

STOCHASTIC PROCESSES AND THE QUANTUM EVOLUTION OF STATES*

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ABSTRACT

Beginning with the statistical description of the results of a duplicated experiment as a set of configurations of some observables together with frequencies of occurrence of each configuration it is shown that an evolution of the system by a stochastic process is obtained when the conditioning parameters of the experiment are altered. It is then shown that any such stochastic process has a representation in terms of linear operators in an abstract vector space with a state vector evolving by an isometric operator \mathbf{S} and commuting Hermitian operators representing observables which evolve by another, unitary, operator \mathbf{U} . This has the structure of conventional quantum theory as in the interaction, or Dirac picture, but here \mathbf{S} is *not* unitary as in conventional theory. This is shown to yield a matrix of transition probabilities that is *not* doubly stochastic as in conventional theory and hence the Pauli master equation does not follow. All implications of this completely irreversible quantum theory have not yet been fully explored, but it points to a new viewpoint in irreversible thermodynamics.

INTRODUCTION

A recent series of papers¹⁻⁶ has developed the idea that much of the formal mathematical structure of physical theory can be deduced directly from the statistical properties of experimental data. The present paper presents that portion of these studies which bears directly on the problem of irreversible physical processes; specifically we point out what appears to be a major flaw in conventional quantum theory and exhibit the proper connection of the quantum mechanical evolution of states to a stochastic process.

DUPLICATED EXPERIMENTS AND TIME

We consider a duplicated experiment with a physical system in which certain parameters are given fixed values and selected properties of the system are measured. Thus suppose that in order to duplicate exactly the conditions of the experiment we must fix values for q_1, q_2, \dots, q_K and $\eta_1, \eta_2, \dots, \eta_J$; then values of (x, y, z, \dots) are measured. Distinct results are represented by sets of numbers, say

$$r_n = (x_n, y_n, z_n, \dots), n = 1, 2, 3, \dots \quad (1)$$

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such that two results, r_n and r_m , are distinct, $r_n \neq r_m$, if they differ in one or more entries. The variables of r are not all independent, say z may be computed from measured values of x and y . Thus if r contains M independent variables the index n is equivalent to M distinct indices, n_1, n_2, \dots, n_M .

If the experiment could be exactly duplicated N times and a particular result r_n were obtained N_n times then we would define the probability for r_n as

$$\Pi_n = \lim_{N \rightarrow \infty} \frac{N_n}{N} \tag{2}$$

Thus a sequence of exact duplications would be summarized as a set of results $r_n, n = 1, 2, \dots$, and a corresponding set of probabilities, $\Pi_n, n = 1, 2, \dots$. In general the spectrum of results is determined by the conditioning parameters, that is $x_n(q, \eta), y_n(q, \eta), \dots$ are functions of the q_i and η_j , and the probability is conditioned by the q_i and η_j that is, $\Pi_n(q, \eta)$.

This statistical description of an experiment does not preclude an exactly deterministic system for which

$$\Pi_n = \delta_{nn'} = \begin{cases} 1, & n = n'(q, \eta) \\ 0, & n \neq n'(q, \eta) \end{cases} \tag{3}$$

but we maintain a general statistical description in which Π_n is not a Kronecker delta.

In reality not all parameters which may condition the outcome of an experiment can be identified and fixed by the experimenter and it is for this reason that we employ a notation indicating two groups of conditioning parameters, those q_1, q_2, \dots, q_K which are identified and fixed and those $\eta_1, \eta_2, \dots, \eta_J$ which are not fixed. Therefore we introduce a one-parameter labelling $\eta_i(t) = \eta_i, i = 1, 2, \dots, J$ such that

$$d\eta_i = \dot{\eta}_i(t)dt, i = 1, 2, \dots, J; dt \neq 0 \tag{4}$$

are never *all* zero. Thus we acknowledge the fact that the external universe is always changing and introduce the notation $x_n(q, t), y_n(q, t), \dots$ and $\Pi_n(a, t)$ for the spectral values of observables and their corresponding probability.

Here t is defined as the time⁵.

