. (23) cannot be attained at any finite time, so that

$$\mathrm{Tr}\boldsymbol{\rho}^2(t_n)<\mathrm{Tr}\boldsymbol{\rho}^2(t_{n-1}), \quad t_n<\infty , \tag{B6}$$

as expressed in Eq. (24). However, because of Eq. (3) we can conclude that an asymptotic statistical operator

$$\boldsymbol{\rho}(\infty)=\lim_{t_n\to\infty}\boldsymbol{\rho}(t_n) \tag{B7}$$

must exist such that

$$\lim_{t_n\to\infty}\mathrm{Tr}\boldsymbol{\rho}^2(t_n)=\mathrm{Tr}\boldsymbol{\rho}^2(\infty) . \tag{B8}$$

APPENDIX C

When the operator $\boldsymbol{\rho}$ is required to have a step-function behavior, its values at the instants of change $\{t_n\}$ differ from those in the immediate neighborhoods. Because [66]

$$\Theta(x)=\begin{cases}1, & x>0\\ \frac{1}{2}, & x=0\\ 0, & x<0 ,\end{cases} \tag{C1}$$

we must then take

$$\boldsymbol{\rho}(t'=t_n)=[\boldsymbol{\rho}(t_n^+)+\boldsymbol{\rho}(t_n^-)]/2 , \tag{C2}$$

which equals $\boldsymbol{\rho}(t_n)$ when $\boldsymbol{\rho}$ is a continuous function of its argument. In the present case, in terms of earlier notation, we write

$$\boldsymbol{\rho}(t_n^+)\equiv\boldsymbol{\rho}(t_n) \tag{C3}$$

and

$$\boldsymbol{\rho}(t_n^-)\equiv\boldsymbol{\rho}(t_{n-1}) , \tag{C4}$$

so that

$$\boldsymbol{\rho}(t'=t_n)=[\boldsymbol{\rho}(t_n)+\boldsymbol{\rho}(t_{n-1})]/2 . \tag{C5}$$

Then, with the aid of Eq. (21), we would obtain

$$\int_0^t dt'\boldsymbol{\rho}(t')=\sum_{n=1}^{\infty}(\tau_n/2)[\boldsymbol{\rho}(t_n)+\boldsymbol{\rho}(t_{n-1})]\Theta(t-t_n) . \tag{C6}$$

As a consequence, we would then have

$$\boldsymbol{\rho}(t_n)-\boldsymbol{\rho}(t_{n-1})=-i\tau_n[\mathbf{H},[\boldsymbol{\rho}(t_n)+\boldsymbol{\rho}(t_{n-1})]/2] \tag{C7}$$

instead of Eq. (43).

Solutions of Eq. (C7) are invertible, as we now show. To do so, we imagine a temporal transformer which is implied by Eq. (C7) but with a change of sign for τ_n and apply it to $\boldsymbol{\rho}(t_n)$. We then obtain

$$\boldsymbol{\rho}(t_n-\tau_n)-\boldsymbol{\rho}(t_n)=i\tau_n[\mathbf{H},[\boldsymbol{\rho}(t_n-\tau_n)+\boldsymbol{\rho}(t_n)]/2] . \tag{C8}$$

When combined with Eq. (C7), it follows that

$$\boldsymbol{\rho}(t_n-\tau_n)-\boldsymbol{\rho}(t_{n-1})=i\tau_n[\mathbf{H},[\boldsymbol{\rho}(t_n-\tau_n)-\boldsymbol{\rho}(t_{n-1})]/2] , \tag{C9}$$

which implies that

$$\boldsymbol{\rho}(t_n-\tau_n)=\boldsymbol{\rho}(t_{n-1}) . \tag{C10}$$

Hence the transformation from $\boldsymbol{\rho}(t_{n-1})$ to $\boldsymbol{\rho}(t_n)$ is then invertible, as asserted.

This constitutes a violation of assumption (ii), Eq. (10), so that the requirement that $\boldsymbol{\rho}$ be an intrinsically discontinuous operator cannot be imposed. The consequent discontinuous behavior expressed in Eq. (19) must be regarded as due to the discontinuous behavior of the time parameter upon which the intrinsically continuous $\boldsymbol{\rho}$ depends.

APPENDIX D

To show that classical dynamical systems must evolve essentially continuously, express Eq. (43) in conventional units and rearrange it to obtain

$$[\boldsymbol{\rho}(t_n)-\boldsymbol{\rho}(t_n-\tau_n)]/\tau_n=i[\boldsymbol{\rho}(t_n),\mathbf{H}]/\hbar , \quad \text{all } n , \tag{D1}$$

where $\hbar=h/2\pi$, h being Planck's constant. Upon exploiting the analogy between the commutator and the classical Poisson bracket [67] and associating the classical dynamical limit with a vanishing value of Planck's constant, it is readily established [68] that

$$\{[\rho(t_n)-\rho(t_n-\tau_n)]/\tau_n\}_{\text{classical}} = \lim_{\hbar\to 0}\{i[\rho(t_n),\mathbf{H}]/\hbar\} = \frac{d\rho(t_n)}{dt_n}\ , \quad \text{(D2)}$$

where the statistical operator has been replaced by its classical counterpart. As a result, we must evidently have

$$\{\tau_n\}_{\text{classical}}=0,\quad \text{all } n\ , \quad \text{(D3)}$$

so that systems which can be adequately described in classical dynamical terms must exhibit essentially continuous evolutionary behavior, as asserted.