Here we have one description of a duplicated experiment in which the results are explicitly identified as time dependent; we may then investigate further the question of whether duplication then has any real meaning, i.e. when not all conditioning parameters are fixed. But an alternative is to consider a time-ordered sequence of measurements of the observables $r = (x, y, z, \dots)$ while those q_1, q_2, \dots, q_K accessible to control are fixed. Thus using any one of the n_i , which is never fixed, as the time-ordering reference [solve this $\eta_i = \eta_i(t)$ for t] we may consider the possibility of defining a probability

$$P(r_{n(1)} \rightarrow r_{n(2)} \rightarrow \dots \rightarrow r_{n(N)} | q)$$

for the time-ordered sequence of results; $r_{n(1)} \rightarrow r_{n(2)} \rightarrow \dots \rightarrow r_{n(N)}$; i.e. $r_{n(1)}$ is observed at time $t_1, r_{n(2)}$ at t_2, \dots etc.

In order properly to define such a probability in mathematical terms it is necessary to construct an event space which forms a sigma algebra and a sigma additive measure over this space. In another paper it is shown that such a probability can be properly defined⁶ if one introduces a certain equivalence relation between 'paths'. Thus the sequence of results $r_{n(1)} \rightarrow r_{n(2)} \rightarrow \dots \rightarrow r_{n(N)}$ is a 'simple path'; a compound path is

$$r_{n(1)} \rightarrow r_{n(2)} \rightarrow \dots \rightarrow (r_{n(k)} \text{ OR } r_{n'(k)}) \rightarrow \dots \rightarrow r_{n(N)}$$

that is, at the k th measurement we are only able to say, either $r_{n(k)}$ OR $r_{n'(k)}$ occurs. The equivalence relation that is introduced is

$$\begin{aligned} & [r_{n(1)} \rightarrow r_{n(2)} \rightarrow \dots \rightarrow (r_{n(k)} \text{ OR } r_{n'(k)}) \rightarrow \dots \rightarrow r_{n(N)}] \\ & = [r_{n(1)} \rightarrow r_{n(2)} \rightarrow \dots \rightarrow r_{n(k)} \rightarrow \dots \rightarrow r_{n(N)}] \\ & \text{OR } [r_{n(1)} \rightarrow r_{n(2)} \rightarrow \dots \rightarrow r_{n'(k)} \rightarrow \dots \rightarrow r_{n(N)}] \end{aligned} \tag{5}$$

That is, the probability for the compound path is required to be equal to the sum of the probabilities for the two simple paths; this defines the equivalence of paths.

With the conditional probability defined by

$$\begin{aligned} P(r_{n(1)} \rightarrow r_{n(2)} \rightarrow \dots \rightarrow C_{(j)} \rightarrow \dots \rightarrow r_{n(N)} | q, C_{(1)} \rightarrow C_{(2)} \rightarrow \dots \rightarrow r_{n(j)} \rightarrow \dots \rightarrow C_{n(N)}) \\ = \frac{P(r_{n(1)} \rightarrow r_{n(2)} \rightarrow \dots \rightarrow r_{n(j)} \rightarrow \dots \rightarrow r_{n(N)} | q)}{P(C_{(1)} \rightarrow C_{(2)} \rightarrow \dots \rightarrow r_{n(j)} \rightarrow \dots \rightarrow C_{n(N)} | q)} \end{aligned} \tag{6}$$

where $C_{(j)}$ stands for $[r_{1(j)}$, OR $r_{2(j)}$ OR $r_{3(j)}$ OR ...], that is *some* result at t_j , and the above equivalence relation, one obtains, by summing over the spectra of $n(1), n(2), \dots, n(N-1)$, the form,

$$\Pi_n(q, t_N) = \sum_{m \neq 1} T_{nm} \Pi_m(q, t_1) \tag{7}$$

where $\Pi_n(q, t_N)$ is identified as

$$\Pi_n(q, t_N) = P(C_{(1)} \rightarrow C_{(2)} \rightarrow \dots \rightarrow C_{(N-1)} \rightarrow r_{n(N)} | q) \tag{8}$$

That is, the probability that some result is obtained at each of t_1, t_2, \dots, t_{N-1} and the specific result $r_{n(N)}$ is obtained at t_N .

Thus a consideration of a time-ordered sequence of measurements leads naturally to a description of the time evolution of the system as a stochastic process. Shortly we will see that this description of time evolution of a system is arrived at by another argument, but first we point out a direct connection of this description to an operator formalism like quantum theory.

PROBABILITY FUNCTIONS IN I^2 AND THE STOCHASTIC OPERATOR

The probability functions introduced above have the properties

$$\Pi_n(q, t) \geq 0 \tag{9}$$

$$T_{nm} \geq 0 \tag{10}$$

together with

$$\sum_{n \geq 1} \Pi_n(q, t) = 1 \tag{11}$$

and

$$\sum_{n \geq 1} T_{nm} = 1 \tag{12}$$

both of which must be identities valid for all q and t configurations.

Because of the non-negative properties of Π_n and T_{nm} we can introduce complex functions $c_n(q, t)$ and $K_{nm}(q, t)$ such that

$$\Pi_n(q, t) = c_n^*(q, t) c_n(q, t) \tag{13}$$

and

$$T_{nm}(q, t) = K_{nm}^*(q, t) K_{nm}(q, t) \tag{14}$$

Then equation 7, with $t_N = t, t_1 = 0$ appears as

$$c_n^*(q, t) c_n(q, t) = \sum_{m \geq 1} K_{nm}^*(q, t) K_{nm}(q, t) c_m^*(q, 0) c_m(q, 0) \tag{15}$$

Since the phases of the $c_n(q, 0)$ and $K_{nm}(q, t)$ are arbitrary these can be chosen such that

$$c_n(q, t) = \sum_{m \geq 1} K_{nm}(q, t) c_m(q, 0) \tag{16}$$

as is proved in the appendix theorem of an earlier paper².

Because the sequences $c_n(q, t), K_{nm}(q, t), n = 1, 2, \dots$, are square summable these have a representation in terms of an abstract vector space and we have here

$$c_n(q, t) = \langle n | q, t \rangle \tag{17}$$

and

$$K_{nm} = \frac{\langle n | \mathbf{K} | m \rangle}{\langle m | \mathbf{K}^\dagger \mathbf{K} | m \rangle^{\frac{1}{2}}} \tag{18}$$

where \mathbf{K} is an abstract operator. These inserted into equation 16 yield

$$\langle n | q, t \rangle = \sum_{m \geq 1} \frac{\langle n | \mathbf{K} | m \rangle}{\langle m | \mathbf{K}^\dagger \mathbf{K} | m \rangle^{\frac{1}{2}}} \langle m | q, 0 \rangle \tag{19}$$

or

$$|q, t \rangle = \mathbf{S} |q, 0 \rangle \tag{20}$$

where

$$\mathbf{S} = \mathbf{K} \mathbf{D} \tag{21}$$

with \mathbf{D} being the diagonal Hermitian operator

$$\mathbf{D} = \sum_{m \geq 1} \frac{|m \rangle \langle m|}{\langle m | \mathbf{K}^\dagger \mathbf{K} | m \rangle^{\frac{1}{2}}} \tag{22}$$

Thus the stochastic evolution of states leads directly to the evolution of a representative state vector by an operator S . In other papers^{4,5} we have shown that

$$S^\dagger S = I \tag{23}$$

but in general

$$S S^\dagger \neq I \tag{24}$$

unless K is a unitary operator. However, no special properties for K need be specified, nor for D either. If D^{-1} exists, then using equation 21 K is given by SD^{-1} , but D^{-1} exists only if $K^\dagger K$ is a diagonal operator and the determinant, $|D|$, exists; this requires that

$$-2 \ln |D| = \sum_{m \geq 1} \ln \langle m | K^\dagger K | m \rangle \tag{25}$$

be a convergent series. We also show elsewhere⁶ that S has a semi-group property. Thus S is an isometric operator for an arbitrary operator K but may be a unitary operator if K is itself a unitary operator, i.e. equations 23 and 24 define an isometric operator. One can readily verify that equations 11 and 12 are identically satisfied by virtue of these forms.

If we define another abstract operator π acting in this vector space as a Hermitian operator having a complete set of eigenvectors $|n\rangle$, $n = 1, 2, \dots$, spanning the space and eigenvalues $\Pi_n(q, t)$, $n = 1, 2, \dots$, that is,

$$\pi |n\rangle = \Pi_n(q, t) |n\rangle, n = 1, 2, \dots \tag{26}$$

then we can show that⁵

$$\pi(q, t) = S \pi(q, 0) S^\dagger \tag{27}$$

is isomorphic to equation 15 and hence is the representation of the stochastic process in the abstract vector format.

This analysis, which proceeds from a consideration of a time-ordered sequence of measurements to the representation of the evolution of the system by an isometric operator in an abstract vector space, fails to indicate how observables are to be represented in the formalism; another approach yields this⁵.