[1] There is a vast literature, but the following four references should suffice for general purposes concerning many aspects of this paper.

[2] G. J. Whitrow, *The Natural Philosophy of Time,* 2nd ed. (Clarendon, Oxford, 1984).

[3] *The Voices of Time,* edited by J. T. Fraser (Braziller, New York, 1966).

[4] *Time in Science and Philosophy,* edited by J. Zeman (Elsevier, New York, 1971).

[5] *Ergodic Theories,* Proceedings of the International School of Physics "Enrico Fermi," Course XIV, edited by P. Caldirola (Academic, New York, 1961).

[6] See, in this connection, H. Mehlberg, *Time in Science and Philosophy* (Ref. [4]), p. 50. The conjectural aspect concerning naturally occurring irreversible processes is stressed here.

[7] We are adopting the terminology of L. Rosenfeld, in *Ergodic Theories* (Ref. [5]), p. 3. A good account of how irreversibility can be reconciled with current temporally reversible laws of physics is given here.

[8] We are expressing an Aristotelian viewpoint here: the times being referred to are taken to be those which reflect changes in the condition of the system. See, for example, *The Natural Philosophy of Time* (Ref. [2]), pp. 25 and 26.

[9] See, for example, E. Hille, *Functional Analysis and Semi-Groups,* American Mathematical Society Colloquium Publication Vol. XXXI (American Mathematical Society, New York, 1948), pp. 387–390, where further references may be found.

[10] *The Natural Philosophy of Time,* G. J. Whitrow (Ref. [2]), p. 200.

[11] *The Natural Philosphy of Time,* G. J. Whitrow (Ref. [2]), p. 215.

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[13] S. Golden and H. C. Longuet-Higgins, J. Chem. Phys. **33**, 1479 (1960).

[14] J. von Neumann, *Mathematical Foundations of Quantum Mechanics,* translated by R. T. Beyer (Princeton University Press, Princeton, 1955), p. 350.

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[17] S. Watanabe, in *The Voices of Time* (Ref. [3]), pp. 540–547.

[18] S. S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Row, Peterson, Evanston, 1961), pp. 505, 506.

[19] *Mathematical Foundations of Quantum Mechanics,* J. von Neumann (Ref. [14]), pp. 34–178.

[20] Unless explicitly stated otherwise, the statistical operators of interest here are assumed not to be temporally invariant.

[21] We follow a convention of regarding time as nonnegative unless otherwise stated explicitly. See, in this connection, the article by R. Schlegel, in *The Voices of Time* (Ref. [3]), pp. 501 and 502.

[22] We assume that all traces exist in what follows.

[23] No undue loss of generality is involved in using a discrete formalism, the sums being regarded as pertinent Stieltjes integrals. We assume convergence of all sums in what follows.

[24] The association of unitary transformations with reversible temporal behavior is well known. See for example, J. von Neumann, *Mathematical Foundations of Quantum Mechanics* (Ref. [14]), p. 351; F. J. Belinfante, *Measurements and Time Reversal in Objective Quantum Theory* (Ref. [16]), pp. 19, 20, 110–120; R. Penrose, *The Emperor's New Mind* (Penguin Books, New York, 1991), pp. 250, 251, and 349.

[25] See, in this connection, R. Penrose, *The Emperor's New Mind* (Ref. [24]), pp. 354–359.

[26] Because the conclusions reached here depend implicitly upon the system involved, the resulting discontinuous behavior and associated temporal discreteness must be regarded as possibly depending on the system, until demonstrated otherwise.

[27] S. Golden, *Quantum Statistical Foundations of Chemical Kinetics* (Clarendon, Oxford, 1969), pp. 69–71.

[28] I. E. Farquhar, *Ergodic Theory in Statistical Mechanics* (Interscience, New York, 1964), pp. 187–191.

[29] See, in this connection, J. von Neumann, *Mathematical Foundations of Quantum Mechanics* (Ref. [14]), pp. 417–445, in which it is pointed out that wave functions yield "mixtures" after appropriate measurements are made. By contrast, the behavior deduced here is inherent and requires no external agents as must be involved in measurement processes. See, also, W. H. Furry, Phys. Rev. **49**, 393 (1936); **49**, 476 (1936).

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[32] See, in this connection, P. Ehrenfest and T. Ehrenfest, *The Conceptual Foundations of the Statistical Approach in Mechanics,* translated by M. J. Moravcsik (Cornell University Press, Ithaca, 1959), pp. 13, 14, and 31–35.

[33] R. C. Tolman, *The Principles of Statistical Mechanics* (Oxford University Press, Oxford, 1955), pp. 134–179.

[34] Appropriate units of the quantities involved are assumed throughout.

[35] See, in this connection, J. von Neumann, *Mathematical Foundations of Quantum Mechanics* (Ref. [14]), pp. 112–115.

[36] A time-dependent Hamiltonian $\mathbf{H}(t)$ could be introduced in Eq. (38), but we shall not do so for the isolated systems of interest here.

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Kinetics (Ref. [27]), pp. 69, 102.
[38] R. Karplus and J. Schwinger, Phys. Rev. **73**, 1020 (1949).
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