OBSERVABLES AND THEIR OPERATORS, AN ALTERNATE VIEWPOINT ON TIME EVOLUTION

Since $\Pi_n(q, t)$ can be represented as $c_n^*(q, t) c_n(q, t)$ we see that the expectation value of any observable is given by

$$\langle x \rangle = \sum_{n \geq 1} x_n(q, t) c_n^*(q, t) c_n(q, t) = C^+ X C \tag{28}$$

where the $x_n(q, t)$ are the measured values of x corresponding to the distinct results r_n . Some $x_m(q, t)$ may thus be equal. Here a matrix notation is introduced with C being the column matrix with elements $c_n(q, t)$ and X the

diagonal matrix with elements $x_n(q, t)$. Also the norm condition, equation 11, appears as

$$C^\dagger C = 1 \tag{29}$$

These forms follow directly from nothing more than the non-negative property of $\Pi_n(q, t)$. Since equation 29 can also be written for any other observable, say y , we see that each observable is represented by a diagonal real matrix and these are all of the same order. Furthermore all diagonal matrices commute, that is

$$XY - YX = 0 \tag{30}$$

for example.

Since this, as well as equations 28 and 29, is invariant under unitary transformation, say

$$C' = VC, \quad X' = VXV^\dagger, \quad Y' = VYV^\dagger \tag{31}$$

with V a unitary matrix, we see

$$C'^\dagger C' = 1, \quad \langle x \rangle = C'^\dagger X' C', \quad X' Y' - Y' X' = 0 \tag{32}$$

and hence in an arbitrary basis the collection of all observables is represented by a collection of commuting Hermitian matrices. This result is completely independent of any arguments about the time evolution of the system, it rests solely on the definition of an expectation value and the non-negative property of a probability.

However, these same forms can be written for *any* values of the q_j and t , say with the q_j and t replaced by $q_j + \delta q_j$ and $t + \delta t$. Thus in a matrix format

$$C_\delta^\dagger C_\delta = 1, \quad \langle x \rangle_\delta = C_\delta^\dagger X_\delta C_\delta, \quad X_\delta Y_\delta - Y_\delta X_\delta = 0, \quad \text{etc.} \tag{33}$$

where the δ subscript indicates the incremented arguments.

Then we introduce linear transformation matrices K and U such that

$$C_\delta = KC, \quad X_\delta = UXU^\dagger, \quad \text{etc.} \tag{34}$$

where X_δ as well as X must be diagonal. Furthermore, in order to preserve commutation⁵ of spectral matrices, every spectral matrix must be transformed by the *same* U and we must have*

$$U^\dagger U = I \tag{35}$$

Thus U must be an isometric matrix and X and X_δ must in general be of different order.

However, if we demand that as all $\delta q_j \rightarrow 0$ and $\delta t \rightarrow 0$

$$\text{limit } X_\delta = X \tag{36}$$

then it can be shown⁵ that U must be unitary and in particular, for infinitesimal δq_j and δt ,

$$U = I + i \sum_{j=1}^K P^{(j)} \delta q_j - iH \delta t \tag{37}$$

* At the time of this writing we have recognized that $U^\dagger U = \alpha I$ with α a scalar is sufficient so further generalization of the theory is possible.

where the $P^{(j)}$ and H are commuting Hermitian matrices. Then every spectral matrix, as X above, must be of a fixed order and all must commute with U to remain diagonal. Thus the spectral matrices of all observables commute with the $P^{(j)}$ and H , and the $P^{(j)}$ and H themselves correspond to observables.

On the other hand we have no basis for requiring $C_\delta \rightarrow C$ as all δq_j and δt go to zero because these quantities contain an arbitrary phase. We point out that the unit norm condition in equations 29 and 33

$$C^\dagger C = 1, \quad C_\delta^\dagger C_\delta = C^\dagger K^\dagger K C = 1 \tag{38}$$

does *not* require K to be unitary or even isometric, because K is uniquely related to C and $K^\dagger K$ inserted into any other matrix product need not leave the product invariant. Equation 38 is satisfied if we impose the less stringent condition on the elements of K ,

$$\sum_{n \geq 1} K_{nm}^* K_{nm} = 1 \tag{39}$$

and *choose* the arbitrary phases of the $c_n(q, t)$ such that⁵

$$\sum_{l \neq m} \sum_{m \geq 1} K_{nm}^* K_{nl} c_m^*(q, t) c_l(q, t) = 0 \tag{40}$$

Then using equation 34 relating the $c_n(q + \delta q, t + \delta t)$ to the $c_n(q, t)$ we find that equation 15 is obtained simply by setting $t = 0$ and $\delta t = t$.

Thus we find the $K_{nm}^* K_{nm}$ to be the transition probabilities in a stochastic equation and again the state of the system evolves by a stochastic process, but now with translation of the q_j as well as t . This alternate analysis is explored at length in another paper⁵.

Most significant is the fact that the state matrix C evolves by one matrix K , for which no special properties are postulated, beyond equation 39, while spectral matrices, like X , evolve by a different matrix, U , which must be unitary or at least isometric.

Carried over to the abstract vector picture we find that in addition to the operators $\mathbf{S}, \mathbf{D}, \mathbf{K}$ and $\boldsymbol{\pi}$ defined above, we also have a Hermitian operator corresponding to each observable in the experiment, as \mathbf{X} for example, and these all commute. We also have the unitary evolution operator \mathbf{U} expressed in terms of commuting Hermitian operators $\mathbf{P}_j, j = 1, 2, \dots, K$ and \mathbf{H} , as

$$\mathbf{U} = \exp \left\{ i \sum_{j=1}^K \mathbf{P}_j \delta q_j - i \mathbf{H} \delta t \right\} \tag{41}$$

In general $\boldsymbol{\pi}$ does not commute with the \mathbf{P}_j and \mathbf{H} , but operators of all observables, as \mathbf{X} for example, must commute with \mathbf{U} and hence with the \mathbf{P}_j and \mathbf{H} as well. In particular, we have from equation 34

$$\mathbf{X}_\delta = \mathbf{U} \mathbf{X} \mathbf{U}^\dagger \tag{42}$$

in the abstract operator format and this yields

$$i \frac{\partial \mathbf{X}}{\partial t} = \mathbf{H} \mathbf{X} - \mathbf{X} \mathbf{H}, \quad -i \frac{\partial \mathbf{X}}{\partial q_j} = \mathbf{P}_j \mathbf{X} - \mathbf{X} \mathbf{P}_j \tag{43}$$

and we see that no operator containing the q_j and t as parameters may represent a *proper* observable.

IRREVERSIBLE QUANTUM THEORY

What we have here is simply an irreversible quantum theory; the isometric operator \mathbf{S} yields a unidirectional evolution of the state vector, but operators of observables evolve by the unitary operator \mathbf{U} . This is essentially the format of the interaction, or Dirac, picture of conventional quantum theory with states evolving by \mathbf{S} and observables by \mathbf{U} , but here \mathbf{S} is not in general unitary.

In this regard we note that from equations 14 and 18 the transition probabilities are given by

$$T_{nm} = \langle n | \mathbf{S} | m \rangle \langle m | \mathbf{S}^\dagger | n \rangle = \frac{\langle n | \mathbf{K} | m \rangle \langle m | \mathbf{K}^\dagger | n \rangle}{\langle m | \mathbf{K}^\dagger \mathbf{K} | m \rangle} \quad (44)$$

and this is *not* a doubly stochastic matrix as in conventional quantum theory unless the operator \mathbf{K} is unitary. As already noted, \mathbf{S} is unitary if \mathbf{K} is unitary, and in fact \mathbf{S} is then equal to \mathbf{K} and we then have the expression familiar to us in conventional quantum theory. The stationary states of quantum theory are those for which $\mathbf{S} = \mathbf{K} = \mathbf{I}$, for then $T_{nm} = \delta_{nm}$ is the identity; i.e. there are then no transitions.

CONCLUSION AND DISCUSSION

At the time of this writing we have not yet constructed an isometric operator \mathbf{S} appropriate to a particular system to illustrate the application of this irreversible quantum theory because the formulation does not yield a general format for the construction of such an operator. Even so we can draw a few specific conclusions. For example, the usual form of the master equation⁷, which is based on a unitary evolution operator for states and hence a doubly stochastic matrix of transition probabilities, must be at best only a good approximation to the proper description of the time evolution of the state probability. Furthermore, having shown that there is a direct logical derivation of this formalism from nothing more than the statistical properties of experimental data we open the way to further generalizations of the theory.

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